Artificial Intelligence 2 Summer Semester 2025

– Lecture Notes –

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FAU Michael Kohlhase: Artificial Intelligence 2

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Chapter 20 Preliminaries



In the broadest sense: A bunch of tools for your toolchest (i.e. various (quasi-mathematical) models, first and foremost)



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- the underlying principles of these models (assumptions, limitations, the math behind them ...)
- the ability to describe real-world problems in terms of these models, where adequate (...and knowing when they are adequate!), and
- the ideas behind effective algorithms that solve these problems (and to understand them well enough to implement them)
- Note: You will likely never get payed to implement an algorithm that e.g. solves Bayesian networks. (They already exist)
 - But you might get payed to recognize that some given problem can be represented as a Bayesian network!
 - Or: you can recognize that it is similar to a Bayesian network, and reuse the underlying principles to develop new specialized tools.



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- ► Employee 1 Deep Learning can do everything: "I just need ≈1.5 million labeled examples of potentially sensitive data, a GPU cluster for training, and a few weeks to train, tweak and finetune the model.

But *then* I can solve the problem... with a confidence of 95%, within 40 seconds of inference per input. Oh, as long as the input isn't longer than 15unit, or I will need to retrain on a bigger input layer..."

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Employee 2 – AI-2 Alumna: "...while you were talking, I quickly built a custom UI for an off-the-shelve <problem> solver that runs on a medium-sized potato and returns a provably correct result in a few milliseconds. For inputs longer than 1000unit, you might need a slightly bigger potato though..."



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- ▶ Moral of the story: Know your *tools* well enough to select the right one for the job.



20.1 Administrative Ground Rules



- Remember: AI-1 dealt with situations with "complete information" and strictly computable, "perfect" solutions to problems.
 (i.e. tree search, logical inference, planning, etc.)
- AI-2 will focus on *probabilistic* scenarios by introducing uncertain situations, and *approximate* solutions to problems. (Bayesian networks, Markov models, machine learning, etc.)



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- Weak Prerequisites for AI-2:

(if you do not have them, study up as needed)

- Al-1 (in particular: PEAS, propositional logic/first-order logic (mostly the syntax), some logic programming) (big Oh and friends)
- (very) elementary complexity theory.

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- basic linear algebra

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- (very) elementary complexity theory.
- rudimentary probability theory
- basic linear algebra
- basic real analysis (aka. calculus)
- Meaning: I will assume you know these things, but some of them we will recap, and what you don't know will make things slightly harder for you, but by no means prohibitively difficult.



(big Oh and friends)

(e.g. from stochastics) (vectors, matrices,...)

(primarily: (partial) derivatives)

(if you do not have them, study up as needed)

- Most crucially Mathematical Literacy: Mathematics is the language that computer scientists express their ideas in! ("A search problem is a tuple (N, S, G, ...) such that...")
- Note: This is a skill that can be *learned*, and more importantly, *practiced!* Not having/honing this skill *will* make things more difficult for you. Be aware of this and, if necessary, work on it it will pay off, not only in this course.



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- ▶ Note: Grades correlate significantly with invested effort; including, but not limited to:
 - time spent on exercises,
 - being here in presence,
 - asking questions,

(learning is 80% perspiration, only 20% inspiration) (humans are social animals ← mirror neurons) (Q/A dialogues activate brains)



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 > being here in presence,
 > asking questions.
 > (learning is 80% perspiration, only 20% inspiration)
 > (humans are social animals ↔ mirror neurons)
 > (Q/A dialogues activate brains)
 - talking to your peers,
 (pool your insights, share your triumphs/frustrations)...

All of these we try to support with the ALEA system. (which also gives us the data to prove this)



(AI-2 is non-trivial)

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► Overall (Module) Grade:

- Grade via the exam (Klausur) $\sim 100\%$ of the grade.
- Up to 10% bonus on-top for an exam with \geq 50% points.
- ▶ Bonus points $\hat{=}$ percentage sum of the best 10 prepuizzes divided by 100.

(< 50% \sim no bonus)



Overall (Module) Grade:

- Grade via the exam (Klausur) \sim 100% of the grade.
- Up to 10% bonus on-top for an exam with \geq 50% points.
- **Exam:** exam conducted in presence on paper!
- Retake Exam: 90 minutes exam six months later.
- ▶ ▲ You have to register for exams in https://campo.fau.de in the first month of classes.
- Note: You can de-register from an exam on https://campo.fau.de up to three working days before exam. (do not miss that if you are not prepared)

(< 50% \rightarrow no bonus)

(~ Oct. 10. 2025) (~ April 10. 2026)

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Preparedness Quizzes

- **PrepQuizzes:** Before every lecture we offer a 10 min online guiz the PrepQuiz about the material from the previous week.
- Motivations: We do this to
 - keep you prepared and working continuously.
 - \triangleright bonus points if the exam has > 50% points
 - update the ALEA learner model.
- ▶ The prepauizes will be given in the ALEA system

```
https://courses.voll-ki.fau.de/guiz-dash/ai-2
```

- You have to be logged into ALEA!
- You can take the prepauliz on your laptop or phone....
- in the lecture or at home
- via WLAN or 4G Network.
- Prepquizzes will only be available 16:15-16:25!

```
(16:15-16:25; starts in week 2)
```

```
(primary)
(potential part of your grade)
               (fringe benefit)
```



- Some degree programs do not "import" the course Artificial Intelligence 1, and thus you may not be able to register for the exam via https://campo.fau.de.
 - Just send me an e-mail and come to the exam,

(we do the necessary admin)

- ► Tell your program coordinator about AI-1/2 so that they remedy this situation
- ▶ In "Wirtschafts-Informatik" you can only take AI-1 and AI-2 together in the "Wahlpflichtbereich".
 - **ECTS** credits need to be divisible by five \leftrightarrow 7.5 + 7.5 = 15.



20.2 Getting Most out of AI-2



- ► Goal: Homework assignments reinforce what was taught in lectures.
- Homework Assignments: Small individual problem/programming/proof task
 - \blacktriangleright but take time to solve (at least read them directly \rightsquigarrow questions)
- Didactic Intuition: Homework assignments give you material to test your understanding and show you how to apply it.
- A Homeworks give no points, but without trying you are unlikely to pass the exam.
- Our Experience: Doing your homework is probably even *more* important (and predictive of exam success) than attending the lecture in person!



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- Our Experience: Doing your homework is probably even *more* important (and predictive of exam success) than attending the lecture in person!
- ► Homeworks will be mainly peer-graded in the ALEA system.
- Didactic Motivation: Through peer grading students are able to see mistakes in their thinking and can correct any problems in future assignments. By grading assignments, students may learn how to complete assignments more accurately and how to improve their future results.(not just us being lazy)

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► Homework Workflow: in ALEA

(see below)

- Homework assignments will be published on thursdays: see https://courses.voll-ki.fau.de/hw/ai-1
- Submission of solutions via the ALEA system in the week after
- Peer grading/feedback (and master solutions) via answer classes.
- ▶ Quality Control: TAs and instructors will monitor and supervise peer grading.



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- ▶ Quality Control: TAs and instructors will monitor and supervise peer grading.
- **Experiment:** Can we motivate enough of you to make peer assessment self-sustaining?
 - ▶ I am appealing to your sense of community responsibility here . . .
 - ▶ You should only expect other's to grade your submission if you grade their's

(cf. Kant's "Moral Imperative")

Make no mistake: The grader usually learns at least as much as the gradee.



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- ► Homework/Tutorial Discipline:

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- Start early! (many assignments need more than one evening's work)
- Don't start by sitting at a blank screen

(talking & study groups help)

- ▶ Humans will be trying to understand the text/code/math when grading it.
- Go to the tutorials, discuss with your TA!

(they are there for you!)



- ► Approach: Weekly tutorials and homework assignments
- **Goal 1:** Reinforce what was taught in the lectures.
- ▶ Goal 2: Allow you to ask any question you have in a protected environment.

(first one in week two) (you need practice)



- ► Approach: Weekly tutorials and homework assignments
- **Goal 1:** Reinforce what was taught in the lectures.

(first one in week two) (you need practice)

(before there is nothing to do)

- **Goal 2:** Allow you to ask any question you have in a protected environment.
- Instructor/Lead TA: Florian Rabe (KWARC Postdoc, Privatdozent)
 - Room: 11.137 @ Händler building, florian.rabe@fau.de
- Tutorials: One each taught by Florian Rabe (lead); Primula Mukherjee, Ilhaam Shaikh, Praveen Kumar Vadlamani, and Shreya Rajesh More.
- Tutorials will start in week 3.
 - > Details (rooms, times, etc) will be announced in time (i.e. not now) on the forum and matrix channel.
- Life-saving Advice: Go to your tutorial, and prepare for it by having looked at the slides and the homework assignments!



- Definition 2.1. Collaboration (or cooperation) is the process of groups of agents acting together for common, mutual benefit, as opposed to acting in competition for selfish benefit. In a collaboration, every agent contributes to the common goal and benefits from the contributions of others.
- ▶ In learning situations, the benefit is "better learning".
- Observation: In collaborative learning, the overall result can be significantly better than in competitive learning.
- ► Good Practice: Form study groups.
 - 1. 🛆 Those learners who work/help most, learn most!
 - 2. 🖄 Freeloaders individuals who only watch learn very little!
- ▶ It is OK to collaborate on homework assignments in Al-2!
- Choose your study group well!

(long- or short-term)

(no bonus points)

(ALeA helps via the study buddy feature)

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- Attendance is not mandatory for the AI-2 course.
- **Note:** There are two ways of learning:
 - Approach B: Read a book/papers
 - Approach I: come to the lectures, be involved, interrupt the instructor whenever you have a question. The only advantage of I over B is that books/papers do not answer questions
- Approach S: come to the lectures and sleep does not work!
- The closer you get to research, the more we need to discuss!

(both are OK, your mileage may vary)



(official version)

(here: lecture notes)

20.3 Learning Resources for AI-2



- **Textbook:** Russel/Norvig: Artificial Intelligence, A modern Approach [RusNor:AIMA09].
 - basically "broad but somewhat shallow"
 - great to get intuitions on the basics of AI

Make sure that you read the edition \geq 3 \leftrightarrow vastly improved over \leq 2.



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Lecture notes will be posted at https://kwarc.info/teaching/AI

- We mostly prepare/update them as we go along
- Please report any errors/shortcomings you notice.
- StudOn Forum: For announcements https://www.studon.fau.de/studon/goto.php?target=lcode_70Bjcaxg
- Matrix Channel: https://matrix.to/#/#ai-12:fau.de for questions, discussion with instructors and among your fellow students. (your channel, use it!) Login via FAU IDM ~ instructions
- Course Videos are at at https://fau.tv/course/id/4225.
- **Do not let the videos mislead you:** Coming to class is highly correlated with passing the exam!

(semantically preloaded \sim research resource)

(improve for the group/successors)



Practical recommendations on Lecture Videos

Excellent Guide: [NorKueRob:lcprs18] (German version at [NorKueRob:vnas18])



A guide for students





Attend lectures.



Take notes.



Be specific.



Catch up.



Ask for help.

Don't cut corners.



NOT a Resource for : LLMs – AI-based tools like ChatGPT

- Definition 3.1. A large language model (LLM) is a computational model capable of language generation or other natural language processing tasks.
- **Example 3.2.** OpenAI's GPT, Google's Bard, and Meta's Llama.



NOT a Resource for : LLMs - AI-based tools like ChatGPT

- Definition 3.6. A large language model (LLM) is a computational model capable of language generation or other natural language processing tasks.
- **Example 3.7.** OpenAI's GPT, Google's Bard, and Meta's Llama.
- Definition 3.8. A chatbot is a software application or web interface that is designed to mimic human conversation through text or voice interactions. Modern chatbots are usually based on LLMs.
- Example 3.9 (ChatGPT talks about AI-1).

tell me about the course AI-1 at FAU Erlangen-Nürnberg	Delete	
AI-1 at FAU Erlangen-Nürnberg typically refers to a foundational course in artificial intelligence offered by the university. While I don't have the specifics of the course details from the latest curriculum, I can provide a general overview of what such a course might include based on common topics covered in introductory AI courses.		
Generally, an introductory AI course would cover the following topics:		
1. Foundations of AI: An overview of what AI is, its history, and its significance in various fields.		
2. Problem Solving and Search Algorithms: Techniques for solving problems through algorithms,		

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(but remains vague)

NOT a Resource for : LLMs - AI-based tools like ChatGPT

- Definition 3.11. A large language model (LLM) is a computational model capable of language generation or other natural language processing tasks.
- **Example 3.12.** OpenAI's GPT, Google's Bard, and Meta's Llama.
- Definition 3.13. A chatbot is a software application or web interface that is designed to mimic human conversation through text or voice interactions. Modern chatbots are usually based on LLMs.
- **Example 3.14 (ChatGPT talks about AI-1).**
- Note: LLM-based chatbots invent every word!
- **Example 3.15 (In the AI-1 exam).** ChatGPT scores ca. 50% of the points.
 - ChatGPT can almost pass the exam . . .
 - But can you?

You will only pass the exam, if you can do Al-1 yourself!

(but remains vague) (suprpisingly often correct)

(We could award it a Master's degree) (the Al-1 exams will be in person on paper)

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NOT a Resource for : LLMs - AI-based tools like ChatGPT

- Definition 3.16. A large language model (LLM) is a computational model capable of language generation or other natural language processing tasks.
- **Example 3.17.** OpenAI's GPT, Google's Bard, and Meta's Llama.
- Definition 3.18. A chatbot is a software application or web interface that is designed to mimic human conversation through text or voice interactions. Modern chatbots are usually based on LLMs.
- Example 3.19 (ChatGPT talks about AI-1).
- Note: LLM-based chatbots invent every word!
- **Example 3.20 (In the AI-1 exam).** ChatGPT scores ca. 50% of the points.
 - ChatGPT can almost pass the exam . . .
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You will only pass the exam, if you can do Al-1 yourself!

- Intuition: AI tools like GhatGPT, CoPilot, etc.
 - can help you solve problems,

hinders learning if used for homeworks/quizzes, etc.

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(but remains vague)

(suprpisingly often correct)

(see also [Shein:iacse24]) (valuable tools in production situations) (like driving instead of jogging)



NOT a Resource for : LLMs – Al-based tools like ChatGPT

- Definition 3.21. A large language model (LLM) is a computational model capable of language generation or other natural language processing tasks.
- Example 3.22. OpenAl's GPT, Google's Bard, and Meta's Llama.
- **Definition 3.23.** A chatbot is a software application or web interface that is designed to mimic human conversation through text or voice interactions. Modern chatbots are usually based on LLMs.

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- Example 3.24 (ChatGPT talks about AI-1).
- Note: LLM-based chatbots invent every word!
- Example 3.25 (In the AI-1 exam). ChatGPT scores ca. 50% of the points.
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You will only pass the exam, if you can do Al-1 yourself!

- Intuition: AI tools like GhatGPT. CoPilot. etc.
 - can help vou solve problems.
 - hinders learning if used for homeworks/quizzes, etc.
- ► What (not) to do:
 - try out these tools to get a first-hand intuition what they can/cannot do
 - challenge yourself while learning so that you can also do it

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(We could award it a Master's degree) (the AI-1 exams will be in person on paper)

(see also [Shein:iacse24])

(but remains vague) (suprpisingly often correct)

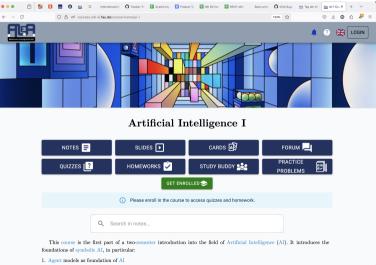
(valuable tools in production situations) (like driving instead of jogging)

(to get most of the brave new Al-supported world)

(mind over matter!)

ALEA in Al-2

 \blacktriangleright We assume that you already know the $\rm ALEA$ system from last semester





- \blacktriangleright We assume that you already know the $\rm ALEA$ system from last semester
- ► Use it for
 - lecture notes
 - flashcards
 - course forum
 - solving and peer-grading homework assignments
 - finding study groups
 - practicing with targeted problems
 - doing the prepquizzes

(notes- vs slides-oriented) (drill yourself on the Al-2 jargon/concepts) (questions, discussions and error reporting)

> (you need not endure AI-2 alone) (e.g. from old exams) (before each lecture)



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Chapter 21 Overview over AI and Topics of AI-II

21.1 What is Artificial Intelligence?



What is Artificial Intelligence? Definition

- Definition 1.1 (According to Wikipedia). Artificial Intelligence (AI) is intelligence exhibited by machines
- Definition 1.2 (also). Artificial Intelligence (AI) is a sub-field of CS that is concerned with the automation of intelligent behavior.
- **BUT:** it is already difficult to define intelligence precisely.
- Definition 1.3 (Elaine Rich). artificial intelligence (AI) studies how we can make the computer do things that humans can still do better at the moment.



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- **Elaine Rich:** Al studies how we can make the computer do things that humans can still do better at the moment.
- This needs a combination of

the ability to learn





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Inference

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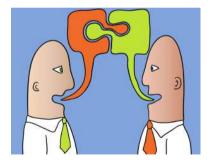
Perception





- **Elaine Rich:** Al studies how we can make the computer do things that humans can still do better at the moment.
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Language understanding



Contraction of the second

What is Artificial Intelligence? Components

- **Elaine Rich:** Al studies how we can make the computer do things that humans can still do better at the moment.
- This needs a combination of

Emotion







in outer space

- in outer space systems need autonomous control:
- remote control impossible due to time lag
- in artificial limbs
- ▶ in household appliances
- ► in hospitals
- for safety/security





▶ in outer space

- in artificial limbs
 - the user controls the prosthesis via existing nerves, can e.g. grip a sheet of paper.
- ▶ in household appliances
- ▶ in hospitals
- for safety/security







- ▶ in outer space
- ▶ in artificial limbs
- ► in household appliances
 - The iRobot Roomba vacuums, mops, and sweeps in corners, ..., parks, charges, and discharges.
 - general robotic household help is on the horizon.
- ▶ in hospitals
- for safety/security





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- ▶ in outer space
- ▶ in artificial limbs
- ► in household appliances
- ▶ in hospitals
 - in the USA 90% of the prostate operations are carried out by RoboDoc
 - Paro is a cuddly robot that eases solitude in nursing homes.
- for safety/security

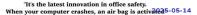






- ▶ in outer space
- in artificial limbs
- ► in household appliances
- ▶ in hospitals
- ▶ for safety/security
 - e.g. Intel verifies correctness of all chips after the "Pentium 5 disaster"







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- **• Observation:** Reserving the term "artificial intelligence" has been quite a land grab!
- But: researchers at the Dartmouth Conference (1956) really thought they would solve/reach AI in two/three decades.
- **Consequence:** Al still asks the big questions.

(and still promises answers soon)

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- ► Another Consequence: Al as a field is an incubator for many innovative technologies.
- ► AI Conundrum: Once AI solves a subfield it is called "CS". (becomes a separate subfield of CS)
- Example 2.1. Functional/Logic Programming, automated theorem proving, Planning, machine learning, Knowledge Representation, ...
- **Still Consequence:** Al research was alternatingly flooded with money and cut off brutally.

The history of AI as a discipline has been very much tied to the amount of funding – that allows us to do research and development.

<u>©</u>

- The history of AI as a discipline has been very much tied to the amount of funding that allows us to do research and development.
- Funding levels are tied to public perception of success

(especially for AI)



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(especially for AI)

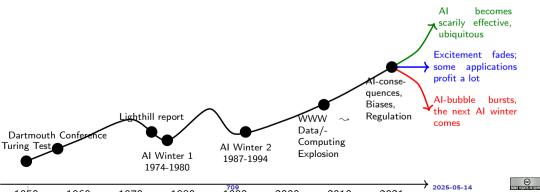
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(especially for AI)

(AI summers and summers)

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- A potted history of AI

FAU



21.3 Ways to Attack the AI Problem



Definition 3.1. Symbolic AI is a subfield of AI based on the assumption that many aspects of intelligence can be achieved by the manipulation of symbols, combining them into meaning-carrying structures (expressions) and manipulating them (using processes) to produce new expressions.



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- Definition 3.6. Statistical AI remedies the two shortcomings of symbolic AI approaches: that all concepts represented by symbols are crisply defined, and that all aspects of the world are knowable/representable in principle. Statistical AI adopts sophisticated mathematical models of uncertainty and uses them to create more accurate world models and reason about them.

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- Definition 3.11. Subsymbolic AI (also called connectionism or neural AI) is a subfield of AI that posits that intelligence is inherently tied to brains, where information is represented by a simple sequence pulses that are processed in parallel via simple calculations realized by neurons, and thus concentrates on neural computing.



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- Definition 3.16. Embodied AI posits that intelligence cannot be achieved by reasoning about the state of the world (symbolically, statistically, or connectivist), but must be embodied i.e. situated in the world, equipped with a "body" that can interact with it via sensors and actuators. Here, the main method for realizing intelligent behavior is by learning from the world.



▶ We can classify the AI approaches by their coverage and the analysis depth (they are complementary)

Deep	symbolic Al-1	not there yet cooperation?
Shallow	no-one wants this	statistical/sub symbolic Al-2
$\begin{array}{c} \text{Analysis} \uparrow \\ \text{Vs.} \\ \text{Coverage} \rightarrow \end{array}$	Narrow	Wide

- ► This semester we will cover foundational aspects of symbolic Al
- next semester concentrate on statistical/subsymbolic AI.

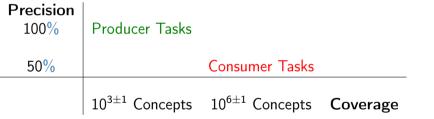
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(deep/narrow processing) (shallow/wide-coverage)



Environmental Niches for both Approaches to AI

- ▶ Observation: There are two kinds of applications/tasks in AI
 - Consumer tasks: consumer grade applications have tasks that must be fully generic and wide coverage. e.g. machine translation like Google Translate)
 - Producer tasks: producer grade applications must be high-precision, but can be domain-specific (e.g. multilingual documentation, machinery-control, program verification, medical technology)



after Aarne Ranta [Ranta:atcp17].

- ► General Rule: Subsymbolic AI is well suited for consumer tasks, while symbolic AI is better suited for producer tasks.
- A domain of producer tasks I am interested in: mathematical/technical documents.



21.4 AI in the KWARC Group



- Observation: The ability to represent knowledge about the world and to draw logical inferences is one of the central components of intelligent behavior.
- **Thus:** reasoning components of some form are at the heart of many AI systems.
- ► KWARC Angle: Scaling up (web-coverage) without dumbing down (too much)
 - Content markup instead of full formalization

Fau

- User support and quality control instead of "The Truth"
- use Mathematics as a test tube $(\triangle$ Mathematics $\hat{=}$ Anything Formal \triangle)
- care more about applications than about philosophy (we cannot help getting this right anyway as logicians)
- ► The KWARC group was established at Jacobs Univ. in 2004, moved to FAU Erlangen in 2016
- See http://kwarc.info for projects, publications, and links

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(too tedious)

(elusive anyway)

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Applications: eMath 3.0, Active Documents, Active Learning, Semantic Spreadsheets/CAD/CAM, Change Mangagement, Global Digital Math Library, Math Search Systems, SMGIoM: Semantic Multilingual Math Glossary, Serious Games,

Foundations of Math:

- ▶ MathML, OpenMath
- advanced Type Theories
- ► MMT: Meta Meta Theory
- Logic Morphisms/Atlas
- Theorem Prover/CAS Interoperability
- Mathematical Models/Simulation

KM & Interaction:

- Semantic Interpretation (aka. Framing)
- math-literate interaction
- MathHub: math archives & active docs
- Active documents: embedded semantic services
- Model-based Education

Semantization:

- ► LATEXWT: LATEX → XWT
- ► STEX: Semantic LATEX
- invasive editors
- Context-Aware IDEs
- Mathematical Corpora
- Linguistics of Math
- ML for Math Semantics Extraction

Foundations: Computational Logic, Web Technologies, OMDoc/MMT

- ▶ We are always looking for bright, motivated KWARCies.
- We have topics in for all levels!

(Enthusiast, Bachelor, Master, Ph.D.)

- List of current topics: https://gl.kwarc.info/kwarc/thesis-projects/
 - Automated Reasoning: Maths Representation in the Large
 - Logics development, (Meta)ⁿ-Frameworks
 - Math Corpus Linguistics: Semantics Extraction
 - Serious Games, Cognitive Engineering, Math Information Retrieval, Legal Reasoning, ...

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- ... last but not least: KWARC is the home of ALEA!
- We always try to find a topic at the intersection of your and our interests.
- ► We also sometimes have positions!.

(HiWi, Ph.D.: $\frac{1}{2}$ E-13, PostDoc: full E-13)



21.5 Agents and Environments in AI2

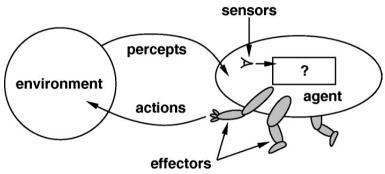


21.5.1 Recap: Rational Agents as a Conceptual Framework



Agents and Environments

- Definition 5.1. An agent is anything that
 - perceives its environment via sensors (a means of sensing the environment)
 - acts on it with actuators (means of changing the environment).
 - Any recognizable, coherent employment of the actuators of an agent is called an action.

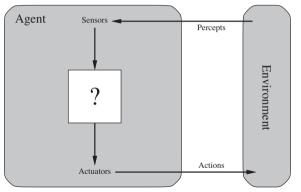


- **Example 5.2.** Agents include humans, robots, softbots, thermostats, etc.
- Remark: The notion of an agent and its environment is intentionally designed to be inclusive. We will classify and discuss subclasses of both later.



Agent Schema: Visualizing the Internal Agent Structure

Agent Schema: We will use the following kind of agent schema to visualize the internal structure of an agent:



Different agents differ on the contents of the white box in the center.



Idea: Try to design agents that are successful!

(aka. "do the right thing")

- ▶ Problem: What do we mean by "successful", how do we measure "success"?
- ▶ Definition 5.3. A performance measure is a function that evaluates a sequence of environments.
- **Example 5.4.** A performance measure for a vacuum cleaner could
 - award one point per "square" cleaned up in time T?
 - award one point per clean "square" per time step, minus one per move?
 - penalize for > k dirty squares?
- Definition 5.5. An agent is called rational, if it chooses whichever action maximizes the expected value of the performance measure given the percept sequence to date.
- Critical Observation: We only need to maximize the expected value, not the actual value of the performance measure!
- Question: Why is rationality a good quality to aim for?



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Consequences of Rationality: Exploration, Learning, Autonomy

Note: A rational agent need not be perfect:	
It only needs to maximize expected value	(rational \neq omniscient)
need not predict e.g. very unlikely but catastrophic events in the future	
Percepts may not supply all relevant information	(rational \neq clairvoyant)
 if we cannot perceive things we do not need to react to them. but we may need to try to find out about hidden dangers 	(exploration)
Action outcomes may not be as expected	(rational \neq successful)
but we may need to take action to ensure that they do (more often)	(learning)
▶ Note: Rationality may entail exploration, learning, autonomy (depending of	on the environment / task)
Definition 5.6. An agent is called autonomous, if it does not rely on the p environment of the designer.	rior knowledge about the

- Autonomy avoids fixed behaviors that can become unsuccessful in a changing environment. (anything
 else would be irrational)
- ▶ The agent may have to learn all relevant traits, invariants, properties of the environment and actions.



- Observation: To design a rational agent, we must specify the task environment in terms of performance measure, environment, actuators, and sensors, together called the PEAS components.
- **Example 5.7.** When designing an automated taxi:
 - Performance measure: safety, destination, profits, legality, comfort, ...
 - Environment: US streets/freeways, traffic, pedestrians, weather, ...
 - Actuators: steering, accelerator, brake, horn, speaker/display, ...
 - Sensors: video, accelerometers, gauges, engine sensors, keyboard, GPS, ...
- **Example 5.8 (Internet Shopping Agent).** The task environment:
 - Performance measure: price, quality, appropriateness, efficiency
 - Environment: current and future WWW sites, vendors, shippers
 - Actuators: display to user, follow URL, fill in form
 - Sensors: HTML pages (text, graphics, scripts)



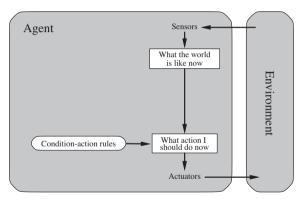
Environment types

- **• Observation 5.9.** Agent design is largely determined by the type of environment it is intended for.
- **Problem:** There is a vast number of possible kinds of environments in Al.
- Solution: Classify along a few "dimensions". (independent characteristics)
- **Definition 5.10.** For an agent *a* we classify the environment *e* of *a* by its type, which is one of the following. We call *e*
 - 1. fully observable, iff the *a*'s sensors give it access to the complete state of the environment at any point in time, else partially observable.
 - 2. deterministic, iff the next state of the environment is completely determined by the current state and *a*'s action, else stochastic.
 - 3. episodic, iff a's experience is divided into atomic episodes, where it perceives and then performs a single action. Crucially, the next episode does not depend on previous ones. Non-episodic environments are called sequential.
 - 4. dynamic, iff the environment can change without an action performed by *a*, else static. If the environment does not change but *a*'s performance measure does, we call *e* semidynamic.
 - 5. discrete, iff the sets of e's state and a's actions are countable, else continuous.
 - 6. single-agent, iff only a acts on e; else multi-agent



Reflex Agents

- ▶ Definition 5.11. An agent $\langle \mathcal{P}, \mathcal{A}, f \rangle$ is called a reflex agent, iff it only takes the last percept into account when choosing an action, i.e. $f(p_1, ..., p_k) = f(p_k)$ for all $p_1, ..., p_k \in \mathcal{P}$.
- ► Agent Schema:



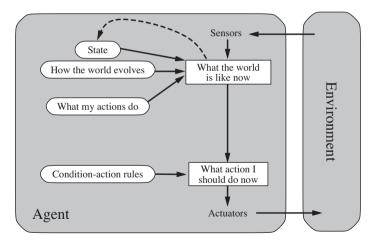
Example 5.12 (Agent Program).

```
procedure Reflex-Vacuum-Agent [location,status] returns an action
if status = Dirty then ...
```



Model-based Reflex Agents: Idea

- ▶ Idea: Keep track of the state of the world we cannot see in an internal model.
- ► Agent Schema:





- ▶ Definition 5.13. A model-based agent (P, A, S, T, s₀, S, a) is an agent (P, A, f) whose actions depend on
 - 1. a world model: a set S of possible states, and a start state $s_0 \in S$.
 - 2. a transition model \mathcal{T} , that predicts a new state $\mathcal{T}(s, a)$ from a state s and an action a.
 - 3. a sensor model S that given a state s and a percept p determine a new state S(s, p).
 - 4. an action function $a: S \rightarrow A$ that given a state selects the next action.

If the world model of a model-based agent A is in state s and A has last taken action a, and now perceives p, then A will transition to state $s' = S(p, \mathcal{T}(s, a))$ and take action a' = a(s'). So, given a sequence p_1, \ldots, p_n of percepts, we recursively define states $s_n = S(\mathcal{T}(s_{n-1}, a(s_{n-1})), p_n)$ with $s_1 = S(s_0, p_1)$. Then $f(p_1, \ldots, p_n) = a(s_n)$.

- Note: As different percept sequences lead to different states, so the agent function f(): P^{*} → A no longer depends only on the last percept.
- Example 5.14 (Tail Lights Again). Model-based agents can do the ??? if the states include a concept of tail light brightness.

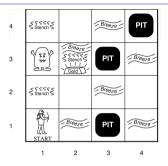


21.5.2 Sources of Uncertainty



Sources of Uncertainty in Decision-Making

Where's that d...Wumpus? And where am I, anyway??



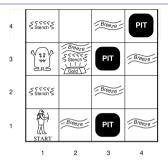
► Non-deterministic actions:

"When I try to go forward in this dark cave, I might actually go forward-left or forward-right."



Sources of Uncertainty in Decision-Making

Where's that d...Wumpus? And where am I, anyway??



Non-deterministic actions:

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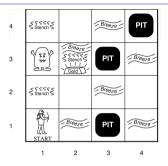
► Partial observability with unreliable sensors:

- "Did I feel a breeze right now?";
- "I think I might smell a Wumpus here, but I got a cold and my nose is blocked."
- "According to the heat scanner, the Wumpus is probably in cell [2,3]."



Sources of Uncertainty in Decision-Making

Where's that d...Wumpus? And where am I, anyway??



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- "Did I feel a breeze right now?";
- "I think I might smell a Wumpus here, but I got a cold and my nose is blocked."
- "According to the heat scanner, the Wumpus is probably in cell [2,3]."

Uncertainty about the domain behavior:

"Are you sure the Wumpus never moves?"



- Robot Localization: Suppose we want to support localization using landmarks to narrow down the area.
- **Example 5.15.** "If you see the Eiffel tower, then you're in Paris."



- Robot Localization: Suppose we want to support localization using landmarks to narrow down the area.
- **Example 5.16.** "If you see the Eiffel tower, then you're in Paris."
- **Difficulty:** Sensors can be imprecise.
 - Even if a landmark is perceived, we cannot conclude with certainty that the robot is at that location.
 - "This is the half-scale Las Vegas copy, you dummy."
 - Even if a landmark is not perceived, we cannot conclude with certainty that the robot is not at that location.
 - "Top of Eiffel tower hidden in the clouds."
- Only the probability of being at a location increases or decreases.



21.5.3 Agent Architectures based on Belief States



Problem: We do not know with certainty what state the world is in!



- **Problem:** We do not know with certainty what state the world is in!
- ▶ Idea: Just keep track of all the possible states it could be in.
- **Definition 5.18.** A model-based agent has a world model consisting of
 - ▶ a belief state that has information about the possible states the world may be in,
 - ▶ a sensor model that updates the belief state based on sensor information, and
 - a transition model that updates the belief state based on actions.



- **Problem:** We do not know with certainty what state the world is in!
- ▶ Idea: Just keep track of all the possible states it could be in.
- **Definition 5.19.** A model-based agent has a world model consisting of
 - ▶ a belief state that has information about the possible states the world may be in,
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- ▶ Idea: The agent environment determines what the world model can be.



- **Problem:** We do not know with certainty what state the world is in!
- ▶ Idea: Just keep track of all the possible states it could be in.
- Definition 5.20. A model-based agent has a world model consisting of
 - ▶ a belief state that has information about the possible states the world may be in,
 - a sensor model that updates the belief state based on sensor information, and
 - a transition model that updates the belief state based on actions.
- Idea: The agent environment determines what the world model can be.
- In a fully observable, deterministic environment,
 - we can observe the initial state and subsequent states are given by the actions alone.
 - Thus the belief state is a singleton (we call its sole member the world state) and the transition model is a function from states and actions to states: a transition function.



- Search-based Agents: In a fully observable, deterministic environment

 - no inference.

(goal $\widehat{=}$ goal state from search problem)

- CSP-based Agents: In a fully observable, deterministic environment
 - goal-based agent withworld state $\widehat{=}$ constraint network,
 - inference $\hat{=}$ constraint propagation.

(goal $\hat{=}$ satisfying assignment)

- ► Logic-based Agents: In a fully observable, deterministic environment
 - ▶ model-based agent with world state $\hat{=}$ logical formula
 - inference $\hat{=}$ e.g. DPLL or resolution.
- ▶ Planning Agents: In a fully observable, deterministic, environment
 - goal-based agent with world state \cong PL0, transition model \cong STRIPS,
 - inference $\hat{=}$ state/plan space search.

(goal: complete plan/execution)



In a fully observable, but stochastic environment,

- the belief state must deal with a set of possible states.
- \blacktriangleright \sim generalize the transition function to a transition relation.



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- ▶ Note: This even applies to online problem solving, where we can just perceive the state. (e.g. when we want to optimize utility)



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 - $\blacktriangleright \sim$ generalize the transition function to a transition relation.
- ▶ Note: This even applies to online problem solving, where we can just perceive the state. (e.g. when we want to optimize utility)
- In a deterministic, but partially observable environment,
 - the belief state must deal with a set of possible states.
 - we can use transition functions.
 - We need a sensor model, which predicts the influence of percepts on the belief state during update.



- In a fully observable, but stochastic environment,
 - the belief state must deal with a set of possible states.
 - $\blacktriangleright \rightsquigarrow$ generalize the transition function to a transition relation.
- ▶ Note: This even applies to online problem solving, where we can just perceive the state. (e.g. when we want to optimize utility)
- In a deterministic, but partially observable environment,
 - the belief state must deal with a set of possible states.
 - we can use transition functions.
 - ▶ We need a sensor model, which predicts the influence of percepts on the belief state during update.
- In a stochastic, partially observable environment,
 - mix the ideas from the last two.

Fau

(sensor model + transition relation)



- ▶ Probabilistic Agents: In a partially observable environment

 - inference $\widehat{=}$ probabilistic inference.



- ▶ Probabilistic Agents: In a partially observable environment

 - inference $\hat{=}$ probabilistic inference.
- ▶ Decision-Theoretic Agents: In a partially observable, stochastic environment

 - inference $\hat{=}$ maximizing expected utility.
- We will study them in detail this semester.



 Basics of probability theory independence,...)

(probability spaces, random variables, conditional probabilities,



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- Probabilistic reasoning: Computing the *a posteriori* probabilities of events given evidence, causal reasoning
 (Representing distributions efficiently, Bayesian networks,...)



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- Probabilistic reasoning: Computing the *a posteriori* probabilities of events given evidence, causal reasoning
 (Representing distributions efficiently, Bayesian networks,...)
- Probabilistic Reasoning over time

(Markov chains, Hidden Markov models,...)

 \Rightarrow We can update our world model episodically based on observations (i.e. sensor data)



Fau

- Basics of probability theory independence,...)
 (probability spaces, random variables, conditional probabilities,
- Probabilistic reasoning: Computing the *a posteriori* probabilities of events given evidence, causal reasoning
 (Representing distributions efficiently, Bayesian networks,...)
- Probabilistic Reasoning over time
- \Rightarrow We can update our world model episodically based on observations (i.e. sensor data)
- Decision theory: Making decisions under uncertainty Markov Decision Procedures,...)
 (Preferences, Utilities, Decision networks,
- $\Rightarrow\,$ We can choose the right action based on our world model and the likely outcomes of our actions

(Markov chains, Hidden Markov models,...)

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Machine learning: Learning from data

(Decision Trees, Classifiers, Neural Networks,...)

(Markov chains, Hidden Markov models,...)



Part 1 Reasoning with Uncertain Knowledge

Chapter 22 Quantifying Uncertainty

22.1 Probability Theory



22.1.1 Prior and Posterior Probabilities

FAU



- Definition 1.1 (Mathematically (slightly simplified)). A probability space or (probability model) is a pair $\langle \Omega, P \rangle$ such that:
 - Ω is a set of outcomes (called the sample space),
 - *P* is a function $\mathcal{P}(\Omega) \rightarrow [0,1]$, such that:
 - $P(\Omega) = 1$ and
 - $P(\bigcup_i A_i) = \sum_i P(A_i)$ for all pairwise disjoint $A_i \in \mathcal{P}(\Omega)$.
 - *P* is called a probability measure.

These properties are called the Kolmogorov axioms.

Intuition: We run some experiment, the outcome of which is any $\omega \in \Omega$.

- For $X \subseteq \Omega$, P(X) is the probability that the result of the experiment is *any one* of the outcomes in X.
- Naturally, the probability that any outcome occurs is 1 (hence $P(\Omega) = 1$).
- ▶ The probability of pairwise disjoint sets of outcomes should just be the sum of their probabilities.
- **Example 1.2 (Dice throws).** Assume we throw a (fair) die two times. Then the sample space Ω is $\{(i,j) | 1 \le i,j \le 6\}$. We define *P* by letting $P(\{A\}) = \frac{1}{36}$ for every $A \in \Omega$. Since the probability of any outcome is the same, we say *P* is uniformly distributed.



Fau

- In practice, we are rarely interested in the *specific* outcome of an experiment, but rather in some *property* of the outcome. This is especially true in the very common situation where we don't even *know* the precise probabilities of the individual outcomes.
- **Example 1.3.** The probability that the *sum* of our two dice throws is 7 is $P(\{(i,j) \in \Omega \mid i+j=7\}) = P(\{(6,1), (1,6), (5,2), (2,5), (4,3), (3,4)\}) = \frac{6}{36} = \frac{1}{6}.$
- ▶ Definition 1.4 (Again, slightly simplified). Let *D* be a set. A random variable is a function $X: \Omega \to D$. We call *D* (somewhat confusingly) the domain of *X*, denoted dom(*X*). For $x \in D$, we define the probability of *x* as $P(X = x) := P(\{\omega \in \Omega \mid X(\omega) = x\})$.
- Definition 1.5. We say that a random variable X is finite domain, iff its domain dom(X) is finite and Boolean, iff dom(X) = {T, F}.

For a Boolean random variable, we will simply write P(X) for P(X = T) and $P(\neg X)$ for P(X = F).



Some Examples

- **Example 1.6.** Summing up our two dice throws is a random variable $S: \Omega \to [2,12]$ with S((i,j)) = i + j. The probability that they sum up to 7 is written as $P(S = 7) = \frac{1}{6}$.
- **Example 1.7.** The first and second of our two dice throws are random variables First, Second: $\Omega \rightarrow [1,6]$ with First((i,j)) = i and Second((i,j)) = j.
- Remark 1.8. Note, that the identity $\Omega \to \Omega$ is a random variable as well.
- Example 1.9. We can model toothache, cavity and gingivitis as Boolean random variables, with the underlying probability space being...?? ~_(")_/~
- Example 1.10. We can model tomorrow's weather as a random variable with domain {sunny, rainy, foggy, warm, cloudy, humid, ...}, with the underlying probability space being...?? -_(\nu)_/^
- ⇒ This is why *probabilistic reasoning* is necessary: We can rarely reduce probabilistic scenarios down to clearly defined, fully known probability spaces and derive all the interesting things from there.
- **But:** The definitions here allow us to *reason* about probabilities and random variables in a *mathematically* rigorous way, e.g. to make our intuitions and assumptions precise, and prove our methods to be *sound*.



Fau

- This is nice and all, but in practice we are interested in "compound" probabilities like: "What is the probability that the sum of our two dice throws is 7, but neither of the two dice is a 3?"
- ▶ Idea: Reuse the syntax of propositional logic and define the logical connectives for random variables!
- **Example 1.11.** We can express the above as: $P(\neg(\text{First} = 3) \land \neg(\text{Second} = 3) \land (S = 7))$
- ▶ Definition 1.12. Let X_1, X_2 be random variables, $x_1 \in \text{dom}(X_1)$ and $x_2 \in \text{dom}(X_2)$. We define:
 - 1. $P(X_1 \neq x_1) := P(\neg (X_1 = x_1)) := P(\{\omega \in \Omega \mid X_1(\omega) \neq x_1\}) = 1 P(X_1 = x_1).$ 2. $P((X_1 = x_1) \land (X_2 = x_2)) := P(\{\omega \in \Omega \mid (X_1(\omega) = x_1) \land (X_2(\omega) = x_2)\})$
 - 2. $P((X_1 = X_1) \land (X_2 = X_2)) := P(\{\omega \in \Omega \mid (X_1(\omega) = X_1) \land (X_2(\omega) = X_2)\})$
 - $=P(\{\omega \in \Omega \mid X_1(\omega) = x_1\} \cap \{\omega \in \Omega \mid X_2(\omega) = x_2\}).$ 3. $P((X_1 = x_1) \lor (X_2 = x_2)) := P(\{\omega \in \Omega \mid (X_1(\omega) = x_1) \lor (X_2(\omega) = x_2)\})$
 - $= P(\{\omega \in \Omega \mid X_1(\omega) = x_1\} \cup \{\omega \in \Omega \mid X_2(\omega) = x_2\}).$

It is also common to write P(A, B) for $P(A \land B)$

► Example 1.13. $P((\text{First} \neq 3) \land (\text{Second} \neq 3) \land (S = 7)) = P(\{(1, 6), (6, 1), (2, 5), (5, 2)\}) = \frac{1}{9}$

- Definition 1.14 (Again slightly simplified). Let (Ω, P) be a probability space. An event is a subset of Ω.
- **Definition 1.15 (Convention).** We call an event (by extension) anything that *represents* a subset of Ω : any statement formed from the logical connectives and values of random variables, on which $P(\cdot)$ is defined.
- Problem 1.1

Remember: We can define $A \lor B := \neg(\neg A \land \neg B)$, $\top := A \lor \neg A$ and $F := \neg T$ – is this compatible with the definition of probabilities on propositional formulae? And why is $P(X_1 \neq x_1) = 1 - P(X_1 = x_1)$?

▶ **Problem 1.2 (Inclusion-Exclusion-Principle)** Show that $P(A \lor B) = P(A) + P(B) - P(A \land B)$.

▶ **Problem 1.3** Show that $P(A) = P(A \land B) + P(A \land \neg B)$



Conditional Probabilities

- ▶ Observation: As we gather new information, our beliefs (*should*) change, and thus our probabilities!
- **Example 1.16.** Your "probability of missing the connection train" increases when you are informed that your current train has 30 minutes delay.
- **Example 1.17.** The "probability of cavity" increases when the doctor is informed that the patient has a toothache.
- Example 1.18. The probability that S = 3 is clearly higher if I know that First = 1 than otherwise or if I know that First = 6!
- **Definition 1.19.** Let A and B be events where $P(B) \neq 0$. The conditional probability of A given B is defined as:

$$P(A \mid B) := \frac{P(A \land B)}{P(B)}$$

We also call P(A) the prior probability of A, and $P(A \mid B)$ the posterior probability.

lumination: If we assume B to hold, then we are only interested in the "part" of Ω where A is true relative to B.

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► Alternatively: We restrict our sample space Ω to the subset of outcomes where *B* holds. We then define a new probability space on this subset by scaling the probability measure so that it sums to 1 – which we do by dividing by P(B). (We "update our beliefs based on new evidence")

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Examples

Example 1.20. If we assume First = 1, then P(S = 3 | (First = 1)) should be precisely $P(Second = 2) = \frac{1}{6}$. We check:

$$P(S = 3 \mid (\text{First} = 1)) = \frac{P((S = 3) \land (\text{First} = 1))}{P(\text{First} = 1)} = \frac{1/36}{1/6} = \frac{1}{6}$$

Example 1.21. Assume the prior probability P(cavity) is 0.122. The probability that a patient has both a cavity and a toothache is $P(cavity \land toothache) = 0.067$. The probability that a patient has a toothache is P(toothache) = 0.15.

If the patient complains about a toothache, we can update our estimation by computing the posterior probability:

$$P(ext{cavity} \mid ext{toothache}) = rac{P(ext{cavity} \wedge ext{toothache})}{P(ext{toothache})} = rac{0.067}{0.15} = 0.45.$$

- Note: We just computed the probability of some underlying *disease* based on the presence of a *symptom*!
- ▶ More Generally: We computed the probability of a *cause* from observing its *effect*.



Some Rules

- Equations on unconditional probabilities have direct analogues for conditional probabilities.
- Problem 1.4 Convince yourself of the following:
 - ▶ $P(A \mid C) = 1 P(\neg A \mid C).$ ▶ $P(A \mid C) = P(A \land B \mid C) + P(A \land \neg B \mid C).$ ▶ $P(A \lor B \mid C) = P(A \mid C) + P(B \mid C) - P(A \land B \mid C).$
- But not on the right hand side!
- Problem 1.5

Find *counterexamples* for the following (false) claims:

$$\blacktriangleright P(A \mid C) = 1 - P(A \mid \neg C)$$

$$\blacktriangleright P(A \mid C) = P(A \mid (B \land C)) + P(A \mid (B \land \neg C)).$$

$$\blacktriangleright P(A \mid (B \lor C)) = P(A \mid B) + P(A \mid C) - P(A \mid (B \land C)).$$



Bayes' Rule

▶ Note: By definition, $P(A | B) = \frac{P(A \land B)}{P(B)}$. In practice, we often know the conditional probability already, and use it to compute the probability of the conjunction instead: $P(A \land B) = P(A | B) \cdot P(B) = P(B | A) \cdot P(A)$.



Bayes' Rule

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- ▶ Theorem 1.23 (Bayes' Theorem). Given propositions A and B where $P(A) \neq 0$ and $P(B) \neq 0$, we have:

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

Proof:
1.
$$P(A \mid B) = \frac{P(A \land B)}{P(B)} = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

...okay, that was straightforward... what's the big deal?



Bayes' Rule

- ▶ Note: By definition, $P(A | B) = \frac{P(A \land B)}{P(B)}$. In practice, we often know the conditional probability already, and use it to compute the probability of the conjunction instead: $P(A \land B) = P(A | B) \cdot P(B) = P(B | A) \cdot P(A)$.
- ▶ Theorem 1.24 (Bayes' Theorem). Given propositions A and B where $P(A) \neq 0$ and $P(B) \neq 0$, we have:

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

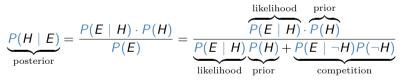
Proof:
1.
$$P(A \mid B) = \frac{P(A \land B)}{P(B)} = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

...okay, that was straightforward... what's the big deal?

- (Somewhat Dubious) Claim: Bayes' Rule is the entire scientific method condensed into a single equation!
- This is an extreme overstatement, but there is a grain of truth in it.



- Say we have a *hypothesis* H about the world.
- We have some prior belief P(H).
- ▶ We gather evidence E. (e.g. "We observe a cosmic microwave background at 2.7K everywhere")
- ▶ Bayes' Rule tells us how to *update our belief* in *H* based on *H*'s ability to *predict E* (the *likelihood* $P(E \mid H)$) *and*, importantly, the ability of *competing hypotheses* to predict the *same* evidence. (This is actually how scientific hypotheses should be evaluated)



... if I keep gathering evidence and update, ultimately the impact of the prior belief will diminish. "You're entitled to your own priors, but not your own likelihoods"

(e.g. "The universe had a beginning")



22.1.2 Independence



Independence

- Question: What is the probability that S = 7 and the patient has a toothache? Or less contrived: What is the probability that the patient has a gingivitis and a cavity?
- Definition 1.25. Two events A and B are called independent, iff P(A ∧ B) = P(A) · P(B). Two random variables X₁, X₂ are called independent, iff for all x₁ ∈ dom(X₁) and x₂ ∈ dom(X₂), the events X₁ = x₁ and X₂ = x₂ are independent. We write A ⊥ B or X₁ ⊥ X₂, respectively.
- Theorem 1.26. Equivalently: Given events A and B with P(B) ≠ 0, then A and B are independent iff P(A | B) = P(A) (equivalently: P(B | A) = P(B)).
 Proof:

1.
$$\Rightarrow$$

By definition, $P(A \mid B) = \frac{P(A \land B)}{P(B)} = \frac{P(A) \cdot P(B)}{P(B)} = P(A)$,
3. \Leftarrow
Assume $P(A \mid B) = P(A)$.
Then $P(A \land B) = P(A \mid B) \cdot P(B) = P(A) \cdot P(B)$.

Note: Independence asserts that two events are "not related" – the probability of one does not depend on the other.

Mathematically, we can determine independence by checking whether $P(A \land B) = P(A) \cdot P(B)$. In practice, this is impossible to check. Instead, we assume independence based on domain knowledge.

Example 1.27.

 First = 2 and Second = 3 are independent - more generally, First and Second are independent (The outcome of the first die does not affect the outcome of the second die) Quick check: P((First = a) ∧ (Second = b)) = ¹/₃₆ = P(First = a) · P(Second = b) √
 First and S are not independent. (The outcome of the first die affects the sum of the two dice.) Counterexample: P((First = 1) ∧ (S = 4)) = ¹/₃₆ ≠ P(First = 1) · P(S = 4) = ¹/₆ · ¹/₃ = ¹/₇₂



Example 1.29.

First = 2 and Second = 3 are independent - more generally, First and Second are independent (The outcome of the first die does not affect the outcome of the second die)
Quick check: P((First = a) ∧ (Second = b)) = ¹/₃₆ = P(First = a) · P(Second = b) √
First and S are not independent. (The outcome of the first die affects the sum of the two dice.) Counterexample: P((First = 1) ∧ (S = 4)) = ¹/₃₆ ≠ P(First = 1) · P(S = 4) = ¹/₆ · ¹/₂ = ¹/₇₂
But: P((First = a) ∧ (S = 7)) = ¹/₃₆ = ¹/₆ · ¹/₆ = P(First = a) · P(S = 7) - so the events First = a and S = 7 are independent. (Why?)



Example 1.31.

- First = 2 and Second = 3 are independent more generally, First and Second are independent (The outcome of the first die does not affect the outcome of the second die)
 Quick check: P((First = a) ∧ (Second = b)) = 1/36 = P(First = a) · P(Second = b) ✓
 First and S are not independent. (The outcome of the first die affects the sum of the two dice.) Counterexample: P((First = 1) ∧ (S = 4)) = 1/36 ≠ P(First = 1) · P(S = 4) = 1/6 · 1/2 = 1/72
 But: P((First = a) ∧ (S = 7)) = 1/36 = 1/6 · 1/6 = P(First = a) · P(S = 7) so the events First = a and S = 7 are independent. (Why?)
- Example 1.32.
 - Are cavity and toothache independent?



Example 1.33.

- First = 2 and Second = 3 are independent more generally, First and Second are independent (The outcome of the first die does not affect the outcome of the second die) Quick check: P((First = a) ∧ (Second = b)) = ¹/₃₆ = P(First = a) · P(Second = b) √
 First and S are not independent. (The outcome of the first die affects the sum of the two dice.) Counterexample: P((First = 1) ∧ (S = 4)) = ¹/₃₆ ≠ P(First = 1) · P(S = 4) = ¹/₆ · ¹/₃ = ¹/₇₂
- **But:** $P((\text{First} = a) \land (S = 7)) = \frac{1}{36} = \frac{1}{6} \cdot \frac{1}{6} = P(\text{First} = a) \cdot P(S = 7) \text{so the events First} = a \text{ and}$ S = 7 are independent. (Why?)

Example 1.34.

Are cavity and toothache independent?

... since cavities can cause a toothache, that would probably be a bad design decision ...



Example 1.35.

- First = 2 and Second = 3 are independent more generally, First and Second are independent (The outcome of the first die does not affect the outcome of the second die) Quick check: P((First = a) ∧ (Second = b)) = 1/36 = P(First = a) · P(Second = b) ✓
 First and S are not independent. (The outcome of the first die affects the sum of the two dice.)
- Counterexample: $P((\text{First} = 1) \land (S = 4)) = \frac{1}{36} \neq P(\text{First} = 1) \cdot P(S = 4) = \frac{1}{6} \cdot \frac{1}{2} = \frac{1}{72}$ **But:** $P((\text{First} = a) \land (S = 7)) = \frac{1}{26} = \frac{1}{6} \cdot \frac{1}{6} = P(\text{First} = a) \cdot P(S = 7)$ - so the events First = a and
- But: $P((\text{First} = \mathbf{a}) \land (5 = 7)) = \frac{1}{36} = \frac{1}{6} \cdot \frac{1}{6} = P(\text{First} = \mathbf{a}) \cdot P(5 = 7) \text{so the events First} = \mathbf{a} \text{ and}$ S = 7 are independent. (Why?)

Example 1.36.

Eau

- Are cavity and toothache independent?
 - \ldots since cavities can cause a toothache, that would probably be a bad design decision \ldots
- Are cavity and gingivitis independent? Cavities do not cause gingivitis, and gingivitis does not cause cavities, so... yes... right?
 (...as far as I know. I'm not a dentist.)

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Example 1.37.

- First = 2 and Second = 3 are independent more generally, First and Second are independent (The outcome of the first die does not affect the outcome of the second die)
 Quick check: P((First = a) ∧ (Second = b)) = ¹/₃₆ = P(First = a) · P(Second = b) ✓
 First and S are not independent. (The outcome of the first die affects the sum of the two dice.)
- Counterexample: $P((\text{First} = 1) \land (S = 4)) = \frac{1}{36} \neq P(\text{First} = 1) \land P(S = 4) = \frac{1}{6} \cdot \frac{1}{2} = \frac{1}{72}$
- But: $P((\text{First} = a) \land (S = 7)) = \frac{1}{36} = \frac{1}{6} \cdot \frac{1}{6} = P(\text{First} = a) \cdot P(S = 7)$ so the events First = a and S = 7 are independent. (Why?)

Example 1.38.

- Are cavity and toothache independent?
 - \ldots since cavities can cause a toothache, that would probably be a bad design decision \ldots
- Are cavity and gingivitis independent? Cavities do not cause gingivitis, and gingivitis does not cause cavities, so... yes... right?
 (...as far as I know. I'm not a dentist.)
- Probably not! A patient who has cavities has probably worse dental hygiene than those who don't, and is thus more likely to have gingivitis as well.
- ~ cavity may be evidence that raises the probability of gingivitis, even if they are not directly causally related.



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- A dentist can diagnose a cavity by using a *probe*, which may (or may not) *catch* in a cavity.
- Say we know from clinical studies that P(cavity) = 0.2, P(toothache | cavity) = 0.6, P(toothache | ¬cavity) = 0.1, P(catch | cavity) = 0.9, and P(catch | ¬cavity) = 0.2.
- ► Assume the patient complains about a toothache, and our probe indeed catches in the aching tooth. What is the likelihood of having a cavity P(cavity | (toothache ∧ catch))?



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- ► Idea: Use Bayes' rule:

 $P(ext{cavity} \mid (ext{toothache} \land ext{catch})) = rac{P(ext{toothache} \land ext{catch} \mid ext{cavity}) \cdot P(ext{cavity})}{P(ext{toothache} \land ext{catch})}$

- ▶ Note: $P(\text{toothache} \land \text{catch}) = P(\text{toothache} \land \text{catch} \mid \text{cavity}) \cdot P(\text{cavity}) + P(\text{toothache} \land \text{catch} \mid \neg \text{cavity}) \cdot P(\neg \text{cavity})$
- ▶ Problem: Now we're only missing $P(\text{toothache} \land \text{catch} \mid (\text{cavity} = b))$ for $b \in \{T, F\}$ Now what?

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- ► Assume the patient complains about a toothache, and our probe indeed catches in the aching tooth. What is the likelihood of having a cavity P(cavity | (toothache ∧ catch))?

► Idea: Use Bayes' rule:

 $P(ext{cavity} \mid (ext{toothache} \land ext{catch})) = rac{P(ext{toothache} \land ext{catch} \mid ext{cavity}) \cdot P(ext{cavity})}{P(ext{toothache} \land ext{catch})}$

- ▶ Note: $P(\text{toothache} \land \text{catch}) = P(\text{toothache} \land \text{catch} \mid \text{cavity}) \cdot P(\text{cavity}) + P(\text{toothache} \land \text{catch} \mid \neg \text{cavity}) \cdot P(\neg \text{cavity})$
- ▶ Problem: Now we're only missing $P(\text{toothache} \land \text{catch} \mid (\text{cavity} = b))$ for $b \in \{\mathsf{T},\mathsf{F}\}$ Now what?
- Are toothache and catch independent, maybe? No: Both have a common (possible) cause, cavity. Also, there's this pesky $P(\cdot | \text{ cavity})$ in the way.....wait a minute...



Conditional Independence – Definition

Assuming the patient has (or does not have) a cavity, the events toothache and catch are independent: Both are caused by a cavity, but they don't influence each other otherwise. i.e. cavity "contains all the information" that links toothache and catch in the first place.



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Definition 1.41. Given events A, B, C with P(C) ≠ 0, then A and B are called conditionally independent given C, iff P(A ∧ B | C) = P(A | C) · P(B | C). Equivalently: iff P(A | (B ∧ C)) = P(A | C), or P(B | (A ∧ C)) = P(B | C).

Let Y be a random variable. We call two random variables X_1, X_2 conditionally independent given Y, iff for all $x_1 \in \text{dom}(X_1)$, $x_2 \in \text{dom}(X_2)$ and $y \in \text{dom}(Y)$, the events $X_1 = x_1$ and $X_2 = x_2$ are conditionally independent given Y = y.



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Assuming the patient has (or does not have) a cavity, the events toothache and catch are independent: Both are caused by a cavity, but they don't influence each other otherwise. i.e. cavity "contains all the information" that links toothache and catch in the first place.

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► Example 1.44. Let's assume toothache and catch are conditionally independent given cavity/¬cavity. Then we can finally compute: $P(\text{cavity} \mid (\text{toothache} \land \text{catch})) = \frac{P(\text{toothache} \land \text{catch} \mid \text{cavity}) \cdot P(\text{cavity})}{P(\text{toothache} \land \text{catch})}$ $= \frac{P(\text{toothache} \mid \text{cavity}) \cdot P(\text{catch} \mid \text{cavity}) \cdot P(\text{cavity})}{P(\text{toothache} \mid \text{cavity}) \cdot P(\text{cavity})}$ $= \frac{0.6 \cdot 0.9 \cdot 0.2}{0.6 \cdot 0.9 \cdot 0.2 + 0.1 \cdot v 0.2 \cdot 0.8} = 0.87$



Conditional Independence

► Lemma 1.45. If A and B are conditionally independent given C, then $P(A \mid (B \land C)) = P(A \mid C)$ Proof: $P(A \mid (B \land C)) = \frac{P(A \land B \land C)}{P(B \land C)} = \frac{P(A \land B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \land C)}{P(B \land C)} = P(A \mid C)$

Question: If A and B are conditionally independent given C, does this imply that A and B are independent?



Conditional Independence

► Lemma 1.46. If A and B are conditionally independent given C, then $P(A \mid (B \land C)) = P(A \mid C)$ Proof: $P(A \mid (B \land C)) = \frac{P(A \land B \land C)}{P(B \land C)} = \frac{P(A \land B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \land C)}{P(B \land C)} = P(A \mid C)$

- Question: If A and B are conditionally independent given C, does this imply that A and B are independent? No. See previous slides for a counterexample.
- Question: If A and B are independent, does this imply that A and B are also conditionally independent given C?



► Lemma 1.47. If A and B are conditionally independent given C, then $P(A \mid (B \land C)) = P(A \mid C)$ Proof: $P(A \mid (B \land C)) = \frac{P(A \land B \land C)}{P(B \land C)} = \frac{P(A \land B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \land C)}{P(B \land C)} = P(A \mid C)$

- Question: If A and B are conditionally independent given C, does this imply that A and B are independent? No. See previous slides for a counterexample.
- ► Question: If A and B are independent, does this imply that A and B are also conditionally independent given C? No. For example: First and Second are independent, but not conditionally independent given S = 4.



► Lemma 1.48. If A and B are conditionally independent given C, then $P(A \mid (B \land C)) = P(A \mid C)$ Proof: $P(A \mid (B \land C)) = \frac{P(A \land B \land C)}{P(B \land C)} = \frac{P(A \land B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \land C)}{P(B \land C)} = P(A \mid C)$

- Question: If A and B are conditionally independent given C, does this imply that A and B are independent? No. See previous slides for a counterexample.
- ► Question: If A and B are independent, does this imply that A and B are also conditionally independent given C? No. For example: First and Second are independent, but not conditionally independent given S = 4.
- Question: Okay, so what if A, B and C are all pairwise independent? Are A and B conditionally independent given C now?



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► Lemma 1.49. If A and B are conditionally independent given C, then $P(A \mid (B \land C)) = P(A \mid C)$ Proof: $P(A \mid (B \land C)) = \frac{P(A \land B \land C)}{P(B \land C)} = \frac{P(A \land B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \land C)}{P(B \land C)} = P(A \mid C)$

- Question: If A and B are conditionally independent given C, does this imply that A and B are independent? No. See previous slides for a counterexample.
- ► Question: If A and B are independent, does this imply that A and B are also conditionally independent given C? No. For example: First and Second are independent, but not conditionally independent given S = 4.
- Question: Okay, so what if A, B and C are all pairwise independent? Are A and B conditionally independent given C now? Still no. Remember: First = a, Second = b and S = 7 are all independent, but First and Second are not conditionally independent given S = 7.
- Question: When can we infer conditional independence from a "more general" notion of independence?

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► Lemma 1.50. If A and B are conditionally independent given C, then $P(A \mid (B \land C)) = P(A \mid C)$ Proof: $P(A \mid (B \land C)) = \frac{P(A \land B \land C)}{P(B \land C)} = \frac{P(A \land B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \mid C) \cdot P(C)}{P(B \land C)} = \frac{P(A \mid C) \cdot P(B \land C)}{P(B \land C)} = P(A \mid C)$

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- Question: When can we infer conditional independence from a "more general" notion of independence?

We need *mutual independence*. Roughly: A set of events is called *mutually* independent, if every event is independent from *any conjunction of the others*. (Not really relevant for this course though)



22.1.3 Conclusion



- Probability spaces serve as a mathematical model (and hence justification) for everything related to probabilities.
- The "atoms" of any statement of probability are the random variables. (Important special cases: Boolean and finite domain)
- We can define probabilities on compund (propositional logical) statements, with (outcomes of) random variables as "propositional variables".
- Conditional probabilities represent posterior probabilities given some observed outcomes.
- Independence and conditional independence are strong assumptions that allow us to simplify computations of probabilities
- Bayes' Theorem (can be used between "causal" and "diagnostic" conditional probabilities)



So much about the math...

- We now have a mathematical setup for probabilities.
- **But:** The math does not tell us what probabilities *are*:
- Assume we can mathematically derive this to be the case: the probability of rain tomorrow is 0.3. What does this even mean?



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- ▶ Objection: And why should I? Is this not purely subjective then?



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- Pragmatically both interpretations amount to the same thing: I should act as if I'm 30% confident that it will rain tomorrow. (Whether by fiat, or because in 30% of comparable cases, it rained.)
- Objection: Still: why should I? And why should my beliefs follow the seemingly arbitrary Kolmogorov axioms?



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- [deFinetti:sssdp31]: If an agent has a belief that violates the Kolmogorov axioms, then there exists a combination of "bets" on propositions so that the agent *always* loses money.
- In other words: If your beliefs are not consistent with the mathematics, and you act in accordance with your beliefs, there is a way to exploit this inconsistency to your disadvantage.



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- In other words: If your beliefs are not consistent with the mathematics, and you act in accordance with your beliefs, there is a way to exploit this inconsistency to your disadvantage.
- \blacktriangleright ... and, more importantly, the AI agents you design! \odot
- I (and my agents) do not bet: That is not true, in a partially observable or non-deterministic world, every action choice is a necessarily bet: The outcome is not sure.



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22.2 Probabilistic Reasoning Techniques



- ▶ This is a CS course. We need to implement this stuff.
- ▶ Do we... implement random variables as functions? Is a probability space a... class maybe?



- ▶ This is a CS course. We need to implement this stuff.
- ▶ Do we... implement random variables as functions? Is a probability space a... class maybe?
- ▶ No: As mentioned, we rarely know the probability space entirely. Instead we will use probability distributions, which are just arrays (of arrays of...) of probabilities.
- And then we represent those as sparsely as possible, by exploiting independence, conditional independence, ...



22.2.1 Probability Distributions



Probability Distributions

- ▶ Definition 2.1. The probability distribution for a random variable X, written P(X), is the vector of probabilities for the (ordered) domain of X.
- ▶ Note: The values in a probability distribution are all positive and sum to 1. (Why?)
- **Example 2.2.** $\mathbb{P}(\text{First}) = \mathbb{P}(\text{Second}) = \langle \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6} \rangle$. (Both First and Second are uniformly distributed)
- ► Example 2.3. The probability distribution P(S) is (¹/₃₆, ¹/₁₈, ¹/₁₂, ¹/₉, ⁵/₃₆, ¹/₆, ⁵/₃₆, ¹/₉, ¹/₁₂, ¹/₁₈, ¹/₃₆). Note the symmetry, with a "peak" at 7 the random variable is (*approximately*, because our domain is discrete rather than continuous) normally distributed (or gaussian distributed, or follows a bell-curve,...).
- Example 2.4. Probability distributions for Boolean random variables are naturally pairs (probabilities for T and F), e.g.:

 $\mathbb{P}(ext{toothache}) = \langle 0.15, 0.85 \rangle$ $\mathbb{P}(ext{cavity}) = \langle 0.122, 0.878 \rangle$

- ► More generally:
- **Definition 2.5.** A probability distribution is a vector v of values $v_i \in [0,1]$ such that $\sum_i v_i = 1$.

The Full Joint Probability Distribution

- ▶ Definition 2.6. Given random variables X₁,...,X_n with domains D₁,...,D_n, the full joint probability distribution, denoted P(X₁,...,X_n), is the n-dimensional array of size |D₁ × ... × D_n| that lists the probabilities of all conjunctions of values of the random variables.
- **Example 2.7.** $\mathbb{P}(cavity, toothache, gingivitis)$ could look something like this:

		toothache		¬toothache
	gingivitis	\neg gingivitis	gingivitis	\neg gingivitis
cavity	0.007	0.06	0.005	0.05
¬cavity	0.08	0.003	0.045	0.75

Example 2.8. $\mathbb{P}(\text{First}, S)$

First $\setminus S$	2	3	4	5	6	7	8	9	10	11	12
1	$\frac{1}{36}$	$\frac{1}{3.6}$	$\frac{1}{3.6}$	$\frac{1}{3.6}$	$\frac{1}{3.6}$	$\frac{1}{36}$	0	0	0	0	0
2	0	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	0	0	0	0
3	0	0	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	0	0	0
4	0	0	0	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	0	0
5	0	0	0	0	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	0
6	0	0	0	0	0	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$
1 .I [']		C T			C (~ •					

Note that if we know the value of First, the value of S is completely determined by the value of Second.



Conditional Probability Distributions

- ▶ **Definition 2.9.** Given random variables X and Y, the conditional probability distribution of X given Y, written $\mathbb{P}(X|Y)$ is the table of all conditional probabilities of values of X given values of Y.
- ► For sets of variables analogously: $\mathbb{P}(X_1, ..., X_n | Y_1, ..., Y_m)$.
- **Example 2.10.** $\mathbb{P}(\text{cavity}|\text{toothache})$:

	toothache	¬toothache				
cavity	$P(\text{cavity} \mid \text{toothache}) = 0.45$	$P(\text{cavity} \mid \neg \text{toothache}) = 0.065$				
¬cavity	$P(\neg \text{cavity} \mid \text{toothache}) = 0.55$	$P(\neg cavity \neg toothache) = 0.935$				

Example 2.11. $\mathbb{P}(\text{First}|S)$

First $\setminus S$	2	3	4	5	6	7	8	9	10	11	12
1	1	$\frac{1}{2}$	1/3	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	0	0	0	0	0
2	0	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{5}$	0	0	0	0
3	0	ō	$\frac{1}{3}$	$\frac{1}{4}$	1 5	$\frac{1}{6}$	<u>1</u> 5	$\frac{1}{4}$	0	0	0
4	0	0	ŏ	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	1	0	0
5	0	0	0	Ō	$\frac{1}{5}$	$\frac{1}{6}$	1 5	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	0
6	0	0	0	0	Ŏ	$\frac{1}{6}$	15	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1

Note: Every "column" of a conditional probability distribution is itself a probability distribution. (Why?)



- > We now "lift" multiplication and division to the level of whole probability distributions:
- ▶ **Definition 2.12.** Whenever we use P in an equation, we take this to mean a system of equations, for each value in the domains of the random variables involved.

Example 2.13.

 P(X, Y) = P(X|Y) · P(Y) represents the system of equations
 P(X = x ∧ Y = y) = P(X = x | Y = y) · P(Y = y) for all x, y in the respective domains.

 P(X|Y) := P(X,Y) represents the system of equations
 P(X = x | (Y = y)) := P((X=x) ∧ (Y=y))

 Bayes' Theorem: P(X|Y) = P(Y|X)·P(X) represents the system of equations
 P(X = x | (Y = y)) = P(Y=y) (X=x))·P(X=x)



- Obviously, the probability distribution contains all the information about a specific random variable we need.
- ▶ **Observation:** The full joint probability distribution of variables X₁,...,X_n contains *all* the information about the random variables *and their conjunctions* we need.
- **Example 2.14.** We can read off the probability P(toothache) from the full joint probability distribution as 0.007 + 0.06 + 0.08 + 0.003 = 0.15, and the probability $P(\text{toothache} \land \text{cavity})$ as 0.007 + 0.06 = 0.067
- We can actually implement this!

(They're just (nested) arrays)

- **But:** just as we often don't have a fully specified probability space to work in, we often don't have a full joint probability distribution for our random variables either.
- ► Also: Given random variables $X_1, ..., X_n$, the full joint probability distribution has $\prod_{i=1}^n |\text{dom}(X_i)|$ entries! (P(First, S) already has 60 entries!)
- So: The rest of this section deals with keeping things small, by computing probabilities instead of storing them all.



Probabilistic reasoning refers to inferring probabilities of events from the probabilities of other events

as opposed to determining the probabilities e.g. *empirically*, by gathering (sufficient amounts of *representative*) data and counting.

- ▶ Note: In practice, we are *primarily* interested in, and have access to, conditional probabilities rather than the unconditional probabilities of conjunctions of events:
 - We don't reason in a vacuum: Usually, we have some evidence and want to infer the posterior probability of some related event. (e.g. infer a plausible *cause* given some *symptom*)
 we are interested in the conditional probability *P*(hypothesis | observation).
 - "80% of patients with a cavity complain about a toothache" (i.e. P(toothache | cavity)) is more the kind of data people actually collect and publish than "1.2% of the general population have both a cavity and a toothache" (i.e. P(cavity ∧ toothache)).
 - Consider the probe catching in a cavity. The probe is a diagnostic tool, which is usually evaluated in terms of its sensitivity P(catch | cavity) and specificity P(¬catch | ¬cavity). (You have probably heard these words a lot since 2020...)

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22.2.2 Naive Bayes



Consider again the dentistry example with random variables cavity, toothache, and catch. We assume cavity causes both toothache and catch, and that toothache and catch are conditionally independent given cavity:



- ▶ We likely know the sensitivity P(catch | cavity) and specificity P(¬catch | ¬cavity), which jointly give us P(catch|cavity), and from medical studies, we should be able to determine P(cavity) (the prevalence of cavities in the population) and P(toothache|cavity).
- This kind of situation is surprisingly common, and therefore deserves a name.





- Definition 2.15. A naive Bayes model (or, less accurately, Bayesian classifier, or, derogatorily, idiot Bayes model) consists of:
 - 1. random variables C, E_1, \ldots, E_n such that all the E_1, \ldots, E_n are conditionally independent given C,
 - 2. the probability distribution $\mathbb{P}(C)$, and
 - 3. the conditional probability distributions $\mathbb{P}(E_i|C)$.

We call C the cause and the E_1, \ldots, E_n the effects of the model.

- Convention: Whenever we draw a graph of random variables, we take the arrows to connect *causes* to their direct *effects*, and assert that unconnected nodes are conditionally independent given all their ancestors. We will make this more precise later.
- ► Can we compute the full joint probability distribution P(cavity, toothache, catch) from this information?



Recovering the Full Joint Probability Distribution

- Lemma 2.16 (Product rule). $\mathbb{P}(X, Y) = \mathbb{P}(X|Y) \cdot \mathbb{P}(Y)$.
- ▶ We can generalize this to more than two variables, by repeatedly applying the product rule:
- **Lemma 2.17 (Chain rule).** For any sequence of random variables X_1, \ldots, X_n :

$$\mathbb{P}(X_1,\ldots,X_n) = \mathbb{P}(X_1|X_2,\ldots,X_n) \cdot \mathbb{P}(X_2|X_3,\ldots,X_n) \cdot \ldots \cdot \mathbb{P}(X_{n-1}|X_n) \cdot P(X_n)$$

Hence:

Theorem 2.18. Given a naive Bayes model with effects E_1, \ldots, E_n and cause C, we have

$$\mathbb{P}(C, E_1, \ldots, E_n) = \mathbb{P}(C) \cdot (\prod_{i=1}^n \mathbb{P}(E_i | C)).$$

- Proof: Using the chain rule:
 - 1. $\mathbb{P}(E_1, \ldots, E_n, C) = \mathbb{P}(E_1 | E_2, \ldots, E_n, C) \cdot \ldots \cdot \mathbb{P}(E_n | C) \cdot \mathbb{P}(C)$

2. Since all the E_i are conditionally independent, we can drop them on the right hand sides of the $\mathbb{P}(E_j|..., C)$

Marginalization

• Great, so now we can compute $\mathbb{P}(C|E_1,...,E_n) = \frac{\mathbb{P}(C,E_1,...,E_n)}{\mathbb{P}(E_1,...,E_n)}$except that we don't know $\mathbb{P}(E_1,...,E_n)$:-/

...except that we can compute the full joint probability distribution, so we can recover it:

► Lemma 2.19 (Marginalization). Given random variables $X_1, ..., X_n$ and $Y_1, ..., Y_m$, we have $\mathbb{P}(X_1, ..., X_n) = \sum_{y_1 \in \text{dom}(Y_1), ..., y_m \in \text{dom}(Y_m)} \mathbb{P}(X_1, ..., X_n, Y_1 = y_1, ..., Y_m = y_m).$

(This is just a fancy way of saying "we can add the relevant entries of the full joint probability distribution")

Example 2.20. Say we observed toothache = T and catch = T. Using marginalization, we can compute

$$P(\operatorname{cavity} \mid (\operatorname{toothache} \wedge \operatorname{catch})) = \frac{P(\operatorname{cavity} \wedge \operatorname{toothache} \wedge \operatorname{catch})}{P(\operatorname{toothache} \wedge \operatorname{catch})}$$
$$= \frac{P(\operatorname{cavity} \wedge \operatorname{toothache} \wedge \operatorname{catch})}{\sum_{\boldsymbol{c} \in \{\operatorname{cavity}, \neg \operatorname{cavity}\}} P(\boldsymbol{c} \wedge \operatorname{toothache} \wedge \operatorname{catch})}$$
$$= \frac{P(\operatorname{cavity}) \cdot P(\operatorname{toothache} \mid \operatorname{cavity}) \cdot P(\operatorname{catch} \mid \operatorname{cavity})}{\sum_{\boldsymbol{c} \in \{\operatorname{cavity}, \neg \operatorname{cavity}\}} P(\boldsymbol{c}) \cdot P(\operatorname{toothache} \mid \boldsymbol{c}) \cdot P(\operatorname{catch} \mid \boldsymbol{c})}$$



Unknowns

▶ What if we don't know catch?

(I'm not a dentist, I don't have a probe...)

- ▶ We split our effects into $\{E_1, ..., E_n\} = \{O_1, ..., O_{n_0}\} \cup \{U_1, ..., U_{n_U}\}$ the observed and unknown random variables.
- Let $D_U := \operatorname{dom}(U_1) \times \ldots \times \operatorname{dom}(U_{n_u})$. Then

$$\mathbb{P}(C|O_{1},...,O_{n_{0}}) = \frac{\mathbb{P}(C,O_{1},...,O_{n_{0}})}{\mathbb{P}(O_{1},...,O_{n_{0}})} \\
= \frac{\sum_{u \in D_{U}} \mathbb{P}(C,O_{1},...,O_{n_{0}},U_{1} = u_{1},...,U_{n_{u}} = u_{n_{u}})}{\sum_{c \in dom(C)} \sum_{u \in D_{U}} \mathbb{P}(O_{1},...,O_{n_{0}},C = c,U_{1} = u_{1},...,U_{n_{u}} = u_{n_{u}})} \\
= \frac{\sum_{u \in D_{U}} \mathbb{P}(C) \cdot (\prod_{i=1}^{n_{0}} \mathbb{P}(O_{i}|C)) \cdot (\prod_{j=1}^{n_{U}} \mathbb{P}(U_{j} = u_{j}|C))}{\sum_{c \in dom(C)} \sum_{u \in D_{U}} P(C = c) \cdot (\prod_{i=1}^{n_{0}} \mathbb{P}(O_{i}|C = c)) \cdot (\prod_{j=1}^{n_{U}} P(U_{j} = u_{j}|(C = c)))} \\
= \frac{\mathbb{P}(C) \cdot (\prod_{i=1}^{n_{0}} \mathbb{P}(O_{i}|C)) \cdot (\sum_{u \in D_{U}} \prod_{j=1}^{n_{U}} \mathbb{P}(U_{j} = u_{j}|C))}{\sum_{c \in dom(C)} P(C = c) \cdot (\prod_{i=1}^{n_{0}} \mathbb{P}(O_{i}|C = c)) \cdot (\sum_{u \in D_{U}} \prod_{j=1}^{n_{U}} P(U_{j} = u_{j}|(C = c)))} \\$$



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Unknowns

Continuing from above:

$$\mathbb{P}(C|O_1,\ldots,O_{n_0}) = \frac{\mathbb{P}(C) \cdot (\prod_{i=1}^{n_0} \mathbb{P}(O_i|C)) \cdot (\sum_{u \in D_U} \prod_{j=1}^{n_U} \mathbb{P}(U_j = u_j|C))}{\sum_{c \in \text{dom}(C)} P(C = c) \cdot (\prod_{i=1}^{n_0} \mathbb{P}(O_i|C = c)) \cdot (\sum_{u \in D_U} \prod_{j=1}^{n_U} P(U_j = u_j \mid (C = c)))}$$

First, note that $\sum_{u \in D_U} \prod_{j=1}^{n_U} P(U_j = u_j \mid (C = c)) = 1$ (We're summing over all possible events on the (conditionally independent) U_1, \ldots, U_{n_U} given C = c)

$$\mathbb{P}(C|O_1,\ldots,O_{n_0}) = \frac{\mathbb{P}(C) \cdot (\prod_{i=1}^{n_0} \mathbb{P}(O_i|C))}{\sum_{c \in \text{dom}(C)} P(C=c) \cdot (\prod_{i=1}^{n_0} \mathbb{P}(O_i|C=c))}$$

- Secondly, note that the *denominator* is
 - 1. the same for any given observations O_1, \ldots, O_{n_0} , independent of the value of C, and
 - 2. the sum over all the numerators in the full distribution.

That is: The denominator only serves to *scale* what is *almost* already the distribution $\mathbb{P}(C|O_1, \ldots, O_{n_0})$ to sum up to 1.



Normalization

Definition 2.21 (Normalization). Given a vector $w := \langle w_1, \ldots, w_k \rangle$ of numbers in [0,1] where $\sum_{i=1}^{k} w_i < 1.$

Then the normalized vector $\alpha(w)$ is defined (component-wise) as

$$(\alpha(w))_i := \frac{w_i}{\sum_{j=1}^k w_j}$$

Note that $\sum_{i=1}^{k} \alpha(w)_i = 1$, i.e. $\alpha(w)$ is a probability distribution.

This finally gives us: **Theorem 2.22 (Inference in a Naive Bayes model).** Let C, E_1, \ldots, E_n a naive Bayes model and $E_1, \ldots, E_n = O_1, \ldots, O_{n_0}, U_1, \ldots, U_{n_{11}}$ Then na

$$\mathbb{P}(C|O_1 = o_1, \ldots, O_{n_o} = o_{n_o}) = \alpha(\mathbb{P}(C) \cdot (\prod_{i=1}^{n_o} \mathbb{P}(O_i = o_i|C)))$$

- ▶ Note, that this is entirely independent of the unknown random variables U_1, \ldots, U_{nu} !
- Also, note that this is just a fancy way of saying "first, compute all the numerators, then divide all of them by their sums".



Putting things together, we get:

$$\begin{split} \mathbb{P}(\text{cavity}|\text{toothache} = \mathsf{T}) &= \alpha(\mathbb{P}(\text{cavity}) \cdot \mathbb{P}(\text{toothache} = \mathsf{T}|\text{cavity})) \\ &= \alpha(\langle P(\text{cavity}) \cdot P(\text{toothache} \mid \text{cavity}), P(\neg \text{cavity}) \cdot P(\text{toothache} \mid \neg \text{cavity}) \rangle) \end{split}$$

Say we have P(cavity) = 0.1, P(toothache | cavity) = 0.8, and P(toothache | ¬cavity) = 0.05. Then

 $\mathbb{P}(\text{cavity}|\text{toothache} = \mathsf{T}) = \alpha(\langle \mathsf{0.1} \cdot \mathsf{0.8}, \mathsf{0.9} \cdot \mathsf{0.05} \rangle) = \alpha(\langle \mathsf{0.08}, \mathsf{0.045} \rangle)$

0.08 + 0.045 = 0.125, hence

$$\mathbb{P}(\mathrm{cavity}|\mathrm{toothache}=\mathsf{T}) = \langle \frac{0.08}{0.125}, \frac{0.045}{0.125} \rangle = \langle 0.64, 0.36 \rangle$$

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Naive Bayes Classification

We can use a naive Bayes model as a very simple *classifier*.

- Assume we want to classify newspaper articles as one of the categories *politics*, *sports*, *business*, *fluff*, etc. based on the words they contain.
- ► Given a large set of articles, we can determine the relevant probabilities by counting the occurrences of the categories P(category), and of words per category i.e. P(word_i|category) for some (huge) list of words (word_i)ⁿ_{i=1}.
- We assume that the occurrence of each word is conditionally independent of the occurrence of any other word given the category of the document. (This assumption is clearly wrong, but it makes the model simple and often works well in practice.)
 (~ "Idiot Bayes model")
- Given a new article, we just count the occurrences k_i of the words in it and compute

$$\mathbb{P}(\text{category}|\text{word}_1 = k_1, \dots, \text{word}_n = k_n) = \alpha(\mathbb{P}(\text{category}) \cdot (\prod_{i=1}^n \mathbb{P}(\text{word}_i = k_i | \text{category})))$$

▶ We then choose the category with the highest probability.



22.2.3 Inference by Enumeration



Inference by Enumeration

- The rules we established for naive Bayes models, i.e. Bayes's theorem, the product rule and chain rule, marginalization and normalization, are general techniques for probabilistic reasoning, and their usefulness is not limited to the naive Bayes models.
- More generally:
- Theorem 2.23. Let Q, E₁,..., E_{n_E}, U₁,..., U_{n_U} be random variables and D := dom(U₁) × ... × dom(U_{n_U}). Then

$$\mathbb{P}(Q|E_1 = e_1, ..., E_{n_E} = e_{n_e}) = \alpha(\sum_{u \in D} \mathbb{P}(Q, E_1 = e_1, ..., E_{n_E} = e_{n_e}, U_1 = u_1, ..., U_{n_U} = u_{n_U}))$$

We call Q the query variable, $E_1, ..., E_{n_E}$ the evidence, and $U_1, ..., U_{n_U}$ the unknown (or hidden) variables, and computing a conditional probability this way enumeration.

- Note that this is just a "mathy" way of saying we
 - 1. sum over all relevant entries of the full joint probability distribution of the variables, and
 - 2. normalize the result to yield a probability distribution.



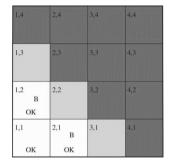
22.2.4 Example – The Wumpus is Back



- We have a maze where
 - Every cell except [1,1] possibly contains a *pit*, with 20% probability.
 - pits cause a breeze in neighboring cells (we forget the wumpus and the gold for now)
- Where should the agent go, if there is a breeze at [1,2] and [2,1]?
- Pure logical inference can conclude nothing about which square is most likely to be safe!

We can model this using the Boolean random variables:

- ▶ $P_{i,j}$ for $i,j \in \{1,2,3,4\}$, stating there is a pit at square [i,j], and
- ▶ $B_{i,j}$ for $(i,j) \in \{(1,1), (1,2), (2,1)\}$, stating there is a breeze at square [i,j]
- \Rightarrow let's apply our machinery!



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- First: Let's try to compute the full joint probability distribution $\mathbb{P}(P_{1,1}, \ldots, P_{4,4}, B_{1,1}, B_{1,2}, B_{2,1}).$
 - 1. By the product rule, this is equal to $\mathbb{T}(2)$

 $\mathbb{P}(B_{1,1}, B_{1,2}, B_{2,1}| P_{1,1}, \ldots, P_{4,4}) \cdot \mathbb{P}(P_{1,1}, \ldots, P_{4,4}).$

- 2. Note that $\mathbb{P}(B_{1,1}, B_{1,2}, B_{2,1}|P_{1,1}, \dots, P_{4,4})$ is either 1 (if all the $B_{i,j}$ are consistent with the positions of the pits $P_{k,l}$) or 0 (otherwise).
- 3. Since the pits are spread independently, we have $\mathbb{P}(P_{1,1}, \ldots, P_{4,4}) = \prod_{i,j=1,1}^{4,4} \mathbb{P}(P_{i,j})$
- \blacktriangleright \rightsquigarrow We know all of these probabilities.

► \sim We can now use enumeration to compute $\mathbb{P}(P_{i,j}| < known >) = \alpha(\sum_{<unknowns>} \mathbb{P}(P_{i,j}, < known >, < unknowns >))$

1,4	2,4	3,4	4,4
1,3	2,3	3,3	4,3
1,2 B OK	2,2	3,2	4,2
1,1 OK	2,1 B OK	3,1	4,1

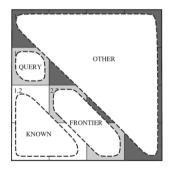


Wumpus Continued

- ▶ **Problem:** We only know $P_{i,j}$ for three fields. If we want to compute e.g. $P_{1,3}$ via enumeration, that leaves $2^{4^2-4} = 4096$ terms to sum over!
- Let's do better.
- Let $b := \neg B_{1,1} \land B_{1,2} \land B_{2,1}$ (All the breezes we know about)
- Let $p := \neg P_{1,1} \land \neg P_{1,2} \land \neg P_{2,1}$. (All the pits we know about)
- Let $F := \{P_{3,1} \land P_{2,2}, \neg P_{3,1} \land P_{2,2}, P_{3,1} \land \neg P_{2,2}, \neg P_{3,1} \land P_{2,2}\}$ (the current "frontier")
- Let O be (the set of assignments for) all the other variables $P_{i,j}$. (i.e. except p, F and our query $P_{1,3}$)

Then the observed breezes b are conditionally independent of O given p and F. (Whether there is a pit anywhere else does not influence the breezes we observe.)

► ⇒
$$P(b \mid P_{1,3}, p, O, F) = P(b \mid P_{1,3}, p, F)$$
. Let's exploit this!



Optimized Wumpus

▶ In particular:

$$\mathbb{P}(P_{1,3}|p,b) = \alpha(\sum_{o \in O, f \in F} \mathbb{P}(P_{1,3}, b, p, f, o)) = \alpha(\sum_{o \in O, f \in F} P(b \mid P_{1,3}, p, o, f) \cdot \mathbb{P}(P_{1,3}, p, f, o))$$

$$= \alpha(\sum_{f \in F} \sum_{o \in O} P(b \mid P_{1,3}, p, f) \cdot \mathbb{P}(P_{1,3}, p, f, o)) = \alpha(\sum_{f \in F} P(b \mid P_{1,3}, p, f) \cdot (\sum_{o \in O} \mathbb{P}(P_{1,3}, p, f, o)))$$

$$= \alpha(\sum_{f \in F} P(b \mid P_{1,3}, p, f) \cdot (\sum_{o \in O} \mathbb{P}(P_{1,3}) \cdot P(p) \cdot P(f) \cdot P(o)))$$

$$= \alpha(\mathbb{P}(P_{1,3}) \cdot P(p) \cdot (\sum_{f \in F} \underbrace{P(b \mid P_{1,3}, p, f)}_{\in \{0,1\}} \cdot P(f) \cdot (\underbrace{\sum_{o \in O} P(o)}_{=1})))$$

 \sim this is just a sum over the frontier. i.e. 4 terms \odot

So: $\mathbb{P}(P_{1,3}|p,b) =$ $\alpha(\langle 0.2 \cdot (0.8)^3 \cdot (1 \cdot 0.04 + 1 \cdot 0.16 + 1 \cdot 0.16 + 0), 0.8 \cdot (0.8)^3 \cdot (1 \cdot 0.04 + 1 \cdot 0.16 + 0 + 0) \rangle) \approx \langle 0.31, 0.69 \rangle$ • Analogously: $\mathbb{P}(P_{3,1}|p,b) = \langle 0.31, 0.69 \rangle$ and $\mathbb{P}(P_{2,2}|p,b) = \langle 0.86, 0.14 \rangle$ $(\Rightarrow avoid [2, 2]!)$ © FAU 2025-05-14

▶ In general, when you want to reason probabilistically, a good heuristic is:

1. Try to frame the full joint probability distribution in terms of the probabilities you know. Exploit product rule/chain rule, independence, conditional independence, marginalization and domain knowledge (as e.g. $\mathbb{P}(b|p, f) \in \{0, 1\}$)

2. Simplify: Start with the equation for enumeration:

$$\mathbb{P}(Q|E_1,...) = \alpha(\sum_{u \in U} \mathbb{P}(Q, E_1, ..., U_1 = u_1, ...))$$

- 3. Substitute by the result of 1., and again, exploit all of our machinery
- 4. Implement the resulting (system of) equation(s)
- **5**. ???
- 6. Profit



- Probability distributions and conditional probability distributions allow us to represent random variables as convenient datastructures in an implementation (Assuming they are finite domain...)
- The full joint probability distribution allows us to compute all probabilities of statements about the random variables contained
 (But possibly inefficient)
- Marginalization and normalization are the specific techniques for extracting the *specific* probabilities we are interested in from the full joint probability distribution.
- The product and chain rule, exploiting (conditional) independence, Bayes' Theorem, and of course domain specific knowledge allow us to do so much more efficiently.
- ▶ Naive Bayes models are one example where all these techniques come together.



Chapter 23 Probabilistic Reasoning: Bayesian Networks

23.1 Introduction



Example 1.1 (From Russell/Norvig).

- I got very valuable stuff at home. So I bought an alarm. Unfortunately, the alarm just rings at home, doesn't call me on my mobile.
- I've got two neighbors, Mary and John, who'll call me if they hear the alarm.
- The problem is that, sometimes, the alarm is caused by an earthquake.
- Also, John might confuse the alarm with his telephone, and Mary might miss the alarm altogether because she typically listens to loud music.

 \sim Random variables: Burglary, Earthquake, Alarm, John, Mary. Given that both John and Mary

call me, what is the probability of a burglary?

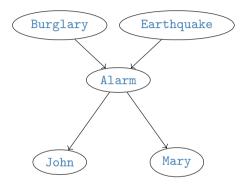
► ~> This is *almost* a naive Bayes model, but with multiple causes (Burglary and Earthquake) for the Alarm, which in turn may cause John and/or Mary.



We assume:

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- We (should) know P(Alarm|Burglary, Earthquake), P(John|Alarm), and P(Mary|Alarm).
- Burglary and Earthquake are independent.
- John and Mary are conditionally independent given Alarm.
- Moreover: Both John and Mary are conditionally independent of any other random variables in the graph given Alarm. (Only Alarm causes them, and everything else only causes them indirectly through Alarm)
- First Step: Construct the full joint probability distribution,
- Second Step: Use enumeration to compute $\mathbb{P}(\text{Burglary}|\text{John} = T, \text{Mary} = T)$.



 $\mathbb{P}(\texttt{John},\texttt{Mary},\texttt{Alarm},\texttt{Burglary},\texttt{Earthquake})$

- $= \mathbb{P}(\texttt{John}|\texttt{Mary},\texttt{Alarm},\texttt{Burglary},\texttt{Earthquake}) \cdot \mathbb{P}(\texttt{Mary}|\texttt{Alarm},\texttt{Burglary},\texttt{Earthquake})$
 - $\mathbf{P}(\texttt{Alarm}|\texttt{Burglary},\texttt{Earthquake}) \cdot \mathbb{P}(\texttt{Burglary}|\texttt{Earthquake}) \cdot \mathbb{P}(\texttt{Earthquake})$
- $= \mathbb{P}(\texttt{John}|\texttt{Alarm}) \cdot \mathbb{P}(\texttt{Mary}|\texttt{Alarm}) \cdot \mathbb{P}(\texttt{Alarm}|\texttt{Burglary},\texttt{Earthquake}) \cdot \mathbb{P}(\texttt{Burglary}) \cdot \mathbb{P}(\texttt{Earthquake})$

▶ We plug into the equation for enumeration:

$$\begin{split} \mathbb{P}(\text{Burglary}|\text{John} = \mathsf{T}, \text{Mary} = \mathsf{T}) = &\alpha(\mathbb{P}(\text{Burglary}) \sum_{a \in \{\mathsf{T},\mathsf{F}\}} P(\text{John} \mid \text{Alarm} = a) \cdot P(\text{Mary} \mid \text{Alarm} = a) \\ &\cdot \sum_{q \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(\text{Alarm} = a|\text{Burglary}, \text{Earthquake} = q) P(\text{Earthquake} = q)) \end{split}$$

Now let's scale things up to arbitrarily many variables!



Bayesian Networks: Definition

Definition 1.2. A Bayesian network consists of

- 1. a directed acyclic graph $\langle \mathcal{X}, \boldsymbol{E} \rangle$ of random variables $\mathcal{X} = \{X_1, \dots, X_n\}$, and
- 2. a conditional probability distribution $\mathbb{P}(X_i | \text{Parents}(X_i))$ for every $X_i \in \mathcal{X}$ (also called the CPT for conditional probability table)

such that every X_i is conditionally independent of any conjunctions of non-descendents of X_i given $Parents(X_i)$.

- Definition 1.3. Let (X, E) be a directed acyclic graph, X ∈ X, and E* the reflexive transitive closure of E. The non-descendents of X are the elements of the set NonDesc(X) := {Y | (X,Y) ∉ E*}\Parents(X).
- Note that the roots of the graph are conditionally independent given the empty set; i.e. they are independent.
- **Theorem 1.4.** The full joint probability distribution of a Bayesian network $\langle \mathcal{X}, E \rangle$ is given by

$$\mathbb{P}(X_1,\ldots,X_n) = \prod_{X_i \in \mathcal{X}} \mathbb{P}(X_i | \text{Parents}(X_i))$$



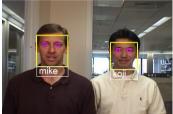
A ubiquitous problem: Observe "symptoms", need to infer "causes". **Medical Diagnosis**



Self-Localization



Face Recognition



Nuclear Test Ban



23.2 Constructing Bayesian Networks



Compactness of Bayesian Networks

▶ Definition 2.1. Given random variables X₁,...,X_n with finite domains D₁,...,D_n, the size of B := ⟨{X₁,...,X_n}, E⟩ is defined as

size(
$$\mathcal{B}$$
):= $\sum_{i=1}^{n} |D_i| \cdot (\prod_{X_j \in \text{Parents}(X_i)} |D_j|)$

Note: size(\mathcal{B}) \cong The total number of entries in the conditional probability distributions.



Compactness of Bayesian Networks

▶ Definition 2.5. Given random variables X₁,...,X_n with finite domains D₁,...,D_n, the size of B := ⟨{X₁,...,X_n}, E⟩ is defined as

size(
$$\mathcal{B}$$
):= $\sum_{i=1}^{n} |D_i| \cdot (\prod_{X_j \in \text{Parents}(X_i)} |D_j|)$

▶ Note: $size(B) \cong$ The total number of entries in the conditional probability distributions.

- ▶ Note: Smaller BN ~> need to assess less probabilities, more efficient inference.
- ▶ **Observation 2.6.** Explicit full joint probability distribution has size $\prod_{i=1}^{n} |D_i|$.
- ▶ Observation 2.7. If $|Parents(X_i)| \le k$ for every X_i , and D_{max} is the largest random variable domain, then $size(B) \le n |D_{max}|^{k+1}$.



Compactness of Bayesian Networks

▶ Definition 2.9. Given random variables X₁,...,X_n with finite domains D₁,...,D_n, the size of B := ⟨{X₁,...,X_n}, E⟩ is defined as

size(
$$\mathcal{B}$$
):= $\sum_{i=1}^{n} |D_i| \cdot (\prod_{X_j \in \text{Parents}(X_i)} |D_j|)$

- ▶ Note: $size(B) \cong$ The total number of entries in the conditional probability distributions.
- \blacktriangleright Note: Smaller BN \rightsquigarrow need to assess less probabilities, more efficient inference.
- ▶ Observation 2.10. Explicit full joint probability distribution has size $\prod_{i=1}^{n} |D_i|$.
- ▶ Observation 2.11. If $|Parents(X_i)| \le k$ for every X_i , and D_{max} is the largest random variable domain, then size(\mathcal{B}) $\le n |D_{max}|^{k+1}$.
- **Example 2.12.** For $|D_{\text{max}}| = 2$, n = 20, k = 4 we have $2^{20} = 1048576$ probabilities, but a Bayesian network of size $\leq 20 \cdot 2^5 = 640 \dots !$
- ▶ In the worst case, $size(B) = n \cdot (\prod_{i=1}^{1} n) |D_i|$, namely if every variable depends on all its predecessors in the chosen variable ordering.
- Intuition: BNs are compact i.e. of small size if each variable is directly influenced only by few of its predecessor variables.

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- ► To keep our Bayesian networks small, we can:
 - 1. Reduce the number of edges: \Rightarrow Order the variables to allow for exploiting conditional independence (causes before effects), or
 - 2. represent the conditional probability distributions efficiently:
 - 2.1 For Boolean random variables X, we only need to store P(X = T | Parents(X))
 - (P(X = F|Parents(X)) = 1 P(X = T|Parents(X))) (Cuts the number of entries in half!)
 - 2.2 Introduce different kinds of nodes exploiting domain knowledge; e.g. deterministic and noisy disjunction nodes.



Reducing Edges: Variable Order Matters

- Given a set of random variables X₁,...,X_n, consider the following (impractical, but illustrative) pseudo-algorithm for constructing a Bayesian network:
- Definition 2.13 (BN construction algorithm).
 - 1. Initialize $BN := \langle \{X_1, \ldots, X_n\}, E \rangle$ where $E = \emptyset$.
 - 2. Fix any variable ordering, X_1, \ldots, X_n .
 - 3. for i := 1, ..., n do
 - a. Choose a minimal set $Parents(X_i) \subseteq \{X_1, \ldots, X_{i-1}\}$ such that

 $\mathbb{P}(X_i|X_{i-1},\ldots,X_1) = \mathbb{P}(X_i|\text{Parents}(X_i))$

- b. For each $X_j \in \text{Parents}(X_i)$, insert (X_j, X_i) into E.
- c. Associate X_i with $\mathbb{P}(X_i | \text{Parents}(X_i))$.
- ► Attention: Which variables we need to include into Parents(X_i) depends on what "{X₁,...,X_{i-1}}" is ... !
- **Thus:** The size of the resulting BN depends on the chosen variable ordering X_1, \ldots, X_n .
- In Particular: The size of a Bayesian network is not a fixed property of the domain. It depends on the skill of the designer.



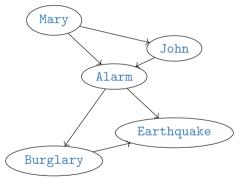
John and Mary Depend on the Variable Order!

Example 2.14. Mary, John, Alarm, Burglary, Earthquake.



John and Mary Depend on the Variable Order!

Example 2.15. Mary, John, Alarm, Burglary, Earthquake.





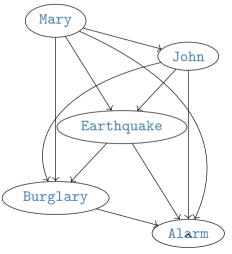
John and Mary Depend on the Variable Order! Ctd.

Example 2.16. Mary, John, Earthquake, Burglary, Alarm.



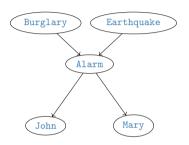
John and Mary Depend on the Variable Order! Ctd.

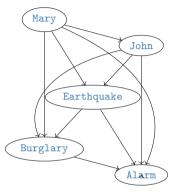
Example 2.17. Mary, John, Earthquake, Burglary, Alarm.





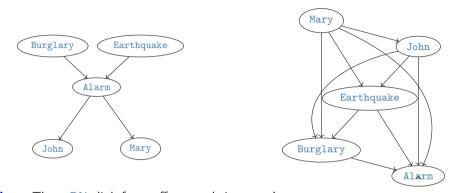
John and Mary, What Went Wrong?







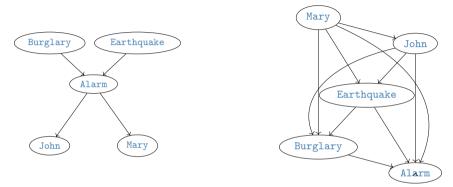
John and Mary, What Went Wrong?



Intuition: These BNs link from effects to their causes!
Even though Mary and John are conditionally independent given Alarm, this is not exploited, since Alarm is not ordered before Mary and John!



John and Mary, What Went Wrong?



Intuition: These BNs link from effects to their causes!

 \Rightarrow Even though Mary and John are conditionally independent given Alarm, this is not exploited, since Alarm is not ordered before Mary and John!

 \Rightarrow **Rule of Thumb:** We should order causes before symptoms.



Representing Conditional Distributions: Deterministic Nodes

▶ **Definition 2.18.** A node X in a Bayesian network is called deterministic, if its value is completely determined by the values of Parents(X).



- ▶ **Definition 2.21.** A node X in a Bayesian network is called deterministic, if its value is completely determined by the values of Parents(X).
- **Example 2.22.** The *sum of two dice throws S* is entirely determined by the values of the two dice *First* and *Second*.



- ▶ **Definition 2.24.** A node X in a Bayesian network is called deterministic, if its value is completely determined by the values of Parents(X).
- **Example 2.25.** The *sum of two dice throws S* is entirely determined by the values of the two dice *First* and *Second*.
- **Example 2.26.** In the *Wumpus* example, the *breezes* are entirely determined by the *pits*



- ▶ **Definition 2.27.** A node X in a Bayesian network is called deterministic, if its value is completely determined by the values of Parents(X).
- **Example 2.28.** The *sum of two dice throws S* is entirely determined by the values of the two dice *First* and *Second*.
- **Example 2.29.** In the *Wumpus* example, the *breezes* are entirely determined by the *pits*
- > ~ *Deterministic* nodes model direct, *causal* relationships.
- ▶ \sim If X is deterministic, then $\mu(X \mid \text{Parents}(X)) \in \{0, 1\}$



- ▶ **Definition 2.30.** A node X in a Bayesian network is called deterministic, if its value is completely determined by the values of Parents(X).
- **Example 2.31.** The *sum of two dice throws S* is entirely determined by the values of the two dice *First* and *Second*.
- **Example 2.32.** In the *Wumpus* example, the *breezes* are entirely determined by the *pits*
- > ~ *Deterministic* nodes model direct, *causal* relationships.
- ▶ \rightsquigarrow If X is deterministic, then $\mu(X \mid \text{Parents}(X)) \in \{0, 1\}$

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▶ \sim we can replace the conditional probability distribution $\mathbb{P}(X|\text{Parents}(X))$ by a boolean function.

Representing Conditional Distributions: Noisy Nodes

Sometimes, values of nodes are "almost deterministic":

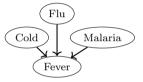
Example 2.33 (Inhibited Causal Dependencies).

Assume the network on the right contains *all* possible causes of fever (Or add a dummy-node for "other causes")

If there is a fever, then *one* of them (at least) must be the cause, but none of them *necessarily* cause a fever: The causal relation between parent and child is inhibited.

 \sim We can model the inhibitions by individual inhibition factors q_d .

- ▶ **Definition 2.34.** The conditional probability distribution of a noisy disjunction node X with Parents(X) = $X_1, ..., X_n$ in a Bayesian network is given by $P(X | X_1, ..., X_n) = 1 - (\prod_{\{j | X_j = T\}} q_j)$, where the q_i are the inhibition factors of $X_i \in \text{Parents}(X)$, defined as $q_i := P(\neg X | \neg X_1, ..., \neg X_{i-1}, X_i, \neg X_{i+1}, ..., \neg X_n)$
- \blacktriangleright \rightarrow Instead of a distribution with 2^k parameters, we only need k parameters!



Representing Conditional Distributions: Noisy Nodes

Example 2.35. Assume the following inhibition factors for **??**:

 $\begin{array}{lll} q_{\rm cold} &=& P(\neg {\rm fever} \mid {\rm cold}, \neg {\rm flu}, \neg {\rm malaria}) = 0.6 \\ q_{\rm flu} &=& P(\neg {\rm fever} \mid \neg {\rm cold}, {\rm flu}, \neg {\rm malaria}) = 0.2 \\ q_{\rm malaria} &=& P(\neg {\rm fever} \mid \neg {\rm cold}, \neg {\rm flu}, {\rm malaria}) = 0.1 \end{array}$

If we model Fever as a noisy disjunction node, then the general rule $P(X_i \mid \text{Parents}(X_i)) = \prod_{\{j \mid X_j = T\}} q_j$ for the CPT gives the following table:

Cold	Flu	Malaria	P(Fever)	$P(\neg \text{Fever})$
F	F	F	0.0	1.0
F	F	Т	0.9	0.1
F	Т	F	0.8	0.2
F	Т	Т	0.98	$0.02 = 0.2 \cdot 0.1$
Т	F	F	0.4	0.6
Т	F	Т	0.94	$0.06 = 0.6 \cdot 0.1$
Т	Т	F	0.88	$0.12 = 0.6 \cdot 0.2$
Т	Т	Т	0.988	$0.012 = 0.6 \cdot 0.2 \cdot 0.1$



- Note that deterministic nodes and noisy disjunction nodes are just two examples of "specialized" kinds of nodes in a Bayesian network.
- ► In general, noisy logical relationships in which a variable depends on k parents can be described by O(k) parameters instead of O(2^k) for the full conditional probability table. This can make assessment (and learning) tractable.
- Example 2.36. The CPCS network [PraProMid:kelbn94] uses noisy-OR and noisy-MAX distributions to model relationships among diseases and symptoms in internal medicine. With 448 nodes and 906 links, it requires only 8,254 values instead of 133,931,430 for a network with full conditional probability distributions.





23.3 Inference in Bayesian Networks



Probabilistic Inference Tasks in Bayesian Networks

- Remember:
- **Definition 3.1 (Probabilistic Inference Task).** Let

 $X_1, \ldots, X_n = Q_1, \ldots, Q_{n_Q}, E_1, \ldots, E_{n_E}, U_1, \ldots, U_{n_U}$ be a set of random variables, a probabilistic inference task.

We wish to compute the conditional probability distribution $\mathbb{P}(Q_1, \ldots, Q_{n_Q} | E_1 = e_1, \ldots, E_{n_E} = e_{n_E})$. We call

- a Q_1, \ldots, Q_{n_Q} the query variables,
- a E_1, \ldots, E_{n_E} the evidence variables, and
- U_1, \ldots, U_{n_U} the hidden variables.

▶ We know the full joint probability distribution: $\mathbb{P}(X_1, ..., X_n) = \prod_{i=1}^n \mathbb{P}(X_i | \text{Parents}(X_i))$

And we know about enumeration:

$$\mathbb{P}(Q_1,...,Q_{n_Q}|E_1 = e_1,...,E_{n_E} = e_{n_E}) = \alpha(\sum_{u \in D_U} \mathbb{P}(Q_1,...,Q_{n_Q},E_1 = e_1,...,E_{n_E} = e_{n_E},U_1 = u_1,...,U_{n_U} = u_{n_U}))$$

(where $D_U = \operatorname{dom}(U_1) \times \ldots \times \operatorname{dom}(U_{n_U})$)

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Remember our example: P(Burglary|John, Mary) (hidden variables: Alarm, Earthquake)

$$= \alpha(\sum_{b_a, b_e \in \{\mathsf{T},\mathsf{F}\}} P(\mathsf{John}, \mathsf{Mary}, \mathsf{Alarm} = b_a, \mathsf{Earthquake} = b_e, \mathsf{Burglary})) \\= \alpha(\sum_{b_a, b_e \in \{\mathsf{T},\mathsf{F}\}} P(\mathsf{John} \mid \mathsf{Alarm} = b_a) \cdot P(\mathsf{Mary} \mid \mathsf{Alarm} = b_a) \\\cdot \mathbb{P}(\mathsf{Alarm} = b_a|\mathsf{Earthquake} = b_e, \mathsf{Burglary}) \cdot P(\mathsf{Earthquake} = b_e) \cdot \mathbb{P}(\mathsf{Burglary}))$$

- ▶ \sim These are 5 factors in 4 summands $(b_a, b_e \in \{\mathsf{T}, \mathsf{F}\})$ over two cases $(\mathsf{Burglary} \in \{\mathsf{T}, \mathsf{F}\})$,
- ▶ \sim 38 arithmetic operations (+3 for α)
- General worst case: $\mathcal{O}(n2^n)$
- Let's do better!



► Some abbreviations: j := John, m := Mary, a := Alarm, e := Earthquake, b := Burglary,

$$\mathbb{P}(b|j,m) = \alpha(\sum_{b_a,b_e \in \{\mathsf{T},\mathsf{F}\}} P(j \mid a = b_a) \cdot P(m \mid a = b_a) \cdot \mathbb{P}(a = b_a|e = b_e, b) \cdot P(e = b_e) \cdot \mathbb{P}(b))$$

Let's "optimize":

Fau

 $\mathbb{P}(b|j,m) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e = b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a = b_a|e = b_e, b) \cdot P(j \mid a = b_a) \cdot P(m \mid a = b_a))))$

 \sim 3 factors in 2 summand + 2 factors in 2 summands + two factors in the outer product, over two cases = 28 arithmetic operations (+3 for α)



- Consider $\mathbb{P}(j|b = \mathsf{T})$.
- Using enumeration:

$$=\alpha(P(b)\cdot(\sum_{b_e\in\{\mathsf{T},\mathsf{F}\}}P(e=b_e)\cdot(\sum_{a_e\in\{\mathsf{T},\mathsf{F}\}}P(a=a_e\mid e=b_e,b)\cdot\mathbb{P}(j|a=a_e)\cdot(\sum_{a_m\in\{\mathsf{T},\mathsf{F}\}}P(m=a_m\mid a=a_m\mid a=a_e)\cdot(\sum_{a_m\in\{\mathsf{T},\mathsf{F}\}}P(m=a_m\mid a=a_m\mid a=a_m\mid a=a_e)\cdot(\sum_{a_m\in\{\mathsf{T},\mathsf{F}\}}P(m=a_m\mid a=a_m\mid a=a_m\mid$$

 $\sim \mathbb{P}(\text{John}|\text{Burglary} = T)$ does not depend on Mary

(duh...)

More generally:

Fau

- ▶ Lemma 3.2. Given a query P(Q₁,...,Q_{n_Q}|E₁ = e₁,...,E_{n_E} = e_{n_E}), we can ignore (and remove) all hidden leaves of the Bayesian network.
- ...doing so yields new leaves, which we can then ignore again, etc., until:
- ▶ Lemma 3.3. Given a query P(Q₁,...,Q_{nQ}|E₁ = e₁,...,E_{nE} = e_{nE}), we can ignore (and remove) all hidden variables that are not ancestors of any of the Q₁,...,Q_{nQ} or E₁,...,E_{nE}.

Enumeration: First Algorithm

• Assume the X_1, \ldots, X_n are topologically sorted

(causes before effects)

 $\begin{aligned} & \text{function ENUMERATE-QUERY}(Q, \langle E_1 = e_1, \dots, E_{n_E} = e_{n_E} \rangle) \\ & P := \langle \rangle \\ & \chi_1, \dots, \chi_n := \text{ variables filtered according to } ??, \text{ topologically sorted} \\ & \text{for all } q \in \text{dom}(Q) \text{ do} \\ & P_i := \text{ENUMALL}(\langle \chi_1, \dots, \chi_n \rangle, \langle E_1 = e_1, \dots, E_{n_E} = e_{n_E}, Q = q \rangle) \\ & \text{return } \alpha(P) \end{aligned}$ $\begin{aligned} & \text{function ENUMALL}(\langle Y_1, \dots, Y_{n_Y} \rangle, \langle A_1 = a_1, \dots, A_{n_A} = a_{n_A} \rangle) \\ & & fn_y = 0 \text{ then return } 1.0 \\ & \text{else if } Y_1 = A_j \text{ then return } P(A_j = a_j \mid \text{Parents}(A_j)) \cdot \text{ENUMALL}(\langle Y_2, \dots, Y_{n_Y} \rangle, \langle A_1 = a_1, \dots, A_{n_A} = a_{n_A} \rangle) \\ & \text{else return } \sum_{y \in \text{dom}(Y_1)} P(Y_1 = y \mid \text{Parents}(Y_1)) \cdot \text{ENUMALL}(\langle Y_2, \dots, Y_{n_Y} \rangle, \langle A_1 = a_1, \dots, A_{n_A} = a_{n_A} \rangle) \\ & a_{n_A}, Y_1 = y \rangle) \end{aligned}$

▶ General worst case Complexity: $O(2^n)$ – better, but still not great



Enumerate-Query($b, \langle j = \mathsf{T}, m = \mathsf{T} \rangle$)

 $\mathbb{P}(b|j = T, m = T) =$



Enumerate-Query($b, \langle j = \mathsf{T}, m = \mathsf{T} \rangle$)

 $\mathbb{P}(b|j = T, m = T) =$



- ► Variable order: *b*, *e*, *a*, *j*, *m*
 - ▶ $P_0 := \text{ENUMALL}(\langle b, e, a, j, m \rangle, \langle j = T, m = T, b = T \rangle)$ ▶ $P_1 := \text{ENUMALL}(\langle b, e, a, j, m \rangle, \langle j = T, m = T, b = F \rangle)$ $\Leftarrow \alpha(\langle P_0, P_1 \rangle)$

 $\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T})=\alpha()$



$$P_{0} := \underbrace{\text{EnumAll}(\langle b, e, a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T} \rangle)}_{=P(b) \cdot \text{EnumAll}(\langle e, a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T} \rangle)}$$

$$P_{1} := \underbrace{\text{EnumAll}(\langle b, e, a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F} \rangle)}_{=P(\neg b) \cdot \text{EnumAll}(\langle e, a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F} \rangle)}$$

$$\Leftrightarrow \alpha(\langle P_{0}, P_{1} \rangle)$$

$$\mathbb{P}(b|j = \mathsf{T}, m = \mathsf{T}) = \alpha(\mathbb{P}(b)\cdot)$$



▶
$$P_0 := P(b) \cdot \text{ENUMALL}(\langle e, a, j, m \rangle, \langle j = T, m = T, b = T \rangle)$$

▶ $P_1 := P(\neg b) \cdot \text{ENUMALL}(\langle e, a, j, m \rangle, \langle j = T, m = T, b = F \rangle)$
 $\Leftarrow \alpha(\langle P_0, P_1 \rangle)$

 $\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T})=\alpha(\mathbb{P}(b)\cdot)$



$$P_{0} := P(b) \cdot \underbrace{\text{EnumAll}(\langle e, a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T} \rangle)}_{=(\sum_{b_{e} \in \{\mathsf{T},\mathsf{F}\}} P(e=b_{e}) \cdot \text{EnumAll}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e=b_{e} \rangle))}$$

$$P_{1} := P(\neg b) \cdot \underbrace{\text{EnumAll}(\langle e, a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F} \rangle)}_{=(\sum_{b_{e} \in \{\mathsf{T},\mathsf{F}\}} P(e=b_{e}) \cdot \text{EnumAll}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e=b_{e} \rangle))}$$

$$\Leftarrow \alpha(\langle P_{0}, P_{1} \rangle)$$

$$\mathbb{P}(b|j = \mathsf{T}, m = \mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e = b_e) \cdot))$$



$$P_{0} := P(b) \cdot \left[+ \begin{array}{c} P(e) \cdot \text{ENUMALL}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{T} \rangle) \\ P(\neg e) \cdot \text{ENUMALL}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{F} \rangle) \end{array} \right]$$

$$P_{1} := P(\neg b) \cdot \left[+ \begin{array}{c} P(e) \cdot \text{ENUMALL}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{T} \rangle) \\ P(\neg e) \cdot \text{ENUMALL}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F} \rangle) \right] \\ \Leftrightarrow \alpha(\langle P_{0}, P_{1} \rangle)$$

$$\mathbb{P}(b|j = \mathsf{T}, m = \mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_{e} \in \{\mathsf{T},\mathsf{F}\}} P(e = b_{e}) \cdot))$$



$$P_{0} := P(b) \cdot \begin{bmatrix} P(e) \cdot & \text{ENUMALL}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{T} \rangle) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid b, e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{T}, e=\mathsf{T}, a=b_{a} \rangle)) \\ P(\neg e) \cdot & \text{ENUMALL}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{F} \rangle) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ P(e) \cdot & \text{ENUMALL}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{T} \rangle) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{T}, a=b_{a} \rangle)) \\ P(\neg e) \cdot & \text{ENUMALL}(\langle a, j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle)) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle))) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle))) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle))) \\ = (\sum_{b_{a} \in \{\mathsf{T}, \mathsf{F}\}} P(a=b_{a} \mid \neg b, \neg e) \cdot \text{ENUMAL}(\langle j, m \rangle \cdot \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{F}, a=b_{a} \rangle))$$

$$\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e=b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_a|e=b_e,b) \cdot \cdot)))$$



FAU

$$P_{0} := P(b) \cdot \begin{bmatrix} + P(a \mid b, e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = T, e = T, a = T \rangle) \\ P(\neg a \mid b, e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = T, e = T, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = T, e = F, a = T \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = T, e = F, a = F \rangle) \\ P(\neg a \mid b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = F, e = F, a = F \rangle) \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot \text{ENUMALL$$

$$\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e=b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_a|e=b_e,b) \cdot \cdot)))$$



Enumeration: Example

Variable order: b, e, a, j, m $P(a \mid b, e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = T, e = T, a = T \rangle)$ $P(e) \cdot \left| + \frac{P(j \mid a) \cdot \text{EnumAll}(\langle m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{T}, a = \mathsf{T} \rangle)}{P(\neg a \mid b, e) \cdot \text{EnumAll}(\langle j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{T}, a = \mathsf{F} \rangle)} \right|$ $=P(j \mid \neg a) \cdot \text{ENUMALL}(\langle m \rangle, \langle j=T, m=T, b=T, e=T, a=F \rangle)$ $P_0 := P(b)$. $P(a \mid b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = T, e = F, a = T \rangle)$ $=P(j \mid a) \cdot \text{ENUMALL}(\langle m \rangle, \langle j=T, m=T, b=T, e=F, a=T \rangle)$ $P(\neg e) \cdot + P(\neg a \mid b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{F}, a = \mathsf{F} \rangle)$ = $P(i \mid \neg a) \cdot \text{ENUMALL}(\langle m \rangle, \langle i = T, m = T, b = T, e = F, a = F \rangle)$ $P(a \mid \neg b, e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{T}, a = \mathsf{T} \rangle)$ + $\frac{=P(j \mid a) \cdot \text{EnumAll}(\langle m \rangle, \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{T}, a=\mathsf{T} \rangle)}{P(\neg a \mid \neg b, e) \cdot \text{EnumAll}(\langle j, m \rangle, \langle j=\mathsf{T}, m=\mathsf{T}, b=\mathsf{F}, e=\mathsf{T}, a=\mathsf{F} \rangle)}$ $=P(j \mid \neg a) \cdot \text{ENUMALL}(\langle m \rangle, \langle j=T, m=T, b=F, e=T, a=F \rangle)$ $\blacktriangleright P_1 := P(\neg b) \cdot | +$ $P(a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)$ = $P(j \mid a)$ ·ENUMALL($\langle m \rangle, \langle j=T, m=T, b=F, e=F, a=T \rangle$) $P(\neg e) \cdot + P(\neg a \mid \neg b, \neg e) \cdot \text{ENUMALL}(\langle j, m \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle)$ $=P(i \mid \neg a) \cdot \text{ENUMALL}(\langle m \rangle, \langle i=T, m=T, b=F, e=F, a=F \rangle)$ œ $\mathsf{FAU}_{\mathcal{O}}(\mathsf{P}_{\mathsf{A}}:\mathsf{P}_{\mathsf{A}}))$ 793 2025-05-14

$$\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e=b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_a|e=b_e,b) \cdot P(j \mid a=b_a) \cdot)))$$

2025-05-14

.

Enumeration: Example

$$P_{0} := P(a \mid b, e) \cdot P(j \mid a) \cdot \underbrace{\operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = T, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = F, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = F, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = F, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = T, e = F, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = T, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle)}_{=P(m \mid a) \cdot \operatorname{ENUMALL}(\langle m \rangle, \langle$$

$$P_{0} := P(b) \cdot \begin{bmatrix} P(e) \cdot \left[+ \begin{array}{c} P(a \mid b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{T}, a = \mathsf{T} \rangle \right) \\ + \begin{array}{c} P(-a \mid b, e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{T}, a = \mathsf{F} \rangle) \\ P(\neg e) \cdot \left[+ \begin{array}{c} P(a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{F}, a = \mathsf{T} \rangle) \\ P(\neg e) \cdot \left[+ \begin{array}{c} P(a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{T}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(-e) \cdot \left[+ \begin{array}{c} P(a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{T}, a = \mathsf{F} \rangle) \\ P(-e) \cdot \left[+ \begin{array}{c} P(a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{T}, a = \mathsf{F} \rangle) \\ P(\neg e) \cdot \left[+ \begin{array}{c} P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg e) \cdot \left[+ \begin{array}{c} P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg e) \cdot \left[+ \begin{array}{c} P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg e) \cdot \left[+ \begin{array}{c} P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg e) \cdot \left[+ \begin{array}{c} P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg a \mid \neg b, \neg e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg a \mid \neg b, \neg e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg a \mid \neg b, \neg e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg a \mid \neg b, \neg e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a = \mathsf{F} \rangle) \\ P(\neg a \mid \neg b, \neg e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = \mathsf{T}, m = \mathsf{T}, b = \mathsf{F}, e = \mathsf{F}, a$$

$$\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e=b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_a|e=b_e,b) \cdot P(j \mid a=b_a) \cdot P(m \mid a=b_a))))$$



FAU

$$P_{0} := P(b) \cdot \begin{bmatrix} P(e) \cdot \begin{bmatrix} + P(a \mid b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = T, e = T, a = T \rangle) \\ + P(\neg a \mid b, e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = T, e = T, a = F \rangle) \\ + P(\neg e) \cdot \begin{bmatrix} + P(a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = T, e = F, a = T \rangle) \\ + P(\neg a \mid b, \neg e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = T, e = F, a = F \rangle) \\ + P(e) \cdot \begin{bmatrix} + P(a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle) \\ + P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle) \\ + P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = F, e = T, a = F \rangle) \\ + P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = F, e = F, a = T \rangle) \\ + P(\neg a \mid \neg b, \neg e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot \text{ENUMALL}(\langle \rangle, \langle j = T, m = T, b = F, e = F, a = F \rangle) \\ \end{pmatrix}$$

$$\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e=b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_a|e=b_e,b) \cdot P(j \mid a=b_a) \cdot P(m \mid a=b_a))))$$



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$$P_{0} := P(b) \cdot \begin{bmatrix} + P(a \mid b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ + P(\neg a \mid b, e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot 1.0 \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ + P(\neg a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \end{bmatrix} \\ P_{1} := P(\neg b) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ + P(\neg a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ + P(\neg a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \end{bmatrix} \\ \Leftrightarrow \alpha(\langle P_{0}, P_{1} \rangle)$$

$$\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e=b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_a|e=b_e,b) \cdot P(j \mid a=b_a) \cdot P(m \mid a=b_a))))$$



$$P_{0} := P(b) \cdot \begin{bmatrix} + P(a \mid b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg a \mid b, e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot 1.0 \\ P(\neg e) \cdot [+ P(a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \end{bmatrix}$$

$$P_{1} := P(\neg b) \cdot \begin{bmatrix} P(e) \cdot [+ P(a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg e) \cdot [+ P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg e) \cdot [+ P(a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \end{bmatrix}$$

$$\approx \underbrace{\alpha(\langle P_{0}, P_{1} \rangle)}_{=\langle \frac{P_{0}}{P_{0}+P_{1}}, \frac{P_{1}}{P_{0}+P_{1}} \rangle}$$

$$\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e=b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_a|e=b_e,b) \cdot P(j \mid a=b_a) \cdot P(m \mid a=b_a))))$$

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$$P_{0} := P(b) \cdot \begin{bmatrix} + P(a \mid b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ + P(\neg a \mid b, e) \cdot P(j \mid \neg a) \cdot P(m \mid \neg a) \cdot 1.0 \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg a \mid b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \end{bmatrix} \\ P_{1} := P(\neg b) \cdot \begin{bmatrix} + P(e) \cdot \begin{bmatrix} + P(a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ + P(\neg a \mid \neg b, e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg e) \cdot \begin{bmatrix} + P(a \mid \neg b, -e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \\ P(\neg e) \cdot P(\neg a \mid \neg b, \neg e) \cdot P(j \mid a) \cdot P(m \mid a) \cdot 1.0 \end{bmatrix} \\ \neq \begin{pmatrix} \frac{P_{0}}{P_{0} + P_{1}}, \frac{P_{1}}{P_{0} + P_{1}} \end{pmatrix}$$

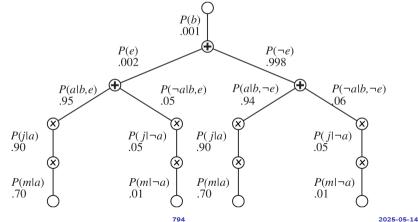
$$\mathbb{P}(b|j=\mathsf{T},m=\mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_{e} \in \{\mathsf{T},\mathsf{F}\}} P(e=b_{e}) \cdot (\sum_{b_{a} \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_{a}|e=b_{e},b) \cdot P(j \mid a=b_{a}) \cdot P(m \mid a=b_{a}))))$$



The Evaluation of $P(b \mid i,m)$ as a "Search Tree"

 $\mathbb{P}(b|j,m) = \alpha(\mathbb{P}(b) \cdot (\sum P(e = b_e) \cdot (\sum \mathbb{P}(a = b_a|e = b_e, b) \cdot P(j \mid a = b_a) \cdot P(m \mid a = b_a))))$ $b_{e} \in \{T, F\}$ $b_{2} \in \{T, F\}$

Note: ENUMERATE-QUERY corresponds to depth-first traversal of an arithmetic expression-tree:

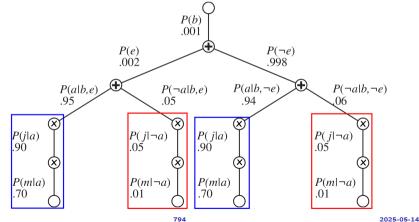




The Evaluation of $P(b \mid i,m)$ as a "Search Tree"

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Note: ENUMERATE-QUERY corresponds to depth-first traversal of an arithmetic expression-tree:





 $\mathbb{P}(b|j,m) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e=b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a=b_a|e=b_e,b) \cdot P(j \mid a=b_a) \cdot P(m \mid a=b_a))))$

The last two factors $P(j \mid a = b_a)$, $P(m \mid a = b_a)$ only depend on a, but are "trapped" behind the summation over e, hence computed twice in two distinct recursive calls to ENUMALL

Idea: Instead of left-to-right (top-down DFS), operate right-to-left (bottom-up) and store intermediate "factors" along with their "dependencies":

$$\alpha(\underbrace{\mathbb{P}(b)}_{f_{7}(b)} \cdot (\underbrace{\sum_{b_{e} \in \{\mathsf{T},\mathsf{F}\}} \underbrace{\mathcal{P}(e=b_{e})}_{f_{5}(e)} \cdot (\underbrace{\sum_{b_{a} \in \{\mathsf{T},\mathsf{F}\}} \underbrace{\mathbb{P}(a=b_{a}|e=b_{e},b)}_{f_{3}(a,b,e)} \cdot \underbrace{\mathcal{P}(j \mid a=b_{a})}_{f_{2}(a)} \cdot \underbrace{\mathcal{P}(m \mid a=b_{a})}_{f_{1}(a)}))}_{f_{4}(b,e)}$$



▶ We only show variable elimination by example: (implementation details get tricky, but the idea is simple)

 $\mathbb{P}(b) \cdot \left(\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} P(e = b_e) \cdot \left(\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a = b_a | e = b_e, b) \cdot P(j \mid a = b_a) \cdot P(m \mid a = b_a)\right)\right)$

- Assume reverse topological order of variables: m, j, a, e, b m is an evidence variable with value T and dependency a, which is a hidden variable. We introduce a new "factor" $f(a) := f_1(a) := \langle P(m \mid a), P(m \mid \neg a) \rangle$. ▶ *j* works analogously, $f_2(a) := \langle P(j \mid a), P(j \mid \neg a) \rangle$. We "multiply" with the existing factor, yielding $f(a) := \langle f_1(a) \cdot f_2(a), f_1(\neg a) \cdot f_2(\neg a) \rangle = \langle P(m \mid a) \cdot P(j \mid a), P(m \mid \neg a) \cdot P(j \mid \neg a) \rangle$ \blacktriangleright a is a hidden variable with dependencies e (hidden) and b (query). 1. We introduce a new "factor" $f_3(a, e, b)$, a 2 × 2 × 2 table with the relevant conditional probabilities $\mathbb{P}(a|e, b)$. 2. We multiply each entry of f₃ with the relevant entries of the existing factor f, yielding f(a, e, b).
 - 3. We "sum out" the resulting factor over a, yielding a new factor $f(e, b) = f(a, e, b) + f(\neg a, e, b)$.

 \sim can speed things up by a factor of 1000! (or more, depending on the order of variables!)

...





- Definition 3.4. A graph G is called singly connected, or a polytree (otherwise multiply connected), if there is at most one undirected path between any two nodes in G.
- Theorem 3.5 (Good News). On singly connected Bayesian networks, variable elimination runs in polynomial time.



- Definition 3.8. A graph G is called singly connected, or a polytree (otherwise multiply connected), if there is at most one undirected path between any two nodes in G.
- Theorem 3.9 (Good News). On singly connected Bayesian networks, variable elimination runs in polynomial time.
- Is our BN for Mary & John a polytree?



(Yes.)

- **Definition 3.12.** A graph G is called singly connected, or a polytree (otherwise multiply connected), if there is at most one undirected path between any two nodes in G.
- Theorem 3.13 (Good News). On singly connected Bayesian networks, variable elimination runs in polynomial time.
- Is our BN for Mary & John a polytree?

(Yes.)

- ► Theorem 3.14 (Bad News). For multiply connected Bayesian networks, probabilistic inference is #P-hard. (#P is harder than NP, i.e. NP ⊆ #P)
- ▶ So?: Life goes on ... In the hard cases, if need be we can throw exactitude to the winds and approximate.
- **Example 3.15.** Sampling techniques as in MCTS.



23.4 Conclusion



Fau

- Bayesian networks (BN) are a wide-spread tool to model uncertainty, and to reason about it. A BN represents conditional independence relations between random variables. It consists of a graph encoding the variable dependencies, and of conditional probability tables (CPTs).
- ▶ Given a variable ordering, the BN is small if every variable depends on only a few of its predecessors.
- Probabilistic inference requires to compute the probability distribution of a set of query variables, given a set of evidence variables whose values we know. The remaining variables are hidden.
- Inference by enumeration takes a BN as input, then applies Normalization+Marginalization, the chain rule, and exploits conditional independence. This can be viewed as a tree search that branches over all values of the hidden variables.
- Variable elimination avoids unnecessary computation. It runs in polynomial time for poly-tree BNs. In general, exact probabilistic inference is #P-hard. Approximate probabilistic inference methods exist.

2025-05-14

Inference by sampling: A whole zoo of methods for doing this exists.



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- **Clustering**: Pre-combining subsets of variables to reduce the running time of inference.



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- Compilation to SAT: More precisely, to "weighted model counting" in CNF formulas. Model counting extends DPLL with the ability to determine the number of satisfying interpretations. Weighted model counting allows to define a mass for each such interpretation (= the probability of an atomic event).



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Fau

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- Dynamic BN: BN with one slice of variables at each "time step", encoding probabilistic behavior over time.
- **Relational BN**: BN with predicates and object variables.
- **First-order BN**: Relational BN with quantification, i.e. probabilistic logic. E.g., the BLOG language developed by Stuart Russel and co-workers.



Chapter 24 Making Simple Decisions Rationally

24.1 Introduction



We now know how to update our world model, represented as (a set of) random variables, given observations. Now we need to act.



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 - How "good" are these consequences?



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► Idea:

Represent actions as "special random variables":

Given disjoint actions a_1, \ldots, a_n , introduce a random variable A with domain $\{a_1, \ldots, a_n\}$. Then we can model/query $\mathbb{P}(X|A = a_i)$.

- Assign numerical values to the possible outcomes of actions (i.e. a function u: dom(X) → ℝ) indicating their desirability.
- Choose the action that maximizes the expected value of u



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Definition 1.4. Decision theory investigates decision problems, i.e. how a utility-based agent *a* deals with choosing among actions based on the desirability of their outcomes given by a real-valued utility function U on states $s \in S$: i.e. $U: S \to \mathbb{R}$.



Decision Theory

- ▶ If our states are random variables, then we obtain a random variable for the utility function:
- ▶ **Observation:** Let $X_i: \Omega \to D_i$ random variables on a probability model $\langle \Omega, P \rangle$ and $f: D_1 \times \ldots \times D_n \to E$. Then $F(x) := f(X_0(x), \ldots, X_n(x))$ is a random variable $\Omega \to E$.



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▶ Definition 1.7. Given a probability model $\langle \Omega, P \rangle$ and a random variable $X : \Omega \to D$ with $D \subseteq \mathbb{R}$, then $E(X) := \sum_{x \in D} P(X = x) \cdot x$ is called the expected value (or expectation) of X. (Assuming the sum/series is actually defined!) Analogously, let e_1, \ldots, e_n a sequence of events. Then the expected value of X given e_1, \ldots, e_n is defined as $E(X|e_1, \ldots, e_n) := \sum_{x \in D} \mu(X = x \mid e_1, \ldots, e_n) \cdot x$.



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- ▶ Definition 1.9. Given a probability model $\langle \Omega, P \rangle$ and a random variable $X : \Omega \to D$ with $D \subseteq \mathbb{R}$, then $E(X) := \sum_{x \in D} P(X = x) \cdot x$ is called the expected value (or expectation) of X. (Assuming the sum/series is actually defined!) Analogously, let e_1, \ldots, e_n a sequence of events. Then the expected value of X given e_1, \ldots, e_n is defined as $E(X|e_1, \ldots, e_n) := \sum_{x \in D} \mu(X = x \mid e_1, \ldots, e_n) \cdot x$.
- Putting things together:

Fau

▶ Definition 1.10. Let $A: \Omega \to D$ a random variable (where D is a set of actions) $X_i: \Omega \to D_i$ random variables (the state), and $U: D_1 \times \ldots \times D_n \to \mathbb{R}$ a utility function. Then the expected utility of the action $a \in D$ is the expected value of U (interpreted as a random variable) given A = a; i.e.

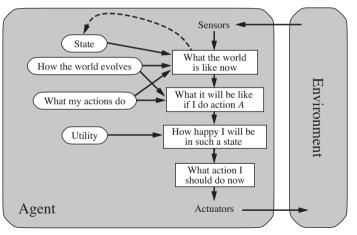
$$\mathbf{EU}(\mathbf{a}) := \sum_{\langle x_1, \dots, x_n \rangle \in D_1 \times \dots \times D_n} \mu(X_1 = x_1, \dots, X_n = x_n \mid A = \mathbf{a}) \cdot U(x_1, \dots, x_n)$$

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Utility-based Agents

- Definition 1.11. A utility-based agent uses a world model along with a utility function that models its preferences among the states of that world. It chooses the action that leads to the best expected utility.
- Agent Schema:



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- Definition 1.12 (MEU principle for Rationality). We call an action rational if it maximizes expected utility (MEU). An utility-based agent is called rational, iff it always chooses a rational action.
- ► Hooray: This solves all of AI.
- **Problem:** There is a long, long way towards an operationalization ;)
- Note: An agent can be entirely rational (consistent with MEU) without ever representing or manipulating utilities and probabilities.
- **Example 1.13.** A reflex agent for tic tac toe based on a perfect lookup table is rational if we take (the negative of) "winning/drawing in *n* steps" as the utility function.
- **Example 1.14 (Al1).** Heuristics in tree search (greedy search, A^*) and game-play (minimax, alpha-beta pruning) maximize "expected" utility.

 \Rightarrow In fully observable, deterministic environments, "expected utility" reduces to a specific determined utility value:

EU(a) = U(T(S(s, e), a)), where e the most recent percept, s the current state, S the sensor function and T the transition function.

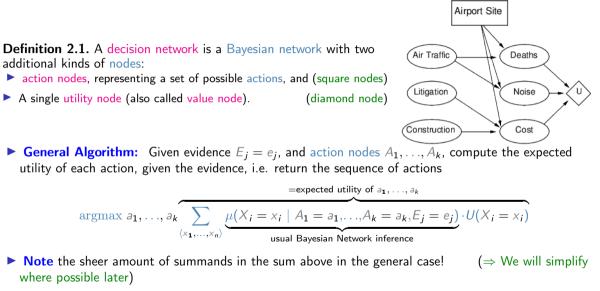
Now let's figure out how to actually assign utilities!



(in principle)

24.2 Decision Networks

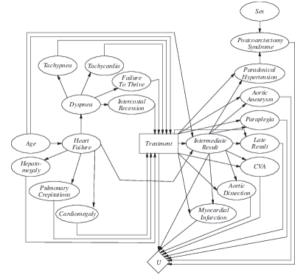






Decision Networks: Example

Example 2.2 (A Decision-Network for Aortic Coarctation). from [Lucas:kadtes96]





24.3 Preferences and Utilities



Preferences in Deterministic Environments

Problem: How do we determine the utility of a state? satisfaction/happiness in a possibly future state...) (We cannot directly measure our (What unit would we even use?)

- Example 3.1. I have to decide whether to go to class today (or sleep in). What is the utility of this lecture?
 (obviously 42)
- Idea: We can let people/agents choose between two states (subjective preference) and derive a utility from these choices.
- ► Example 3.2. "Give me your cell-phone or I will give you a bloody nose". ~> To make a decision in a deterministic environment, the agent must determine whether it prefers a state without phone to one with a bloody nose?
- **Definition 3.3.** Given states A and B (we call them prizes) an agent can express preferences of the form
 - $\blacktriangleright A \succ B \qquad A \text{ prefered over } B$
 - $\blacktriangleright A \sim B \qquad \text{indifference between } A \text{ and } B$
 - $\blacktriangleright A \succeq B \qquad B \text{ not prefered over } A$
 - i.e. Given a set \mathcal{S} (of states), we define binary relations \succ and \sim on \mathcal{S} .



- Problem: In nondeterministic environments we do not have full information about the states we choose between.
- Example 3.4 (Airline Food). "Do you want chicken or pasta" (but we cannot see through the tin foil)

Definition 3.5.

Let S a set of states. We call a random variable X with domain $\{A_1, \ldots, A_n\} \subseteq S$ a lottery and write $[p_1, A_1; \ldots; p_n, A_n]$, where $p_i = P(X = A_i)$.

- ► Idea: A lottery represents the result of a nondeterministic action that can have outcomes A_i with prior probability p_i. For the binary case, we use [p,A;1-p,B]. We can then extend preferences to include lotteries, as a measure of how *strongly* we prefer one prize over another.
- **Convention:** We assume S to be *closed under lotteries*, i.e. lotteries themselves are also states. That allows us to consider lotteries such as [p,A;1-p,[q,B;1-q,C]].



FAU

Note: Preferences of a rational agent must obey certain constraints – An agent with rational preferences can be described as an MEU-agent.

▶ Definition 3.6. We call a set > of preferences rational, iff the following constraints hold:

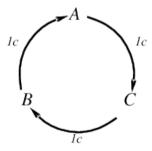
Orderability	$A \succ B \lor B \succ A \lor A \sim B$
Transitivity	$A \succ B \land B \succ C \Rightarrow A \succ C$
Continuity	$A \succ B \succ C \Rightarrow (\exists p.[p,A;1-p,C] \sim B)$
Substitutability	$A \sim B \Rightarrow [p,A;1-p,C] \sim [p,B;1-p,C]$
Monotonicity	$A \succ B \Rightarrow ((p > q) \Leftrightarrow [p,A;1-p,B] \succ [q,A;1-q,B])$
Decomposability	$[p,A;1-p,[q,B;1-q,C]] \sim [p,A;((1-p)q),B;((1-p)(1-q)),C]$

From a set of rational preferences, we can obtain a meaningful utility function.

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Rational preferences contd.

- ▶ Violating the rationality constraints from ??? leads to self-evident irrationality.
- **Example 3.7.** An agent with intransitive preferences can be induced to give away all its money:
 - ▶ If $B \succ C$, then an agent who has C would pay (say) 1 cent to get B
 - ▶ If $A \succ B$, then an agent who has B would pay (say) 1 cent to get A
 - ▶ If $C \succ A$, then an agent who has A would pay (say) 1 cent to get C





24.4 Utilities



► **Theorem 4.1.** (*Ramsey, 1931; von Neumann and Morgenstern, 1944*) Given a rational set of preferences there exists a real valued function U such that $U(A) \ge U(B)$, iff $A \succeq B$ and $U([p_1, S_1; ...; p_n, S_n]) = \sum_i p_i U(S_i)$

This is an existence theorem, uniqueness not guaranteed.

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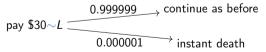
- ▶ Note: Agent behavior is *invariant* w.r.t. positive linear transformations, i.e. an agent with utility function $U'(x) = k_1 U(x) + k_2$ where $k_1 > 0$ behaves exactly like one with U.
- Observation: With deterministic prizes only (no lottery choices), only a total ordering on prizes can be determined.
- Definition 4.2. We call a total ordering on states a value function or ordinal utility function. (If we don't need to care about *relative* utilities of states, e.g. to compute non-trivial expected utilities, that's all we need anyway!)



- Intuition: Utilities map states to real numbers.
- Question: Which numbers exactly?
- Definition 4.3 (Standard approach to assessment of human utilities). Compare a given state A to a standard lottery L_p that has
 - "best possible prize" u_{\top} with probability p
 - "worst possible catastrophe" u_{\perp} with probability 1 p

adjust lottery probability p until $A \sim L_p$. Then U(A) = p.

Example 4.4. Choose $u_{\top} \cong$ current state, $u_{\perp} \cong$ instant death





▶ Definition 4.5. Normalized utilities: $u_{\top} = 1$, $u_{\perp} = 0$. (Not very meaningful, but at least it's independent of the specific problem...)



Definition 4.8. Normalized utilities: $u_{\perp} = 1$, $u_{\perp} = 0$.

Obviously: Money function (see later))
 (Not very meaningful, but at least it's independent of the specific problem...)
 (Very intuitive, often easy to determine, but actually not well-suited as a utility function (see later))



- **Definition 4.11.** Normalized utilities: $u_{\top} = 1$, $u_{\perp} = 0$.
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- Definition 4.12. Micromorts: one millionth chance of instant death. (useful for Russian roulette, paying to reduce product risks, etc.)
- **But:** Not necessarily a good measure of risk, if the risk is "merely" severe injury or illness...



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- Definition 4.15. Micromorts: one millionth chance of instant death. (useful for Russian roulette, paying to reduce product risks, etc.)
- **But:** Not necessarily a good measure of risk, if the risk is "merely" severe injury or illness...
- The following measure is better

(more informative)

 Definition 4.16. QALYs: quality adjusted life years QALYs are useful for medical decisions involving substantial risk.



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Problem: What is the monetary value of a micromort?



- **Problem:** What is the monetary value of a micromort?
- Just ask people: What would you pay to avoid playing Russian roulette with a million-barrelled revolver? (Usually: quite a lot!)



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- Just ask people: What would you pay to avoid playing Russian roulette with a million-barrelled revolver? (Usually: quite a lot!)
- But their behavior suggests a lower price:
 - Driving in a car for 370km incurs a risk of one micromort;
 - Over the life of your car say, 150,000km that's 400 micromorts.
 - People appear to be willing to pay about 10,000€ more for a safer car that halves the risk of death. (~ 25€ per micromort)

This figure has been confirmed across many individuals and risk types.



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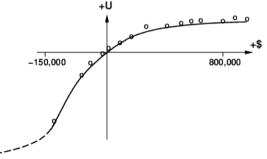
This figure has been confirmed across many individuals and risk types.

Of course, this argument holds only for small risks. Most people won't agree to kill themselves for 25M€. (Also: People are pretty bad at estimating and comparing risks, especially if they are small.) (Various cognitive biases and heuristics are at work here!)



Money vs. Utility

- Money does not behave as a utility function should.
- Given a lottery *L* with expected monetary value EMV(L), usually U(L) < U(EMV(L)), i.e., people are risk averse.
- **Utility curve:** For what probability p am I indifferent between a prize x and a lottery [p, M; 1-p, 0 for large numbers M?
- > Typical empirical data, extrapolated with risk prone behavior for debitors:



Empirically: Comes close to the logarithm on the natural numbers.
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24.5 Multi-Attribute Utility



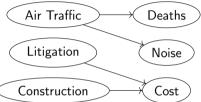
- ▶ **Recap:** So far we understand how to obtain utility functions $u: S \to \mathbb{R}$ on states $s \in S$ from (rational) preferences.
- **But** in practice, our actions often impact *multiple* distinct "attributes" that need to be weighed against each other.
 - \Rightarrow Lotteries become complex very quickly
- ▶ **Definition 5.1.** Let $X_1, ..., X_n$ be random variables with domains $D_1, ..., D_n$. Then we call a function $u: D_1 \times ... \times D_n \to \mathbb{R}$ a (multi-attribute) utility function on attributes $X_1, ..., X_n$.
- ▶ Note: In the general (worst) case, a multi-attribute utility function on *n* random variables with domain sizes *k* each requires *kⁿ* parameters to represent.
- But: A utility function on multiple attributes often has "internal structure" that we can exploit to simplify things.

For example, the distinct attributes are often "independent" with respect to their utility (a higher-quality product is better than a lower-quality one that costs the same, and a cheaper product is better than an expensive one of the same quality)



Multi-Attribute Utility: Example

Example 5.2 (Assessing an Airport Site).



- Attributes: Deaths, Noise, Cost.
- Question: What is U(Deaths, Noise, Cost) for a projected airport?

▶ How can complex utility function be assessed from preference behaviour?

- Idea 1: Identify conditions under which decisions can be made without complete identification of U(X1,...,Xn).
- ▶ Idea 2: Identify various types of *independence* in preferences and derive consequent canonical forms for $U(X_1, ..., X_n)$.

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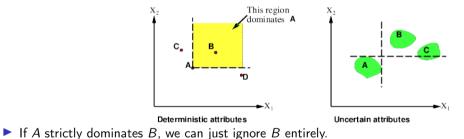
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Strict Dominance

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First Assumption: *U* is often *monotone* in each argument.

- (wlog. growing)
- Definition 5.3. (Informally) An action B strictly dominates an action A, iff every possible outcome of B is at least as good as every possible outcome of A,

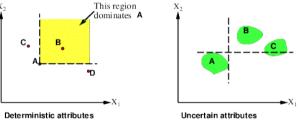


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- **Definition 5.4.** (Informally) An action B strictly dominates an action A, iff every possible outcome of B is at least as good as every possible outcome of A,



- If A strictly dominates B, we can just ignore B entirely.
- **Observation:** Strict dominance seldom holds in practice (life is difficult) but is useful for narrowing down the field of contenders.



▶ **Definition 5.5.** Let X_1, X_2 distributions with domains $\subseteq \mathbb{R}$.

 X_1 stochastically dominates X_2 iff for all $t \in \mathbb{R}$, we have $P(X_1 \ge t) \ge P(X_2 \ge t)$, and for some t, we have $P(X_1 \ge t) > P(X_2 \ge t)$.

▶ Observation 5.6. If U is monotone in X_1 , and $\mathbb{P}(X_1|a)$ stochastically dominates $\mathbb{P}(X_1|b)$ for actions a, b, then a is always the better choice than b, with all other attributes X_i being equal. ⇒ If some action $\mathbb{P}(X_i|a)$ stochastically dominates $\mathbb{P}(X_i|b)$ for all attributes X_i , we can ignore b.



Fau

Definition 5.8. Let X_1, X_2 distributions with domains $\subseteq \mathbb{R}$.

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- **Observation 5.9.** If U is monotone in X_1 , and $\mathbb{P}(X_1|a)$ stochastically dominates $\mathbb{P}(X_1|b)$ for actions a, b, then a is always the better choice than b, with all other attributes X_i being equal.
 - \Rightarrow If some action $\mathbb{P}(X_i|a)$ stochastically dominates $\mathbb{P}(X_i|b)$ for all attributes X_i , we can ignore b.
- **Observation:** Stochastic dominance can often be determined without exact distributions using *qualitative* reasoning.
- ► Example 5.10 (Construction cost increases with distance). If airport location S₁ is closer to the city than S₂ ~→ S₁ stochastically dominates S₂ on cost.q

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- **Recall:** In deterministic environments an agent has a value function.
- **Definition 5.11.** X_1 and X_2 preferentially independent of X_3 iff preference between $\langle x_1, x_2, z \rangle$ and $\langle x'_1, x'_2, z \rangle$ does not depend on z. (i.e. the tradeoff between x_1 and x_2 is independent of z)
- Example 5.12. E.g., (Noise, Cost, Safety): are preferentially independent (20,000 suffer, 4.6 G\$, 0.06 deaths/mpm) vs.(70,000 suffer, 4.2 G\$, 0.06 deaths/mpm)
- ► Theorem 5.13 (Leontief, 1947). If every pair of attributes is preferentially independent of its complement, then every subset of attributes is preferentially independent of its complement: mutual preferential independence.
- ▶ **Theorem 5.14 (Debreu, 1960).** Mutual preferential independence implies that there is an additive value function: $V(S) = \sum_i V_i(X_i(S))$, where V_i is a value function referencing just one variable X_i .
- Hence assess n single-attribute functions.

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(often a good approximation)

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Example 5.15. The value function for the airport decision might be

 $V(noise, cost, deaths) = -noise \cdot 10^4 - cost - deaths \cdot 10^{12}$

- Definition 5.16. X is utility independent of Y iff preferences over lotteries in X do not depend on particular values in Y
- Definition 5.17. A set X is mutually utility independent (MUI), iff each subset is utility independent of its complement.



- Definition 5.19. X is utility independent of Y iff preferences over lotteries in X do not depend on particular values in Y
- Definition 5.20. A set X is mutually utility independent (MUI), iff each subset is utility independent of its complement.
- ► Theorem 5.21. For a MUI set of attributes X, there is a multiplicative utility function of the form: [Keeney:muf74]

$$U = \sum_{\{\{X_0, \dots, X_k\} \subseteq \mathcal{X}\}} \prod_{i=1}^k U_i(X_i = x_i)$$

 \Rightarrow U can be represented using n single-attribute utility functions.

System Support: Routine procedures and software packages for generating preference tests to identify various canonical families of utility functions.



- ▶ There are multiple ways to improve inference in decision networks:
- Exploit "inner structure" of the utility function to simplify the computation,
- eliminate dominated actions,

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- Iabel pairs of nodes with stochastic dominance: If (the utility of) some attribute dominates (the utility of) another attribute, focus on the dominant one (e.g. if price is always more important than quality, ignore quality whenever the price between two choices differs)
- various techniques for variable elimination,
- policy iteration (more on that when we talk about Markov decision procedures)

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24.6 The Value of Information



We now know how to exploit the information we have to make decisions. But if we knew more, we might be able to make even better decisions in the long run - potentially at the cost of gaining utility. (exploration vs. exploitation)

Example 6.1 (Medical Diagnosis).

- > We do not expect a doctor to already know the results of the diagnostic tests when the patient comes in.
- Tests are often expensive, and sometimes hazardous.

(directly or by delaying treatment)

- ► Therefore: Only test, if
 - knowing the results lead to a significantly better treatment plan,
 - information from test results is not drowned out by a-priori likelihood.
- Definition 6.2. Information value theory is concerned with agent making decisions on information gathering rationally.



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Value of Information by Example

- ▶ Idea: Compute the expected gain in utility from acquring information.
- ► Example 6.3 (Buying Oil Drilling Rights). There are n blocks of drilling rights available, exactly one block actually has oil worth k∈, in particular:
 - The prior probability of a block having oil is $\frac{1}{n}$ each (mutually exclusive).
 - The current price of each block is $\frac{k}{n} \in$.
 - A "consultant" offers an accurate survey of block (say) 3. How much should we be willing to pay for the survey?



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 - The current price of each block is $\frac{k}{n} \in$.
 - A "consultant" offers an accurate survey of block (say) 3. How much should we be willing to pay for the survey?
- Solution: Compute the expected value of the best action given the information, minus the expected value of the best action without information.

Example 6.6 (Oil Drilling Rights contd.).

- Survey may say "oil in block 3 with probability $\frac{1}{n}$ " \rightarrow we buy block 3 for $\frac{k}{n} \in$ and make a profit of $(k \frac{k}{n}) \in$.
- Survey may say "no oil in block 3 with probability $\frac{n-1}{n}$ " \rightsquigarrow we buy another block, and make an expected profit of $\frac{k}{n-1} \frac{k}{n} \in .$
- Without the survery, the expected profit is 0
- Expected profit is $\frac{1}{n} \cdot \frac{(n-1)k}{n} + \frac{n-1}{n} \cdot \frac{k}{n(n-1)} = \frac{k}{n}$.
- ▶ So, we should pay up to $\frac{k}{n} \in$ for the information.

(as much as block 3 is worth!)

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▶ **Definition 6.7.** Let A the set of available actions and F a random variable. Given evidence $E_i = e_i$, let α be the action that maximizes expected utility a priori, and α_f the action that maximizes expected utility given F = f, i.e.: $\alpha = \underset{a \in A}{\operatorname{argmax}} \operatorname{EU}(a|E_i = e_i)$ and $\alpha_f = \underset{a \in A}{\operatorname{argmax}} \operatorname{EU}(a|E_i = e_i, F = f)$ The value of perfect information (VPI) on F given evidence $E_i = e_i$ is defined as

$$\operatorname{VPI}_{E_i=e_i}(F) := \left(\sum_{f \in \operatorname{dom}(F)} P(F = f \mid E_i = e_i) \cdot \operatorname{EU}(\alpha_f \mid E_i = e_i, F = f)\right) - \operatorname{EU}(\alpha \mid E_i = e_i)$$

▶ Intuition: The VPI is the expected gain from knowing the value of *F* relative to the current expected utility, and considering the relative probabilities of the possible outcomes of *F*.



- Observation 6.8 (VPI is Non-negative). $VPI_E(F) \ge 0$ for all j and E
- ▶ Observation 6.9 (VPI is Non-additive). $VPI_E(F, G) \neq VPI_E(F) + VPI_E(G)$

Observation 6.10 (VPI is Order-independent).

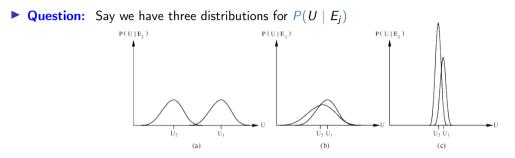
(in expectation, not post hoc)

(consider, e.g., obtaining F twice)

 $\operatorname{VPI}_{F}(F, G) = \operatorname{VPI}_{F}(F) + \operatorname{VPI}_{F,F}(G) = \operatorname{VPI}_{F}(G) + \operatorname{VPI}_{F,G}(F)$

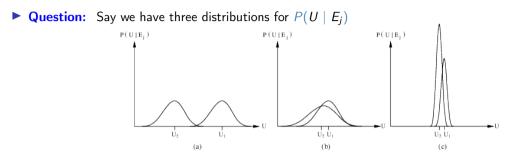
Note: When more than one piece of evidence can be gathered, maximizing VPI for each to select one is not always optimal ~ evidence-gathering becomes a sequential decision problem.





Qualitatively: What is the value of information (VPI) in these three cases?

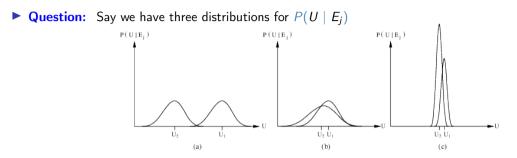




Qualitatively: What is the value of information (VPI) in these three cases?

- ► Answers: qualitatively:
 - a) Choice is obvious (a_1 almost certainly better) \sim information worth little





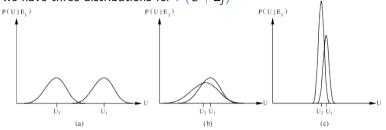
Qualitatively: What is the value of information (VPI) in these three cases?

- ► Answers: qualitatively:
 - a) Choice is obvious (a_1 almost certainly better) \sim information worth little
 - b) Choice is non-obvious (unclear) \sim information worth a lot



Qualitative behavior of VPI

Question: Say we have three distributions for $P(U \mid E_i)$



Qualitatively: What is the value of information (VPI) in these three cases?

Answers: gualitatively:

- a) Choice is obvious (a_1 almost certainly better) \sim information worth little
- b) Choice is non-obvious (unclear) \sim information worth a lot
- c) Choice is non-obvious (unclear) but makes little difference \sim information worth little Note two things
- The difference between (b) and (c) is the width of the distribution, i.e. how close the possible outcomes are together
- \triangleright The fact that U_2 has a high peak in (c) means that its expected value is known with higher certainty than (irrelevant to the argument) U_1 . FAU © 2025-05-14

A simple Information-Gathering Agent

Definition 6.11. A simple information gathering agent.

```
function Information–Gathering–Agent (percept) returns an action

persistent: D, a decision network

integrate percept into D

j := \underset{k}{\operatorname{argmax}} \operatorname{VPI}_{E}(E_{k})/\operatorname{Cost}(E_{k})

if \operatorname{VPI}_{E}(E_{j}) > \operatorname{Cost}(E_{j}) return Request(E_{j})

else return the best action from D
```

The next percept after $\text{Request}(E_j)$ provides a value for E_j .

- Problem: The information gathering implemented here is myopic, i.e. only acquires a single evidence variable, or acts immediately. (cf. greedy search)
- But it works relatively well in practice. (e.g. outperforms humans for selecting diagnostic tests)
- Strategies for nonmyopic information gathering exist

(gathers info before acting)

(Not discussed in this course)



- An MEU agent maximizes expected utility.
- Decision theory provides a framework for rational decision making.
- Decision networks augment Bayesian networks with action nodes and a utility node.
- rational preferences allow us to obtain a utility function (orderability, transitivity, continuity, substitutability, monotonicity, decomposability)
- multi-attribute utility functions can usually be "destructured" to allow for better inference and representation (can be monotone, attributes may dominate others, actions may dominate others, may be multiplicative,...)
- information value theory tells us when to explore rather than exploit, using
- ▶ VPI (value of perfect information) to determine how much to "pay" for information.



2025-05-14

Chapter 25 Temporal Probability Models

2025-05-14

25.1 Modeling Time and Uncertainty



Stochastic Processes

The world changes in *stochastically predictable ways*. **Example 1.1**.

- The weather changes, but the weather tomorrow is somewhat predictable given today's weather and other factors, (which in turn (somewhat) depends on yesterday's weather, which in turn...)
- ▶ the stock market changes, but the stock price tomorrow is probably related to today's price,

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A patient's blood sugar changes, but their blood sugar is related to their blood sugar 10 minutes ago (in particular if they didn't eat anything in between)

How do we model this?

Fau



The world changes in *stochastically predictable ways*. **Example 1.4.**

- The weather changes, but the weather tomorrow is somewhat predictable given today's weather and other factors, (which in turn (somewhat) depends on yesterday's weather, which in turn...)
- ▶ the stock market changes, but the stock price tomorrow is probably related to today's price,
- A patient's blood sugar changes, but their blood sugar is related to their blood sugar 10 minutes ago (in particular if they didn't eat anything in between)

How do we model this?

Definition 1.5. Let $\langle \Omega, P \rangle$ a probability space and $\langle S, \preceq \rangle$ a (not necessarily *totally*) ordered set. A sequence of random variables $(X_t)_{t \in S}$ with dom $(X_t) = D$ is called a stochastic process over the time structure S.

Intuition: X_t models the outcome of the random variable X at time step t. The sample space Ω corresponds to the set of all possible sequences of outcomes.

Note: We will almost exclusively use $\langle S, \preceq \rangle = \langle \mathbb{N}, \leq \rangle$.

Definition 1.6. Given a stochastic process X_t over S and $a, b \in S$ with $a \leq b$, we write $X_{a:b}$ for the sequence $X_a, X_{a+1}, \ldots, X_{b-1}, X_b$ and $E_{a:b}^{=e}$ for $E_a = e_a, \ldots, E_b = e_b$.



Example 1.7 (Umbrellas). You are a security guard in a secret underground facility, want to know it if is raining outside. Your only source of information is whether the director comes in with an umbrella.

- ▶ We have a stochastic process Rain₀, Rain₁, Rain₂, ... of hidden variables, and
- ▶ a related stochastic process Umbrella₀, Umbrella₁, Umbrella₂, ... of evidence variables.

...and a combined stochastic process $\langle \text{Rain}_0, \text{Umbrella}_0 \rangle$, $\langle \text{Rain}_1, \text{Umbrella}_1 \rangle$,... Note that Umbrella_t only depends on Rain_t , not on e.g. Umbrella_{t-1} (except indirectly through Rain_t) / Rain_{t-1}).

Definition 1.8. We call a stochastic process of *hidden* variables a state variable.



Idea: Construct a Bayesian network from these variables ...without everything exploding in size...?



Markov Processes

Idea: Construct a Bayesian network from these variables ...without everything exploding in size...?

Definition 1.11. Let $(X_t)_{t \in S}$ a stochastic process. X has the (*n*th order) Markov property iff X_t only depends on a bounded subset of $X_{0:t-1}$ – i.e. for all $t \in S$ we have $\mathbb{P}(X_t|X_0, \ldots X_{t-1}) = \mathbb{P}(X_t|X_{t-n}, \ldots X_{t-1})$ for some $n \in S$. A stochastic process with the Markov property for some n is called a (*n*th order) Markov process.

FAU :



(parents?)

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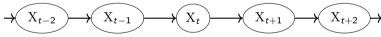
Markov Processes

Idea: Construct a Bayesian network from these variables ...without everything exploding in size...?

Definition 1.13. Let $(X_t)_{t \in S}$ a stochastic process. X has the (*n*th order) Markov property iff X_t only depends on a bounded subset of $X_{0:t-1}$ – i.e. for all $t \in S$ we have $\mathbb{P}(X_t|X_0, \ldots, X_{t-1}) = \mathbb{P}(X_t|X_{t-n}, \ldots, X_{t-1})$ for some $n \in S$. A stochastic process with the Markov property for some n is called a (*n*th order) Markov process.

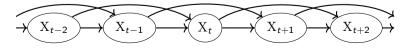
Important special cases: **Definition 1.14.**

First-order Markov property: $\mathbb{P}(X_t|X_{0:t-1}) = \mathbb{P}(X_t|X_{t-1})$



A first order Markov process is called a Markov chain.

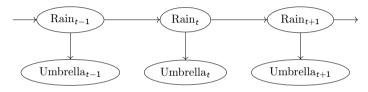
Second-order Markov property: $\mathbb{P}(X_t|X_{0:t-1}) = \mathbb{P}(X_t|X_{t-2}, X_{t-1})$



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(parents?)

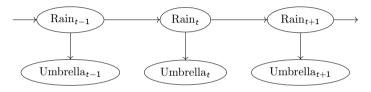
Example 1.15 (Umbrellas continued). We model the situation in a Bayesian network:



Problem: This network does not actually have the First-order Markov property...



Example 1.16 (Umbrellas continued). We model the situation in a Bayesian network:



Problem: This network does not actually have the First-order Markov property...

Possible fixes: We have two ways to fix this:

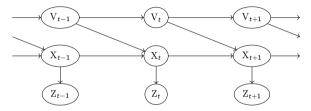
- 1. Increase the order of the Markov process.
- 2. Add more state variables, e.g., Temp_t , Pressure_t .

(more dependencies \Rightarrow more complex inference) (more information sources)



Markov Process Example: Robot Motion

Example 1.17 (Random Robot Motion). Assume we want to track a robot wandering randomly on the X/Y plane, whose position we can only observe roughly (e.g. by approximate GPS coordinates:) Markov chain



- the velocity V_i may change unpredictably.
- ▶ the exact position X_i depends on previous position X_{i-1} and velocity V_{i-1}
- ▶ the position X_i influences the observed position Z_i.

Example 1.18 (Battery Powered Robot). If the robot has a battery, the Markov property is violated!

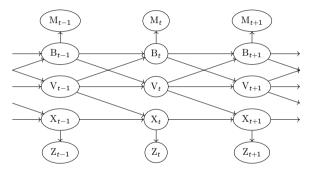
- Battery exhaustion has a systematic effect on the change in velocity.
- This depends on how much power was used by all previous manoeuvres.



Markov Process Example: Robot Motion

Idea: We can restore the Markov property by including a state variable for the charge level B_t . (Better still: Battery level sensor)

Example 1.19 (Battery Powered Robot Motion).



- ▶ Battery level B_i is influenced by previous level B_{i-1} and velocity V_{i-1} .
- ▶ Velocity V_i is influenced by previous level B_{i-1} and velocity V_{i-1} .
- Battery meter M_i is only influenced by Battery level B_i.



Stationary Markov Processes as Transition Models

Remark 1.20. Given a stochastic process with state variables X_t and evidence variables E_t , then $\mathbb{P}(X_t|X_{0:t})$ is a transition model and $\mathbb{P}(E_t|X_{0:t}, \mathbb{E}_{1:t-1})$ a sensor model in the sense of a model-based agent.

Note that we assume that the X_t do not depend on the E_t .

Also note that with the Markov property, the transition model simplifies to $\mathbb{P}(X_t|X_{t-n})$.

Problem: Even with the Markov property the transition model is infinite.



 $(t \in \mathbb{N})$

Stationary Markov Processes as Transition Models

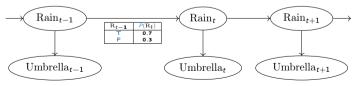
Remark 1.23. Given a stochastic process with state variables X_t and evidence variables E_t , then $\mathbb{P}(X_t|X_{0:t})$ is a transition model and $\mathbb{P}(E_t|X_{0:t}, \mathbb{E}_{1:t-1})$ a sensor model in the sense of a model-based agent.

Note that we assume that the X_t do not depend on the E_t .

Also note that with the Markov property, the transition model simplifies to $\mathbb{P}(X_t|X_{t-n})$.

Problem: Even with the Markov property the transition model is infinite. $(t \in \mathbb{N})$ **Definition 1.24.** A Markov chain is called stationary if the transition model is independent of time, i.e. $\mathbb{P}(X_t|X_{t-1})$ is the same for all t.

Example 1.25 (Umbrellas are stationary). $\mathbb{P}(\text{Rain}_t | \text{Rain}_{t-1})$ does not depend on t. (need only one table)



Contraction of the second

Stationary Markov Processes as Transition Models

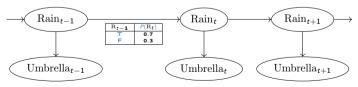
Remark 1.26. Given a stochastic process with state variables X_t and evidence variables E_t , then $\mathbb{P}(X_t|X_{0:t})$ is a transition model and $\mathbb{P}(E_t|X_{0:t}, \mathbb{E}_{1:t-1})$ a sensor model in the sense of a model-based agent.

Note that we assume that the X_t do not depend on the E_t .

Also note that with the Markov property, the transition model simplifies to $\mathbb{P}(X_t|X_{t-n})$.

Problem: Even with the Markov property the transition model is infinite. $(t \in \mathbb{N})$ **Definition 1.27.** A Markov chain is called stationary if the transition model is independent of time, i.e. $\mathbb{P}(X_t|X_{t-1})$ is the same for all t.

Example 1.28 (Umbrellas are stationary). $\mathbb{P}(\text{Rain}_t | \text{Rain}_{t-1})$ does not depend on t. (need only one table)



Don't confuse "stationary" (Markov processes) with "static" (environments).
 We restrict ourselves to stationary Markov processes in Al-2.



Markov Sensor Models

Recap: The sensor model $\mathbb{P}(E_t | X_{0:t}, E_{1:t-1})$ allows us (using Bayes rule et al) to update our belief state about X_t given the observations $E_{0:t}$.

Problem: The evidence variables E_t could depend on any of the variables $X_{0:t}, E_{1:t-1}...$



Markov Sensor Models

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Problem: The evidence variables E_t could depend on any of the variables $X_{0:t}, E_{1:t-1}...$

Definition 1.31. We say that a sensor model has the sensor Markov property, iff $\mathbb{P}(E_t|X_{0:t}, \mathbb{E}_{1:t-1}) = \mathbb{P}(E_t|X_t) - i.e.$, the sensor model depends only on the current state.

Assumptions on Sensor Models: We usually assume the sensor Markov property and make it stationary as well: $\mathbb{P}(\mathcal{E}_t|X_t)$ is fixed for all t.



Markov Sensor Models

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Problem: The evidence variables E_t could depend on any of the variables $X_{0:t}$, $E_{1:t-1}$...

Definition 1.33. We say that a sensor model has the sensor Markov property, iff $\mathbb{P}(E_t|X_{0:t}, \mathbb{E}_{1:t-1}) = \mathbb{P}(E_t|X_t) - i.e.$, the sensor model depends only on the current state.

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Definition 1.34 (Note).

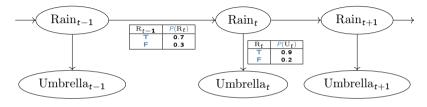
- ▶ If a Markov chain X is stationary and discrete, we can represent the transition model as a matrix $T_{ij} := P(X_t = j \mid X_{t-1} = i).$
- ▶ If a sensor model has the sensor Markov property, we can represent each observation $E_t = e_t$ at time t as the diagonal matrix O_t with $O_{tii} := P(E_t = e_t | X_t = i)$.
- ► A pair (X, E) where X is a (stationary) Markov chains, E_i only depends on X_i, and E has the sensor Markov property is called a (stationary) Hidden Markov Model (HMM). (X and E are single variables)

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Umbrellas, the full Story

Example 1.35 (Umbrellas, Transition & Sensor Models).



This is a hidden Markov model

Observation 1.36. If we know the initial prior probabilities $\mathbb{P}(X_0)$ ($\widehat{=}$ time t = 0), then we can compute the full joint probability distribution as

$$\mathbb{P}(X_{0:t}, \mathsf{E}_{1:t}) = \mathbb{P}(X_0) \cdot \left(\prod_{i=1}^t \mathbb{P}(X_i | X_{i-1}) \cdot \mathbb{P}(\mathcal{E}_i | X_i)\right)$$

FAU



25.2 Inference: Filtering, Prediction, and Smoothing



Inference tasks

Definition 2.1. Given a Markov process with state variables X_t and evidence variables E_t , we are interested in the following Markov inference tasks:

- ► Filtering (or monitoring) P(X_t | E^{=e}_{1:t}): Given the sequence of observations up until time t, compute the likely state of the world at *current* time t.
- Prediction (or state estimation) P(X_{t+k} | E^{=e}_{1:t}) for k > 0: Given the sequence of observations up until time t, compute the likely *future* state of the world at time t + k.
- Smoothing (or hindsight) $\mathbb{P}(X_{t-k}|E_{1:t}^{=e})$ for 0 < k < t: Given the sequence of observations up until time *t*, compute the likely *past* state of the world at time t k.
- Most likely explanation $\underset{X_{1:t}}{\operatorname{argmax}} (P(X_{1:t}^{=x} | E_{1:t}^{=e}))$: Given the sequence of observations up until time t, compute the most likely sequence of states that led to these observations.

Note: The most likely sequence of states is *not* (necessarily) the sequence of most likely states ;-) In this section, we assume X and E to represent *multiple* variables, where X jointly forms a Markov chain and the E jointly have the sensor Markov property. In the case where X and E are stationary *single* variables, we have a stationary hidden Markov model and can use the matrix forms.



Note:

- Using the full joint probability distribution, we can compute any conditional probability we want, but not necessarily efficiently.
- ▶ We want to use filtering to update our "world model" $\mathbb{P}(X_t)$ based on a new observation $E_t = e_t$ and our *previous* world model $\mathbb{P}(X_{t-1})$.
- $\Rightarrow \text{ We want a function } \mathbb{P}(X_t | E_{1:t}^{=e}) = F(e_t, \underbrace{\mathbb{P}(X_{t-1} | E_{1:t-1}^{=e})}_{F(e_{t-1}, \dots)})$

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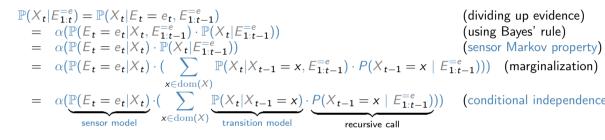
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- Using the full joint probability distribution, we can compute any conditional probability we want, but not necessarily efficiently.
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Spoiler:

$$F(e_t, \mathbb{P}(X_{t-1}|E_{1:t-1}^{=e})) = \alpha(\mathsf{O}_t \cdot \mathsf{T}^{\mathsf{T}} \cdot \mathbb{P}(X_{t-1}|E_{1:t-1}^{=e}))$$







$$\begin{split} \mathbb{P}(X_t | E_{1:t}^{=e}) &= \mathbb{P}(X_t | E_t = e_t, E_{1:t-1}^{=e}) & \text{(dividing up evidence)} \\ &= \alpha(\mathbb{P}(E_t = e_t | X_t, E_{1:t-1}^{=e}) \cdot \mathbb{P}(X_t | E_{1:t-1}^{=e})) & \text{(using Bayes' rule)} \\ &= \alpha(\mathbb{P}(E_t = e_t | X_t) \cdot \mathbb{P}(X_t | E_{1:t-1}^{=e})) & \text{(sensor Markov property)} \\ &= \alpha(\mathbb{P}(E_t = e_t | X_t) \cdot (\sum_{x \in \text{dom}(X)} \mathbb{P}(X_t | X_{t-1} = x, E_{1:t-1}^{=e}) \cdot \mathbb{P}(X_{t-1} = x | E_{1:t-1}^{=e}))) & \text{(marginalization)} \\ &= \alpha(\underbrace{\mathbb{P}(E_t = e_t | X_t)}_{\text{sensor model}} \cdot (\sum_{x \in \text{dom}(X)} \underbrace{\mathbb{P}(X_t | X_{t-1} = x)}_{\text{transition model}} \cdot \underbrace{\mathbb{P}(X_{t-1} = x | E_{1:t-1}^{=e})}_{\text{recursive call}})) & \text{(conditional independence)} \\ \end{split}$$

Reminder: In a stationary HMM, we have the matrices $T_{ij} = P(X_t = j \mid X_{t-1} = i)$ and $O_{t_{ii}} = P(E_t = e_t \mid X_t = i)$. Then interpreting $\mathbb{P}(X_{t-1} \mid E_{1:t-1}^{=e})$ as a vector, the above corresponds exactly to the matrix multiplication $\alpha(O_t \cdot T^T \cdot \mathbb{P}(X_{t-1} \mid E_{1:t-1}^{=e}))$

Definition 2.3. We call the inner part of the above expression the forward algorithm, i.e. $\mathbb{P}(X_t | E_{1:t}^{=e}) = \alpha(\text{FORWARD}(e_t, \mathbb{P}(X_{t-1} | E_{1:t-1}^{=e}))) =: f_{1:t}.$

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Filtering the Umbrellas

Example 2.4. Let's assume:

▶ $\mathbb{P}(\mathbb{R}_0) = \langle 0.5, 0.5 \rangle$, (Note that with growing *t* (and evidence), the impact of the prior at *t* = 0 vanishes anyway)

$$P(\mathbf{R}_{t+1} \mid \mathbf{R}_t) = 0.6, \ P(\neg \mathbf{R}_{t+1} \mid \neg \mathbf{R}_t) = 0.8, \ P(\mathbf{U}_t \mid \mathbf{R}_t) = 0.9 \text{ and } P(\neg \mathbf{U}_t \mid \neg \mathbf{R}_t) = 0.85$$

$$\Rightarrow \ \mathsf{T} = \begin{pmatrix} 0.6 & 0.4 \\ 0.2 & 0.8 \end{pmatrix}$$

▶ The director carries an umbrella on days 1 and 2, and *not* on day 3.

$$\Rightarrow O_1 = O_2 = \begin{pmatrix} 0.9 & 0 \\ 0 & 0.15 \end{pmatrix} \text{ and } O_3 = \begin{pmatrix} 0.1 & 0 \\ 0 & 0.85 \end{pmatrix}.$$

Then:



 $\begin{aligned} & \textbf{Example 2.5. } f_{1:1} := \mathbb{P}(\mathbb{R}_{1} | \mathbb{U}_{1} = \mathsf{T}) = \langle 0.8, 0.2 \rangle \\ & \blacktriangleright f_{1:2} := \mathbb{P}(\mathbb{R}_{2} | \mathbb{U}_{2} = \mathsf{T}, \mathbb{U}_{1} = \mathsf{T}) = \alpha(\mathbb{O}_{2} \cdot \mathsf{T}^{\mathsf{T}} \cdot f_{1:1}) = \alpha(\mathbb{P}(\mathbb{U}_{2} = \mathsf{T} | \mathbb{R}_{2}) \cdot (\sum_{b \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(\mathbb{R}_{2} | \mathbb{R}_{1} = b) \cdot f_{1:1}(b))) \\ & = \alpha(\langle 0.9, 0.15 \rangle \cdot (\langle 0.6, 0.4 \rangle \cdot 0.8 + \langle 0.2, 0.8 \rangle \cdot 0.2)) = \alpha(\langle 0.468, 0.072 \rangle) = \langle 0.87, 0.13 \rangle \\ & \vdash f_{1:3} := \mathbb{P}(\mathbb{R}_{3} | \mathbb{U}_{3} = \mathsf{F}, \mathbb{U}_{2} = \mathsf{T}, \mathbb{U}_{1} = \mathsf{T}) = \alpha(\mathbb{O}_{3} \cdot \mathsf{T}^{\mathsf{T}} \cdot f_{1:2}) \\ & = \alpha(\mathbb{P}(\mathbb{U}_{3} = \mathsf{F} | \mathbb{R}_{3}) \cdot (\sum_{b \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(\mathbb{R}_{3} | \mathbb{R}_{2} = b) \cdot f_{1:2}(b))) \\ & = \alpha(\langle 0.1, 0.85 \rangle \cdot (\langle 0.6, 0.4 \rangle \cdot 0.87 + \langle 0.2, 0.8 \rangle \cdot 0.13)) = \alpha(\langle 0.0547, 0.3853 \rangle) = \langle 0.12, 0.88 \rangle \end{aligned}$

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Prediction in Markov Chains

Prediction: $\mathbb{P}(X_{t+k}|E_{1:t}^{=e})$ for k > 0.

Intuition: Prediction is filtering without new evidence - i.e. we can use filtering until t, and then continue as follows:

Lemma 2.6. By the same reasoning as filtering:

$$\mathbb{P}(X_{t+k+1}|E_{1:t}^{=e}) = \sum_{x \in \text{dom}(X)} \underbrace{\mathbb{P}(X_{t+k+1}|X_{t+k} = x)}_{\text{transition model}} \cdot \underbrace{\mathcal{P}(X_{t+k} = x \mid E_{1:t}^{=e})}_{\text{recursive call}} \underbrace{= \mathsf{T}^{\mathsf{T}} \cdot \mathbb{P}(X_{t+k} = x \mid E_{1:t}^{=e})}_{\text{HMM}}$$

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$$\mathbb{P}(X_{t+k+1}|E_{1:t}^{=e}) = \sum_{x \in \operatorname{dom}(X)} \underbrace{\mathbb{P}(X_{t+k+1}|X_{t+k}=x)}_{transition \ model} \cdot \underbrace{\mathcal{P}(X_{t+k}=x \mid E_{1:t}^{=e})}_{recursive \ call} \underbrace{= \mathsf{T}^{\mathsf{T}} \cdot \mathbb{P}(X_{t+k}=x|E_{1:t}^{=e})}_{HMM}$$

Observation 2.9. As $k \to \infty$, $\mathbb{P}(X_{t+k}|E_{1:t}^{=e})$ converges towards a fixed point called the stationary distribution of the Markov chain. (which we can compute from the equation $S = \mathsf{T}^T \cdot S$)

 \rightsquigarrow the impact of the evidence vanishes.

 \sim The stationary distribution only depends on the transition model.

 \sim There is a small window of time (depending on the transition model) where the evidence has enough impact to allow for prediction beyond the mere stationary distribution, called the mixing time of the Markov chain.

 \sim Predicting the future is difficult, and the further into the future, the more difficult it is (Who knew...)

FAU

Smoothing: $\mathbb{P}(X_{t-k}|E_{1:t}^{=e})$ for k > 0. Intuition: Use filtering to compute $\mathbb{P}(X_t|E_{1:t-k}^{=e})$, then recurse *backwards* from *t* until t - k.

$$\mathbb{P}(X_{t-k}|E_{1:t}^{=e}) = \mathbb{P}(X_{t-k}|E_{t-(k-1):t}^{=e}, E_{1:t-k}^{=e}) = \alpha(\mathbb{P}(E_{t-(k-1):t}^{=e}|X_{t-k}, E_{1:t-k}^{=e}) \cdot \mathbb{P}(X_{t-k}|E_{1:t-k}^{=e})) = \alpha(\mathbb{P}(E_{t-(k-1):t}^{=e}|X_{t-k}) \cdot \mathbb{P}(X_{t-k}|E_{1:t-k}^{=e})) = \alpha(\mathbb{P}(E_{t-(k-1):t}^{=e}|X_{t-k}) \cdot \mathbb{P}(X_{t-k}|E_{1:t-k}^{=e})) = \alpha(f_{1:t-k} \times b_{t-(k-1):t}) \cdot \mathbb{P}(X_{t-k}|E_{1:t-k}^{=e})) = \alpha(f_{1:t-k} \times b_{t-(k-1):t}) = \alpha(f_{1:t-k} \times b_{t-(k-1):t}) = \alpha(f_{1:t-k} \times b_{t-(k-1):t})) = \alpha(f_{1:t-k} \times b_{t-(k-1):t}) = \alpha(f_{1:t-k} \times b_{t-(k-1):t})) = \alpha(f_{1:t-k} \times b_{t-(k-1):t}) = \alpha(f_{1:t-k} \times b_{t-(k-1):t}) = \alpha(f_{1:t-k} \times b_{t-(k-1):t}) = \alpha(f_{1:t-k} \times b_{t-(k-1):t})) = \alpha(f_{1:t-k} \times b_{t-(k-1):t}) =$$

(Divide the evidence) (Bayes Rule) (cond. independence)

(where \times denotes component-wise multiplication)

Smoothing (continued)

FAU

Definition 2.10 (Backward message). $b_{t-k:t} = \mathbb{P}(E_{t-k:t}^{=e}|X_{t-(k+1)})$

$$= \sum_{x \in dom(X)} \mathbb{P}(E_{t-k:t}^{=e} | X_{t-k} = x, X_{t-(k+1)}) \cdot \mathbb{P}(X_{t-k} = x | X_{t-(k+1)})$$

$$= \sum_{x \in dom(X)} P(E_{t-k:t}^{=e} | X_{t-k} = x) \cdot \mathbb{P}(X_{t-k} = x | X_{t-(k+1)})$$

$$= \sum_{x \in dom(X)} P(E_{t-k} = e_{t-k}, E_{t-(k-1):t}^{=e} | X_{t-k} = x) \cdot \mathbb{P}(X_{t-k} = x | X_{t-(k+1)})$$

$$= \sum_{x \in dom(X)} \frac{P(E_{t-k} = e_{t-k} | X_{t-k} = x)}{\text{sensor model}} \cdot \frac{P(E_{t-(k-1):t}^{=e} | X_{t-k} = x)}{\mathbb{E}^{t-(k-1):t}} \cdot \frac{\mathbb{P}(X_{t-k} = x | X_{t-(k+1)})}{\mathbb{E}^{t-(k-1):t}}$$

Note: in a stationary hidden Markov model, we get the matrix formulation $b_{t-k:t} = T \cdot O_{t-k} \cdot b_{t-(k-1):t}$



Smoothing (continued)

Definition 2.12 (Backward message). $\mathbf{b}_{t-k;t} = \mathbb{P}(\mathcal{E}_{t-k;t}^{=e} | X_{t-(k+1)})$

$$= \sum_{x \in dom(X)} \mathbb{P}(E_{t-k:t}^{=e} | X_{t-k} = x, X_{t-(k+1)}) \cdot \mathbb{P}(X_{t-k} = x | X_{t-(k+1)})$$

$$= \sum_{x \in dom(X)} P(E_{t-k:t}^{=e} | X_{t-k} = x) \cdot \mathbb{P}(X_{t-k} = x | X_{t-(k+1)})$$

$$= \sum_{x \in dom(X)} P(E_{t-k} = e_{t-k}, E_{t-(k-1):t}^{=e} | X_{t-k} = x) \cdot \mathbb{P}(X_{t-k} = x | X_{t-(k+1)})$$

$$= \sum_{x \in dom(X)} \underbrace{P(E_{t-k} = e_{t-k} | X_{t-k} = x)}_{\text{sensor model}} \cdot \underbrace{P(E_{t-(k-1):t}^{=e} | X_{t-k} = x)}_{=b_{t-(k-1):t}} \cdot \underbrace{\mathbb{P}(X_{t-k} = x | X_{t-(k+1)})}_{\text{transition model}}$$

Note: in a stationary hidden Markov model, we get the matrix formulation $b_{t-k:t} = T \cdot O_{t-k} \cdot b_{t-(k-1):t}$ **Definition 2.13.** We call the associated algorithm the backward algorithm, i.e. $\mathbb{P}(X_{t-k}|E_{1:t}^{=e}) = \alpha(\text{FORWARD}(e_{t-k}, f_{1:t-(k+1)}) \times \text{BACKWARD}(e_{t-(k-1)}, b_{t-(k-2):t})).$ $f_{1:t-k}$ $b_{t-(k-1):t}$ As a starting point for the recursion, we let $b_{t+1:t}$ the uniform vector with 1 in every component. FAU 845



Smoothing example

Fau

$$\mathbb{P}(\mathtt{R}_1|\mathtt{U}_1=\mathsf{T},\mathtt{U}_2=\mathsf{T},\mathtt{U}_3=\mathsf{F})=\alpha(\mathsf{f}_{1:1}\times\mathsf{b}_{2:3})$$

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Definition 2.15. Forward backward algorithm: returns the sequence of posterior distributions $\mathbb{P}(X_1) \dots \mathbb{P}(X_t)$ given evidence e_1, \dots, e_t :

function FORWARD-BACKWARD($\langle e_1, \ldots, e_t \rangle, \mathbb{P}(X_0)$) $f := \langle \mathbb{P}(X_0) \rangle$ $b := \langle 1, 1, \ldots \rangle$ $S := \langle \mathbb{P}(X_0) \rangle$ for $i = 1, \ldots, t$ do $f_i := FORWARD(f_{i-1}, e_i)$ for $i = t, \ldots, 1$ do $S_i := \alpha(f_i \times b)$ $b := BACKWARD(b, e_i)$ return S

/* filtering */

/* smoothing */

Time complexity linear in t (polytree inference), Space complexity $O(t \cdot |f|)$.



Idea: If T and O_i are invertible, we can avoid storing all forward messages in the smoothing algorithm by running filtering backwards:

$$f_{1:i+1} = \alpha(\mathsf{O}_{i+1} \cdot \mathsf{T}^T \cdot \mathsf{f}_{1:i})$$
$$\Rightarrow f_{1:i} = \alpha(\mathsf{T}^{T^{-1}} \cdot \mathsf{O}_{i+1}^{-1} \cdot \mathsf{f}_{1:i+1})$$

- \Rightarrow we can trade space complexity for time complexity:
- ▶ In the first for-loop, we only compute the final $f_{1:t}$
- ▶ In the second for-loop, we compute both $f_{1:i}$ and $b_{t-i:t}$

 \Rightarrow constant space.

But: Requires that both matrices are invertible, i.e. *every observation must be possible in every state*. (Possible hack: increase the probabilities of 0 to "negligibly small")

(No need to store the intermediate results) (Only one copy of $f_{1:i}$, $b_{t-i:t}$ is stored)



Most Likely Explanation

Smoothing allows us to compute the sequence of most likely states X_1, \ldots, X_t given $E_{1:t}^{=e}$. What if we want the most likely sequence of states? i.e. $\max_{t \in [1,t]} (P(X_{1:t}^{=x} | E_{1:t}^{=e}))$?

Example 2.16. Given the sequence $U_1, U_2, \neg U_3, U_4, U_5$, the most likely state for R_3 is F, but the most likely sequence *might* be that it rained throughout...

Prominent Application: In speech recognition, we want to find the most likely word sequence, given what we have heard. (can be quite noisy)

Idea:

- For every $x_t \in \text{dom}(X)$ and $0 \le i \le t$, recursively compute the most likely path X_1, \ldots, X_i ending in $X_i = x_i$ given the observed evidence.
- remember the x_{i-1} that most likely leads to x_i.
- Among the resulting paths, pick the one to the $X_t = x_t$ with the most likely path,
- ▶ and then recurse backwards.

 \sim we want to know $\max_{X_1,\dots,X_{t-1}} \mathbb{P}(X_{1:t-1}^{=x}, X_t | E_{1:t}^{=e})$, and then pick the X_t with the maximal value.



Most Likely Explanation (continued)

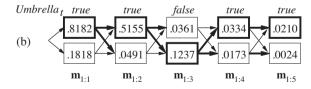
By the same reasoning as for filtering:

$$\max_{x_1,\dots,x_{t-1}} \mathbb{P}(X_{1:t-1}^{=x}, X_t | E_{1:t}^{=e})$$

$$= \alpha(\underbrace{\mathbb{P}(E_t = e_t | X_t)}_{\text{sensor model}} \cdot \max_{x_{t-1}} (\underbrace{\mathbb{P}(X_t | X_{t-1} = x_{t-1})}_{\text{transition model}} \cdot \underbrace{\max_{x_1,\dots,x_{t-2}} (\mathbb{P}(X_{1:t-2}^{=x}, X_{t-1} = x_{t-1} | E_{1:t-1}^{=e}))))$$

$$=:\max_{x_1,\dots,x_{t-2}} (\mathbb{P}(X_{1:t-2}^{=x}, X_{t-1} = x_{t-1} | E_{1:t-1}^{=e})))$$

 $m_{1:t}(i)$ gives the maximal probability that the most likely path up to t leads to state $X_t = i$. Note that we can leave out the α , since we're only interested in the maximum. **Example 2.17.** For the sequence [T, T, F, T, T]:



bold arrows: best predecessor measured by "best preceding sequence probability \times transition probability" FAU = 850 2025-05-14 Definition 2.18. The Viterbi algorithm now proceeds as follows:

```
function VITERBI(\langle e_1, \ldots, e_t \rangle, \mathbb{P}(X_0))
     m := \mathbb{P}(X_0)
                                                                                                                                                                                     /* m1·i */
                                                                                                             /* the most likely predecessor of each possible x_i */
     prev := \langle \rangle
     for i = 1, \ldots, t do
            m' := \max_{X_{i-1}} \left( \mathbb{P}(E_i = e_i | X_i) \cdot \mathbb{P}(X_i | X_{i-1} = X_{i-1}) \cdot m_{X_{i-1}} \right)
            \operatorname{prev}_{i-1} := \operatorname{argmax} \left( \mathbb{P}(E_i = e_i | X_i) \cdot \mathbb{P}(X_i | X_{i-1} = x_{i-1}) \cdot m_{x_i} \right)
                                   \times i - 1
            m \longleftarrow m'
     P := \langle 0, 0, \dots, \text{ argmax } m_x \rangle
                              (x \in dom(X))
     for i = t - 1, ..., 0 do
           P_i := \operatorname{prev}_{i, P_{i+1}}
     return P
```

Observation 2.19. Viterbi has linear time complexity and linear space complexity (needs to keep the most likely sequence leading to each state).



25.3 Hidden Markov Models – Extended Example





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Example: Robot Localization using Common Sense

Example 3.1 (Robot Localization in a Maze). A robot has four sonar sensors that tell it about obstacles in four directions: N, S, W, E.

We write the result where the sensor that detects obstacles in the north, south, and east as N S E.

We filter out the impossible states:

\odot	0	٥	0		0	0	0	٥	٥		\odot	٥	0		۰
		0	0		0			٥		٥		٥			
	0	0	٥		0			0	0	0	0	0			0
\odot	٥		٥	0	٥		\odot	٥	0	٥		0	0	٥	۰

a) Possible robot locations after $e_1 = N S W$

Remark 3.2. This only works for perfect sensors. What if our sensors are imperfect?

(else no impossible states)



Example: Robot Localization using Common Sense

Example 3.3 (Robot Localization in a Maze). A robot has four sonar sensors that tell it about obstacles in four directions: N, S, W, E.

We write the result where the sensor that detects obstacles in the north, south, and east as N S E.

We filter out the impossible states:

Γ	•	\odot	0	0		0	0	0	0	0		٥	٥	0		٥
			0	0		0			0		0		0			
Γ		0	0	0		0			0	0	0	0	0			0
Ľ	0	0		0	0	0		0	0	0	0		0	0	0	0

b) Possible robot locations after $e_1 = N S W$ and $e_2 = N S$

Remark 3.4. This only works for perfect sensors. What if our sensors are imperfect?

(else no impossible states)



HMM Example: Robot Localization (Modeling)

Example 3.5 (HMM-based Robot Localization). We have the following setup:

- A hidden Random variable X_t for robot location
- Let N(i) be the set of neighboring fields of the field $X_i = x_i$
- ► The Transition matrix for the move action

$$P(X_{t+1} = j \mid X_t = i) = \mathsf{T}_{ij} = \begin{cases} \frac{1}{|\mathcal{N}(i)|} & \text{if } j \in \mathcal{N}(i) \\ 0 & \text{else} \end{cases}$$

We do not know where the robot starts: P(X₀) = 1/n (here n = 42)
 Evidence variable E_t: four bit presence/absence of obstacles in N, S, W, E. Let d_{it} be the number of wrong bits and ε the error rate of the sensor. Then

$$P(E_t = e_t \mid X_t = i) = O_{tii} = (1 - \epsilon)^{4 - d_{it}} \cdot \epsilon^{d_{it}}$$

(We assume the sensors are independent)

For example, the probability that the sensor on a square with obstacles in north and south would produce N S E is $(1 - \epsilon)^3 \cdot \epsilon^1$.

We can now use filtering for localization, smoothing to determine e.g. the starting location, and the Viterbi algorithm to find out how the robot got to where it is now.

FAU

(domain: 42 empty squares)

(T has $42^2 = 1764$ entries)



We use HMM filtering equation $f_{1:t+1} = \alpha \cdot O_{t+1} T^t f_{1:t}$ to compute posterior distribution over locations. (i.e. robot localization)

0	•	0	0		0	•	0	ο	0		0	0	0		0
		0	0		0			0		0		0			
	0	0	0		0			0	0	0	0	0			0
0	0		0	0	0		0	0	0	0		0	0	0	0

Example 3.6. Redoing ???, with $\epsilon = 0.2$.

a) Posterior distribution over robot location after $E_1 = N S W$

Still the same locations as in the "perfect sensing" case, but now other locations have non-zero probability.



We use HMM filtering equation $f_{1:t+1} = \alpha \cdot O_{t+1} T^t f_{1:t}$ to compute posterior distribution over locations. (i.e. robot localization)

0	0	0	0		0	•	0	0	0		0	0	0		0
		0	0		0			0		0		0			
	0	0	0		0			0	0	0	0	0			0
0	0		0	0	0		0	0	0	0		0	0	0	0

Example 3.7. Redoing ???, with $\epsilon = 0.2$.

b) Posterior distribution over robot location after $\mathrm{E}_1=\mathrm{N}\;\mathrm{S}\;\mathrm{W}$ and $\mathrm{E}_2=\mathrm{N}\;\mathrm{S}$

Still the same locations as in the "perfect sensing" case, but now other locations have non-zero probability.

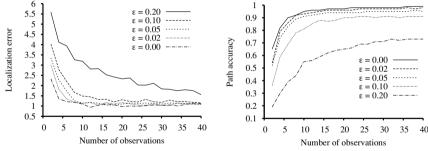


HMM Example: Further Inference Applications

Idea: We can use smoothing: $b_{k+1:t} = TO_{k+1}b_{k+2:t}$ to find out where it started and the Viterbi algorithm to find the most likely path it took.

Example 3.8.Performance of HMM localization vs. observation length





Localization error (Manhattan distance from true location)

Viterbi path accuracy (fraction of correct states on Viterbi path)

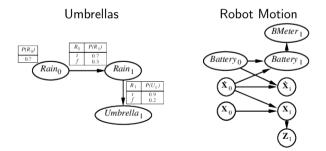
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25.4 Dynamic Bayesian Networks



Dynamic Bayesian networks

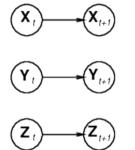
- ▶ **Definition 4.1.** A Bayesian network D is called dynamic (a DBN), iff its random variables are indexed by a time structure. We assume that D is
 - time sliced, i.e. that the time slices D_t the subgraphs of *t*-indexed random variables and the edges between them are isomorphic.
 - ▶ a stationary Markov chain, i.e. that variables X_t can only have parents in \mathcal{D}_t and \mathcal{D}_{t-1} .
- \triangleright X_t, E_t contain arbitrarily many variables in a replicated Bayesian network.
- Example 4.2.

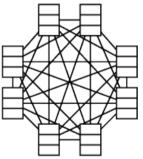


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DBNs vs. HMMs

- Observation 4.3.
 - Every HMM is a single-variable DBN.
 - Every DBN can be turned into an HMM. dependencies)
 - ▶ DBNs have sparse dependencies ~→ exponentially fewer parameters;





(combine variables into tuple \Rightarrow lose information about

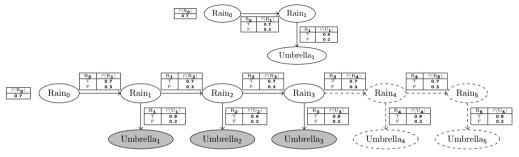
► Example 4.4 (Sparse Dependencies). With 20 Boolean state variables, three parents each, a DBN has 20 · 2³ = 160 parameters, the corresponding HMM has 2²⁰ · 2²⁰ ≈ 10¹².



(trivially)

Exact inference in DBNs

Definition 4.5 (Naive method). Unroll the network and run any exact algorithm.



- **Problem:** Inference cost for each update grows with *t*.
- **Definition 4.6.** Rollup filtering: add slice t + 1, "sum out" slice t using variable elimination.

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- ▶ **Observation:** Largest factor is $\mathcal{O}(d^{n+1})$, update cost $\mathcal{O}(d^{n+2})$, where d is the maximal domain size.
- **Note:** Much better than the HMM update cost of $\mathcal{O}(d^{2n})$



Fau

- ► Temporal probability models use state and evidence variables replicated over time.
- Markov property and stationarity assumption, so we need both
 - ▶ a transition model and $P(X_t|X_{t-1})$
 - a sensor model $P(E_t|X_t)$.
- Tasks are filtering, prediction, smoothing, most likely sequence; (all done recursi cost per time step)
- Hidden Markov models have a single discrete state variable;
- DBNs subsume HMMs, exact update intractable.

(all done recursively with constant

2025-05-14

(used for speech recognition)

Chapter 26 Making Complex Decisions

We will now combine the ideas of stochastic process with that of acting based on maximizing expected utility:

- Markov decision processes (MDPs) for sequential environments.
- Value/policy iteration for computing utilities in MDPs.
- Partially observable MDP (POMDPs).
- Decision theoretic agents for POMDPs.

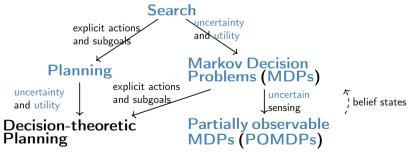


26.1 Sequential Decision Problems



Sequential Decision Problems

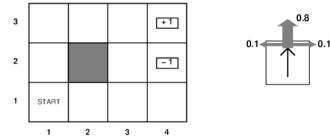
- Definition 1.1. In sequential decision problems, the agent's utility depends on a sequence of decisions (or their result states).
- Definition 1.2. Utility functions on action sequences are often expressed in terms of immediate rewards that are incurred upon reaching a (single) state.
- Methods: depend on the environment:
 - ▶ If it is fully observable ~> Markov decision process (MDPs)
 - else \rightarrow partially observable MDP (POMDP).
- Sequential decision problems incorporate utilities, uncertainty, and sensing.
- Preview: Search problems and planning tasks are special cases.





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Example 1.3 (Running Example: The 4x3 World). A (fully observable) 4 × 3 environment with non-deterministic actions:



- States $s \in S$, actions $a \in As$.
- ▶ Transition model: $P(s' | s,a) \cong$ probability that *a* in *s* leads to *s'*.
- reward function:

 $R(s) := \begin{cases} -0.04 & \text{if (small penalty) for nonterminal states} \\ \pm 1 & \text{if for terminal states} \end{cases}$

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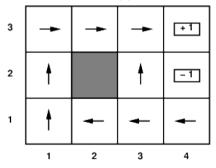


- Motivation: Let us (for now) consider sequential decision problems in a fully observable, stochastic environment with a Markovian transition model on a *finite* set of states and an additive reward function. (We will switch to partially observable ones later)
- **Definition 1.4.** A Markov decision process (MDP) (S, A, T, s_0, R) consists of
 - ▶ a set of S of states (with initial state $s_0 \in S$),
 - for every state s, a set of actions As.
 - ▶ a transition model $\mathcal{T}(s, a) = \mathbb{P}(S|s, a)$, and
 - a reward function $R: S \to \mathbb{R}$; we call R(s) a reward.
- Idea: We use the rewards as a utility function: The goal is to choose actions such that the expected cumulative rewards for the "foreseeable future" is maximized ⇒ need to take future actions and future states into account



Solving MDPs

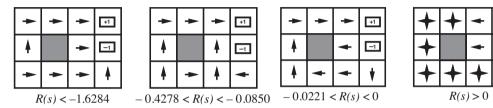
- In MDPs, the aim is to find an optimal policy $\pi(s)$, which tells us the best action for every possible state s. (because we can't predict where we might end up, we need to consider all states)
- ▶ Definition 1.5. A policy π for an MDP is a function mapping each state s to an action a ∈ As. An optimal policy is a policy that maximizes the expected total rewards. (for some notion of "total"...)
- **Example 1.6.** Optimal policy when state penalty R(s) is 0.04:



Note: When you run against a wall, you stay in your square.



Example 1.7. Optimal policy depends on the reward function R(s).

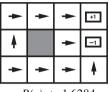


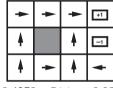
Question: Explain what you see in a qualitative manner!

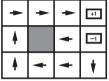
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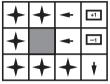
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Example 1.8. Optimal policy depends on the reward function R(s).









R(s) > 0

R(s) < -1.6284

-0.4278 < R(s) < -0.0850

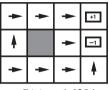
-0.0221 < R(s) < 0

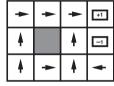
- Question: Explain what you see in a qualitative manner!
- Answer: Careful risk/reward balancing is characteristic of MDPs.
 - 1. $-\infty \leq R(s) \leq -1.6284 \sim$ Life is so painful that agent heads for the next exit.

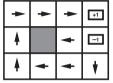


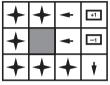
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Example 1.9. Optimal policy depends on the reward function R(s).









R(s) < -1.6284

-0.4278 < R(s) < -0.0850

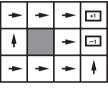
-0.0221 < R(s) < 0

R(s) > 0

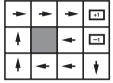
- Question: Explain what you see in a qualitative manner!
- Answer: Careful risk/reward balancing is characteristic of MDPs.
 - 1. $-\infty \le R(s) \le -1.6284 \rightarrow$ Life is so painful that agent heads for the next exit.
 - 2. $-0.4278 \le R(s) \le -0.0850$, life is quite unpleasant; the agent takes the shortest route to the +1 state and is willing to risk falling into the -1 state by accident. In particular, the agent takes the shortcut from (3,1).

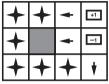


Example 1.10. Optimal policy depends on the reward function R(s).



*	٨	4	+1
4		4	Ţ
•	+	4	+





R(s) < -1.6284

-0.4278 < R(s) < -0.0850

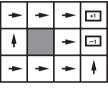
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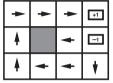
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 - 3. Life is slightly dreary $(-0.0221 < R(s) < 0) \sim$ take no risks at all. In (4,1) and (3,2) head directly away from the $-1 \sim$ cannot fall in by accident.

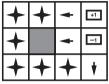


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 - 3. Life is slightly dreary $(-0.0221 < R(s) < 0) \sim$ take no risks at all. In (4,1) and (3,2) head directly away from the $-1 \sim$ cannot fall in by accident.
 - 4. If R(s) > 0, then life is positively enjoyable \sim avoid both exits \sim reap infinite rewards.



26.2 Utilities over Time



Why rewards?

- ▶ **Recall:** We cannot observe/assess utility functions, only preferences ~> induce utility functions from rational preferences
- ▶ Problem: In MDPs we need to understand preferences between sequences of states.
- Definition 2.1. We call preferences on reward sequences stationary, iff

 $[r, r_0, r_1, r_2, \ldots] \succ [r, r'_0, r'_1, r'_2, \ldots] \Leftrightarrow [r_0, r_1, r_2, \ldots] \succ [r'_0, r'_1, r'_2, \ldots]$

(i.e. rewards over time are "independent" of each other)

Good news:

Theorem 2.2. For stationary preferences, there are only two ways to combine rewards over time.

- additive rewards: $U([s_0, s_1, s_2, ...]) = R(s_0) + R(s_1) + R(s_2) + \cdots$
- ► discounted rewards: $U([s_0, s_1, s_2, ...]) = R(s_0) + \gamma R(s_1) + \gamma^2 R(s_2) + \cdots$ where $0 \le \gamma \le 1$ is called discount factor.
- \Rightarrow we can reduce utilities over time to rewards on individual states



Utilities of State Sequences

Problem: Infinite lifetimes \rightsquigarrow additive rewards may become infinite.

Possible Solutions:

1. Finite horizon: terminate utility computation at a fixed time T

$$U([s_0,\ldots,s_\infty])=R(s_0)+\cdots+R(s_T)$$

 \rightsquigarrow nonstationary policy: $\pi(s)$ depends on time left.

- 2. If there are absorbing states: for any policy π agent eventually "dies" with probability $1 \rightarrow \text{expected}$ utility of every state is finite.
- 3. Discounting: assuming $\gamma <$ 1, $R(s) \leq R_{\max}$,

$$U([s_0, s_1, \ldots]) = \sum_{t=0}^{\infty} \gamma^t R(s_t) \le \sum_{t=0}^{\infty} \gamma^t R_{\max} = R_{\max}/(1-\gamma)$$

Smaller $\gamma \rightsquigarrow$ shorter horizon.

We will only consider discounted rewards in this course



Discounted rewards are both convenient and (often) realistic:

- stationary preferences imply (additive rewards or) discounted rewards anyway,
- discounted rewards lead to finite utilities for (potentially) infinite sequences of states (we can compute expected utilities for the entire future),
- discounted rewards lead to stationary policies, which are easier to compute and often more adequate (unless we know that remaining time matters),
- discounted rewards mean we value short-term gains over long-term gains (all else being equal), which is often realistic (e.g. the same amount of money gained early gives more opportunity to spend/invest >> potentially more utility in the long run)
- ▶ we can interpret the discount factor as a measure of *uncertainty about future rewards* ⇒ more robust measure in uncertain environments.

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Remember: Given a sequence of states $S = s_0, s_1, s_2, ...$, and a discount factor $0 \le \gamma < 1$, the utility of the sequence is

$$U(S) = \sum_{t=0}^{\infty} \gamma^t R(s_t)$$

Definition 2.3. Given a policy π and a starting state s_0 , let $S_{s_0}^{\pi}$ be the random variable giving the sequence of states resulting from executing π at every state starting at s_0 . (Since the environment is stochastic, we don't know the exact sequence.)

Then the expected utility obtained by executing π starting in s_0 is given by

 $U^{\pi}(s_0) := \mathrm{EU}(S^{\pi}_{s_0}).$

We define the optimal policy $\pi_{s_0}^* := \operatorname{argmax} U^{\pi}(s_0)$.



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We define the optimal policy $\pi_{s_0}^* := \underset{\pi}{\operatorname{argmax}} U^{\pi}(s_0).$

Note: This is perfectly well-defined, but almost always computationally infeasible. (requires considering *all possible (potentially infinite) sequences of states*)

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Observation 2.5. $\pi_{s_0}^*$ is independent of the state s_0 . *Proof sketch:* If π_a^* and π_b^* reach point *c*, then there is no reason to disagree from that point on – or with π_c^* , and we expect optimal policies to "meet at some state" sooner or later. **(A)** ?? does not hold for finite horizon policies!



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Definition 2.9. We call $\pi^* := \pi_s^*$ for some *s* the optimal policy. **Definition 2.10.** The utility U(s) of a state *s* is $U^{\pi^*}(s)$.



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Definition 2.12. We call $\pi^* := \pi_s^*$ for some *s* the optimal policy. **Definition 2.13.** The utility U(s) of a state *s* is $U^{\pi^*}(s)$.

Remark: $R(s) \cong$ "immediate reward", whereas $U \cong$ "long-term reward".

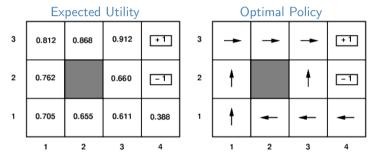
Given the utilities of the states, choosing the best action is just MEU: maximize the expected utility of the immediate successor states

$$\pi^*(s) = \operatorname*{argmax}_{a \in A(s)} \left(\sum_{s'} P(s' \mid s, a) \cdot U(s') \right)$$

 \Rightarrow given the "true" utilities, we can compute the optimal policy and vice versa.



Example 2.14 (Running Example Continued).



▶ Question: Why do we go left in (3,1) and not up?

(follow the utility)



26.3 Value/Policy Iteration



Dynamic programming: the Bellman equation

- ▶ **Problem:** We have defined U(s) via the optimal policy: $U(s) := U^{\pi^*}(s)$, but how to compute it without knowing π^* ?
- **Observation:** A simple relationship among utilities of neighboring states:

expected sum of rewards = current reward + $\gamma \cdot$ exp. reward sum after best action

Theorem 3.1 (Bellman equation (1957)).

$$U(s) = R(s) + \gamma \cdot \max_{a \in A(s)} \sum_{s'} U(s') \cdot P(s' \mid s, a)$$

We call this equation the Bellman equation

Example 3.2. $U(1,1) = -0.04$	
+ $\gamma \max\{0.8U(1,2) + 0.1U(2,1) + 0.1U(1,1),$	up
0.9U(1,1) + 0.1U(1,2)	left
0.9U(1,1) + 0.1U(2,1)	down
$0.8U(2,1) + 0.1U(1,2) + 0.1U(1,1)\}$	right

Problem: One equation/state $\sim n$ nonlinear (max isn't) equations in *n* unknowns. \sim cannot use linear algebra techniques for solving them.

FAU



Value Iteration Algorithm

- ► Idea: We use a simple iteration scheme to find a fixpoint:
 - $1. \ \ {\rm start \ with \ arbitrary \ utility \ values,}$
 - 2. update to make them locally consistent with the Bellman equation,
 - 3. everywhere locally consistent \rightsquigarrow global optimality.

Definition 3.3. The value iteration algorithm for utilitysutility function is given by

```
function VALUE-ITERATION (mdp, \epsilon) returns a utility fn.

inputs: mdp, an MDP with states S, actions A(s), transition model P(s' | s,a),

rewards R(s), and discount \gamma

\epsilon, the maximum error allowed in the utility of any state

local variables: U, U', vectors of utilities for states in S, initially zero

\delta, the maximum change in the utility of any state in an iteration

repeat

U := U'; \delta := 0

for each state s in S do

U'[s] := R(s) + \gamma \cdot \max_{a \in A(s)} (\sum_{s'} U[s'] \cdot P(s' | s,a))

if |U'[s] - U[s]| > \delta then \delta := |U'[s] - U[s]|

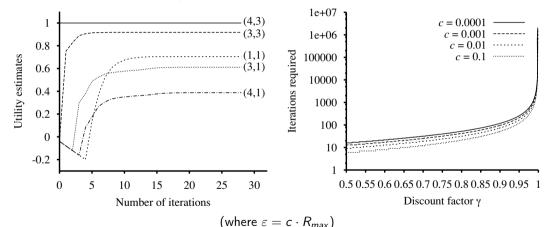
until \delta < \epsilon(1 - \gamma)/\gamma

return U
```

▶ **Remark:** Retrieve the optimal policy with $\pi[s] := \underset{a \in A(s)}{\operatorname{argmax}} (\sum_{s'} U[s'] \cdot P(s' \mid s, a))$

Fau





Example 3.4 (Iteration on 4x3).



- ▶ Definition 3.5. The maximum norm is defined as ||U|| = max |U(s)|, so ||U V|| = maximum difference between U and V.
- ▶ Let U^t and U^{t+1} be successive approximations to the true utility U during value iteration.
- **Theorem 3.6.** For any two approximations U^t and V^t

 $\left\| \boldsymbol{U}^{t+1} - \boldsymbol{V}^{t+1} \right\| \leq \gamma \left\| \boldsymbol{U}^{t} - \boldsymbol{V}^{t} \right\|$

I.e., any distinct approximations get closer to each other over time In particular, any approximation gets closer to the true U over time \Rightarrow value iteration converges to a unique, stable, optimal solution.

► Theorem 3.7. If $\|U^{t+1} - U^t\| < \epsilon$, then $\|U^{t+1} - U\| < 2\epsilon\gamma/1 - \gamma$

(once the change in U^t becomes small, we are almost done.)

Remark: The policy resulting from U^t may be optimal long before the utilities convergence!



Fau

- ▶ **Recap:** Value iteration computes utilities ~→ optimal policy by MEU.
- This even works if the utility estimate is inaccurate.
- ▶ Idea: Search for optimal policy and utility values simultaneously [Howard:dpmp60]: Iterate
 - **>** policy evaluation: given policy π_i , calculate $U_i = U^{\pi_i}$, the utility of each state were π_i to be executed.
 - **b** policy improvement: calculate a new MEU policy π_{i+1} using 1 lookahead Terminate if policy improvement yields no change in computed utilities.
- **Observation 3.8.** Upon termination U_i is a fixpoint of Bellman update \sim Solution to Bellman equation $\sim \pi_i$ is an optimal policy.
- ▶ Observation 3.9. Policy improvement improves policy and policy space is finite ~> termination.

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(\leftrightarrow policy loss small)

Definition 3.10. The policy iteration algorithm is given by the following pseudocode:

```
function POLICY-ITERATION(mdp) returns a policy

inputs: mdp, and MDP with states S, actions A(s), transition model P(s' | s,a)

local variables: U a vector of utilities for states in S, initially zero

\pi a policy indexed by state, initially random,

repeat

U := POLICY-EVALUATION(\pi, U, mdp)

unchanged? := true

foreach state s in X do

if max (\sum_{s'} P(s' | s,a) \cdot U(s')) > \sum_{s'} P(s' | s, \pi[s]) \cdot U(s') then do

\pi[s] := \operatorname{argmax} (\sum_{s'} P(s' | s,b) \cdot U(s'))

unchanged? := false

until unchanged?
```



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Policy Evaluation

- **Problem:** How to implement the POLICY–EVALUATION algorithm?
- **Solution:** To compute utilities given a fixed π : For all *s* we have

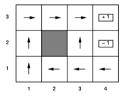
$$U(s) = R(s) + \gamma(\sum_{s'} U(s') \cdot P(s' \mid s, \pi(s)))$$

(i.e. Bellman equation with the maximum replaced by the current policy π)

Example 3.11 (Simplified Bellman Equations for π).

$$U_i(1,1) = -0.04 + 0.8U_i(1,2) + 0.1U_i(1,1) + 0.1U_i(2,1)$$

$$U_i(1,2) = -0.04 + 0.8U_i(1,3) + 0.1U_i(1,2)$$



► Observation 3.12. n simultaneous linear equations in n unknowns, solve in O(n³) with standard linear algebra methods.



- ► Value iteration requires many iterations, but each one is cheap.
- Policy iteration often converges in few iterations, but each is expensive.
- ldea: Use a few steps of value iteration (but with π fixed), starting from the value function produced the last time to produce an approximate value determination step.
- Often converges much faster than pure VI or PI.
- Leads to much more general algorithms where Bellman value updates and Howard policy updates can be performed locally in any order.
- Remark: Reinforcement learning algorithms operate by performing such updates based on the observed transitions made in an initially unknown environment.



26.4 Partially Observable MDPs

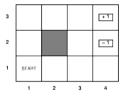


- ▶ Definition 4.1. A partially observable MDP (a POMDP for short) is a MDP together with an observation model *O* that has the sensor Markov property and is stationary: $O(s, e) = P(e \mid s)$.
- Example 4.2 (Noisy 4x3 World).

Add a partial and/or noisy sensor. e.g. count number of adjacent walls with 0.1 error If sensor reports 1, we are in (3,?)

$$(1 \le w \le 2)$$

(noise)
(probably)





- Definition 4.4. A partially observable MDP (a POMDP for short) is a MDP together with an observation model O that has the sensor Markov property and is stationary: O(s, e) = P(e | s).
- Example 4.5 (Noisy 4x3 World).

Add a partial and/or noisy sensor.a \blacksquare e.g. count number of adjacent walls $(1 \le w \le 2)$ awith 0.1 error(noise)aIf sensor reports 1, we are in (3,?)(probably)a

Problem: Agent does not know which state it is in \sim makes no sense to talk about policy $\pi(s)$!

1 2 3



- Definition 4.7. A partially observable MDP (a POMDP for short) is a MDP together with an observation model O that has the sensor Markov property and is stationary: O(s, e) = P(e | s).
- Example 4.8 (Noisy 4x3 World).

Add a partial and/or noisy sensor.a $\overset{3}{}$ $\overset{*}{}$ e.g. count number of adjacent walls $(1 \le w \le 2)$ a $\overset{2}{}$ with 0.1 error(noise)aaIf sensor reports 1, we are in (3,?)(probably)aa

- **Problem:** Agent does not know which state it is in \sim makes no sense to talk about policy $\pi(s)$!
- Theorem 4.9 (Astrom 1965). The optimal policy in a POMDP is a function π(b) where b is the belief state (probability distribution over states).
- ▶ Idea: Convert a POMDP into an MDP in belief state space, where $\mathcal{T}(b, a, b')$ is the probability that the new belief state is b' given that the current belief state is b and the agent does a. I.e., essentially a filtering update step.

1 2 3



POMDP: Filtering at the Belief State Level

- **Recap:** Filtering updates the belief state for new evidence.
- ► For POMDPs, we also need to consider actions.

(but the effect is the same)

▶ If *b* is the previous belief state and agent does action A = a and then perceives E = e, then the new belief state is

$$b' = lpha(\mathbb{P}(E = e|s') \cdot (\sum_{s} \mathbb{P}(s'|S = s, A = a) \cdot b(s)))$$

We write b' = FORWARD(b, a, e) in analogy to recursive state estimation.

- Fundamental Insight for POMDPs: The optimal action only depends on the agent's current belief state. (good, it does not know the state!)
- **Consequence:** The optimal policy can be written as a function $\pi^*(b)$ from belief states to actions.
- Definition 4.10. The POMDP decision cycle is to iterate over
 - 1. Given the current belief state *b*, execute the action $a = \pi^*(b)$
 - 2. Receive percept e.
 - 3. Set the current belief state to FORWARD(b, a, e) and repeat.
- ▶ Intuition: POMDP decision cycle is search in belief state space.



Fau

- ▶ Recap: The POMDP decision cycle is search in belief state space.
- **• Observation 4.11.** Actions change the belief state, not just the (physical) state.
- ▶ Thus POMDP solutions automatically include information gathering behavior.
- **Problem:** The belief state is continuous: If there are *n* states, *b* is an *n*-dimensional real-valued vector.
- **Example 4.12.** The belief state of the 4x3 world is a 11 dimensional continuous space. (11 states)
- Theorem 4.13. Solving POMDPs is very hard! (actually, PSPACE hard)
- In particular, none of the algorithms we have learned applies.
- ► The real world is a POMDP (with initially unknown transition model *T* and sensor model *O*)

(discreteness assumption)

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Reducing POMDPs to Belief-State MDPs I

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- Idea: Calculating the probability that an agent in belief state b reaches belief state b' after executing action a.
 - if we knew the action and the subsequent percept e, then b' = FORWARD(b, a, e). (deterministic update to the belief state)
 - but we don't, since b' depends on e.
- Idea: To compute P(e | a,b) the probability that e is perceived after executing a in belief state b
 sum up over all actual states the agent might reach:

$$P(e \mid a,b) = \sum_{s'} P(e \mid a,s',b) \cdot P(s' \mid a,b)$$
$$= \sum_{s'} P(e \mid s') \cdot P(s' \mid a,b)$$
$$= \sum_{s'} P(e \mid s') \cdot (\sum_{s} P(s' \mid s,a), b(s))$$

(let's calculate $P(e \mid a, b)$)

Reducing POMDPs to Belief-State MDPs II

Write the probability of reaching b' from b, given action a, as P(b' | b,a), then

$$P(b' \mid b,a) = P(b' \mid a,b) = \sum_{e} P(b' \mid e,a,b) \cdot P(e \mid a,b)$$

= $\sum_{e} P(b' \mid e,a,b) \cdot (\sum_{s'} P(e \mid s') \cdot (\sum_{s} P(s' \mid s,a), b(s)))$

where $P(b' \mid e, a, b)$ is 1 if b' = FORWARD(b, a, e) and 0 otherwise.

- **• Observation:** This equation defines a transition model for belief state space!
- ▶ Idea: We can also define a reward function for belief states:

$$\rho(b) := \sum_{s} b(s) \cdot R(s)$$

i.e., the expected reward for the actual states the agent might be in.



- ▶ Together, P(b' | b,a) and $\rho(b)$ define an (observable) MDP on the space of belief states.
- **Theorem 4.14.** An optimal policy $\pi^*(b)$ for this MDP, is also an optimal policy for the original *POMDP*.
- Upshot: Solving a POMDP on a physical state space can be reduced to solving an MDP on the corresponding belief state space.
- **Remember:** The belief state is always observable to the agent, by definition.



Ideas towards Value-Iteration on POMDPs

- **Recap:** The value iteration algorithm from ??? computes one utility value per state.
- ▶ **Problem:** We have infinitely many belief states ~> be more creative!
- **• Observation:** Consider an optimal policy π^*
 - ▶ applied in a specific belief state *b*: π^* generates an action,
 - ▶ for each subsequent percept, the belief state is updated and a new action is generated ...

For this specific *b*: $\pi^* \cong$ a conditional plan!

Idea: Think about conditional plans and how the expected utility of executing a fixed conditional plan varies with the initial belief state. (instead of optimal policies)

Definition 4.15. Given a set of percepts E and a set of actions A, a conditional plan is either an action $a \in A$, or a tuple $\langle a, E', p_1, p_2 \rangle$ such that $a \in A, E' \subseteq E$, and p_1, p_2 are conditional plans. It represents the strategy "First execute a, If we subsequently perceive $e \in E'$, continue with p_1 , otherwise continue with p_2 ."

The depth of a conditional plan p is the maximum number of actions in any path from p before reaching a single action plan.



Expected Utilities of Conditional Plans on Belief States

- **• Observation 1:** Let p be a conditional plan and $\alpha_p(s)$ the utility of executing p in state s.
 - the expected utility of p in belief state b is $\sum_{s} b(s) \cdot \alpha_{p}(s) \cong b \cdot \alpha_{p}$ as vectors.
 - the expected utility of a fixed conditional plan varies linearly with b
 - \blacktriangleright \sim the "best conditional plan to execute" corresponds to a hyperplane in belief state space.



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Observation 2: We can replace the *original* actions by conditional plans on those actions! Let π* be the subsequent optimal policy. At any given belief state b,

- π^* will choose to execute the conditional plan with highest expected utility
- the expected utility of b under the π^* is the utility of that plan:

$$U(b) = U^{\pi^*}(b) = \max_b (b \cdot \alpha_p)$$

- If the optimal policy π* chooses to execute p starting at b, then it is reasonable to expect that it might choose to execute p in belief states that are very close to b;
- ▶ if we bound the depth of the conditional plans, then there are only finitely many such plans
- the continuous space of belief states will generally be divided into regions, each corresponding to a particular conditional plan that is optimal in that region.



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- ▶ if we bound the depth of the conditional plans, then there are only finitely many such plans
- the continuous space of belief states will generally be divided into regions, each corresponding to a particular conditional plan that is optimal in that region.
- ▶ Observation 3 (conbined): The utility function *U*(*b*) on belief states, being the maximum of a collection of hyperplanes, is piecewise linear and convex.



A simple Illustrating Example I

Example 4.16. A world with states S_0 and S_1 , where $R(S_0) = 0$ and $R(S_1) = 1$ and two actions:

- "Stay" stays put with probability 0.9
- "Go" switches to the other state with probability 0.9.
- ▶ The sensor reports the correct state with probability 0.6.

Obviously, the agent should "Stay" when it thinks it's in state S_1 and "Go" when it thinks it's in state S_0 .

The belief state has dimension 1.

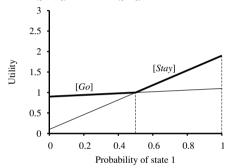
(the two probabilities sum up to 1)

► Consider the one-step plans [*Stay*] and [*Go*] and their direct utilities:

$$\begin{aligned} \alpha_{([Stay])}(S_0) &= 0.9R(S_0) + 0.1R(S_1) = 0.1 \\ \alpha_{([stay])}(S_1) &= 0.9R(S_1) + 0.1R(S_0) = 0.9 \\ \alpha_{([go])}(S_0) &= 0.9R(S_1) + 0.1R(S_0) = 0.9 \\ \alpha_{([go])}(S_1) &= 0.9R(S_0) + 0.1R(S_1) = 0.1 \end{aligned}$$

A simple Illustrating Example II

• Let us visualize the hyperplanes $b \cdot \alpha_{([Stay])}$ and $b \cdot \alpha_{([Go])}$.



The maximum represents the utility function for the finite-horizon problem that allows just one action
 in each "piece" the optimal action is the first action of the corresponding plan.

• Here the optimal one-step policy is to "Stay" when b(1) > 0.5 and "Go" otherwise.



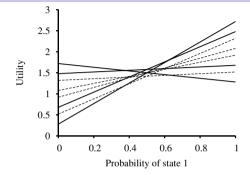
- compute the utilities for conditional plans of depth 2 by considering
 - each possible first action,
 - each possible subsequent percept, and then
 - each way of choosing a depth-1 plan to execute for each percept:

There are eight of depth 2:

[Stay, if P = 0 then Stay else Stay fi], [Stay, if P = 0 then Stay else Go fi], ...



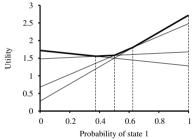
A simple Illustrating Example IV



Four of them (dashed lines) are suboptimal for the whole belief space We call them dominated

(they can be ignored)





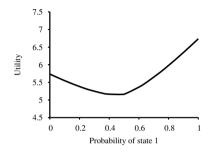
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▶ There are four undominated plans, each optimal in their region

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A simple Illustrating Example VI



- ▶ Idea: Repeat for depth 3 and so on.
- ▶ Theorem 4.17 (POMDP Plan Utility). Let *p* be a depth-*d* conditional plan whose initial action is a and whose depth-*d* − 1-subplan for percept *e* is p.e, then

$$\alpha_{p}(s) = R(s) + \gamma(\sum_{s'} P(s' \mid s, a)(\sum_{e} P(e \mid s') \cdot \alpha_{p.e}(s')))$$

This recursion naturally gives us a value iteration algorithm,



Definition 4.18. The POMDP value iteration algorithm for POMDPs is given by recursively updating

$$\alpha_{p}(s) = R(s) + \gamma(\sum_{s'} P(s' \mid s, a)(\sum_{e} P(e \mid s') \cdot \alpha_{p.e}(s')))$$

Observations: The complexity depends primarily on the generated plans:

• Given |A| actions and |E| possible observations, there are are $|A|^{|E|^{d-1}}$ distinct depth-d plans.

The elimination of dominated plans is essential for reducing this doubly exponential growth (but they are already constructed)

Hopelessly inefficient in practice - even the 3x4 POMDP is too hard!

(144 undominated)



26.5 Online Agents with POMDPs

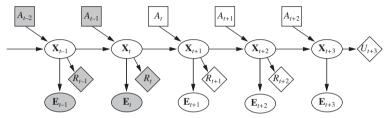


- Idea: Let's try to use the computationally efficient representations (dynamic Bayesian networks and decision networks) for POMDPs.
- Definition 5.1. A dynamic decision network (DDN) is a graph-based representation of a POMDP, where
 - Transition and sensor model are represented as a DBN.
 - Action nodes and utility nodes are added as in decision networks.
- In a DDN, a filtering algorithm is used to incorporate each new percept and action and to update the belief state representation.
- Decisions are made in DDN by projecting forward possible action sequences and choosing the best one.
- DDNs like the DBNs they are based on are factored representations v typically exponential complexity advantages!



Structure of DDNs for POMDPs

DDN for POMDPs: The generic structure of a dymamic decision network at time t is



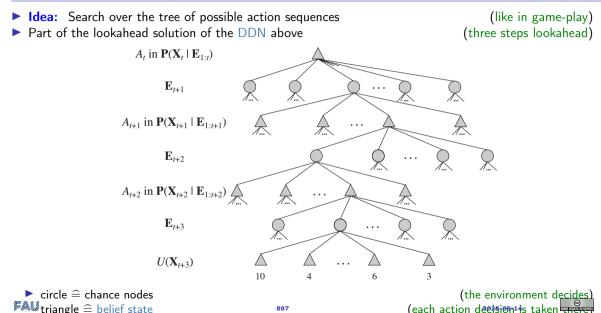
- POMDP state S_t becomes a set of random variables X_t
- there may be multiple evidence variables E_t
- Action at time t denoted by A_t . agent must choose a value for A_t .
- Transition model: $\mathbb{P}(X_{t+1}|X_t, A_t)$; sensor model: $\mathbb{P}(E_t|X_t)$.
- Reward functions R_t and utility U_t of state S_t .
- **Problem:** How do we compute with that?
- Answer: All POMDP algorithms can be adapted to DDNs!

Fau

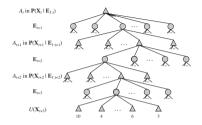


(only need CPTs)

Lookahead: Searching over the Possible Action Sequences



Designing Online Agents for POMDPs



Belief state at triangle computed by filtering with actions/percepts leading to it

- ► for decision A_{t+i} will use percepts $E_{t+1:t+i}$ (even if values at time t unknown)
- thus a POMDP agent automatically takes into account the value of information and executes information gathering actions where appropriate.
- ▶ Observation: Time complexity for exhaustive search up to depth *d* is $\mathcal{O}(|A|^d \cdot |E|^d)$ ($|A| \cong$ number of actions, $|E| \cong$ number of percepts)
- **Upshot:** Much better than POMDP value iteration with $\mathcal{O}(|A|^{|E|^{d-1}})$.
- **Empirically:** For problems in which the discount factor γ is not too close to 1, a shallow search is often good enough to give near-optimal decisions.



- Decision theoretic agents for sequential environments
- Building on temporal, probabilistic models/inference
- ► MDPs for fully observable case.
- ▶ Value/Policy Iteration for MDPs ~→ optimal policies.
- POMDPs for partially observable case.
- ► POMDPs ADP on belief state space.
- ▶ The world is a POMDP with (initially) unknown transition and sensor models.

(dynamic Bayesian networks)



Part 2 Machine Learning



Chapter 27 Learning from Observations

Learning agents

Inductive learning

- Decision tree learning
- Measuring learning performance
- Computational Learning Theory
- Linear regression and classification
- Neural Networks
- Support Vector Machines

27.1 Forms of Learning

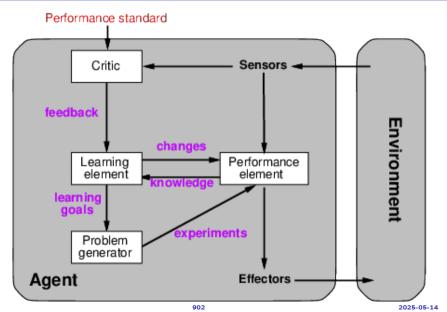


- Learning is essential for unknown environments:
 - i.e., when designer lacks omniscience.
 - ► The world is a POMDP with (initially) unknown transition and sensor models.
- Learning is useful as a system construction method.
 - ▶ i.e., expose the agent to reality rather than trying to write it down
- ► Learning modifies the agent's decision mechanisms to improve performance.

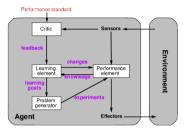


Recap: Learning Agents

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Recap: Learning Agents (continued)



- **Definition 1.1.** Performance element is what we called "agent" up to now.
- Definition 1.2. Critic/learning element/problem generator do the "improving".
- Definition 1.3. Performance standard is fixed;

(outside the environment)

- We can't adjust performance standard to flatter own behaviour!
- No standard *in the environment*: e.g. ordinary chess and suicide chess look identical.
- Essentially, certain kinds of percepts are "hardwired" as good/bad (e.g.,pain, hunger)
- **Definition 1.4.** Learning element may use knowledge already acquired in the performance element.
- Definition 1.5. Learning may require experimentation actions an agent might not normally consider such as dropping rocks from the Tower of Pisa.



- Supervised learning: There's an unknown function $f: A \to B$ called the target function. We do know a set of pairs $T := \{\langle a_i, f(a_i) \rangle\}$ of examples. The goal is to find a hypothesis $h \in \mathcal{H} \subseteq A \to B$ based on T, that is "approximately" equal to f. (Most of the techniques we will consider)
- Unsupervised learning: Given a set of data A, find a pattern in the data; i.e. a function f: A → B for some predetermined B.
 (Primarily clustering/dimensionality reduction)
- Reinforcement learning: The agent receives a reward for each action performed. T he goal is to iteratively adapt the action function to maximize the total reward. (Useful in e.g. game play)



27.2 Supervised Learning



Definition 2.1. A supervised (or inductive) learning problem consists of the following data:

- ▶ A set of hypotheses \mathcal{H} consisting of functions $A \rightarrow B$,
- a set of examples T ⊆ A × B called the training set, such that for every a ∈ A, there is at most one b ∈ B with (a, b) ∈ T,
 (⇒ T is a function on some subset of A)

We assume there is an unknown function $f: A \to B$ called the target function with $T \subseteq f$. **Definition 2.2.** Inductive learning algorithms solve inductive learning problems by finding a hypothesis $h \in \mathcal{H}$ such that $h \sim f$ (for some notion of similarity).

Definition 2.3. We call a supervised learning problem with target function $A \rightarrow B$ a classification problem if *B* is finite, and call the members of *B* classes. We call it a regression problem if $B = \mathbb{R}$.



- ▶ Idea: Construct/adjust hypothesis $h \in H$ to agree with a training set T.
- ▶ Definition 2.4. We call *h* consistent with *f* (on a set $T \subseteq \text{dom}(f)$), if it agrees with *f* (on all examples in *T*).
- Example 2.5 (Curve Fitting).

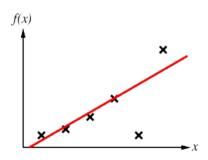
Training Set f(x)xxxxxxxx

Ockham's-razor: maximize a combination of consistency and simplicity.



- ▶ Idea: Construct/adjust hypothesis $h \in H$ to agree with a training set T.
- ▶ **Definition 2.6.** We call *h* consistent with *f* (on a set $T \subseteq \text{dom}(f)$), if it agrees with *f* (on all examples in *T*).
- Example 2.7 (Curve Fitting).

Linear Hypothesis partially, approximatively consistent

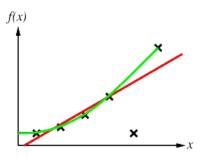


Ockham's-razor: maximize a combination of consistency and simplicity.



- ▶ Idea: Construct/adjust hypothesis $h \in H$ to agree with a training set T.
- ▶ Definition 2.8. We call *h* consistent with *f* (on a set $T \subseteq \text{dom}(f)$), if it agrees with *f* (on all examples in *T*).
- Example 2.9 (Curve Fitting).

Quadratic Hypothesis partially consistent

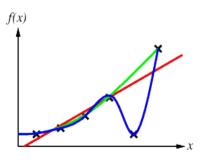


Ockham's-razor: maximize a combination of consistency and simplicity.



- ▶ Idea: Construct/adjust hypothesis $h \in H$ to agree with a training set T.
- ▶ Definition 2.10. We call *h* consistent with *f* (on a set $T \subseteq \text{dom}(f)$), if it agrees with *f* (on all examples in *T*).
- **Example 2.11 (Curve Fitting).**

Degree-4 Hypothesis consistent

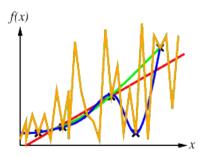


► Ockham's-razor: maximize a combination of consistency and simplicity.



- ▶ Idea: Construct/adjust hypothesis $h \in H$ to agree with a training set T.
- ▶ Definition 2.12. We call *h* consistent with *f* (on a set $T \subseteq \text{dom}(f)$), if it agrees with *f* (on all examples in *T*).
- **Example 2.13 (Curve Fitting).**

High-degree Hypothesis consistent



Ockham's-razor: maximize a combination of consistency and simplicity.



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- Observation: Whether we can find a consistent hypothesis for a given training set depends on the chosen hypothesis space.
- **Definition 2.14.** We say that an supervised learning problem is realizable, iff there is a hypothesis $h \in \mathcal{H}$ consistent with the training set \mathcal{T} .
- Problem: We do not always know whether a given learning problem is realizable, unless we have prior knowledge. (depending on the hypothesis space)
- **Solution:** Make \mathcal{H} large, e.g. the class of all Turing machines.
- Tradeoff: The computational complexity of the supervised learning problem is tied to the size of the hypothesis space. E.g. consistency is not even decidable for general Turing machines.
- Much of the research in machine learning has concentrated on simple hypothesis spaces.
- **Preview:** We will concentrate on propositional logic and related languages first.

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- **Problem:** We want to learn a hypothesis that fits the future data best.
- ▶ Intuition: This only works, if the training set is "representative" for the underlying process.
- Idea: We think of examples (seen and unseen) as a sequence, and express the "representativeness" as a stationarity assumption for the probability distribution.
- Method: Each example before we see it is a random variable E_j , the observed value $e_j = (x_j, y_j)$ samples its distribution.
- Definition 2.15. A sequence of E₁,..., E_n of random variables is independent and identically distributed (short IID), iff they are
 - independent, i.e. $\mathbb{P}(E_j|E_{(j-1)}, E_{(j-2)}, \ldots) = \mathbb{P}(E_j)$ and
 - identically distributed, i.e. $\mathbb{P}(E_i) = \mathbb{P}(E_j)$ for all *i* and *j*.
- **Example 2.16.** A sequence of die tosses is IID. (fair or loaded does not matter)
- **Stationarity Assumption:** We assume that the set \mathcal{E} of examples is IID in the future.



27.3 Learning Decision Trees



Attribute-based Representations

Definition 3.1. In attribute-based representations, examples are described by

- attributes: (simple) functions on input samples,
- their values, and
- classifications.

(think pre classifiers on examples) (classify by attributes)

(Boolean, discrete, continuous, etc.)

Example 3.2 (In a Restaurant). Situations where I will/won't wait for a table:

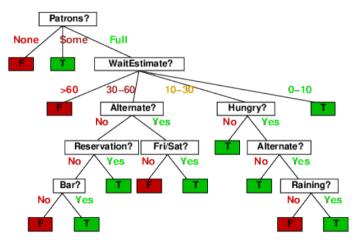
•			/								
– ,	Attributes										Target
Example	Alt	Bar	Fri	Hun	Pat	Price	Rain	Res	Type	Est	WillWait
X1	Т	F	F	Т	Some	\$\$\$	F	Т	French	0–10	Т
X ₂	Т	F	F	Т	Full	\$	F	F	Thai	30–60	F
X3	F	Т	F	F	Some	\$	F	F	Burger	0–10	Т
X_{4}	Т	F	Т	Т	Full	\$	F	F	Thai	10-30	Т
X_{5}	Т	F	Т	F	Full	\$\$\$	F	Т	French	>60	F
\times_{6}	F	Т	F	Т	Some	\$\$	Т	Т	Italian	0–10	Т
X_7	F	Т	F	F	None	\$	Т	F	Burger	0–10	F
X8	F	F	F	Т	Some	\$\$	Т	Т	Thai	0–10	Т
Xg	F	Т	Т	F	Full	\$	Т	F	Burger	>60	F
X10	Т	Т	Т	Т	Full	\$\$\$	F	Т	Italian	10-30	F
X11	F	F	F	F	None	\$	F	F	Thai	0–10	F
X ₁₂	Т	Т	Т	Т	Full	\$	F	F	Burger	30–60	Т

Definition 3.3. For a boolean classification we say that an example is positive (T) or negative (F) depending on its class.



Decision Trees

- Decision trees are one possible representation for hypotheses.
- **Example 3.4 (Restaurant continued).** Here is the "true" tree for deciding whether to wait:

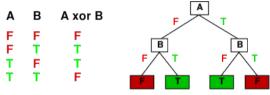




- Definition 3.5. A decision tree for a given attribute-based representation is a tree, where the non-leaf nodes are labeled by attributes, their outgoing edges by disjoint sets of attribute values, and the leaf nodes are labeled by the classifications.
- Definition 3.6. We call an attribute together with a set of attribute values (an inner node) with outgoing edge label an attribute test.
- ▶ the target function is a function $A_1 \times \ldots \times A_n \rightarrow C$, where A_i are the domains of the attributes and *C* is the set of classifications.



- ▶ Decision trees can express any function of the input attributes $\Rightarrow H = A_1 \times \ldots \times A_n$
- **Example 3.7.** For Boolean functions, a path from the root to a leaf corresponds to a row in a truth table:



 \Rightarrow a decision tree corresponds to a truth table

(Formula in DNF)

Trivially, for any training set there is a consistent hypothesis with one path to a leaf for each example, but it probably won't generalize to new examples.

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Solution: Prefer to find more *compact* decision trees.



Decision Tree learning

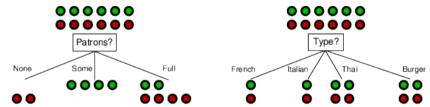
- ▶ Aim: Find a small decision tree consistent with the training examples.
- Idea: (recursively) choose "most significant" attribute as root of (sub)tree.
- Definition 3.8. The following algorithm performs decision tree learning (DTL)

```
function DTL(examples, attributes, default) returns a decision tree
  if examples is empty then return default
   else if all examples have the same classification then return the classification
   else if attributes is empty then return MODE(examples)
   else
      best := Choose–Attribute(attributes. examples)
      tree := a new decision tree with root test best
      m := MODE(examples)
      for each value v; of best do
         examples<sub>i</sub> := {elements of examples with best = v_i}
         subtree := DTL(examples_i, attributes \setminus best, m)
         add a branch to tree with label v; and subtree subtree
     return tree
```

MODE(examples) = most frequent value in example.



- Idea: A good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative".
- Example 3.9.



Attribute "Patrons?" is a better choice, it gives gives information about the classification.

► Can we make this more formal? ~> Use information theory!

(up next)



27.4 Using Information Theory



Intuition: Information answers questions – the less I know initially, the more Information is contained in an answer.

Definition 4.1. Let $\langle p_1, \ldots, p_n \rangle$ the distribution of a random variable *P*. The information (also called entropy) of *P* is

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$$I(\langle p_1, \ldots, p_n \rangle) := \sum_{i=1}^n -p_i \cdot \log_2(p_i)$$

Note: For $p_i = 0$, we consider $p_i \cdot \log_2(p_i) = 0$ The unit of information is a bit, where $1b := l(\langle \frac{1}{2}, \frac{1}{2} \rangle) = 1$ **Example 4.2 (Information of a Coin Toss).**

► For a fair coin toss we have $I(\langle \frac{1}{2}, \frac{1}{2} \rangle) = -\frac{1}{2}\log_2(\frac{1}{2}) - \frac{1}{2}\log_2(\frac{1}{2}) = 1b.$

• With a loaded coin (99% heads) we have $I(\langle \frac{1}{100}, \frac{99}{100} \rangle) = 0.08b$. *Rightarrow* Information goes to 0 as head probability goes to 1.

"How likely is the outcome actually going to tell me something informative?"

 $(\log_2(0))$ is undefined)



Information Gain in Decision Trees

Idea: Suppose we have p examples classified as positive and n examples as negative. We can then estimate the probability distribution of the classification C with $\mathbb{P}(C) = \langle \frac{p}{p+n}, \frac{n}{p+n} \rangle$, and need $I(\mathbb{P}(C))$ bits to correctly classify a new example.

Example 4.3. For 12 restaurant examples and p = n = 6, we need $I(\mathbb{P}(\text{WillWait})) = I(\langle \frac{6}{12}, \frac{6}{12} \rangle) = 1b$ of information. (i.e. exactly the information which of the two classes)

Treating attributes also as random variables, we can compute how much information is needed *after* knowing the value for one attribute:

Example 4.4. If we know Pat = Full, we only need $I(\mathbb{P}(WillWait|Pat = Full)) = I(\langle \frac{4}{6}, \frac{2}{6} \rangle) \approx 0.9$ bits of information.

Note: The expected number of bits needed after an attribute test on A is

$$\sum_{a} P(A = a) \cdot I(\mathbb{P}(C|A = a))$$

Definition 4.5. The information gain from an attribute test A is

$$\operatorname{Gain}(A) := I(\mathbb{P}(C)) - \sum_{a} P(A = a) \cdot I(\mathbb{P}(C|A = a))$$



Information Gain (continued)

▶ **Definition 4.6.** Assume we know the results of some attribute tests $b := B_1 = b_1 \land ... \land B_n = b_n$. Then the conditional information gain from an attribute test A is

$$\operatorname{Gain}(A|b) := I(\mathbb{P}(C|b)) - \sum_{a} P(A = a \mid b) \cdot I(\mathbb{P}(C|a, b))$$

Example 4.7. If the classification C is Boolean and we have p positive and n negative examples, the information gain is

$$\operatorname{Gain}(A) = I(\langle \frac{p}{p+n}, \frac{n}{p+n} \rangle) - \sum_{a} \frac{p_{a}+n_{a}}{p+n} I(\langle \frac{p_{a}}{p_{a}+n_{a}}, \frac{n_{a}}{p_{a}+n_{a}} \rangle)$$

where p_a and n_a are the positive and negative examples with A = a. • Example 4.8.

► Idea: Choose the attribute that maximizes information gain.

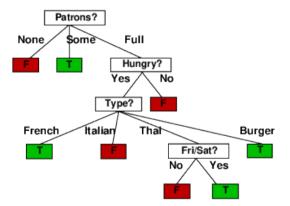
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Restaurant Example contd.

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Example 4.9. Decision tree learned by DTL from the 12 examples using information gain maximization for Choose—Attribute:



Result: Substantially simpler than "true" tree – a more complex hypothesis isn't justified by small amount of data.

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27.5 Evaluating and Choosing the Best Hypothesis



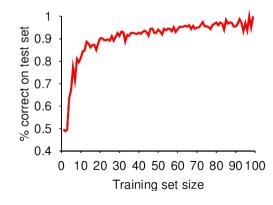
Performance measurement

• **Question:** How do we know that $h \ge f$?

(Hume's Problem of Induction)

 $1. \ Use \ theorems \ of \ computational/statistical \ learning \ theory.$

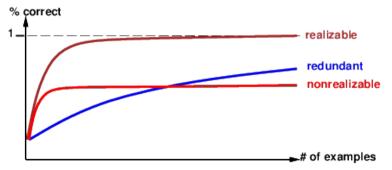
- 2. Try *h* on a new test set of examples. (use same distribution over example space as training set)
- ▶ Definition 5.1. The learning curve $\hat{=}$ percentage correct on test set as a function of training set size.
- Example 5.2. Restaurant data; graph averaged over 20 trials





Performance measurement contd.

- Observation 5.3. The learning curve depends on
 - realizable (can express target function) vs. non-realizable non-realizability can be due to missing attributes or restricted hypothesis class (e.g., thresholded linear function)
 - redundant expressiveness (e.g., lots of irrelevant attributes)



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- **• Observation:** Sometimes a learned hypothesis is more specific than the experiments warrant.
- Definition 5.4. We speak of overfitting, if a hypothesis h describes random error in the (limited) training set rather than the underlying relationship. Underfitting occurs when h cannot capture the underlying trend of the data.
- Qualitatively: Overfitting increases with the size of hypothesis space and the number of attributes, but decreases with number of examples.
- Idea: Combat overfitting by "generalizing" decision trees computed by DTL.



- **Idea:** Combat overfitting by "generalizing" decision trees \sim prune "irrelevant" nodes.
- **Definition 5.5.** For decision tree pruning repeat the following on a learned decision tree:
 - Find a terminal test node *n* (only result leaves as children)
 - ▶ If test is irrelevant, i.e. has low information gain, prune it by replacing *n* by with a leaf node.
- **Question:** How big should the information gain be to split (\rightsquigarrow keep) a node?
- ► Idea: Use a statistical significance test.
- Definition 5.6. A result has statistical significance, if the probability they could arise from the null hypothesis (i.e. the assumption that there is no underlying pattern) is very low (usually 5%).



Determining Attribute Irrelevance

- ► For decision tree pruning, the null hypothesis is that the attribute is irrelevant.
- Compute the probability that the example distribution (p positive, n negative) for a terminal node deviates from the expected distribution under the null hypothesis.
- For an attribute A with d values, compare the actual numbers p_k and n_k in each subset s_k with the expected numbers (expected if A is irrelevant)

$$\widehat{p}_k = p \cdot rac{p_k + n_k}{p + n}$$
 and $\widehat{n}_k = n \cdot rac{p_k + n_k}{p + n}$.

A convenient measure of the total deviation is

(sum of squared errors)

$$\Delta = \sum_{k=1}^{d} \frac{\left(p_k - \widehat{p}_k\right)^2}{\widehat{p}_k} + \frac{\left(n_k - \widehat{n}_k\right)^2}{\widehat{n}_k}$$

- ▶ Lemma 5.7 (Neyman-Pearson). Under the null hypothesis, the value of Δ is distributed according to the χ^2 distribution with d 1 degrees of freedom. [NeyPea:pmtsh33]
- ► Definition 5.8. Decision tree pruning with Pearson's χ^2 with d-1 degrees of freedom for Δ is called χ^2 pruning. $(\chi^2$ values from stats library.)
- **Example 5.9.** The *type* attribute has four values, so three degrees of freedom, so $\Delta = 7.82$ would reject the null hypothesis at the 5% level.

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- **Recall:** We want to learn a hypothesis that fits the future data best.
- ▶ Definition 5.10. Given an inductive learning problem with a set of examples $T \subseteq AB$, we define the error rate of a hypothesis $h \in H$ as the fraction of errors:

$$\frac{|\{\langle x, y \rangle \in T \mid h(x) \neq y\}|}{|T|}$$

- **Caveat:** A low error rate on the training set does not mean that a hypothesis generalizes well.
- ▶ Idea: Do not use homework questions in the exam.
- **Definition 5.11.** The practice of splitting the data available for learning into
 - 1. a training set from which the learning algorithm produces a hypothesis h and
 - 2. a test set, which is used for evaluating h

is called holdout cross validation.

Fau

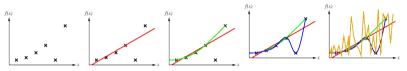
(no peeking at test set allowed)



▶ Question: What is a good ratio between training set and test set size?

- small training set \sim poor hypothesis.
- small test set \rightsquigarrow poor estimate of the accuracy.
- ▶ **Definition 5.12.** In *k* fold cross validation, we perform *k* rounds of learning, each with 1/*k* of the data as test set and average over the *k* error rates.
- ▶ Intuition: Each example does double duty: for training and testing.
- ▶ k = 5 and k = 10 are popular \sim good accuracy at k times computation time.
- **Definition 5.13.** If $k = |\operatorname{dom}(f)|$, then k fold cross validation is called leave one out cross validation (LOOCV).

- Definition 5.14. The model selection problem is to determine given data a good hypothesis space.
- **Example 5.15.** What is the best polynomial degree to fit the data



Observation 5.16. We can solve the problem of "learning from observations f" in a two-part process:

- 1. model selection determines a hypothesis space \mathcal{H} ,
- 2. optimization solves the induced inductive learning problem.
- Idea: Solve the two parts together by iteration over "size". (they inform each other)
- ▶ Problem: Need a notion of "size" ↔ e.g. number of nodes in a decision tree.
- Concrete Problem: Find the "size" that best balances overfitting and underfitting to optimize test set accuracy.



Model Selection Algorithm (Wrapper)

▶ Definition 5.17. The model selection algorithm (MSA) jointly optimizes model selection and optimization by partitioning and cross-validation:

```
function CROSS-VALIDATION-WRAPPER(Learner, k, examples) returns a hypothesis
  local variables: errT, an array, indexed by size, storing training—set error rates
                 errV, an array, indexed by size, storing validation-set error rates
  for size = 1 to \infty do
   errT[size], errV[size] := CROSS–VALIDATION(Learner,size,k,examples)
  if errT has converged then do
      best size := the value of size with minimum errV[size]
      return Learner(best size,examples)
```

```
function CROSS–VALIDATION(Learner, size, k, examples) returns two values:
        average training set error rate, average validation set error rate
  fold errT := 0; fold errV := 0
  for fold = 1 to k do
      training set, validation set := PARTITION(examples,fold,k)
      h := \text{Learner}(size, training set)
      fold errT := fold errT + ERROR - RATE(h, training set)
      fold errV := fold errV + ERROR-RATE(h, validation set)
  return fold errT/k, fold errV/k
```

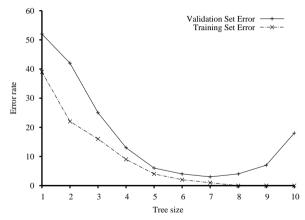
function PARTITION(*examples*, fold, k) returns two sets:

a validation set of size |examples|/k and the rest; the split is different for each fold value



Error Rates on Training/Validation Data

Example 5.18 (An Error Curve for Restaurant Decision Trees). Modify DTL to be breadth-first, information gain sorted, stop after k nodes.



Stops when training set error rate converges, choose optimal tree for validation curve.(here a tree with 7 nodes)

So far we have been minimizing error rates.

(better than maximizing ©)

(not only minimize error rates)

- Example 5.19 (Classifying Spam). It is much worse to classify ham (legitimate mails) as spam than vice versa. (message loss)
- ▶ Recall Rationality: Decision-makers should maximize expected utility (MEU).
- So: Machine learning should maximize "utility".

Fau

- machine learning traditionally deals with utilities in form of "loss functions".
- ▶ **Definition 5.20.** The loss function *L* is defined by setting $L(x, y, \hat{y})$ to be the amount of utility lost by prediction $h(x) = \hat{y}$ instead of f(x) = y. If *L* is independent of *x*, we often use $L(y, \hat{y})$.
- **Example 5.21.** L(spam, ham) = 1, while L(ham, spam) = 10.

• Note: L(y, y) = 0.

(no loss if you are exactly correct)

► Definition 5.22 (Popular general loss functions). absolute value loss $L_1(y, \hat{y}) := |y - \hat{y}|$ small error squared error loss $L_2(y, \hat{y}) := (y - \hat{y})^2$ ditto, but 0/1 loss $L_{0/1}(y, \hat{y}) := 0$, if $y = \hat{y}$, else 1 error rate

small errors are good ditto, but differentiable error rate

- ▶ Idea: Maximize expected utility by choosing hypothesis h that minimizes expected loss over all $(x,y) \in f$.
- **Definition 5.23.** Let \mathcal{E} be the set of all possible examples and $\mathbb{P}(X, Y)$ the prior probability distribution over its components, then the expected generalization loss for a hypothesis *h* with respect to a loss function *L* is

GenLoss_L(h):=
$$\sum_{(x,y)\in\mathcal{E}} L(y,h(x)) \cdot P(x,y)$$

and the best hypothesis $h^* := \underset{h \in \mathcal{H}}{\operatorname{argmin}} \operatorname{GenLoss}_L(h).$



Empirical Loss

- **Problem:** P(X, Y) is unknown \sim learner can only estimate generalization loss:
- **Definition 5.24.** Let L be a loss function and E a set of examples with #(E) = N, then we call

$$\operatorname{EmpLoss}_{L,E}(h) := \frac{1}{N} \left(\sum_{(x,y) \in E} L(y, h(x)) \right)$$

the empirical loss and $\widehat{h}^* := \underset{h \in \mathcal{H}}{\operatorname{argmin}} \operatorname{EmpLoss}_{L, \mathcal{E}}(h)$ the estimated best hypothesis.

- There are four reasons why \hat{h}^* may differ from f:
 - 1. Realizablility: then we have to settle for an approximation \hat{h}^* of f.
 - 2. Variance: different subsets of f give different $\hat{h}^* \rightarrow$ more examples.
 - 3. Noise: if f is non deterministic, then we cannot expect perfect results.
 - 4. Computational complexity: if \mathcal{H} is too large to systematically explore, we make due with subset and get an approximation.

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Regularization

Idea: Directly use empirical loss to solve model selection. Minimize the weighted sum of empirical loss and hypothesis complexity.

▶ Definition 5.25. Let $\lambda \in \mathbb{R}$, $h \in \mathcal{H}$, and *E* a set of examples, then we call

 $\operatorname{Cost}_{L,E}(h) := \operatorname{EmpLoss}_{L,E}(h) + \lambda \operatorname{Complexity}(h)$

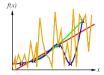
the total cost of h on E.

Definition 5.26. The process of finding a total cost minimizing hypothesis

 $\widehat{h}^* := \operatorname*{argmin}_{h \in \mathcal{H}} \operatorname{Cost}_{L, E}(h)$

is called regularization; Complexity is called the regularization function or hypothesis complexity. **Example 5.27 (Regularization for Polynomials).**

A good regularization function for polynomials is the sum of squares of exponents. \sim keep away from wriggly curves!





(finding a good \mathcal{H}) (to avoid overfitting).

EAU

- **Remark:** In regularization, empirical loss and hypothesis complexity are not measured in the same scale $\rightsquigarrow \lambda$ mediates between scales.
- **Idea:** Measure both in the same scale \sim use information content, i.e. in bits.
- **Definition 5.28.** Let $h \in \mathcal{H}$ be a hypothesis and E a set of examples, then the description length of (h, E) is computed as follows:
 - 1. encode the hypothesis as a Turing machine program, count bits.
 - 2. count data bits:
 - \blacktriangleright correctly predicted example \rightsquigarrow 0b
 - ► incorrectly predicted example ~> according to size of error.

The minimum description length or MDL hypothesis minimizes the total number of bits required.

- This works well in the limit, but for smaller problems there is a difficulty in that the choice of encoding for the program affects the outcome.
 - e.g., how best to encode a decision tree as a bit string?



 Traditional methods in statistics and early machine learning concentrated on small-scale learning (50-5000 examples)

- Generalization error mostly comes from
 - approximation error of not having the true f in the hypothesis space
 - estimation error of too few training examples to limit variance.
- ▶ In recent years there has been more emphasis on large-scale learning.
 - Generalization error is dominated by limits of computation
 - there is enough data and a rich enough model that we could find an h that is very close to the true f,
 - but the computation to find it is too complex, so we settle for a sub-optimal approximation.
 - ▶ Hardware advances (GPU farms, Amazon EC2, Google Data Centers, ...) help.

(millions of examples)

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27.6 Computational Learning Theory



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- ▶ Main Question: How can we be sure that our learning algorithm has produced a hypothesis that will predict the correct value for previously unseen inputs?
- **Formally:** How do we know that the hypothesis h is close to the target function f if we don't know what f is?

Other - more recent - Questions:

- How many examples do we need to get a good h?
- What hypothesis space \mathcal{H} should we use?
- If the \mathcal{H} is very complex, can we even find the best *h*, or do we have to settle for a local maximum in \mathcal{H} .
- How complex should h be?
- How do we avoid overfitting?
- "Computational Learning Theory" tries to answer these using concepts from AI, statistics, and theoretical CS.



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Basic idea of Computational Learning Theory:

- Any hypothesis h that is seriously wrong will almost certainly be "found out" with high probability after a small number of examples, because it will make an incorrect prediction.
- ▶ Thus, if *h* is consistent with a sufficiently large set of training examples is unlikely to be seriously wrong.
- $\blacktriangleright \sim h$ is probably approximately correct.
- Definition 6.1. Any learning algorithm that returns hypotheses that are probably approximately correct is called a PAC learning algorithm.
- ▶ Derive performance bounds for PAC learning algorithms in general, using the
- ► Stationarity Assumption (again): We assume that the set *E* of possible examples is IID ~> we have a fixed distribution P(E) = P(X, Y) on examples.

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Simplifying Assumptions: f is a function (deterministic) and $f \in \mathcal{H}$.



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- Start with PAC theorems for Boolean functions, for which $L_{0/1}$ is appropriate.
- Definition 6.2. The error rate error(h) of a hypothesis h is the probability that h misclassifies a new example.

$$\operatorname{error}(h) := \operatorname{GenLoss}_{L_{0/1}}(h) = \sum_{(x,y) \in \mathcal{E}} L_{0/1}(y,h(x)) \cdot P(x,y)$$

Intuition: $\operatorname{error}(h)$ is the probability that *h* misclassifies a new example.

- ▶ This is the same quantity as measured in the learning curves above.
- ▶ Definition 6.3. A hypothesis h is called approximatively correct, iff error(h) ≤ e for some small e > 0. We write H_b:={h ∈ H | error(h) > e} for the "seriously bad" hypotheses.



- ▶ Let's compute the probability that $h_b \in H_b$ is consistent with the first *N* examples.
- We know $\operatorname{error}(h_b) > \epsilon$
 - $\sim P(h_b \text{ agrees with } N \text{ examples}) \leq (1 \epsilon)^N.$ (independence) $\sim P(\mathcal{H}_b \text{ contains consistent hyp.}) \leq |\mathcal{H}_b| \cdot (1 - \epsilon)^N \leq |\mathcal{H}| \cdot (1 - \epsilon)^N.$ ($\mathcal{H}_b \subseteq \mathcal{H}$) $\sim \text{ to bound this by a small } \delta, \text{ show the algorithm } N \geq \frac{1}{\epsilon} \cdot (\log_2(\frac{1}{\delta}) + \log_2(|\mathcal{H}|)) \text{ examples.}$
- Definition 6.4. The number of required examples as a function of ε and δ is called the sample complexity of H.

► Example 6.5. If H is the set of n-ary Boolean functions, then |H| = 2^{2ⁿ}.
 ~ sample complexity grows with O(log₂(2^{2ⁿ})) = O(2ⁿ).
 There are 2ⁿ possible examples,
 ~ PAC learning for Boolean functions needs to see (nearly) all examples.



- ▶ Problem: PAC learning for Boolean functions needs to see (nearly) all examples.
 - \blacktriangleright H contains enough hypotheses to classify any given set of examples in all possible ways.
 - ▶ In particular, for any set of N examples, the set of hypotheses consistent with those examples contains equal numbers of hypotheses that predict x_{N+1} to be positive and hypotheses that predict x_{N+1} to be negative.
- ▶ Idea/Problem: restrict the *H* in some way

► Three Ways out of this Dilemma:

- 1. bring prior knowledge into the problem.
- 2. prefer simple hypotheses.

Fau

3. focus on "learnable subsets" of \mathcal{H} .

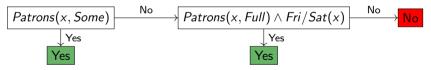
(but we may lose realizability)

```
(???)
(e.g. decision tree pruning)
(next)
```

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- ▶ Idea: Apply PAC learning to a "learnable hypothesis space".
- Definition 6.6. A decision list consists of a sequence of tests, each of which is a conjunction of literals.
 - ▶ If a test succeeds when applied to an example description, the decision list specifies the value to be returned.
 - If the test fails, processing continues with the next test in the list.
- **Remark:** Like decision trees, but restricted branching, but more complex tests.
- **Example 6.7 (A decision list for the Restaurant Problem).**



Lemma 6.8. Given arbitrary size conditions, decision lists can represent arbitrary Boolean functions.
 This directly defeats our purpose of finding a "learnable subset" of H.



- ▶ Definition 6.9. The set of decision lists where tests are of conjunctions of at most k literals is denoted by k-DL.
- **Example 6.10.** The decision list from **??** is in 2–DL.
- **• Observation 6.11.** k-DL contains k-DT, the set of decision trees of depth at most k.
- **Definition 6.12.** We denote the set of k-DL decision lists with at most n Boolean attributes with k-DL(n). The set of conjunctions of at most k literals over n attributes is written as Conj(k, n).
- ► Decision lists are constructed of optional yes/no tests, so there are at most 3^{|Conj(k,n)|} distinct sets of component tests. Each of these sets of tests can be in any order, so |k-DL(n)| ≤ 3^{|Conj(k,n)|} · |Conj(k,n)|!



Decision Lists: Learnable Subsets (Sample Complexity)

► The number of conjunctions of *k* literals from *n* attributes is given by

$$\operatorname{Conj}(k,n)| = \sum_{i=1}^{k} \binom{2n}{i}$$

thus $|\operatorname{Conj}(k, n)| = \mathcal{O}(n^k)$. Hence, we obtain (after some work)

 $|k-\mathsf{DL}(n)|=2^{\mathcal{O}(n^k\log_2(n^k))}$

▶ Plug this into the equation for the sample complexity: $N \ge \frac{1}{\epsilon} \cdot (\log_2(\frac{1}{\delta}) + \log_2(|\mathcal{H}|))$ to obtain

$$N \geq rac{1}{\epsilon} \cdot (\log_2(rac{1}{\delta}) + \log_2(\mathcal{O}(n^k \log_2(n^k))))$$

Intuitively: Any algorithm that returns a consistent decision list will PAC learn a k-DL function in a reasonable number of examples, for small k.



Idea: Use a greedy search algorithm that repeats

1. find test that agrees exactly with some subset E of the training set,

- 2. add it to the decision list under construction and removes E,
- 3. construct the remainder of the DL using just the remaining examples,

until there are no examples left.

▶ Definition 6.13. The following algorithm performs decision list learning

```
function DLL(E) returns a decision list, or failure

if E is empty then return (the trivial decision list) No

t := a test that matches a nonempty subset E_t of E

such that the members of E_t are all positive or all negative

if there is no such t then return failure

if the examples in E_t are positive then o := Yes else o := No

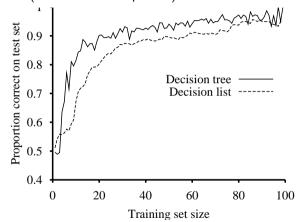
return a decision list with initial test t and outcome o and remaining tests given by

DLL(E \setminus E_t)
```



Decision Lists Learning in Comparison

Learning curves: for DLL (and DTL for comparison)



Upshot: The simpler DLL works quite well!

27.7 Regression and Classification with Linear Models

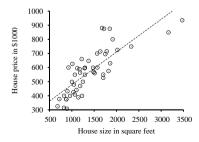


Univariate Linear Regression

- **Definition 7.1.** A univariate or unary function is a function with one argument.
- ▶ **Recall:** A mapping f between vector spaces is called linear, iff it preserves rmodule/plus and rmodule/scalar multiplication, i.e. $f(\alpha \cdot v_1 + v_2) = \alpha \cdot f(v_1) + f(v_2)$.
- Observation 7.2. A univariate, linear function f: ℝ → ℝ is of the form f(x) = w₁x + w₀ for some w_i ∈ ℝ.
- **Definition 7.3.** Given a vector $w := (w_0, w_1)$, we define $h_w(x) := w_1 x + w_0$.
- ▶ Definition 7.4. Given a set of examples E ⊆ ℝ×ℝ, the task of finding h_w that best fits E is called linear regression.

Example 7.5.

Examples of house price vs. square feet in houses sold in Berkeley in July 2009. Also: linear function hypothesis that minimizes squared error loss y = 0.232x + 246.





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Univariate Linear Regression by Loss Minimization

▶ Idea: Minimize squared error loss over $\{(x_i, y_i) | i \le N\}$

(used already by Gauss)

$$Loss(h_w) = \sum_{j=1}^{N} L_2(y_j, h_w(x_j)) = \sum_{j=1}^{N} (y_j - h_w(x_j))^2 = \sum_{j=1}^{N} (y_j - (w_1 x_j + w_0))^2$$

Task: find $w^* := \operatorname{argmin} \operatorname{Loss}(h_w)$.

Recall: $\sum_{j=1}^{N} (y_j - (w_1 x_j + w_0))^2$ is minimized, when the partial derivatives wrt. the w_i are zero, i.e. when

$$\frac{\partial}{\partial w_0} \left(\sum_{j=1}^N \left(y_j - \left(w_1 x_j + w_0 \right) \right)^2 \right) = 0 \quad \text{and} \quad \frac{\partial}{\partial w_1} \left(\sum_{j=1}^N \left(y_j - \left(w_1 x_j + w_0 \right) \right)^2 \right) = 0$$

Observation: These equations have a unique solution:

$$w_{1} = \frac{N(\sum_{j} x_{j} y_{j}) - (\sum_{j} x_{j})(\sum_{j} y_{j})}{N(\sum_{j} x_{j}^{2}) - (\sum_{j} x_{j})^{2}} \qquad w_{0} = \frac{(\sum_{j} y_{j}) - w_{1}(\sum_{j} x_{j})}{N}$$

Remark: Closed-form solutions only exist for linear regression, for other (differentiable) hypothesis spaces use gradient descent methods for adjusting/learning weights.

FAU



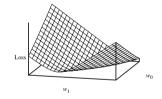
Remark: Many forms of learning involve adjusting weights to minimize loss.

Definition 7.6. The weight space of a parametric model is the space of all possible combinations of parameters (called the weights). Loss minimization in a weight space is called weight fitting.

```
The weight space of univariate linear regression is \mathbb{R}^2.

\sim graph the loss function over \mathbb{R}^2.

Note: it is convex.
```



Observation 7.7. The squared error loss function is convex for any linear regression problem ~> there are no local minima.



Gradient Descent Methods

- ▶ If we do not have closed form solutions for minimizing loss, we need to search.
- ▶ Idea: Use local search (hill climbing) methods.
- ▶ **Definition 7.8.** The gradient descent algorithm for finding a minimum of a continuous function *F* is hill climbing in the direction of the steepest descent, which can be computed by the partial derivatives of *F*.

```
function gradient-descent(F,w,\alpha) returns a local minimum of F
inputs: a differentiable function F and initial weights w.
loop until w converges do
for each w<sub>i</sub> do
w_i \leftarrow w_i - \alpha \frac{\partial}{\partial w_i} F(w)
end for
end loop
```

The parameter α is called the learning rate. It can be a fixed constant or it can decay as learning proceeds.



► Let's try gradient descent for Loss.

▶ Work out the partial derivatives for one example (*x*,*y*):

$$\frac{\partial \text{Loss}(w)}{\partial w_i} = \frac{\partial (y - h_w(x))^2}{\partial w_i} = 2(y - h_w(x)) \frac{\partial (y - (w_1 x + w_0))}{\partial w_i}$$

and thus

$$\frac{\partial \text{Loss}(w)}{\partial w_0} = -2(y - h_w(x)) \qquad \frac{\partial \text{Loss}(w)}{\partial w_1} = -2(y - h_w(x))x$$

Plug this into the gradient descent updates:

$$w_{0} \longleftarrow w_{0} - \alpha \cdot (-2(y - h_{w}(x))) \qquad w_{1} \longleftarrow w_{1} - \alpha \cdot -2((y - h_{w}(x))) \cdot x$$



- Analogously for *n* training examples (x_j, y_j) :
- Definition 7.9.

Fau

$$w_0 \leftarrow w_0 - \alpha(\sum_j -2(y_j - h_w(x_j))) \quad w_1 \leftarrow w_1 - \alpha(\sum_j -2(y_j - h_w(x_n))x_n)$$

These updates constitute the batch gradient descent learning rule for univariate linear regression.

- Convergence to the unique global loss minimum is guaranteed (as long as we pick α small enough) but may be very slow.
- Doing batch gradient descent on random subsets of the examples of fixed batch size n is called stochastic gradient descent (SGD). (More computationally efficient than updating for every example)

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Multivariate Linear Regression

- **Definition 7.10.** A multivariate or *n*-ary function is a function with one or more arguments.
- We can use it for multivariate linear regression.

Idea: Every example $\vec{x_j}$ is an *n* element vector and the hypothesis space is the set of functions

$$h_{sw}(\vec{x}_j) = w_0 + w_1 x_{j,1} + \ldots + w_n x_{j,n} = w_0 + \sum_i w_i x_{j,i}$$

Trick: Invent $x_{j,0} := 1$ and use matrix notation:

$$h_{sw}(\vec{x}_j) = \vec{w} \cdot \vec{x}_j = \vec{w}^t \vec{x}_j = \sum_i w_i x_{j,i}$$

- **Definition 7.11.** The best vector of weights, w^{*}, minimizes squared-error loss over the examples: $w^* := \underset{w}{\operatorname{argmin}} (\sum_j L_2(y_j)(w \cdot \vec{x_j})).$
- Gradient descent will reach the (unique) minimum of the loss function; the update equation for each weight w_i is

$$w_i \leftarrow w_i - \alpha(\sum_j x_{j,i}(y_j - h_w(\vec{x}_j)))$$



- ▶ We can also solve analytically for the w^{*} that minimizes loss.
- Let \vec{y} be the vector of outputs for the training examples, and X be the data matrix, i.e., the matrix of inputs with one *n*-dimensional example per row.

Then the solution $w^* = (X^T X)^{-1} X^T \vec{y}$ minimizes the squared error.



- **Remark:** Univariate linear regression does not overfit, but in the multivariate case there might be "redundant dimensions" that result in overfitting.
- ▶ Idea: Use regularization with a complexity function based on weights.
- ▶ Definition 7.12. Complexity(h_w) = $L_q(w) = \sum_i |w_i|^q$
- **Caveat:** Do not confuse this with the loss functions L_1 and L_2 .
- **Problem:** Which q should we pick? (L_1 and L_2 minimize sum of absolute values/squares)
- Answer: It depends on the application.

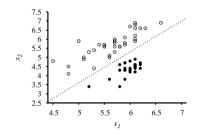
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Remark: L₁-regularization tends to produce a sparse model, i.e. it sets many weights to 0, effectively declaring the corresponding attributes to be irrelevant.
 Hypotheses that discard attributes can be easier for a human to understand, and may be less likely to overfit. (see [RusNor:AIMA03])

Linear Classifiers with a hard Threshold

- ▶ Idea: The result of linear regression can be used for classification.
- **Example 7.13 (Nuclear Test Ban Verification).**

Plots of seismic data parameters: body wave magnitude x_1 vs. surface wave magnitude x_2 . White: earthquakes, black: underground explosions **Also**: h_{w^*} as a decision boundary $x_2 = 17x_1 - 4.9$.

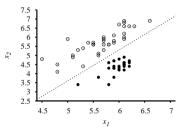


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Linear Classifiers with a hard Threshold

- ▶ Idea: The result of linear regression can be used for classification.
- **Example 7.16 (Nuclear Test Ban Verification).**

Plots of seismic data parameters: body wave magnitude x_1 vs. surface wave magnitude x_2 . White: earthquakes, black: underground explosions **Also**: h_{w^*} as a decision boundary $x_2 = 17x_1 - 4.9$.



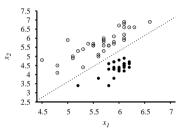
- Definition 7.17. A decision boundary is a line (or a surface, in higher dimensions) that separates two classes of points. A linear decision boundary is called a linear separator and data that admits one are called linearly separable.
- **Example 7.18 (Nuclear Tests continued).** The linear separator for **??**is defined by
 - $-4.9 + 1.7x_1 x_2 = 0$, explosions are characterized by $-4.9 + 1.7x_1 x_2 > 0$, earthquakes by $-4.9 + 1.7x_1 x_2 < 0$.



Linear Classifiers with a hard Threshold

- ▶ Idea: The result of linear regression can be used for classification.
- **Example 7.19 (Nuclear Test Ban Verification).**

Plots of seismic data parameters: body wave magnitude x_1 vs. surface wave magnitude x_2 . White: earthquakes, black: underground explosions **Also**: h_{w^*} as a decision boundary $x_2 = 17x_1 - 4.9$.



- Definition 7.20. A decision boundary is a line (or a surface, in higher dimensions) that separates two classes of points. A linear decision boundary is called a linear separator and data that admits one are called linearly separable.
- **Example 7.21 (Nuclear Tests continued).** The linear separator for **??**is defined by
 - $-4.9 + 1.7x_1 x_2 = 0$, explosions are characterized by $-4.9 + 1.7x_1 x_2 > 0$, earthquakes by $-4.9 + 1.7x_1 x_2 < 0$.
- ► Useful Trick: If we introduce dummy coordinate $x_0 = 1$, then we can write the classification hypothesis as $h_w(x) = 1$ if $w \cdot x > 0$ and 0 otherwise.



Linear Classifiers with a hard Threshold (Perceptron Rule)

- ▶ So $h_w(x) = 1$ if $w \cdot x > 0$ and 0 otherwise is well-defined, how to choose w?
- ► Think of h_w(x) = T(w·x), where T(z) = 1, if z > 0 and T(z) = 0 otherwise. We call T a threshold function.
- **Problem:** \mathcal{T} is not differentiable and $\frac{\partial \mathcal{T}}{\partial z} = 0$ where defined \rightsquigarrow
 - ▶ No closed-form solutions by setting $\frac{\partial T}{\partial z} = 0$ and solving.
 - Gradient-descent methods in weight-space do not work either.
- ▶ We can learn weights by iterating over the following rule:
- Definition 7.22. Given an example (x,y), the perceptron learning rule is

$$w_i \leftarrow w_i + \alpha \cdot (y - h_w(x)) \cdot x_i$$

- \blacktriangleright as we are considering 0/1 classification, there are three possibilities:
 - 1. If $y = h_w(x)$, then w_i remains unchanged.
 - 2. If y = 1 and $h_w(x) = 0$, then w_i is in/decreased if x_i is positive/negative. (we want to make $w \cdot x$ bigger so that $\mathcal{T}(w \cdot x) = 1$)
 - 3. If y = 0 and $h_w(x) = 1$, then w_i is de/increased if x_i is positive/negative. (we want to make $w \cdot x$ smaller so that $\mathcal{T}(w \cdot x) = 0$)

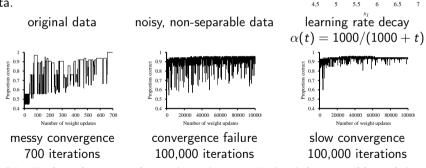
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Learning Curves for Linear Classifiers (Perceptron Rule)

Example 7.23.

Learning curves (plots of total training set accuracy vs. number of iterations) for the perceptron rule on the earthquake/explosions data.



7.5

6.5

5.5 x 5

> 4.5 4 3.5

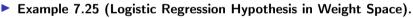
> 2.5

Theorem 7.24. Finding the minimal-error hypothesis is NP-hard, but possible with learning rate decay.

Linear Classification with Logistic Regression

- **So far:** Passing the output of a linear function through a threshold function \mathcal{T} yields a linear classifier.
- **Problem:** The hard nature of \mathcal{T} brings problems:
 - \blacktriangleright $\mathcal T$ is not differentiable nor continuous \rightsquigarrow learning via perceptron rule becomes unpredictable.
 - \blacktriangleright \mathcal{T} is "overly precise" near the boundary \leftrightarrow need more graded judgments.
- ▶ Idea: Soften the threshold, approximate it with a differentiable function.

We use the standard logistic function $I(x) = \frac{1}{1+e^{-x}}$ So we have $h_w(x) = I(w \cdot x) = \frac{1}{1+e^{-(w \cdot x)}}$



Plot of a logistic regression hypothesis for the earthquake/explosion data. The value at (w_0, w_1) is the probability of belonging to the class labeled 1.

We speak of the cliff in the classifier intuitively.





Logistic Regression

- **Definition 7.26.** The process of weight fitting in $h_w(x) = \frac{1}{1+e^{-(w \cdot x)}}$ is called logistic regression.
- ▶ There is no easy closed form solution, but gradient descent is straightforward,
- ▶ As our hypotheses have continuous output, use the squared error loss function L_2 .
- ► For an example (x,y) we compute the partial derivatives:

 $\frac{\partial}{\partial w}$

$$\begin{aligned} \frac{\partial}{\partial w_i} ((y - h_w(x))^2) \\ &= 2 \cdot h_w(x) \cdot \frac{\partial}{\partial w_i} (y - h_w(x)) \\ &= -2 \cdot h_w(x) \cdot l'(w \cdot x) \cdot \frac{\partial}{\partial w_i} (w \cdot x) \\ &= -2 \cdot h_w(x) \cdot l'(w \cdot x) \cdot x_i \end{aligned}$$

(via chain rule)



Logistic Regression (continued)

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► The derivative of the logistic function satisfies l'(z) = l(z)(1 - l(z)), thus

$$l'(w \cdot x) = l(w \cdot x)(1 - l(w \cdot x)) = h_w(x)(1 - h_w(x))$$

Definition 7.27. The rule for logistic update (weight update for minimizing the loss) is

$$w_i \leftarrow w_i + \alpha \cdot (y - h_w(x)) \cdot h_w(x) \cdot (1 - h_w(x)) \cdot x_i$$

Example 7.28 (Redoing the Learning Curves). original data noisy, non-separable data learning rate decay $\alpha(t) = 1000/(1000 + t)$ 0.9 0.9 0.9 0.8 0.8 0.8 0.7 0.7 0.6 0.6 0.6 0.5 0.5 0.5 0 1000 2000 5000 20000 40000 60000 80000 10000 20000 2000 4000 40000 60000 80000 10000 Number of weight updates Number of weight undates Number of weight updates convergence failure slow convergence messy convergence 5000 iterations 100.000 iterations 100.000 iterations **Upshot:** Logistic update seems to perform better than perceptron update.

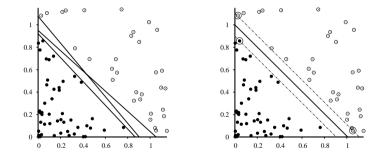
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27.8 Support Vector Machines



Support Vector Machines

Definition 8.1. Given a linearly separable data set E the maximum margin separator is the linear separator s that maximizes the margin, i.e. the distance of the E from s. **Example 8.2.** All lines on the left are valid linear separators:



We expect the maximum margin separator on the right to generalize best **Note:** To find the maximum margin separator, we only need to consider the innermost points (circled above).

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Definition 8.3. Support-vector machines (SVMs; also support-vector networks) are supervised learning models for classification and regression.

SVMs construct a maximum margin separator by prioritizing critical examples (support vectors).

SVMs are still one of the most popular approaches for "off-the-shelf" supervised learning.

Setting:

- ▶ We have a training set $E = \{\langle x_1, y_1 \rangle, ..., \langle x_n, y_n \rangle\}$ where $x_i \in \mathbb{R}^p$ and $y_i \in \{-1, 1\}$ (instead of $\{1, 0\}$)
- ▶ The goal is to find a *hyperplane* in \mathbb{R}^p that maximally separates the two classes (i.e. $y_i = -1$ from $y_i = 1$)
- **Remember** A hyperplane can be represented as the set $\{x \mid (w \cdot x) + b = 0\}$ for some vector w and scalar b. (w is orthogonal to the plane, b determines the offset from the origin)



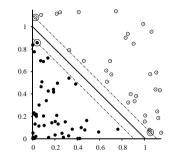
Finding the Maximum Margin Separator (Separable Case)

Idea: The margin is bounded by the two hyperplanes described by $\{x | (w \cdot x) + b + 1 = 0\}$ (lower boundary) and $\{x | (w \cdot x) + b - 1 = 0\}$ (upper boundary).

 \Rightarrow The distance between them is $\frac{2}{\|\mathbf{w}\|_2}$.

Constraints: To maximize the margin, minimize $||w||_2$ while keeping x_i out of the margin:

$$(\mathbf{w} \cdot \mathbf{x}_i) + b \ge 1$$
 for $y_i = 1$ and $(\mathbf{w} \cdot \mathbf{x}_i) + b \le -1$ for $y_i = -1$
 $\Rightarrow y_i((\mathbf{w} \cdot \mathbf{x}_i) - b) \ge 1$ for $1 \le i \le n$.
 \Rightarrow This is an optimization problem.



Theorem 8.4 (SVM equation). Let $\alpha = \underset{\alpha}{\operatorname{argmax}} \left(\sum_{j} \alpha_{j} - \frac{1}{2} \left(\sum_{j,k} \alpha_{j} \alpha_{k} y_{j} y_{k}(x_{j} \cdot x_{k})\right)\right)$ under the constraints $\alpha_{j} \geq 0$ and $\sum_{j} \alpha_{j} y_{j} = 0$. The maximum margin separator is given by $w = \sum_{j} \alpha_{j} x_{j}$ and $b = w \cdot x_{i} - y_{i}$ for any x_{i} where $\alpha_{i} \neq 0$.

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Proof sketch: By the duality principle for optimization problems

Finding the Maximum Margin Separator (Separable Case)

$$\alpha = \operatorname*{argmax}_{\alpha} \left(\sum_{j} \alpha_{j} - \frac{1}{2} (\sum_{j,k} \alpha_{j} \alpha_{k} y_{j} y_{k} (x_{j} \cdot x_{k})) \right), \text{where } \alpha_{j} \geq 0, \quad \sum_{j} \alpha_{j} y_{j} = 0$$

Important Properties:

- The weights α_j associated with each data point are zero except at the support vectors (the points closest to the separator),
- The expression is convex \sim the single global maximum can found efficiently,
- Data enter the expression only in the form of dot products of point pairs → once the optimal α_i have been calculated, we have h(x) = sign(∑_i α_jy_j(x·x_j) − b)
- There are good software packages for solving such quadratic programming optimizations

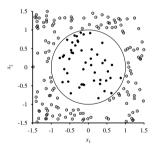
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Support Vector Machines (Kernel Trick)

What if the data is not linearly separable?

Idea: Transform the data into a *feature space* where they are. **Definition 8.5.** A feature for data in \mathbb{R}^p is a function $\mathbb{R}^p \to \mathbb{R}^q$.

Example 8.6 (Projecting Up a Non-Separable Data Set). The true decision boundary is $x_1^2 + x_2^2 \le 1$.



 \sim use the feature "distance from center"



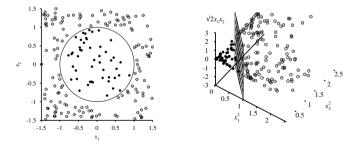
Support Vector Machines (Kernel Trick continued)

Idea: Replace $x_i \cdot x_j$ by some other product on the feature space in the SVM equation

Definition 8.7. A kernel function is a function $K : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ of the form $K(x_1, x_2) = \langle F(x_1), F(x_2) \rangle$ for some feature F and inner product $\langle \cdot, \cdot \rangle$ on the codomain of F.

Smart choices for a kernel function often allow us to compute $K(x_i, x_j)$ without needing to compute F at all.

Example 8.8. If we encode the distance from the center as the feature $F(x) = \langle x_1^2, x_2^2, \sqrt{2}x_1x_2 \rangle$ and define the kernel function as $K(x_i, x_j) = F(x_i) \cdot F(x_j)$, then this simplifies to $K(x_i, x_j) = (x_i \cdot x_j)^2$





Support Vector Machines (Kernel Trick continued)

Generally: We can learn non-linear separators by solving

$$\underset{\alpha}{\operatorname{argmax}} \left(\sum_{j} \alpha_{j} - \frac{1}{2} (\sum_{j,k} \alpha_{j} \alpha_{k} y_{j} y_{k} \mathcal{K}(\mathsf{x}_{j},\mathsf{x}_{k})) \right)$$

where K is a kernel function

Definition 8.9. Let $X = \{x_1, ..., x_n\}$. A symmetric function $K : X \times X \to \mathbb{R}$ is called positive definite iff the matrix $K_{i,j} = K(x_i, x_j)$ is a positive definite matrix. **Theorem 8.10 (Mercer's Theorem).** Every positive definite function K on X is a kernel function on X for some feature F.

Definition 8.11. The function $K(x_j, x_k) = (1 + (x_j \cdot x_j))^d$ is a kernel function corresponding to a feature space whose dimension is exponential in d. It is called the polynomial kernel.



27.9 Artificial Neural Networks



Brains

Neural networks

Perceptrons

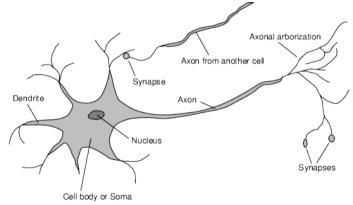
Multilayer perceptrons

Applications of neural networks



Brains

Axiom 9.1 (Neuroscience Hypothesis). Mental activity consists consists primarily of electrochemical activity in networks of brain cells called neurons.



- **Definition 9.2.** The animal brain is a biological neural network
 - with 10^{11} neurons of > 20 types, 10^{14} synapses, (1ms) (10ms) cycle time.
 - Signals are noisy "spike trains" of electrical potential.



- One approach to artificial intelligence is to model and simulate brains. (and hope that AI comes along naturally)
- Definition 9.3. The AI subfield of neural networks (also called connectionism, parallel distributed processing, and neural computation) studies computing systems inspired by the biological neural networks that constitute brains.
- Neural networks are attractive computational devices, since they perform important AI tasks most importantly learning and distributed, noise-tolerant computation – naturally and efficiently.

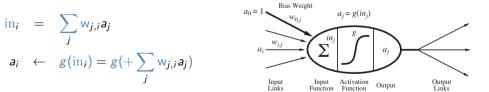


Neural Networks - McCulloch-Pitts "unit"

Definition 9.4. An artificial neural network is a directed graph such that every edge $a_i \rightarrow a_j$ is associated with a weight $w_{i,j} \in \mathbb{R}$, and each node a_j with parents a_1, \ldots, a_n is associated with a function $f(w_{1,j}, \ldots, w_{n,j}, x_1, \ldots, x_n) \in \mathbb{R}$. We call the output of a node's function its activation, the matrix $w_{i,j}$ the weight matrix, the nodes units and the edges links.

In 1943 McCulloch and Pitts proposed a simple model for a neuron/brain:

Definition 9.5. A McCulloch-Pitts unit first computes a weighted sum of all inputs and then applies an activation function g to it.



If g is a threshold function, we call the unit a perceptron unit, if g is a logistic function a sigmoid perceptron unit.

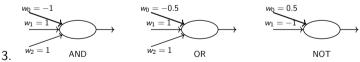
A McCulloch-Pitts network is a neural network with McCulloch-Pitts units.

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- McCulloch-Pitts units are a gross oversimplification of real neurons, but its purpose is to develop understanding of what neural networks of simple units can do.
- Theorem 9.6 (McCulloch and Pitts). Every Boolean function can be implemented as McCulloch-Pitts networks.
- Proof: by construction
 - 1. Recall that $a_i \leftarrow g(\sum_j w_{j,i}a_j)$. Let g(r) = 1 iff r > 0, else 0.

2. As for linear regression we use $a_0 = 1 \rightarrow w_{0,i}$ as a bias weight (or intercept) threshold)



4. Any Boolean function can be implemented as a DAG of McCulloch-Pitts units.



(determines the

- \blacktriangleright We have models for neurons \leadsto connect them to neural networks.
- **Definition 9.7.** A neural network is called a feed-forward network, if it is acyclic.
- ▶ Intuition: Feed-forward networks implement functions, they have no internal state.
- Definition 9.8. Feed-forward networks are usually organized in layers: a *n* layer network has a partition {L₀,...,L_n} of the nodes, such that edges only connect nodes from subsequent layer. L₀ is called the input layer and its members input units, and L_n the output layer and its members output units. Any unit that is not in the input layer or the output layer is called hidden.



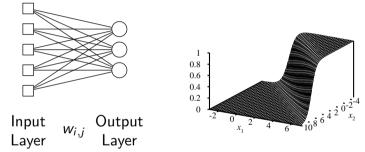
- **Definition 9.9.** A neural network is called recurrent (a RNNs), iff it has cycles.
 - Hopfield networks have symmetric weights (w_{i,j} = w_{j,i}) g(x) = sign(x), a_i = ±1; (holographic associative memory)
 - Boltzmann machines use stochastic activation functions.
- ► Recurrent neural networks have cycles with delay ~> have internal state (like flip-flops), can oscillate etc.

Recurrent neural networks follow largely the same principles as feed-forward networks, so we will not go into details here.



Single-layer Perceptrons

- Definition 9.10. A perceptron network is a feed-forward network of perceptron units. A single layer perceptron network is called a perceptron.
- Example 9.11.

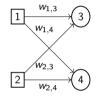


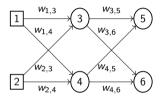
- All input units are directly connected to output units.
- ► Output units all operate separately, no shared weights ~> treat as the combination of n perceptron units.
- ► Adjusting weights moves the location, orientation, and steepness of cliff.



Feed-forward Neural Networks (Example)

- ▶ Feed-forward network $\hat{=}$ a parameterized family of nonlinear functions:
- **Example 9.12.** We show two feed-forward networks:





a) single layer (perceptron network) b) 2 layer feed-forward network

$$\begin{aligned} \mathbf{a}_5 &= g(\mathbf{w}_{3,5} \cdot \mathbf{a}_3 + \mathbf{w}_{4,5} \cdot \mathbf{a}_4) \\ &= g(\mathbf{w}_{3,5} \cdot g(\mathbf{w}_{1,3} \cdot \mathbf{a}_1 + \mathbf{w}_{2,3}\mathbf{a}_2) + \mathbf{w}_{4,5} \cdot g(\mathbf{w}_{1,4} \cdot \mathbf{a}_1 + \mathbf{w}_{2,4}\mathbf{a}_2)) \end{aligned}$$

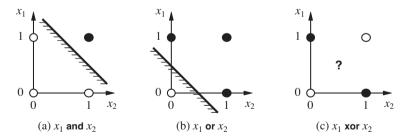
Idea: Adjusting weights changes the function: do learning this way!



Expressiveness of Perceptrons

- Consider a perceptron with g = step function (Rosenblatt, 1957, 1960)
- Can represent AND, OR, NOT, majority, etc., but not XOR
- Represents a linear separator in input space:

$$\sum_{j} w_{j} x_{j} > 0 \quad \text{or} \quad \mathsf{W}, \times > 0$$



Minsky & Papert (1969) pricked the first neural network balloon!



(and thus no adders)

For learning, we update the weights using gradient descent based on the generalization loss function. Let e.g. $L(w) = (y - h_w(x))^2$ (the squared error loss). We compute the gradient:

$$\frac{\partial L(\mathbf{w})}{\partial w_{j,k}} = 2 \cdot (y_k - h_w(x)_k) \cdot \frac{\partial (y - h_w(x))}{\partial w_{j,k}} = 2 \cdot (y_k - h_w(x)_k) \cdot \frac{\partial}{\partial w_{j,k}} (y - g(\sum_{j=0}^n w_{j,k} x_j))$$
$$= -2 \cdot (y_k - h_w(x)_k) \cdot g'(\mathbf{in}_k) \cdot x_j$$

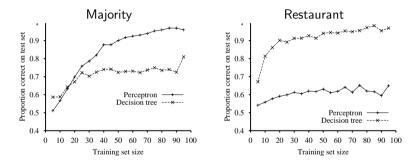
 \sim Replacing the constant factor -2 by a learning rate parameter α we get the update rule:

$$\mathbf{w}_{j,k} \leftarrow \mathbf{w}_{j,k} + \alpha \cdot (\mathbf{y}_k - \mathbf{h}_{\mathbf{w}}(\mathbf{x})_k) \cdot \mathbf{g}'(\mathrm{in}_k) \cdot \mathbf{x}_j$$



Perceptron learning contd.

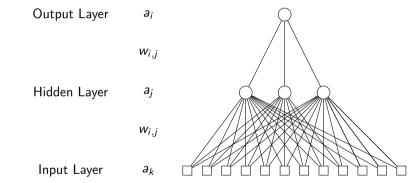
The perceptron learning rule converges to a consistent function - for any linearly separable data set



Perceptron learns the majority function easily, where DTL is hopeless. Conversely, DTL learns the restaurant function easily, where a perceptron is hopeless. (not representable)



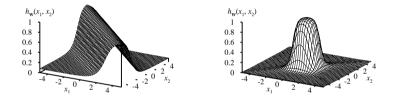
Definition 9.13. In multi layer perceptrons (MLPs), layers are usually fully connected; numbers of hidden units typically chosen by hand.



Definition 9.14. Some MLPs have residual connections, i.e. connections that skip layers.



▶ All continuous functions w/ 2 layers, all functions w/ 3 layers.



- Combine two opposite-facing threshold functions to make a ridge.
- Combine two perpendicular ridges to make a bump.
- Add bumps of various sizes and locations to fit any surface.
- Proof requires exponentially many hidden units.

(cf. DTL proof)



Learning in Multilayer Networks

Note: The *output layer* of a multilayer neural network is a single-layer perceptron whose input is the output of the last hidden layer.

 \sim We can use the perceptron learning rule to update the weights of the output layer; e.g. for a squared error loss function: $w_{j,k} \leftarrow w_{j,k} + \alpha \cdot (y_k - h_w(x)_k) \cdot g'(in_k) \cdot a_j$ What about the hidden layers?

Idea: The hidden node j is "responsible" for some fraction of the error proportional to the weight $w_{j,k}$. \sim Back-propagate the error $\Delta_k = (y_k - h_w(x)_k) \cdot g'(in_j)$ from node k in the output layer to the hidden node j.

Let's justify this:

$$\frac{\partial L(\mathbf{w})_{k}}{\partial \mathbf{w}_{i,j}} = -2 \cdot \underbrace{(y_{k} - h_{\mathbf{w}}(\mathbf{x})_{k}) \cdot g'(\mathbf{in}_{k})}_{=:\Delta_{k}} \cdot \frac{\partial \mathbf{in}_{k}}{\partial \mathbf{w}_{i,j}} \quad \text{(as before)}$$

$$= -2 \cdot \Delta_{k} \cdot \frac{\partial (\sum_{\ell} \mathbf{w}_{\ell,k} \mathbf{a}_{\ell})}{\partial \mathbf{w}_{i,j}} = -2 \cdot \Delta_{k} \cdot \mathbf{w}_{j,k} \cdot \frac{\partial \mathbf{a}_{j}}{\partial \mathbf{w}_{i,j}} = -2 \cdot \Delta_{k} \cdot \mathbf{w}_{j,k} \cdot \frac{\partial g(\mathbf{in}_{j})}{\partial \mathbf{w}_{i,j}}$$

$$= -2 \cdot \underbrace{\Delta_{k} \cdot \mathbf{w}_{j,k} \cdot g'(\mathbf{in}_{j})}_{=:\Delta_{j,k}} \cdot \mathbf{a}_{i}$$



Learning in Multilayer Networks (Hidden Layers)

$$\frac{\partial L(\mathbf{w})_k}{\partial \mathbf{w}_{i,j}} = -2 \cdot \underbrace{\Delta_k \cdot \mathbf{w}_{j,k} \cdot g'(\mathrm{in}_j)}_{=:\Delta_{j,k}} \cdot \mathbf{a}_i$$

Idea: The total "error" of the hidden node j is the sum of all the connected nodes k in the next layer **Definition 9.15.** The back-propagation rule for hidden nodes of a multilayer perceptron is $\Delta_j \leftarrow g'(\text{in}_j) \cdot (\sum_i w_{j,i} \Delta_i)$ And the update rule for weights in a hidden layer is $w_{k,j} \leftarrow w_{k,j} + \alpha \cdot a_k \cdot \Delta_j$

Remark: Most neuroscientists deny that back-propagation occurs in the brain.

The back-propagation process can be summarized as follows:

- 1. Compute the Δ values for the output units, using the observed error.
- 2. Starting with output layer, repeat the following for each layer in the network, until the earliest hidden layer is reached:
 - 2.1 Propagate the Δ values back to the previous (hidden) layer.
 - 2.2 Update the weights between the two layers.



Backprogagation Learning Algorithm

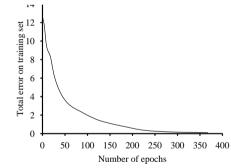
Definition 9.16. The back-propagation learning algorithm is given the following pseudocode

```
function BACK–PROP–LEARNING(examples, network) returns a neural network
  inputs: examples, a set of examples, each with input vector x and output vector y
            network, a multilayer network with L layers, weights w_{i,i}, activation function g
  local variables: \Delta, a vector of errors, indexed by network node
  foreach weight w_{i,i} in network do
    w_{i,j} := a small random number
  repeat
    foreach example (x, y) in examples do
       /* Propagate the inputs forward to compute the outputs */
      foreach node i in the input layer do a_i := x_i
         for l = 2 to L do
           foreach node j in layer / do
             in_i := \sum_i w_{i,i} a_i
             a_i := g(in_i)
       /* Propagate deltas backward from output laver to input laver */
      foreach node i in the output layer do \Delta[i] := g'(in_i) \cdot (y_i - a_i)
      for l = l - 1 to 1 do
         foreach node i in layer l do \Delta[i] := g'(in_i) \cdot (\sum_i w_{i,j} \Delta[j])
       /* Update every weight in network using deltas */
      foreach weight w_{i,j} in network do w_{i,j} := w_{i,j} + \alpha \cdot a_i \cdot \Delta[j]
  until some stopping criterion is satisfied
  return network
```

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Back-Propagation – Properties

- Sum gradient updates for all examples in some "batch" and apply gradient descent.
- Learning curve for 100 restaurant examples: finds exact fit.

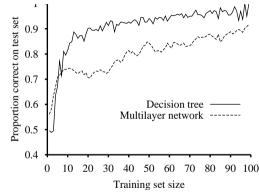


Typical problems: slow convergence, local minima.



Back-Propagation - Properties (contd.)

Example 9.17. Learning curve for MLPs with 4 hidden units:



- **Experience shows:** MLPs are quite good for complex pattern recognition tasks, but resulting hypotheses cannot be understood easily.
- This makes MLPs ineligible for some tasks, such as credit card and loan approvals, where law requires clear unbiased criteria.



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0	1	2	3	ч	5	6	7	8	9
0	1	Э	3	4	J	6	7	9	3

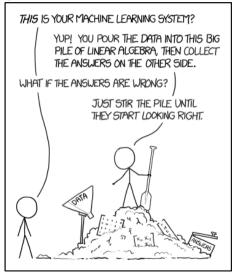
- ▶ 400-300-10 unit MLP = 1.6% error
- ▶ LeNet: 768–192–30–10 unit MLP = 0.9% error
- Current best (kernel machines, vision algorithms) $\approx 0.6\%$ error

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- neural networks can be extremely powerful (hypothesis space intractably complex)
- Perceptrons (one-layer networks) insufficiently expressive for most applications
- Multi-layer networks are sufficiently expressive; can be trained by gradient descent, i.e., error back-propagation
- Many applications: speech, driving, handwriting, fraud detection, etc.
- Engineering, cognitive modelling, and neural system modelling subfields have largely diverged
- Drawbacks: take long to converge, require large amounts of data, and are difficult to *interpret* (Why is the output what it is?)

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► A Skepticists View: see https://xkcd.com/1838/





- Learning needed for unknown environments, lazy designers.
- Learning agent = performance element + learning element.
- Learning method depends on type of performance element, available feedback, type of component to be improved, and its representation.
- For supervised learning, the aim is to find a simple hypothesis that is approximately consistent with training examples
- Decision tree learning using information gain.
- Learning performance = prediction accuracy measured on test set
- PAC learning as a general theory of learning boundaries.
- Linear regression (hypothesis space of univariate linear functions).
- Linear classification by linear regression with hard and soft thresholds.



Chapter 28 Statistical Learning

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- Definition 0.1. Statistical learning has the goal to learn the correct probability distribution of a random variable.
- Example 0.2.
 - Bayesian learning, i.e. learning probabilistic models (e.g. the CPTs in Bayesian networks) from observations.
 - Maximum a posteriori and maximum likelihood learning
 - Bayesian network learning
 - ML Parameter Learning with Complete Data
 - Naive Bayes Models/Learning



28.1 Full Bayesian Learning



Example 1.1. Suppose there are five kinds of bags of candies:

- 1. 10% are h_1 : 100% cherry candies
- 2. 20% are h_2 : 75% cherry candies + 25% lime candies
- 3. 40% are h_3 : 50% cherry candies + 50% lime candies
- 4. 20% are h_4 : 25% cherry candies + 75% lime candies
- 5. 10% are h_5 : 100% lime candies

Then we observe candies drawn from some bag:

........

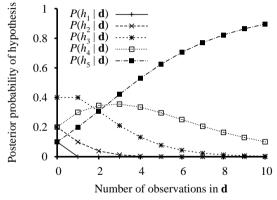
What kind of bag is it? What flavour will the next candy be?

Note: Every hypothesis is itself a probability distribution over the random variable "flavour".

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Candy Flavors: Posterior probability of hypotheses

► Example 1.2. Let d_i be the event that the *i*th drawn candy is green. The probability of hypothesis h_i after n limes are observed (= d_{1:n} =: d) is



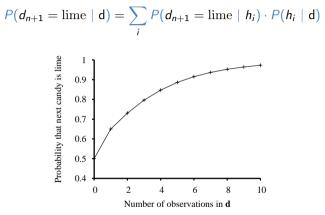
if the observations are IID, i.e. $P(d \mid h_i) = \prod_j P(d_j \mid h_i)$ and the hypothesis prior is as advertised.(e.g. $P(d \mid h_3) = 0.5^{10} = 0.1\%)$ The posterior probabilities start with the hypothesis priors, change with data.

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Candy Flavors: Prediction Probability

• We calculate that the n + 1-th candy is lime:



 \sim we compute the expected value of *the probability of the next candy being lime* over all hypotheses (i.e. distributions). \sim "meta-distribution"

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Full Bayesian Learning

- ▶ Idea: View learning as Bayesian updating of a probability distribution over the hypothesis space:
 - ▶ *H* is the hypothesis variable with values $h_1, h_2, ...$ and prior $\mathbb{P}(H)$.
 - *j*th observation d_j gives the outcome of random variable D_j .
 - $d := d_1, \ldots, d_N$ constitutes the training set of a inductive learning problem.
- Definition 1.3. Bayesian learning calculates the probability of each hypothesis and makes predictions based on this:
 - Given the data so far, each hypothesis has a posterior probability:

 $P(h_i \mid d) = \alpha(P(d \mid h_i) \cdot P(h_i))$

where $P(d | h_i)$ is called the likelihood (of the data under each hypothesis) and $P(h_i)$ the hypothesis prior.

Bayesian predictions use a likelihood-weighted average over the hypotheses:

$$\mathbb{P}(\mathbf{X}|\mathsf{d}) = \sum_{i} \mathbb{P}(\mathbf{X}|\mathsf{d}, h_i) \cdot P(h_i \mid \mathsf{d}) = \sum_{i} \mathbb{P}(\mathbf{X}|h_i) \cdot P(h_i \mid \mathsf{d})$$

 Observation: No need to pick one best-guess hypothesis for Bayesian predictions! (and that is all an agent cares about)



- **• Observation:** The Bayesian prediction eventually agrees with the true hypothesis.
 - > The probability of generating "uncharacteristic" data indefinitely is vanishingly small.
 - Proof sketch: Argument analogous to PAC learning.
- **Problem:** Summing over the hypothesis space is often intractable.
- **Example 1.4.** There are $2^{2^6} = 18,446,744,073,709,551,616$ Boolean functions of 6 arguments.
- **Solution:** Approximate the learning methods to simplify.



28.2 Approximations of Bayesian Learning

Maximum A Posteriori (MAP) Approximation

- **Goal:** Get rid of summation over the space of all hypotheses in predictions.
- ► Idea: Make predictions wrt. the "most probable hypothesis"!
- **Definition 2.1.** For maximum a posteriori learning (MAP learning) choose the MAP hypothesis h_{MAP} that maximizes $P(h_i \mid d)$.
 - I.e., maximize $P(d \mid h_i) \cdot P(h_i)$ or (even better) $\log_2(P(d \mid h_i)) + \log_2(P(h_i))$.
- ▶ Predictions made according to a MAP hypothesis h_{MAP} are approximately Bayesian to the extent that $P(X|d) \approx P(X|h_{MAP})$.
- **Example 2.2.** In our candy example, $h_{MAP} = h_5$ after three limes in a row
 - ▶ a MAP learner then predicts that candy 4 is lime with probability 1.
 - compare with Bayesian prediction of 0.8.

- (see prediction curves above)
- As more data arrive, the MAP and Bayesian predictions become closer, because the competitors to the MAP hypothesis become less and less probable.
- ► For deterministic hypotheses, $P(d | h_i)$ is 1 if consistent, 0 otherwise $\rightarrow MAP =$ simplest consistent hypothesis.
- Remark: Finding MAP hypotheses is often much easier than Bayesian learning, because it requires solving an optimization problem instead of a large summation (or integration) problem.



(cf. science)

▶ Idea: Reinterpret the log terms $\log_2(P(d \mid h_i)) + \log_2(P(h_i))$ in MAP learning:

- Maximizing $P(\mathbf{d} \mid h_i) \cdot P(h_i) \cong \text{minimizing } -\log_2(P(\mathbf{d} \mid h_i)) \log_2(P(h_i)).$
- ▶ $-\log_2(P(d \mid h_i)) \cong$ number of bits to encode data given hypothesis.
- ▶ $-\log_2(P(h_i)) \cong$ additional bits to encode hypothesis.
- ▶ Indeed if hypothesis predicts the data exactly e.g. h_5 in candy example then $\log_2(1) = 0 \rightarrow$ preferred hypothesis.
- ▶ This is more directly modeled by the following approximation to Bayesian learning:
- ▶ Definition 2.3. In minimum description length learning (MDL learning) the MDL hypothesis *h*_{MDL} minimizes the information entropy of the hypothesis likelihood.



(???)

- ▶ Observation: For large data sets, the prior becomes irrelevant. (we might not trust it anyways)
- Idea: Use this to simplify learning.
- Definition 2.4. Maximum likelihood learning (ML learning): choose the ML hypothesis h_{ML} maximizing P(d | h_i). (simply get the best fit to the data)
- ML learning is the "standard" (non Bayesian) statistical learning method.



28.3 Parameter Learning for Bayesian Networks



ML Parameter Learning in Bayesian Nets

Bayesian networks (with continuous random variables) often feature nodes with a particular parametric distribution $D(\theta)$ (e.g. normal, binomial, Poisson, etc.). How do we learn the parameters of these distributions from data?

Example 3.1. We get a candy bag from a new manufacturer; what is the fraction θ of cherry candies? (Note: We use the probability itself as the parameter. This is somewhat boring, but simple.)



New Facet: Any θ is possible: continuum of hypotheses h_{θ} θ is a parameter for this simple (binomial) family of models; We call h_{θ} a MLP hypothesis and the process of learning θ MLP learning.

Example 3.2. Suppose we unwrap *N* candies, *c* cherries and $\ell = N - c$ limes. These are IID observations, so the likelihood is $P(d \mid h_{\theta}) = \prod_{i=1}^{N} P(d_i \mid h_{\theta}) = \theta^c \cdot (1 - \theta)^{\ell}$



ML Parameter Learning in Bayes Nets

Trick: When optimizing a product, optimize the logarithm instead! $(\log_2(!) \text{ is monotone and turns products into sums})$ **Definition 3.3.** The log likelihood is the binary logarithm of the likelihood. $L(d|h):=\log_2(P(d | h))$

Example 3.4. Compute the log likelihood as

$$L(\mathbf{d}|h_{\theta}) = \log_2(P(\mathbf{d} \mid h_{\theta})) = \sum_{j=1}^{N} \log_2(P(\mathbf{d}_j \mid h_{\theta})) = c \log_2(\theta) + \ell \log_2(1-\theta)$$

Maximize this w.r.t. θ

$$\frac{\partial}{\partial \theta}(L(\mathsf{d}|h_{\theta})) = \frac{c}{\theta} - \frac{\ell}{1-\theta} = 0 \rightsquigarrow \theta = \frac{c}{c+\ell} = \frac{c}{N}$$

In English: h_{θ} asserts that the actual proportion of cherries in the bag is equal to the observed proportion in the candies unwrapped so far! (...exactly what we should expect!) (\Rightarrow Generalize to more interesting parametric models later) **Warning:** This causes problems with 0 counts!



(using ??)

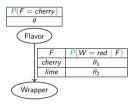
Cooking Recipe:

- 1. Write down an expression for the likelihood of the data as a function of the parameter(s).
- 2. Write down the derivative of the log likelihood with respect to each parameter.
- 3. Find the parameter values such that the derivatives are zero



Multiple Parameters Example

Example 3.5. Red/green wrapper depends probabilistically on flavour:



Likelihood for, e.g., cherry candy in green wrapper:

$$P(F = cherry, W = green \mid h_{\theta,\theta_{1},\theta_{2}})$$

= $P(F = cherry \mid h_{\theta,\theta_{1},\theta_{2}}) \cdot P(W = green \mid F = cherry, h_{\theta,\theta_{1},\theta_{2}})$
= $\theta \cdot (1 - \theta_{1})$

• Ovservation: For N candies, r_c red-wrapped cherry candies, etc. we have

$$P(\mathsf{d} \mid h_{\theta,\theta_{1},\theta_{2}}) = \theta^{\mathsf{c}} \cdot (1-\theta)^{\ell} \cdot \theta_{1}^{r_{\mathsf{c}}} \cdot (1-\theta_{1})^{g_{\mathsf{c}}} \cdot \theta_{2}^{r_{\ell}} \cdot (1-\theta_{2})^{g_{\ell}}$$

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Minimize the log likelihood:

$$L = c \log_2(\theta) + \ell \log_2(1-\theta) + r_c \log_2(\theta_1) + g_c \log_2(1-\theta_1) + r_\ell \log_2(\theta_2) + g_\ell \log_2(1-\theta_2)$$

Derivatives of L contain only the relevant parameter:

$$\begin{array}{rcl} \frac{\partial l}{\partial \theta} & = & \frac{c}{\theta} - \frac{\ell}{1 - \theta} = 0 & \rightsquigarrow & \theta = \frac{c}{c + \ell} \\ \frac{\partial l}{\partial \theta_1} & = & \frac{r_c}{\theta_1} - \frac{g_c}{1 - \theta_1} = 0 & \rightsquigarrow & \theta_1 = \frac{r_c}{r_c + g_c} \\ \frac{\partial l}{\partial \theta_2} & = & \frac{r_\ell}{\theta_2} - \frac{g_\ell}{1 - \theta_2} = 0 & \rightsquigarrow & \theta_2 = \frac{r_\ell}{r_\ell + g_\ell} \end{array}$$

- **Upshot:** With complete data, *parameters can be learned separately* in Bayesian networks.
- Remaining Problem: Have to be careful with zero values! (division by zero)

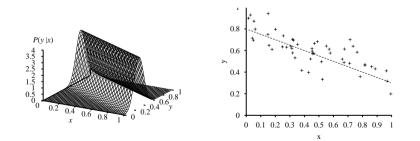


Example: Linear Gaussian Model

A continuous random variable Y has the *linear-Gaussian distribution* with respect to a continuous random variable X, if the outcome of Y is determined by a linear function of the outcome of X plus gaussian noise with a fixed variance σ , i.e.

$$P(y_1 \le Y \le y_2 \mid X = x) = \int_{y_1}^{y_2} N(y; \theta_1 x + \theta_2, \sigma^2) \, \mathrm{d}y = \int_{y_1}^{y_2} \frac{1}{\sigma \sqrt{2\pi}} \cdot e^{-\frac{1}{2} \cdot \left(\frac{y - (\theta_1 x + \theta_2)}{\sigma}\right)^2} \, \mathrm{d}y$$

 \sim assuming σ given, we have two parameter θ_1 and $\theta_2 \sim$ Hypothesis space is $\mathbb{R} \times \mathbb{R}$



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$$P(y_1 \le Y \le y_2 \mid X = x) = \int_{y_1}^{y_2} \frac{1}{\sigma\sqrt{2\pi}} \cdot e^{-\frac{1}{2} \cdot \left(\frac{y - (\theta_1 x + \theta_2)}{\sigma}\right)^2} \, dy$$

 \sim Given observations $X = X, Y = y$, maximize $\prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(y_i - (\theta_1 x_i + \theta_2))^2}{2\sigma^2}}$ w.r.t. θ_1, θ_2 . (we can ignore the integral for this)

- 1/-

Using the log likelihood, this is equivalent to minimizing $\sum_{i=1}^{N} (y_i - (\theta_1 x_i + \theta_2))^2 \sim \text{minimizing the sum of squared errors gives the ML solution}$



- ► Full Bayesian learning gives best possible predictions but is intractable.
- ▶ MAP learning balances complexity with accuracy on training data.
- Maximum likelihood learning assumes uniform prior, OK for large data sets:
 - 1. Choose a parameterized family of models to describe the data. \sim requires substantial insight and sometimes new models.
 - 2. Write down the likelihood of the data as a function of the parameters. \sim may require summing over hidden variables, i.e., inference.
 - 3. Write down the derivative of the log likelihood w.r.t. each parameter.
 - Find the parameter values such that the derivatives are zero.
 → may be hard/impossible; modern optimization techniques help.
- Naive Bayes models as a fall-back solution for machine learning:
 - conditional independence of all attributes as simplifying assumption.



Chapter 29 Reinforcement Learning

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29.1 Reinforcement Learning: Introduction & Motivation



- ▶ So far: We have studied "learning from examples". (functions, logical theories, probability models)
- Now: How can agents learn "what to do" in the absence of labeled examples of "what to do". We call this problem unsupervised learning.
- Example 1.1 (Playing Chess). Learn transition models for own moves and maybe predict opponent's moves.
- Problem: The agent needs to have some feedback about what is good/bad cannot decide "what to do" otherwise. (recall: external performance standard for learning agents)
- **Example 1.2.** The ultimate feedback in chess is whether you win, lose, or draw.
- Definition 1.3. We call a learning situation where there are no labeled examples unsupervised learning and the feedback involved a reward or reinforcement.
- **Example 1.4.** In soccer, there are intermediate reinforcements in the shape of goals, penalties, ...



- Definition 1.5. Reinforcement learning is a type of unsupervised learning where an agent learns how to behave in an environment by performing actions and seeing the results.
- Recap: In ??? we introduced rewards as parts of MDPs (Markov decision processes) to define optimal policies.
 - an optimal policy maximizes the expected total reward.
- Idea: The task of reinforcement learning is to use observed rewards to come up with an optimal policy.
- In MDPs, the agent has total knowledge about the environment and the reward function, in reinforcement learning we do not assume this.
 (~ POMDPs+reward-learning)
- **Example 1.6.** You play a game without knowing the rules, and at some time the opponent shouts "*you lose!*"



- Reinforcement Learning solves all of AI: An agent is placed in an environment and must learn to behave successfully therein.
- **KISS:** We will only look at simple environments and simple agent designs:
 - A utility-based agent learns a utility function on states and uses it to select actions that maximize the expected outcome utility.
 (passive learning)
 - A Q-learning agent learns an action-utility function, or Q-function, giving the expected utility of taking a given action in a given state.
 (active learning)
 - A reflex agent learns a policy that maps directly from states to actions.



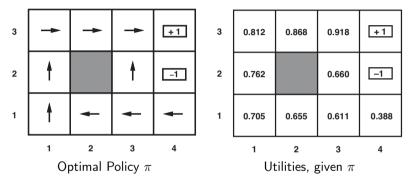
29.2 Passive Learning



- Definition 2.1 (To keep things simple). Agent uses a state-based representation in a fully observable environment:
 - In passive learning, the agent's policy π is fixed: in state s, it always executes the action $\pi(s)$.
 - ▶ Its goal is simply to learn how good the policy is that is, to learn the utility function $U^{\pi}(s)$.
- The passive learning task is similar to the policy evaluation task (part of the policy iteration algorithm) but the agent does not know
 - the transition model P(s' | s,a), which specifies the probability of reaching state s' from state s after doing action a,
 - the reward function R(s), which specifies the reward for each state.



Example 2.2 (Passive Learning). We use the 4 × 3 world introduced above



• The agent executes a set of trials in the environment using its policy π .

- In each trial, the agent starts in state (1,1) and experiences a sequence of state transitions until it reaches one of the terminal states, (4,2) or (4,3).
- Its percepts supply both the current state and the reward received in that state.



Fau

Example 2.3. Typical trials might look like this:

1. $(1,1)_{-0.4} \rightsquigarrow (1,2)_{-0.4} \rightsquigarrow (1,3)_{-0.4} \rightsquigarrow (1,2)_{-0.4} \rightsquigarrow (1,3)_{-0.4} \rightsquigarrow (2,3)_{-0.4} \rightsquigarrow (3,3)_{-0.4} \rightsquigarrow (4,3)_{+1}$ 2. $(1,1)_{-0.4} \rightsquigarrow (1,2)_{-0.4} \rightsquigarrow (1,3)_{-0.4} \rightsquigarrow (2,3)_{-0.4} \rightsquigarrow (3,3)_{-0.4} \rightsquigarrow (3,2)_{-0.4} \rightsquigarrow (3,3)_{-0.4} \rightsquigarrow (4,3)_{+1}$ 3. $(1,1)_{-0.4} \rightsquigarrow (2,1)_{-0.4} \rightsquigarrow (3,1)_{-0.4} \rightsquigarrow (3,2)_{-0.4} \rightsquigarrow (4,2)_{-1}$.

Definition 2.4. The utility is defined to be the expected sum of (discounted) rewards obtained if policy π is followed.

$$U^{\pi}(s) := E\left[\sum_{t=0}^{\infty} \gamma^{t} R(S_{t})\right]$$

where R(s) is the reward for a state, S_t (a random variable) is the state reached at time t when executing policy π , and $S_0 = s$. (for 4×3 we take the discount factor $\gamma = 1$)

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- A simple method for direct utility estimation was invented in the late 1950s in the area of adaptive control theory.
- Definition 2.5. The utility of a state is the expected total reward from that state onward (called the expected reward to go).
- **Idea:** Each trial provides a sample of the reward to go for each state visited.
- **Example 2.6.** The first trial in ??? provides a sample total reward of 0.72 for state (1,1), two samples of 0.76 and 0.84 for (1,2), two samples of 0.80 and 0.88 for (1,3), ...
- Definition 2.7. The direct utility estimation algorithm cycles over trials, calculates the reward to go for each state, and updates the estimated utility for that state by keeping the running average for that for each state in a table.
- **Observation 2.8.** In the limit, the sample average will converge to the true expectation (utility) from *???*.
- Remark 2.9. Direct utility estimation is just supervised learning, where each example has the state as input and the observed reward to go as output.
- **Upshot:** We have reduced reinforcement learning to an inductive learning problem.



Adaptive Dynamic Programming

- Problem: The utilities of states are not independent in direct utility estimation!
- The utility of each state equals its own reward plus the expected utility of its successor states.
- **So:** The utility values obey a Bellman equation for a fixed policy π .

$$U^{\pi}(s) = R(s) + \gamma \cdot \left(\sum_{s'} P(s' \mid s, \pi(s)) \cdot U^{\pi}(s')\right)$$

- Observation 2.10. By ignoring the connections between states, direct utility estimation misses opportunities for learning.
- **Example 2.11.** Recall trial 2 in ???; state (3,3) is new.
 - $2 (1,1)_{-0,4} \sim (1,2)_{-0,4} \sim (1,3)_{-0,4} \sim (2,3)_{-0,4} \sim (3,3)_{-0,4} \sim (3,2)_{-0,4} \sim (3,3)_{-0,4} \sim (4,3)_{+1}$ (known high utility from trial 1)
 - The next transition reaches (3,3),
 - **b** Bellman equation: \sim high $U^{\pi}(3,2)$ because $(3,2)_{-0,4} \sim (3,3)$
 - But direct utility estimation learns nothing until the end of the trial.
- ▶ Intuition: Direct utility estimation searches for U in a hypothesis space that too large \leftrightarrow many functions that violate the Bellman equations.
- Thus the algorithm often converges very slowly.



Adaptive Dynamic Programming

- Idea: Take advantage of the constraints among the utilities of states by
 - learning the transition model that connects them,
 - solving the corresponding Markov decision process using a dynamic programming method.

This means plugging the learned transition model $P(s'|s, \pi(s))$ and the observed rewards R(s) into the Bellman equations to calculate the utilities of the states.

- As above: These equations are linear (no maximization involved) (solve with any any linear algebra package).
- **• Observation 2.12.** Learning the model itself is easy, because the environment is fully observable.
- Corollary 2.13. We have a supervised learning task where the input is a state-action pair and the output is the resulting state.
 - ▶ In the simplest case, we can represent the transition model as a table of probabilities.
 - Count how often each action outcome occurs and estimate the transition probability P(s' | s,a) from the frequency with which s' is reached by action a in s.
- Example 2.14. In the 3 trials from ???, Right is executed 3 times in (1,3) and 2 times the result is (2,3), so P((2,3) | (1,3), Right) is estimated to be 2/3.



Passive ADP Learning Algorithm

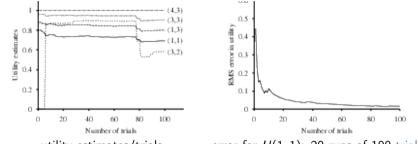
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Definition 2.15. The passive ADP algorithm is given by
  function PASSIVE-ADP-AGENT(percept) returns an action
    inputs: percept, a percept indicating the current state s' and reward signal r'
    persistent: \pi a fixed policy
        mdp. an MDP with model P, rewards R, discount \gamma
        U, a table of utilities, initially empty
        N_{\rm sa}, a table of frequencies for state—action pairs, initially zero
        N_{s'|sa}, a table of outcome frequencies given state—action pairs, initially zero
        s, a, the previous state and action, initially null
     if s' is new then U[s'] := r'; R[s'] := r'
     if s is not null then
        increment N_{sa}[s, a] and N_{s'|sa}[s', s, a]
        for each t such that N_{sllsa}[t, s, a] is nonzero do
           P(t|s,a) := N_{s'|sa}[t,s,a]/N_{sa}[s,a]
     U := \text{POLICY} - \text{EVALUATION}(\pi.mdp)
     if s'.TERMINAL? then s, a := null else s, a := s', \pi[s']
     return a
```

POLICY-EVALUATION computes $U^{\pi}(s) := E\left[\sum_{t=0}^{\infty} \gamma^{t} R(s_{t})\right]$ in a MDP.



Passive ADP Convergence

Example 2.16 (Passive ADP learning curves for the 4x3 world). Given the optimal policy from ???



utility estimates/trials

error for U(1, 1): 20 runs of 100 trials

Note the large changes occurring around the 78^{th} trial – this is the first time that the agent falls into the -1 terminal state at (4,2).

Observation 2.17. The ADP agent is limited only by its ability to learn the transition model. (intractable for large state spaces)

- **Example 2.18.** In backgammon, roughly 10⁵⁰ equations in 10⁵⁰ unknowns.
- Idea: Use this as a baseline to compare passive learning algorithms

FAU



29.3 Active Reinforcement Learning



- **Recap:** A passive learning agent has a fixed policy that determines its behavior.
- An active agent must also decide what actions to take.
- ▶ Idea: Adapt the passive ADP algorithm to handle this new freedom.
 - learn a complete model with outcome probabilities for all actions, rather than just the model for the fixed policy. (use PASSIVE-ADP-AGENT)
 - choose actions; the utilities to learn are defined by the optimal policy, they obey the Bellman equation:

$$U(s) = R(s) + \gamma \cdot \max_{a \in A(s)} (\sum_{s'} U(s') \cdot P(s' \mid s, a))$$

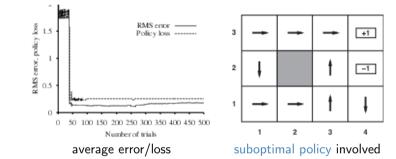
- solve with value/policy iteration techniques from ???.
- choose a good action, e.g.
 - by one-step lookahead to maximize expected utility, or
 - if agent uses policy iteration and has optimal policy, execute that.

This agent/algorithm is greedy, since it only optimizes the next step!



Greedy ADP Learning (Evaluation)

Example 3.1 (Greedy ADP learning curves for the 4x3 world).



The agent follows the optimal policy for the learned model at each step.

- It does not learn the true utilities or the true optimal policy!
- instead, in the 39th trial, it finds a policy that reaches the +1 reward along the lower route via (2,1), (3,1), (3,2), and (3,3).
- After experimenting with minor variations, from the 276th trial onward it sticks to that policy, never learning the utilities of the other states and never finding the optimal route via (1,2), (1,3), and (2,3).



- Observation 3.2. Greedy active ADP learning agents very seldom converge against the optimal solution
 - The learned model is not the same as the true environment,
 - What is optimal in the learned model need not be in the true environment.
- ▶ What can be done? The agent does not know the true environment.
- Idea: Actions do more than provide rewards according to the learned model
 - they also contribute to learning the true model by affecting the percepts received.
 - By improving the model, the agent may reap greater rewards in the future.
- **Observation 3.3.** An agent must make a tradeoff between
 - exploitation to maximize its reward as reflected in its current utility estimates and
 - exploration to maximize its long term well-being.

Pure exploitation risks getting stuck in a rut. Pure exploration to improve one's knowledge is of no use if one never puts that knowledge into practice.

Compare with the information gathering agent from ???.



Chapter 30 Knowledge in Learning

30.1 Logical Formulations of Learning



Recap: Learning from examples.

(last chapter)

- ▶ Idea: Construct a function with the input/output behavior observed in data.
- ► Method: Search for suitable functions in the hypothesis space. (e.g. decision trees)
- **• Observation 1.1.** Every learning task begins from zero. (except for the choice of hypothesis space)
- **Problem:** We have to forget everything before we can learn something new.
- Idea: Utilize prior knowledge about the world! (represented e.g. in logic)



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- ▶ Recall: Examples are composed of descriptions (of the input sample) and classifications.
- ▶ Idea: Represent examples and hypotheses as logical formulae.
- **Example 1.2.** For attribute-based representations, we can use PL¹: we use predicate constants for Boolean attributes and classification and function constants for the other attributes.
- ▶ Definition 1.3. Logic based inductive learning tries to learn an hypothesis h that explains the classifications of the examples given their description, i.e. $h, D \models C$ (the explanation constraint), where
 - $\blacktriangleright \ \mathcal{D}$ is the conjunction of the descriptions, and
 - \blacktriangleright C the conjunction of their classifications.

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- ▶ Idea: We solve the explanation constraint $h, D \models C$ for h where h ranges over some hypothesis space.
- ▶ Refinement: Use Occam's razor or additional constraints to avoid h = C. (too easy otherwise/boring; see below)



Example 1.4 (Restaurant Example again). Descriptions are conjunctions of literals built up from

- ▶ predicates Alt, Bar, Fri/Sat, Hun, Rain, and res
- equations about the functions Pat, Price, Type, and Est.

For instance the first example X_1 from ???, can be described as

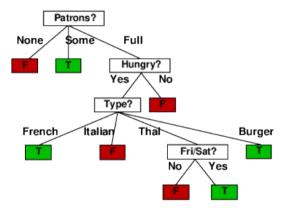
 $\operatorname{Alt}(X_1) \wedge \neg \operatorname{Bar}(X_1) \wedge \operatorname{Fri}/\operatorname{Sat}(X_1) \wedge \operatorname{Hun}(X_1) \wedge \ldots$

The classification is given by the goal predicate WillWait, in this case $WillWait(X_1)$ or $\neg WillWait(X_1)$.



A logical Formulation of Learning (Restaurant Tree)

Example 1.5 (Restaurant Example again; Tree). The induced decision tree from ???



C

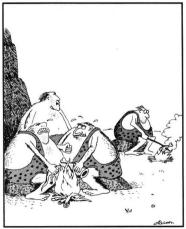
Example 1.6 (Restaurant Example again; Tree). The induced decision tree from ??? can be represented as

 $\begin{aligned} \forall r. WillWait(r) &\Leftrightarrow Pat(r, Some) \\ &\lor Pat(r, Full) \land Hun(r) \land Type(r, French) \\ &\lor Pat(r, Full) \land Hun(r) \land Type(r, Thai) \land Fri/Sat(r) \\ &\lor Pat(r, Full) \land Hun(r) \land Type(r, Burger) \end{aligned}$

Method: Construct a disjunction of all the paths from the root to the positive leaves interpreted as conjunctions of the attributes on the path.

Note: The equivalence takes care of positive and negative examples.

Example 1.7. Learning from very few examples using background knowledge: 1. Caveman Zog and the fish on a stick:



"Hey! Look what Zog do!"



Example 1.9. Learning from very few examples using background knowledge:

- 1. Caveman Zog and the fish on a stick:
- 2. Generalizing from one Brazilian:

Upon meeting her first Brazilian - Fernando - who speaks Portugese, Sarah

- learns/generalizes that all Brazilians speak Portugese,
- but not that all Brazilians are called Fernando.



Example 1.11. Learning from very few examples using background knowledge:

- $1. \ \mbox{Caveman Zog}$ and the fish on a stick:
- 2. Generalizing from one Brazilian:
- 3. General rules about effectiveness of antibiotics:
 - When Sarah gifted in diagnostics, but clueless in pharmacology observes a doctor prescribing the antibiotic Proxadone for an inflamed foot, she learns/infers that Proxadone is effective against this ailment.
- **• Observation:** The methods/algorithms from ??? cannot replicate this.



(whv?)

Example 1.13. Learning from very few examples using background knowledge:

1025

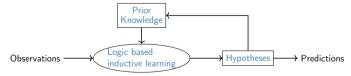
- 1. Caveman Zog and the fish on a stick:
- 2. Generalizing from one Brazilian:
- 3. General rules about effectiveness of antibiotics:
- Observation: The methods/algorithms from ??? cannot replicate this.
- Missing Piece: The background knowledge!
- Problem: To use background knowledge, need a method to obtain it.
- Question: How to use knowledge to learn more efficiently?

(why?)

(use learning)



- **Example 1.15.** Learning from very few examples using background knowledge:
 - 1. Caveman Zog and the fish on a stick:
 - 2. Generalizing from one Brazilian:
 - 3. General rules about effectiveness of antibiotics:
- **Observation:** The methods/algorithms from ??? cannot replicate this.
- Missing Piece: The background knowledge!
- ▶ Problem: To use background knowledge, need a method to obtain it.
- Question: How to use knowledge to learn more efficiently?
- Answer: Cumulative development: collect knowledge and use it in learning!

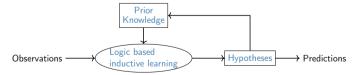


(why?)

(use learning)



- **Example 1.17.** Learning from very few examples using background knowledge:
 - $1. \ \mbox{Caveman Zog}$ and the fish on a stick:
 - 2. Generalizing from one Brazilian:
 - 3. General rules about effectiveness of antibiotics:
- **Observation:** The methods/algorithms from ??? cannot replicate this.
- Missing Piece: The background knowledge!
- ▶ Problem: To use background knowledge, need a method to obtain it.
- Question: How to use knowledge to learn more efficiently?
- Answer: Cumulative development: collect knowledge and use it in learning!



Definition 1.18. We call the body of knowledge accumulated by (a group of) agents their background knowledge. It acts as prior knowledge in logic based learning processes.

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(why?)

(use learning)

- Explanation based learning (EBL)
- Relevance based learning (RBL)
- Knowledge based inductive learning (KBIL)



 ▶ Definition 1.19. Deduction
 ⇒ knowledge extension

 ▶ Example 1.20. *rains* ⇒ wet_street rains wet_street



Definition 1.25. Deduction
 ² knowledge extension
 ² Met_street
 ² Newledge extension
 ² Knowledge extensio



 Definition 1.31. Deduction
 ^a knowledge extension
 Example 1.32. ^{rains ⇒ wet_street rains}/_{wet_street} D

 Definition 1.33. Abduction
 ^a explanation

 Example 1.34. ^{rains ⇒ wet_street wet_street}/_{rains} A

 Definition 1.35. Induction
 ^a learning general rules from examples

 Example 1.36. ^{wet_street rains}/_{rains ⇒ wet_street} /



30.2 Inductive Logic Programming

C

- ▶ Idea: Background knowledge and new hypothesis combine to explain the examples.
- **Example 2.1.** Inferring disease *D* from the symptoms is not enough to explain the prescription of medicine *M*.

Need a new general rule: "*M is effective against D*"

(induction from example)

Definition 2.2. Knowledge based inductive learning (KBIL) replaces the explanation constraint by the KBIL constraint:

 $Background \land Hypothesis \land Descriptions \vDash Classifications$



- Definition 2.3. Inductive logic programming (ILP) is logic based inductive learning method that uses logic programming as a uniform representation for examples, background knowledge and hypotheses. Given an encoding of the known background knowledge and a set of examples represented as a logical knowledge base of facts, an ILP system will derive a hypothesised logic program which entails all the positive and none of the negative examples.
- Main field of study for KBIL algorithms.
- Prior knowledge plays two key roles:
 - 1. The effective hypothesis space is reduced to include only those theories that are consistent with what is already known.
 - 2. Prior knowledge can be used to reduce the size of the hypothesis explaining the observations.
 - Smaller hypotheses are easier to find.
- Observation: ILP systems can formulate hypotheses in first-order logic.
 - $\rightsquigarrow\,$ Can learn in environments not understood by simpler systems.



- Combines inductive methods with the power of first-order representations.
- Offers a rigorous approach to the general KBIL problem.
- ▶ Offers complete algorithms for inducing general, first-order theories from examples.



30.2.1 An Example



General knowledge-based induction problem

$Background \land Hypothesis \land Descriptions \vDash Classifications$

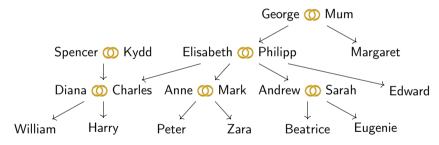
Example 2.4 (Learning family relations from examples).

- Observations are an extended family tree
 - mother, father and married relations
 - male and female properties
- ► Target predicates: grandparent, BrotherInLaw, Ancestor
- $\, \sim \,$ The goal is to find a logical formula that serves as a $\mathit{definition}$ of the target predicates
- equivalently: A Prolog program that computes the value of the target predicate
- $\rightsquigarrow\,$ We obtain a perfectly comprehensible hypothesis

British Royalty Family Tree (not quite not up to date)

> The facts about kinship and relations can be visualized as a family tree:

FAU



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Example

- Descriptions include facts like
 - father(Philip, Charles)
 - mother(Mum, Margaret)
 - married(Diana, Charles)
 - male(Philip)
 - female(Beatrice)
- Sentences in classifications depend on the target concept being learned (in the example: 12 positive, 388 negative)
 - grandparent(Mum, Charles)
 - ¬grandparent(Mum, Harry)
- **Goal:** Find a set of sentences for hypothesis such that the entailment constraint is satisfied.
- **Example 2.5.** Without background knowledge, define grandparent in terms of mother and father.

 $grandparent(x, y) \Leftrightarrow (\exists z. mother(x, z) \land mother(z, y)) \lor (\exists z. mother(x, z) \land father(z, y)) \lor \ldots \lor (\exists z. father(x, z) \land father(z, y)) \lor (\exists z. mother(z, y$



Fau

- **• Observation:** Decision tree learning will get nowhere!
 - To express Grandparent as a (Boolean) attribute, pairs of people need to be objects Grandparent((Mum, Charles)).
 - But then the example descriptions can not be represented

FirstElementIsMotherOfElizabeth(*(Mum, Charles)*)

- ► A large disjunction of specific cases without any hope of generalization to new examples.
- **Generally:** Attribute-based learning algorithms are incapable of learning relational predicates.

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Background knowledge

• Observation: A little bit of background knowledge helps a lot.

Example 2.6. If the background knowledge contains

 $\operatorname{parent}(x, y) \Leftrightarrow \operatorname{mother}(x, y) \lor \operatorname{father}(x, y)$

then Grandparent can be reduced to

Fau

 $grandparent(x, y) \Leftrightarrow (\exists z. parent(x, z) \land parent(z, y))$

- Definition 2.7. A constructive induction algorithm creates new predicates to facilitate the expression of explanatory hypotheses.
- **Example 2.8.** Use constructive induction to introduce a predicate parent to simplify the definitions of the target predicates.

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30.2.2 Top-Down Inductive Learning: FOIL



- ▶ Bottom-up learning; e.g. Decision-tree learning: start from the observations and work backwards.
 - Decision tree is gradually grown until it is consistent with the observations.
- Top-down learning method
 - start from a general rule and specialize it on every example.



- Split positive and negative examples
 - $\blacktriangleright Positive: \langle George, Anne \rangle, \langle Philip, Peter \rangle, \langle Spencer, Harry \rangle$
 - $\blacktriangleright \text{ Negative: } \langle \textit{George}, \textit{Elizabeth} \rangle, \langle \textit{Harry}, \textit{Zara} \rangle, \langle \textit{Charles}, \textit{Philip} \rangle$
- Construct a set of Horn clauses with head grandfather(x, y) such that the positive examples are instances of the grandfather relationship.
 - Start with a clause with an empty body \Rightarrow grandfather(x, y).
 - All examples are now classified as positive, so specialize to rule out the negative examples: Here are 3 potential additions:
 - 1. father $(x, y) \Rightarrow$ grandfather(x, y)
 - 2. $parent(x, z) \Rightarrow grandfather(x, y)$
 - 3. father(x, z) \Rightarrow grandfather(x, y)
 - ► The first one incorrectly classifies the 12 positive examples.
 - The second one is incorrect on a larger part of the negative examples.
 - ▶ Prefer the third clause and specialize to $father(x, z) \land parent(z, y) \Rightarrow grandfather(x, y)$.



```
function Foil(examples,target) returns a set of Horn clauses
inputs: examples, set of examples
target, a literal for the goal predicate
local variables: clauses, set of clauses, initially empty
while examples contains positive examples do
clause := New-Clause(examples,target)
remove examples covered by clause from examples
add clause to clauses
return clauses
```



FOIL

function Extend—Example(example,literal) returns a new example
if example satisfies literal
then return the set of examples created by extending example with each
possible constant value for each new variable in literal
else return the empty set

function New-Literals(*clause*) **returns** a set of possibly ''useful'' literals **function** Choose-Literal(*literals*) **returns** the ''best'' literal from *literals*



FOIL: Choosing Literals

- ▶ New-Literals: Takes a clause and constructs all possibly "useful" literals
- father(x, z) \Rightarrow grandfather(x, y)
- Add literals using predicates
 - Negated or unnegated
 - Use any existing predicate (including the goal)
 - Arguments must be variables
 - Each literal must include at least one variable from an earlier literal or from the head of the clause
 - ▶ Valid: Mother(z, u), Married(z, z), grandfather(v, x)
 - Invalid: Married(u, v)
- Equality and inequality literals
 - E.g. $z \neq x$, empty list
- Arithmetic comparisons
 - E.g. x > y, threshold values



- ▶ The way New-Literal changes the clauses leads to a very large branching factor.
- Improve performance by using type information:
 - E.g., parent(x, n) where x is a person and n is a number
- Choose-Literal uses a heuristic similar to information gain.
- Ockham's razor to eliminate hypotheses.
 - If the clause becomes longer than the total length of the positive examples that the clause explains, this clause is not a valid hypothesis.
- Most impressive demonstration

Fau

Learn the correct definition of list-processing functions in Prolog from a small set of examples, using previously learned functions as background knowledge.

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30.2.3 Inverse Resolution



Definition 2.9. Inverse resolution in a nutshell

- Classifications follows from *Background* \land *Hypothesis* \land *Descriptions*.
- This can be proven by resolution.
- Run the proof backwards to find hypothesis.



Definition 2.10. Inverse resolution in a nutshell

- ► Classifications follows from *Background* ∧ *Hypothesis* ∧ *Descriptions*.
- This can be proven by resolution.
- Run the proof backwards to find hypothesis.
- **Problem:** How to run the resolution proof backwards?



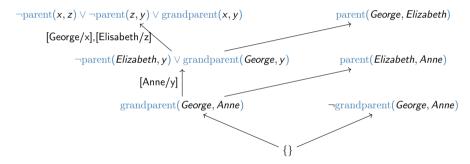
Definition 2.11. Inverse resolution in a nutshell

- ► Classifications follows from *Background* ∧ *Hypothesis* ∧ *Descriptions*.
- This can be proven by resolution.
- Run the proof backwards to find hypothesis.
- Problem: How to run the resolution proof backwards?
- **Recap:** In ordinary resolution we take two clauses $C_1 = L \vee R_1$ and $C_2 = \neg L \vee R_2$ and resolve them to produce the resolvent $C = R_1 \vee R_2$.
- ▶ Idea: Two possible variants of inverse resolution:
 - Take resolvent C and produce two clauses C_1 and C_2 .
 - Take C and C_1 and produce C_2 .



Generating Inverse Proofs (Example)

- $1. \ \mbox{Start}$ with an example classified as both positive and negative
- $2. \ \mbox{Invent clauses that resolve with a fact in our knowledge base}$



 $\neg \operatorname{parent}(x, z) \lor \neg \operatorname{parent}(z, y) \lor \operatorname{grandparent}(x, y)$ is equivalent to $\operatorname{parent}(x, z) \land \operatorname{parent}(z, y) \Rightarrow \operatorname{grandparent}(x, y)$ (Need a contradiction)



- lnverse resolution is a search algorithm: For any C and C_1 there can be several or even an infinite number of clauses C_2 .
- **Example 2.12.** Instead of parent(*George*, *Elizabeth*) there were numerous alternatives we could have picked!
- ▶ The clauses C₁ that participate in each step can be chosen from Background, Descriptions, Classifications or from hypothesized clauses already generated.
- ▶ ILP needs restrictions to make the search manageable
 - Eliminate function symbols
 - Generate only the most specific hypotheses
 - Use Horn clauses
 - All hypothesized clauses must be consistent with each other
 - Each hypothesized clause must agree with the observations

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- ► An inverse resolution procedure is a complete algorithm for learning first-order theories:
 - If some unknown hypothesis generates a set of examples, then an inverse resolution procedure can generate hypothesis from the examples.
- Can inverse resolution infer the law of gravity from examples of falling bodies?
 - Yes, given suitable background mathematics!
- Monkey and typewriter problem: How to overcome the large branching factor and the lack of structure in the search space?



- Inverse resolution is capable of generating new predicates:
 - Resolution of C_1 and C_2 into C eliminates a literal that C_1 and C_2 share.
 - This literal might contain a predicate that does not appear in C.
 - When working backwards, one possibility is to generate a new predicate from which to construct the missing literal.



Example 2.13.

P can be used in later inverse resolution steps.

- **Example 2.14.** mother(x, y) \Rightarrow P(x, y) or father(x, y) \Rightarrow P(x, y) leading to the "Parent" relationship.
- Inventing new predicates is important to reduce the size of the definition of the goal predicate.
- Some of the deepest revolutions in science come from the invention of new predicates. (e.g. Galileo's invention of acceleration)



- ▶ ILP systems have outperformed knowledge free methods in a number of domains.
- Molecular biology: the GOLEM system has been able to generate high-quality predictions of protein structures and the therapeutic efficacy of various drugs.
- GOLEM is a completely general-purpose program that is able to make use of background knowledge about any domain.



Part 3 Natural Language

- Definition 2.15. A natural language is any form of spoken or signed means of communication that has evolved naturally in humans through use and repetition without conscious planning or premeditation.
- ▶ In other words: the language you use all day long, e.g. English, German, ...
- Why Should we care about natural language?:
 - Even more so than thinking, language is a skill that only humans have.
 - It is a miracle that we can express complex thoughts in a sentence in a matter of seconds.
 - It is no less miraculous that a child can learn tens of thousands of words and complex syntax in a matter of a few years.



Natural Language and AI

- ► Without natural language capabilities (understanding and generation) no Al!
- Ca. 100.000 years ago, humans learned to speak, ca. 7.000 years ago, to write.
- Alan Turing based his test on natural language:
 - We want AI agents to be able to communicate with humans.
 - ▶ We want AI agents to be able to acquire knowledge from written documents.
- In this part, we analyze the problem with specific information-seeking tasks:
 - Language models
 - Text classification
 - Information retrieval
 - Information extraction

(Which strings are English/Spanish/etc.) (E.g. spam detection) (aka. Search Engines) (finding objects and their relations in texts)

(for good reason)



Chapter 31 Natural Language Processing

31.1 Introduction to NLP



- **Generally:** Studying of natural languages and development of systems that can use/generate these.
- Definition 1.1. Natural language processing (NLP) is an engineering field at the intersection of computer science, AI, and linguistics which is concerned with the interactions between computers and human (natural) languages. Most challenges in NLP involve:
 - Natural language understanding (NLU) that is, enabling computers to derive meaning (representations) from human or natural language input.
 - Natural language generation (NLG) which aims at generating natural language or speech from meaning representation.
- ▶ For communication with/among humans we need both NLU and NLG.



- Language Assistance:
 - written language: Spell/grammar/style-checking,
 - spoken language: dictation systems and screen readers,
 - multilingual text: machine-supported text and dialog translation, eLearning.



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 - information extraction, question answering.

(e.g. Google/Bing) (e.g. http://ask.com)

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- Dialog Systems/Interfaces:
 - information systems: at airport, tele-banking, e-commerce, call centers,
 - dialog interfaces for computers, robots, cars.

(e.g. Google/Bing)
(e.g. http://ask.com)

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 - search and classification of documents,
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- Dialog Systems/Interfaces:
 - information systems: at airport, tele-banking, e-commerce, call centers,
 - dialog interfaces for computers, robots, cars.
- Observation: The earlier technologies largely rely on pattern matching, the latter ones need to compute the meaning of the input utterances, e.g. for database lookups in information systems.

(e.g. Google/Bing) (e.g. http://ask.com)

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(e.g. Siri/Alexa)



31.2 Natural Language and its Meaning



Observation: Different (academic) disciplines specialize the notion of semantics (of natural language) in different ways.



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- **Philosophy:** has a long history of trying to answer it, e.g.
 - Platon \sim cave allegory. Aristotle \sim syllogisms.
 - ► Frege/Russell ~> sense vs. referent.

("Michael Kohlhase" vs. "Odvsseus")

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- Linguistics/Language Philosophy: We need semantics e.g. in translation "Der Geist ist willig aber das Fleisch ist schwach!" vs. "Der Schnaps ist gut, aber der Braten ist verkocht!"

("Michael Kohlhase" vs. "Odvsseus")

(meaning counts)



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▶ Psychology/Cognition: Semantics = "what is in our brains"

("Michael Kohlhase" vs. "Odysseus")

(meaning counts) (→ mental models)



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- ▶ Psychology/Cognition: Semantics = "what is in our brains"
- Mathematics has driven much of modern logic in the quest for foundations.
 - Logic as "foundation of mathematics" solved as far as possible
 - In daily practice syntax and semantics are not differentiated (much).

("Michael Kohlhase" vs. "Odysseus")

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- Mathematics has driven much of modern logic in the quest for foundations.
 - Logic as "foundation of mathematics" solved as far as possible
 - In daily practice syntax and semantics are not differentiated (much).
- ► Logic@AI/CS tries to define meaning and compute with them.
 - makes syntax explicit in a formal language
 - defines truth/validity by mapping sentences into "world"
 - gives rules of truth-preserving reasoning

("Michael Kohlhase" vs. "Odysseus")

(meaning counts) (→ mental models)

(applied semantics) (formulae, sentences) (interpretation) (inference)



Idea: Machine translation is very simple!

(we have good lexica)

- ► Example 2.1. "Peter liebt Maria." ~ "Peter loves Mary."
- \land this only works for simple examples!
- ▶ Example 2.2. "Wirf der Kuh das Heu über den Zaun." ☆"Throw the cow the hay over the fence." (differing grammar; Google Translate)
- **Example 2.3.** A Grammar is not the only problem
 - "Der Geist ist willig, aber das Fleisch ist schwach!"
 - "Der Schnaps ist gut, aber der Braten ist verkocht!"
- Observation 2.4. We have to understand the meaning for high-quality translation!



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Language and Information

- ▶ Observation: Humans use words (sentences, texts) in natural languages to represent and communicate information.
- **But:** What really counts is not the words themselves, but the meaning information they carry.

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Language and Information

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- Example 2.7 (Word Meaning).

"Newspaper"



▶ For questions/answers, it would be very useful to find out what words (sentences/texts) mean.



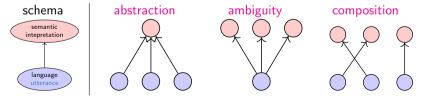
Language and Information

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- **Example 2.9 (Word Meaning).**

"Newspaper"



- ▶ For questions/answers, it would be very useful to find out what words (sentences/texts) mean.
- ▶ Definition 2.10. Interpretation of natural language utterances: three problems



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Example 2.11 (Abstraction).



"*Car*" and "*automobile*" have the same meaning.

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Language and Information (Examples)

Example 2.14 (Abstraction). "Car" and " Example 2.15 (Ambiguity). A "bank" car feature.

"Car" and "automobile" have the same meaning.

A "*bank*" can be a financial institution or a geographical feature.



Language and Information (Examples)

Example 2.17 (Abstraction). "*Car*" and "*automobile*" have the same meaning. Example 2.18 (Ambiguity). A "bank" can be a financial institution or a geographical feature **Example 2.19 (Composition).**

"Every student sleeps" $\rightsquigarrow \forall x.student(x) \Rightarrow sleep(x)$



Context Contributes to the Meaning of NL Utterances

- ▶ Observation: Not all information conveyed is linguistically realized in an utterance.
- **Example 2.20.** "The lecture begins at 11:00 am." What lecture? Today?
- **Definition 2.21.** We call a piece *i* of information linguistically realized in an utterance *U*, iff, we can trace *i* to a fragment of *U*.
- Definition 2.22 (Possible Mechanism). Inferring the missing pieces from the context and world knowledge:

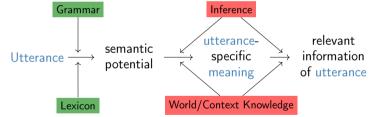


We call this process semantic/pragmatic analysis.



Context Contributes to the Meaning of NL Utterances

- **Example 2.23.** "*It starts at eleven.*" What starts?
- Before we can resolve the time, we need to resolve the anaphor "it".
- Possible Mechanism: More Inference!



 \sim Semantic/pragmatic analysis is quite complex!

(prime topic of AI-2)



31.3 Looking at Natural Language



Fun with Diamonds (are they real?) [Davidson:tam67]

Example 3.1. We study the truth conditions of adjectival complexes:

"This is a diamond."



 $(\models diamond)$

Example 3.2. We study the truth conditions of adjectival complexes:

- "This is a diamond."
- "This is a blue diamond."

 $(\models diamond)$ $(\models diamond, \models blue)$

C

Example 3.3. We study the truth conditions of adjectival complexes:

- "This is a diamond."
- "This is a blue diamond."
- "This is a big diamond."

 $(\models diamond)$ $(\models diamond, \models blue)$ $(\models diamond, \not\models big)$



Example 3.4. We study the truth conditions of adjectival complexes:

- "This is a diamond."
- "This is a blue diamond."
- "This is a big diamond."
- "This is a fake diamond."

 $(\models diamond)$ $(\models diamond, \models blue)$ $(\models diamond, \not\models big)$ $(\models \neg diamond)$

Example 3.5. We study the truth conditions of adjectival complexes:

- "This is a diamond."
- "This is a blue diamond."
- "This is a big diamond."
- "This is a fake diamond."
- "This is a fake blue diamond."

 $(\models diamond)$ $(\models diamond, \models blue)$ $(\models diamond, \not\models big)$ $(\models \neg diamond)$ $(\models blue?, \models diamond?)$



Example 3.6. We study the truth conditions of adjectival complexes:

- "This is a diamond."
- "This is a blue diamond."
- "This is a big diamond."
- "This is a fake diamond."
- "This is a fake blue diamond."
- "Mary knows that this is a diamond."

 $(\models diamond)$ $(\models diamond, \models blue)$ $(\models diamond, \not\models big)$ $(\models \neg diamond)$ $(\models blue?, \models diamond?)$ $(\models diamond)$

©

Example 3.7. We study the truth conditions of adjectival complexes:

- "This is a diamond."
- "This is a blue diamond."
- "This is a big diamond."
- "This is a fake diamond."
- "This is a fake blue diamond."
- "Mary knows that this is a diamond."
- "Mary believes that this is a diamond."

```
(\models diamond)
(\models diamond, \models blue)
(\models diamond, \not\models big)
(\models \neg diamond)
(\models blue?, \models diamond?)
(\models diamond)
(\not\models diamond)
```

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- **Definition 3.8.** We call an utterance ambiguous, iff it has multiple meanings, which we call readings.
- **Example 3.9.** All of the following sentences are ambiguous:
 - "John went to the bank."

(river or financial?)



- **Definition 3.10.** We call an utterance ambiguous, iff it has multiple meanings, which we call readings.
- **Example 3.11.** All of the following sentences are ambiguous:
 - "John went to the bank."
 - "You should have seen the bull we got from the pope."

(river or financial?) (three readings!)



- **Definition 3.12.** We call an utterance ambiguous, iff it has multiple meanings, which we call readings.
- **Example 3.13.** All of the following sentences are ambiguous:
 - "John went to the bank."
 - "You should have seen the bull we got from the pope."
 - "I saw her duck."

(river or financial?) (three readings!) (animal or action?)

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- **Definition 3.14.** We call an utterance ambiguous, iff it has multiple meanings, which we call readings.
- **Example 3.15.** All of the following sentences are ambiguous:
 - "John went to the bank."
 - "You should have seen the bull we got from the pope."
 - "I saw her duck."
 - "John chased the gangster in the red sports car."

(river or financial?) (three readings!) (animal or action?) (three-way too!)



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Example 3.16. "*Every man loves a woman.*"

(Keira Knightley or his mother!)



- **Example 3.21.** "Every man loves a woman."
- **Example 3.22.** "Every car has a radio."

(Keira Knightley or his mother!) (only one reading!)



Example 3.26. "Every man loves a woman." (Keira Knightley or his mother!)
 Example 3.27. "Every car has a radio." (only one reading!)
 Example 3.28. "Some student in every course sleeps in every class at least some of the time." (how many readings?)



- Example 3.31. "Every man loves a woman." (Keira Knightley or his mother!)
 Example 3.32. "Every car has a radio." (only one reading!)
 Example 3.33. "Every car has a radio." (base of the time." (base of the time.")
- Example 3.33. "Some student in every course sleeps in every class at least some of the time." (how many readings?)
- **Example 3.34.** "*The president of the US* is having an affair with an intern." (2002 or 2000?)



- Example 3.36. "Every man loves a woman." (Keira Knightley or his mother!)
 Example 3.37. "Every car has a radio." (only one reading!)
 Example 3.38. "Some student in every course sleeps in every class at least some of the time." (how many readings?)
- Example 3.39. "The president of the US is having an affair with an intern." (2002 or 2000?)
 Example 3.40. "Everyone is here." (who is everyone?)



More Context: Anaphora – Challenge for Pragmatic Analysis

Example 3.41 (Anaphoric References).

"John is a bachelor. His wife is very nice."

(Uh, what?, who?)



Example 3.45 (Anaphoric References).

- "John is a bachelor. His wife is very nice."
- "John likes his dog Spiff even though he bites him sometimes."

(Uh, what?, who?) (who bites?)



Example 3.49 (Anaphoric References).

- "John is a bachelor. His wife is very nice."
- "John likes his dog Spiff even though he bites him sometimes."
- "John likes Spiff. Peter does too."

(Uh, what?, who?) (who bites?) (what to does Peter do?)



Example 3.53 (Anaphoric References).

- "John is a bachelor. His wife is very nice."
- "John likes his dog Spiff even though he bites him sometimes."
- "John likes Spiff. Peter does too."
- "John loves his wife. Peter does too."

(Uh, what?, who?) (who bites?) (what to does Peter do?) (whom does Peter love?)



Example 3.57 (Anaphoric References).

- "John is a bachelor. His wife is very nice."
- "John likes his dog Spiff even though he bites him sometimes."
- "John likes Spiff. Peter does too."
- "John loves his wife. Peter does too."
- "John loves golf, and Mary too."

(Uh, what?, who?) (who bites?) (what to does Peter do?) (whom does Peter love?) (who does what?)



Example 3.61 (Anaphoric References).

- "John is a bachelor. His wife is very nice."
- "John likes his dog Spiff even though he bites him sometimes."
- "John likes Spiff. Peter does too."
- "John loves his wife. Peter does too."
- "John loves golf, and Mary too."

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(Uh, what?, who?) (who bites?)

(what to does Peter do?) (whom does Peter love?)

(who does what?)

Definition 3.62. A word or phrase is called anaphoric (or an anaphor), if its interpretation depends upon another phrase in context. In a narrower sense, an anaphor refers to an earlier phrase (its antecedent), while a cataphor to a later one (its postcedent).

Definition 3.63. The process of determining the antecedent or postcedent of an anaphoric phrase is called anaphor resolution.

Definition 3.64. An anaphoric connection between anaphor and its antecedent or postcedent is called direct, iff it can be understood purely syntactically. An anaphoric connection is called indirect or a bridging reference if additional knowledge is needed.



Example 3.65 (Anaphoric References).

- "John is a bachelor. His wife is very nice."
- "John likes his dog Spiff even though he bites him sometimes."
- "John likes Spiff. Peter does too."
- "John loves his wife. Peter does too."
- "John loves golf, and Mary too."

(Uh, what?, who?) (who bites?) (what to does Peter do?)

- (whom does Peter love?)
 - (who does what?)
- Definition 3.66. A word or phrase is called anaphoric (or an anaphor), if its interpretation depends upon another phrase in context. In a narrower sense, an anaphor refers to an earlier phrase (its antecedent), while a cataphor to a later one (its postcedent).

Definition 3.67. The process of determining the antecedent or postcedent of an anaphoric phrase is called anaphor resolution.

Definition 3.68. An anaphoric connection between anaphor and its antecedent or postcedent is called direct, iff it can be understood purely syntactically. An anaphoric connection is called indirect or a bridging reference if additional knowledge is needed.

- Anaphora are another example, where natural languages use the inferential capabilities of the hearer/reader to "shorten" utterances.
- Anaphora challenge pragmatic analysis, since they can only be resolved from the context using world knowledge.



Example 3.69. Consider the following sentences involving definite description:
 1. "The king of America is rich."

(true or false?)

How do the interact with your context and world knowledge?

Example 3.70. Consider the following sentences involving definite description:

- 1. "The king of America is rich."
- 2. "The king of America isn't rich."

(true or false?) (false or true?)

How do the interact with your context and world knowledge?



Example 3.71. Consider the following sentences involving definite description:

- 1. "The king of America is rich."
- 2. "The king of America isn't rich."
- 3. "If America had a king, the king of America would be rich."

How do the interact with your context and world knowledge?

(true or false?) (false or true?) (true or false!)



Example 3.72. Consider the following sentences involving definite description:

- 1. "The king of America is rich."
- 2. "The king of America isn't rich."
- 3. "If America had a king, the king of America would be rich."
- 4. "The king of Buganda is rich."

How do the interact with your context and world knowledge?

(true or false?) (false or true?) (true or false!) (Where is Buganda?)

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Example 3.73. Consider the following sentences involving definite description:

- 1. "The king of America is rich."
- 2. "The king of America isn't rich."
- 3. "If America had a king, the king of America would be rich."
- 4. "The king of Buganda is rich."
- 5. "... Joe Smith... The CEO of Westinghouse announced budget cuts."

How do the interact with your context and world knowledge?

(true or false?) (false or true?) (true or false!) (Where is Buganda?) (CEO=J.S.!)

Fau



Example 3.74. Consider the following sentences involving definite description:

- 1. "The king of America is rich."
- 2. "The king of America isn't rich."
- 3. "If America had a king, the king of America would be rich."
- 4. "The king of Buganda is rich."
- 5. "... Joe Smith... The CEO of Westinghouse announced budget cuts."

How do the interact with your context and world knowledge?

- The interpretation or whether they make sense at all dep
- ▶ Note: Last two examples feed back into the context or even world knowledge:
 - ▶ If 4. is uttered by an Africa expert, we add ""Buganda exists and is a monarchy" to our world knowledge
 - We add "Joe Smith is the CEO of Westinghouse to the context/world knowledge" (happens all the time in newpaper articles)

(true or false?) (false or true?) (true or false!) (Where is Buganda?) (CEO=J.S.!)

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31.4 Language Models



Natural Languages vs. Formal Language

- **Recap:** A formal language is a set of strings.
- **Example 4.1.** Programming languages like Java or C⁺⁺ are formal languages.
- ▶ Remark 4.2. Natural languages like English, German, or Spanish are not.
- **Example 4.3.** Let us look at concrete examples
 - "Not to be invited is sad!"
 - "To not be invited is sad!"

(definitely English) (controversial)

- ▶ Idea: Let's be lenient, instead of a hard set, use a probability distribution.
- Definition 4.4. A (statistical) language model is a probability distribution over sequences of characters or words.
- ▶ Idea: Try to learn/derive language models from text corpora.
- Definition 4.5. A text corpus (or simply corpus; plural corpora) is a large and structured collection of natural language texts called documents.
- **Definition 4.6.** In corpus linguistics, corpora are used to do statistical analysis and hypothesis testing, checking occurrences or validating linguistic rules within a specific natural language.



N-gram Character Models

- ▶ Written text is composed of characters letters, digits, punctuation, and spaces.
- ► Idea: Let's study language models for sequences of characters.
- ► As for Markov processes, we write P(c_{1:N}) for the probability of a character sequence c₁...c_n of length N.
- **Definition 4.7.** We call an character sequence of length *n* an *n* gram (unigram, bigram, trigram for n = 1, 2, 3).
- **Definition 4.8.** An *n* gram model is a Markov process of order n 1.
- ▶ *Remark 4.9.* For a trigram model, $P(c_i | c_{1:i-1}) = P(c_i | c_{(i-2)}, c_{(i-1)})$. Factoring with the chain rule and then using the Markov property, we obtain

$$P(\mathbf{c}_{1:N}) = \prod_{i=1}^{N} P(\mathbf{c}_i \mid \mathbf{c}_{1:i-1}) = \prod_{i=1}^{N} P(\mathbf{c}_i \mid \mathbf{c}_{(i-2)}, \mathbf{c}_{(i-1)})$$

▶ Thus, a trigram model for a language with 100 characters, $P(c_i | c_{i-2:i-1})$ has 1.000.000 entries. It can be estimated from a corpus with 10^7 characters.



Applications of N-Gram Models of Character Sequences

- ► What can we do with *N* gram models?
- **Definition 4.10.** The problem of language identification is given a text, determine the natural language it is written in.
- Remark 4.11. Current technology can classify even short texts like "Hello, world", or "Wie geht es Dir" correctly with more than 99% accuracy.
- ► One approach: Build a trigram language model P(c_i|c_{i-2:i-1}, ℓ) for each candidate language ℓ by counting trigrams in a ℓ-corpus.

Apply Bayes' rule and the Markov property to get the most likely language:

$$\ell^* = \operatorname{argmax}_{\ell} \left(P(\ell \mid c_{1:N}) \right)$$

=
$$\operatorname{argmax}_{\ell} \left(P(\ell) \cdot P(c_{1:N} \mid \ell) \right)$$

=
$$\operatorname{argmax}_{\ell} \left(P(\ell) \cdot \left(\prod_{i=1}^{N} P(c_i \mid c_{i-2:i-1}, \ell) \right) \right)$$

The prior probability $P(\ell)$ can be estimated, it is not a critical factor, since the trigram language models are extremely sensitive.

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Other Applications of Character N-Gram Models

- Spelling correction is a direct application of a single-language language model: Estimate the probability of a word and all off-by-one variants.
- Definition 4.12. Genre classification means deciding whether a text is a news story, a legal document, a scientific article, etc.
- Remark 4.13. While many features help make this classification, counts of punctuation and other character n-gram features go a long way [KesNunSch:adtg97].
- Definition 4.14. Named entity recognition (NER) is the task of finding names of things in a document and deciding what class they belong to.
- **Example 4.15.** In "*Mr. Sopersteen was prescribed aciphex.*" NER should recognize that "*Mr. Sopersteen*" is the name of a person and "*aciphex*" is the name of a drug.
- Remark 4.16. Character-level language models are good for this task because they can associate the character sequence "ex" with a drug name and "steen" with a person name, and thereby identify words that they have never seen before.



- ▶ Idea: *n* gram models apply to word sequences as well.
- **Problems:** The method works identically, but
 - 1. There are many more words than characters.
 - 2. And what is a word anyways?

(100 vs. 10⁵ in Englisch) (space/punctuation-delimited substrings?)

3. Data sparsity: we do not have enough data! For a language model for 10⁵ words in English, we have 10¹⁵ trigrams.

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4. Most training corpora do not have all words.



- Definition 4.17. Out of vocabulary (OOV) words are unknown words that appear in the test corpus but not training corpus.
- Remark 4.18. OOV words are usually content words such as names and locations which contain information crucial to the success of NLP tasks.
- Idea: Model OOV words by
 - 1. adding a new word token, e.g. $\langle UNK \rangle$ to the vocabulary,
 - 2. in the training corpus, replacing the respective first occurrence of a previously unknown word by <UNK>,
 - 3. counting *n* grams as usual, treating $\langle UNK \rangle$ as a regular word.

This trick can be refined if we have a word classifier, then use a new token per class, e.g. $\langle EMAIL \rangle$ or $\langle NUM \rangle$.



What can Word *N*-Gram Models do?

- **Example 4.19 (Test** *n*-grams). Build unigram, bigram, and trigram language models over the words [RusNor:AIMA03], randomly sample sequences from the models.
 - 1. Unigram: "logical are as are confusion a may right tries agent goal the was"
 - 2. Bigram: "systems are very similar computational approach would be represented"
 - 3. Trigram: "planning and scheduling are integrated the success of naive bayes model"
- Clearly there are differences, how can we measure them to evaluate the models?



What can Word *N*-Gram Models do?

- Example 4.23 (Test *n*-grams). Build unigram, bigram, and trigram language models over the words [RusNor:AIMA03], randomly sample sequences from the models.
 - 1. Unigram: "logical are as are confusion a may right tries agent goal the was ..."
 - 2. Bigram: "systems are very similar computational approach would be represented"
 - 3. Trigram: "planning and scheduling are integrated the success of naive bayes model"
- Clearly there are differences, how can we measure them to evaluate the models?
- **Definition 4.24.** The perplexity of a sequence $c_{1:N}$ is defined as

 $\operatorname{Perplexity}(c_{1:N}) := P(c_{1:N})^{-(\frac{1}{N})}$

▶ Intuition: The reciprocal of probability, normalized by sequence length.

Example 4.25. For a language with n characters or words and a language model that predicts that all are equally likely, the perplexity of any sequence is n. If some characters or words are more likely than others, and the model reflects that, then the perplexity of correct sequences will be less than n.

Example 4.26. In ???, the perplexity was 891 for the unigram model, 142 for the bigram model and 91 for the trigram model.



31.5 Part of Speech Tagging



- Recall: n-grams can predict that a word sequence like "a black cat" is more likely than "cat black a". (as trigram 1. appears 0.000014% in a corpus and 2. never)
- Native Speakers However: Will tell you that "a black cat" matches a familiar pattern: article-adjective-noun, while "cat black a" does not!
- **Example 5.1.** Consider "the fulvous kitten" a native speaker reasons that it
 - follows the determiner-adjective-noun pattern
 - "fulvous" (\triangleq brownish yellow) ends in "ous" \rightsquigarrow adjective

So by generalization this is (probably) correct English.

- **Observation:** The order of syntactical categories of words plays a role in English!
- **Problem:** How can we compute them?

(up next)



FAU

- Definition 5.2. Part-of-speech tagging (also POS tagging, POST, or grammatical tagging) is the process of marking up a word in corpus with tags (called POS tags) as corresponding to a particular part of speech (a category of words with similar syntactic properties) based on both its definition and its context.
- Example 5.3. A sentence tagged with POS tags from the Penn treebank: From the start , it took a person with great qualities to succeed IN DT NN , PRP VBD DT NN IN JJ NNS TO VB
 "From" is tagged as a preposition (IN)
 "the" as a determiner (DT)
 ...
- Observation: Even though POS tagging is uninteresting in its own right, it is useful as a first step in many NLP tasks.
- Example 5.4. In text-to-speech synthesis, a POS tag of "noun" for "record" helps determine the correct pronunciation (as opposed to the tag "verb")

(see below)

The Penn Treebank POS tags

Example 5.5. The following 45 POS tags are used by the Penn treebank:

Tag	Word	Description	Tag	Word	Description
CC	and	Coordinating conjunction	PRP\$	your	Possessive pronoun
CD	three	Cardinal number	RB	quickly	Adverb
DT	the	Determiner	RBR	quicker	Adverb, comparative
EX	there	Existential there	RBS	quickest	Adverb, superlative
FW	per se	Foreign word	RP	off	Particle
IN	of	Preposition	SYM	+	Symbol
JJ	purple	Adjective	TO	to	to
JJR	better	Adjective, comparative	UH	eureka	Interjection
JJS	best	Adjective, superlative	VB	talk	Verb, base form
LS	1	List item marker	VBD	talked	Verb, past tense
MD	should	Modal	VBG	talking	Verb, gerund
NN	kitten	Noun, singular or mass	VBN	talked	Verb, past participle
NNS	kittens	Noun, plural	VBP	talk	Verb, non-3rd-sing
NNP	Ali	Proper noun, singular	VBZ	talks	Verb, 3rd-sing
NNPS	Fords	Proper noun, plural	WDT	which	Wh-determiner
PDT	all	Predeterminer	WP	who	Wh-pronoun
POS	's	Possessive ending	WP\$	whose	Possessive wh-pronoun
PRP	you	Personal pronoun	WRB	where	Wh-adverb
\$	\$	Dollar sign	#	#	Pound sign
**	24	Left quote		2	Right quote
([Left parenthesis)]	Right parenthesis
,		Comma		1	Sentence end
:	;	Mid-sentence punctuation			



Idea: Treat the POS tags in a sentence as state variables C_{1:n} in a HMM: the words are the evidence variables W_{1:n}, use prediction for POS tagging.

- ► The HMM is a generative model that
 - starts in the tag predicted by the prior probability (usually IN)
 - and then, for each step makes two choices:
 - what word e.g. "From" should be emitted
 - what state e.g. DT should come next
- ► This works, but there are problems
 - the HMM does not consider context other than the current state
 - it does not have any idea what the sentence is trying to convey
- ▶ Idea: Use the Viterbi algorithm to find the most probable sequence of hidden states (POS tags)
- ▶ POS taggers based on the Viterbi algorithm can reach an F_1 score of up to 97%.

The Viterbi algorithm for POS tagging – Details

- ▶ We need a transition model $P(C_t | C_{t-1})$: the probability of one POS tag following another.
- **Example 5.6.** $P(C_t = VB | C_{t-1} = MD) = 0.8$ means that given a modal verb (e.g. "would") the following word is a verb (e.g. "think") with probability 0.8.
- Question: Where does the number 0.8 come from?
- Answer: From counts in the corpus with appropriate smoothing! There are 13124 instances of MD in the Penn treebank and 10471 are followed by a VB.
- For the sensor model $P(W_t = would | C_t = MD) = 0.1$ means that if we choose a modal verb, we will choose "would" 10% of the time.
- These numbers also come from the corpus with appropriate smoothing.
- Limitations: HMM models only know about the transition and sensor models In particular, we cannot take into account that e.g. words ending in "ous" are likely adjectives.
- We will see methods based on neural networks later.



31.6 Text Classification



- Problem: Often we want to (ideally) automatically see who can best deal with a given document (e.g. e-mails in customer service)
- Definition 6.1. Given a set of categories the task of deciding which one a given document belongs to is called text classification or categorization.
- **Example 6.2.** Language identification and genre classification are examples of text classification.
- **Example 6.3.** Sentiment analysis classifying a product review as positive or negative.
- **Example 6.4.** Spam detection classifying an email message as spam or ham (i.e. non-spam).



Spam Detection

- **Definition 6.5.** Spam detection classifying an email message as spam or ham (i.e. non-spam)
- **General Idea:** Use NLP/machine learning techniques to learn the categories.
- **Example 6.6.** We have lots of examples of spam/ham, e.g.

Spam (from my spam folder) Ham (in my inbox) Wholesale Fashion Watches -57% today. De-The practical significance of hypertree width signer watches for cheap in identifying more ... You can buy ViagraFr\$1.85 All Medications Abstract: We will motivate the problem of at unbeatable prices! ... social identity clustering: ... WE CAN TREAT ANYTHING YOU SUF-Good to see you my friend. Hey Peter, It FER FROM JUST TRUST US was good to hear from you. ... Sta.rt earn*ing the salary yo,u d-eserve by PDS implies convexity of the resulting optio'btaining the prope, r crede'ntials! mization problem (Kernel Ridge ...

- Specifically: What are good features to classify e-mails by?
 - n-grams like "for cheap" and "You can buy" indicate spam
 - character-level features: capitalization, punctuation
- We have two complementary ways of talking about classification: ► Note:
 - using language models
 - using machine learning



(but also occur in ham)

(e.g. in "vo, u d-eserve")

(up next)



Idea: Define two *n*-gram language models:

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1. one for $\mathsf{P}(\mathrm{Message}|\mathrm{spam})$ by training on the spam folder

2. one for P(Message|ham) by training on the inbox

Then we can classify a new message m with an application of Bayes' rule:

 $\underset{c \in \{\text{spam,ham}\}}{\operatorname{argmax}} (P(c \mid m)) = \underset{c \in \{\text{spam,ham}\}}{\operatorname{argmax}} (P(m \mid c)P(c))$

where P(c) is estimated just by counting the total number of spam and ham messages.

This approach works well for spam detection, just as it did for language identification.

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Classifier Success Measures: Precision, Recall, and F1 score

- ▶ We need a way to measure success in classification tasks.
- ▶ Definition 6.7. Let $f_C: S \to \mathbb{B}$ be a binary classifier for a class $C \subseteq S$, then we call $a \in S$ with $f_C(a) = T$ a false positive, iff $a \notin C$ and $f_C(a) = F$ a false negative, iff $a \in C$. False positives and negatives are errors of f_C . True positives and negatives occur when f_C correctly indicates actual membership in S.
- ▶ Definition 6.8. The precision of f_C is defined as $\frac{\#(TP)}{\#(TP)+\#(FP)}$ and the recall is $\frac{\#(TP)}{\#(TP)+\#(FN)}$, where *TP* is the set of true positives and *FN/FP* the sets of false negatives and false positives of f_C .
- Intuitively these measure the rates of:
 - true positives in class C.
 (precision high, iff few false positives)
 - true positives in $f_c^{-1}(T)$. (recall high, iff few true positives forgotten, i.e. few false negatives)
- Definition 6.9. The F₁ score combines precision and recall into a single number: (harmonic mean)
 2 precision · recall
 (precision + recall)
- **• Observation:** Classifiers try to reach precision and recall $\rightsquigarrow F_1$ score of 1.
 - $\blacktriangleright\,$ if that is impossible, compromize on one \rightsquigarrow F_β score .
 - The F_{β} score generalizes the F_1 score by weighing the precision β times as important as recall.

(application-dependent)



31.7 Information Retrieval

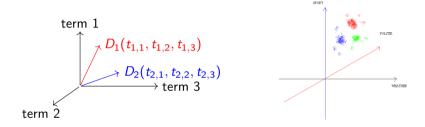


- Definition 7.1. An information need is an individual or group's desire to locate and obtain information to satisfy a conscious or unconscious need.
- **Definition 7.2.** An information object is medium that is mainly used for its information content.
- Definition 7.3. Information retrieval (IR) deals with the representation, organization, storage, and maintenance of information objects that provide users with easy access to the relevant information and satisfy their various information needs.
 - **Observation (Hjørland 1997):** Information need is closely related to relevance: If something is relevant for a person in relation to a given task, we might say that the person needs the information for that task.
- Definition 7.4. Relevance denotes how well an information object meets the information need of the user. Relevance may include concerns such as timeliness, authority or novelty of the object.
- **Observation:** We normally come in contact with IR in the form of web search.
- Definition 7.5. Web search is a fully automatic process that responds to a user query by returning a sorted document list relevant to the user requirements expressed in the query.
- **Example 7.6.** Google and Bing are web search engines, their query is a bag of words and documents are web pages, PDFs, images, videos, shopping portals.



- Idea: For web search, we usually represent documents and queries as bags of words over a fixed vocabulary V. Given a query Q, we return all documents that are "similar".
- ▶ Definition 7.7. Given a vocabulary (a list) V of words, a word w ∈ V, and a document d, then we define the raw term frequency (often just called the term frequency) of w in d as the number of occurrences of w in d.
- ▶ Definition 7.8. A multiset of words in V = {t₁,...,t_n} is called a bag of words (BOW), and can be represented as a word frequency vectors in N^{|V|}: the vector of raw word frequencies.
- ► Example 7.9. If we have two documents: d₁ = "Have a good day!" and d₂ = "Have a great day!", then we can use V = "Have", "a", "good", "great", "day" and can represent "good" as (0,0,1,0,0), "great" as (0,0,0,1,0), and d₁ a (1,1,1,0,1). Words outside the vocabulary are ignored in the BOW approach. So the document
 - $d_3 =$ "What a day, a good day" is represented as (0, 2, 1, 0, 2).

▶ Idea: Query and document are similar, iff the angle between their word frequency vectors is small.



Lemma 7.10 (Euclidean Dot Product Formula). $A \cdot B = ||A||_2 ||B||_2 \cos \theta$, where θ is the angle between A and B.

Definition 7.11. The cosine similarity of A and B is $\cos \theta = \frac{A \cdot B}{\|A\|_2 \|B\|_2}$.



TF-IDF: Term Frequency/Inverse Document Frequency

- **Problem:** Word frequency vectors treat all the words equally.
- Example 7.12. In an query "the brown cow", the "the" is less important than "brown cow". (because "the" is less specific)
- Idea: Introduce a weighting factor for the word frequency vector that de-emphasizes the dimension of the more (globally) frequent words.
- We need to normalize the word frequency vectors first:
- ▶ Definition 7.13. Given a document d and a vocabulary word $t \in V$, the normalized term frequency (confusingly often called just term frequency) tf(t, d) is the raw term frequency divided by |d|.
- ▶ Definition 7.14. Given a document collection $D = \{d_1, ..., d_N\}$ and a word t the inverse document frequency is given by $idf(t, D) := log_{10}(\frac{N}{|\{d \in D \mid t \in d\}|})$.
- **Definition 7.15.** We define $\operatorname{tfidf}(t, d, D) := \operatorname{tf}(t, d) \cdot \operatorname{idf}(t, D)$.
- ▶ Idea: Use the tfidf-vector with cosine similarity for information retrieval instead.
- ▶ **Definition 7.16.** Let *D* be a document collection with vocabulary $V = \{t_1, ..., t_{|V|}\}$, then the tfidf-vector $\overline{\text{tfidf}}(d, D) \in \mathbb{N}^{|V|}$ is defined by $\overline{\text{tfidf}}(d, D)_i := \text{tfidf}(t_i, d, D)$.



• Let $D := \{d_1, d_2\}$ be a document corpus over the vocabulary

 $V = \{$ "this", "is", "a", "sample", "another", "example" $\}$

with word frequency vectors $\langle 1, 1, 1, 2, 0, 0 \rangle$ and $\langle 1, 1, 0, 0, 2, 3 \rangle$.

Then we compute for the word "this"

•
$$tf("this", d_1) = \frac{1}{5} = 0.2 and tf("this", d_2) = \frac{1}{7} \approx 0.14$$
,

- idf is constant over D, we have $\operatorname{idf}("this", D) = \log_{10}(\frac{2}{2}) = 0$,
- thus tfidf("this", d_1, D) = 0 = tfidf("this", d_2, D).

("*this*" occurs in both)

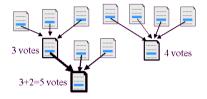
- ▶ The word "example" is more interesting, since it occurs only in d₂
 - $tf("example", d_1) = \frac{0}{5} = 0$ and $tf("example", d_2) = \frac{3}{7} \approx 0.429$.
 - $idf("example", D) = \log_{10}(\frac{2}{1}) \approx 0.301,$
 - ▶ thus tfidf("example", d_1 , D) = 0 · 0.301 = 0 and tfidf("example", d_2 , D) \approx 0.429 · 0.301 = 0.129.



(thrice)

Ranking Search Hits: e.g. Google's Page Rank

- **Problem:** There are many hits, need to sort them
- ▶ Idea: A web site is important, ... if many other hyperlink to it.



- ▶ Refinement: ..., if many important web pages hyperlink to it.
- **Definition 7.17.** Let A be a web page that is hyperlinked from web pages S_1, \ldots, S_n , then the page rank PR of A is defined as

$$\operatorname{PR}(A) = 1 - d + d\left(\frac{\operatorname{PR}(S_1)}{C(S_1)} + \dots + \frac{\operatorname{PR}(S_n)}{C(S_n)}\right)$$

where C(W) is the number of links in a page W and d = 0.85.

▶ Remark 7.18. PR(A) is the probability of reaching A by random browsing.

FAU



(e.g. by importance)

31.8 Information Extraction



- Definition 8.1. Information extraction is the process of acquiring information by skimming a text and looking for occurrences of a particular class of object and for relationships among objects.
- **Example 8.2.** Extracting instances of addresses from web pages, with attributes for street, city, state, and zip code;
- **Example 8.3.** Extracting instances of storms from weather reports, with attributes for temperature, wind speed, and precipitation.
- **Observation:** In a limited domain, this can be done with high accuracy.



Attribute-Based Information Extraction

- Definition 8.4. In attribute-based information extraction we assume that the text refers to a single object and the task is to extract a factored representation.
- **Example 8.5 (Computer Prices).** Extracting from the text "*IBM ThinkBook 970. Our price:* \$399.00" the attribute-based representation

{Manufacturer=IBM, Model=ThinkBook970,Price=\$399.00}.

- ► Idea: Try a template-based approach for each attribute.
- Definition 8.6. A template is a finite automaton that recognizes the information to be extracted. The template often consists of three sub-automata per attribute: the prefix pattern followed by the target pattern (it matches the attribute value) and the postfix pattern.
- Example 8.7 (Extracing Prices with Regular Expressions). When we want to extract computer price information, we could use regular expressions for the automata, concretely, the
 - prefix pattern: .*price[:]?
 - target pattern: [\$][0-9]+([.][0-9][0-9])?
 - postfix pattern: + shipping
- ► Alternative: take all the target matches and choose among them.
- Example 8.8. For "List price \$99.00, special sale price \$78.00, shipping \$3.00." take the lowest price that is within 50% of the highest price. ~ "\$78.00"



Relational Information Extraction

- Question: Can we also do structured representations?
- ► Answer: That is the next step up from attribute-based information extraction.
- ▶ **Definition 8.9.** The task of a relational extraction system is to extract multiple objects and the relationships among them from a text.
- **Example 8.10.** When these systems see the text "*\$249.99,*" they need to determine not just that it is a price, but also which object has that price.
- Example 8.11. FASTUS is a typical relational extraction system, which handles news stories about corporate mergers and acquisitions. It can read the story Bridgestone Sports Co. said Friday it has set up a joint venture in Taiwan with a local concern and a Japanese trading house to produce golf clubs to be shipped to Japan.

and extract the relations:

```
e \in JointVentures \land Product(e, "golfclubs) \land Date(e, "Friday")
```

```
Member(e, "BridgestoneSportsCo") \land Member(e, "alocalconcern")
```

```
Member(e, "aJapanesetradinghouse")
```



Advertisement: Logic-Based Natural Language Semantics

Advanced Course: "Logic-Based Natural Language Semantics" (next semester)

- Wed. 10:15-11:50 and Thu 12:15-13:50
- Contents:

Fau

- Foundations of Natural Language Semantics (NLS)
- Montague's Method of Fragments
- Implementing Fragments in GLF
- Inference Systems for Natural Language Pragmatics
- Advanced logical systems for NLS
- Grading: Attendance & Wakefulness, Project/Homework, Oral Exam.
- **Course Intent:** Groom students for bachelor/master theses and as KWARC research assistants.

(expected: < 10 Students)

(Alternating Lectures and hands-on Lab Sessions)

(Grammar, Semantics Constr., Logic) (Grammatical Framework and MMT) (tableau machine) (modal, higher-order, dynamic Logics)

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Chapter 32 Deep Learning for NLP

- Observation: Symbolic and statistical systems have demonstrated success on many NLP tasks, but their performance is limited by the endless complexity of natural language.
- Idea: Given the vast amount of text in machine-readable form, can data-driven machine-learning base approaches do better?
- ▶ In this chapter, we explore this idea, using and extending the methods from ???.
- Overview:
 - 1. Word embeddings
 - 2. Recurrent neural networks for NLP
 - 3. Sequence-to-sequence models
 - 4. Transformer Architecture
 - 5. Pretraining and transfer learning.



32.1 Word Embeddings



Word Embeddings

Problem: For ML methods in NLP, we need numerical data.

(not words)

- ▶ Idea: Embed words or word sequences into real vector spaces.
- ▶ Definition 1.1. A word embedding is a mapping from words in context into a real vector space ℝⁿ used for natural language processing.
- Definition 1.2. A vector is called one hot, iff all components are 0 except for one 1. We call a word embedding one hot, iff all of its vectors are.

One hot word embeddings are rarely used for actual tasks, but often used as a *starting point* for better word embeddings.

- Example 1.3 (Vector Space Methods in Information Retrieval). Word frequency vectors are induced by adding up one hot word embeddings.
- ► Example 1.4. Given a corpus D the context the tf idf word embedding is given by $\operatorname{tfidf}(t, d, D) := \operatorname{tf}(t, d) \cdot \log_{10}(\frac{|D|}{|\{d \in D \mid t \in d\}|})$, where $\operatorname{tf}(t, d)$ is the term frequency of word t in document d.
- ▶ Intuition behind these two: Words that occur in similar documents are similar.



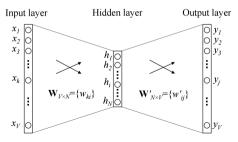
Word2Vec

Idea: Use *feature extraction* to map words to vectors in \mathbb{R}^N :

Train a neural network on a "dummy task", throw away the output layer, use the previous layer's output (of size N) as the word embedding

First Attempt: Dimensionality Reduction: Train to predict the original one hot vector:

- ► For a vocabulary size V, train a network with a single hidden layer; i.e. three layers of sizes (V, N, V). The first two layers will compute our embeddings.
- Feed the one hot encoded input word into the network, and train it on the one hot vector itself, using a softmax activation function at the output layer. (softmax normalizes a vector into a probability distribution)



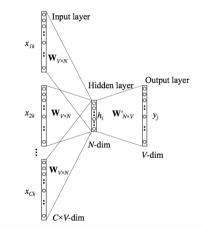


Word2Vec: The Continuous Bag Of Words (CBOW) Algorithm

Distributional Semantics: "a word is characterized by the company it keeps".

Better Idea: Predict a word from its context:

- ► For a context window size n, take all sequences of 2n + 1 words in our corpus (e.g. the brown cow jumps over the moon for n = 3) as training data. We call the word at the center (jumps) the target word, and the remaining words the context words.
- For every such sentence, pass all context words (one-hot encoded) through the first layer of the network, yielding 2n vectors.
- Pass their average into the output layer (average pooling layer) with a softmax activation function, and train the network to predict the target word. (sum pooling also works)



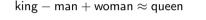
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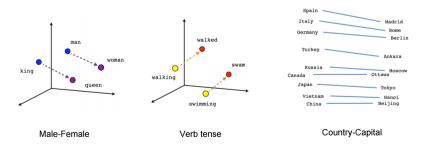
Properties

Vector embeddings like CBOW have interesting properties:

- Similarity: Using e.g. cosine similarity $(A \cdot B \cdot \cos(\theta))$ to compare vectors, we can find words with similar meanings.
- Semantic and syntactic relationships emerge as arithmetic relations:



 $\mathsf{germany}-\mathsf{country}+\mathsf{capitol}\approx\mathsf{berlin}$





- ▶ Observation: Word embeddings are crucial as first steps in any NN-based NLP methods.
- In practice it is often sufficient to use generic, pretrained word embeddings
- Definition 1.5. Common pretrained i.e. trained for generic NLP applications word embeddings include
 - Word2vec: the original system that established the concept
 - GloVe (Global Vectors)
 - ► FASTTEXT

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(see above)

- (embeddings for 157 languages) k) (up next)
- But we can also train our own word embedding (together with main task)



Learning POS tags and Word embeddings simultaneously

Specific word embeddings are trained on a carefully selected corpus and tend to emphasize the characteristics of the task.

Example 1.6. POS tagging – even though simple – is a good but non-trivial example. Recall that many words can have multiple POS tags, e.g. "*cut*" can be

- a present tense verb (transitive or intransitive)
- a past tense verb
- a infinitive verb
- a past participle
- ► an adjective
- ▶ a noun.

If a nearby temporal adverb refers to the past \sim this occurrence may be a past tense verb.

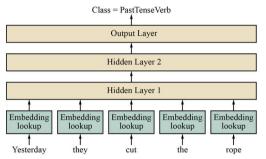
Note: CBOW treats all context words identically reagrdless of *order*, but in POS tagging the exact *positions* of the words matter.

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POS/Embedding Network

Idea: Start with a random (or pretrained) embedding of the words in the corpus and just concatenate them over some context window size



Layer 1 has (in this case) 5 · N inputs, Output layer is one hot over POS classes.

- The embedding layers treat all words the same, but the first hidden layer will treat them differently depending on the position.
- The embeddings will be finetuned for the POS task during training.

Note: Better positional encoding techniques exist (e.g. sinusoidal), but for fixed small context window sizes, this works well. C FAU

32.2 Recurrent Neural Networks



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- word embeddings give a good representation of words in isolation.
- ► But natural language of word sequences ← surrounding words provide context!
- ► For simple tasks like POS tagging, a fixed-size window of e.g. 5 words is sufficient.
- Observation: For advanced tasks like question answering we need more context!
- Example 2.1. In the sentence "Eduardo told me that Miguel was very sick so I took him to the hospital", the pronouns "him" refers to "Miguel" and not "Eduardo". (14 words of context)
- Observation: Language models with *n*-grams or *n*-word feed-forward networks have problems: Either the context is too small or the model has too many parameters! (or both)
- ▶ Observation: Feed-forward networks N also have the problem of asymmetry: whatever N learns about a word w at position n, it has to relearn about w at position $m \neq n$.
- Idea: What about recurrent neural networks nets with cycles?

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(up next)

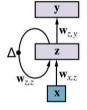
RNNs for Time Series

► Idea: RNNs – neural networks with cycles – have memory → use that for more context in neural NLP.

Example 2.2 (A simple RNN).

It has an input layer x, a hidden layer z with recurrent connections and delay Δ , and an output layer y as shown on the right. Defining Equations for time step t:

$$\begin{aligned} \mathbf{z}_t &= \mathbf{g}_{\mathbf{z}}(\mathbf{W}_{\mathbf{z},\mathbf{z}}\mathbf{z}_{t-1} + \mathbf{W}_{\mathbf{x},\mathbf{z}}\mathbf{x}_t) \\ \mathbf{y}_t &= \mathbf{g}_{\mathbf{y}}(\mathbf{W}_{\mathbf{z},\mathbf{y}}\mathbf{z}_t) \end{aligned}$$

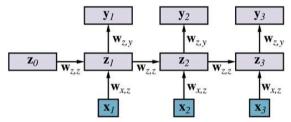


where g_z and g_y are the activation functions for the hidden and output layers.

Intuition: RNNs are a bit like HMMs and dynamic Bayesian Networks: They make a Markov assumption: the hidden state z suffices to capture the input from all previous inputs.

▶ Side Benefit: RNNs solve the asymmetry problem \leftrightarrow , the $W_{z,z}$ are the same at every step.

- **Idea:** For training, unroll a RNN into a feed-forward network \sim back-propagation.
- **Example 2.3.** The RNN from **??** unrolled three times.



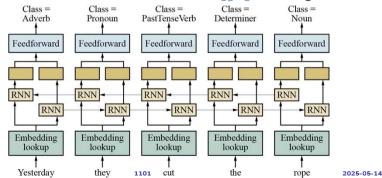
Problem: The weight matrices $W_{x,z}$, $W_{z,z}$, and $W_{z,y}$ are shared over all time slides.

Definition 2.4. The back-propagation through time algorithm carefully maintains the identity of W_{z,z} over all steps



Bidirectional RNN for more Context

- Observation: RNNs only take left context i.e. words before into account, but we may also need right context – the words after.
- Example 2.5. For "Eduardo told me that Miguel was very sick so I took <u>him</u> to the hospital" the pronoun "him" resolves to "Miguel" with high probability. If the sentence ended with "to see Miguel", then it should be "Eduardo".
- Definition 2.6. A bidirectional RNN concatenates a separate right-to-left model onto a left-to-right model
- **Example 2.7.** Bidirectional RNNs can be used for POS tagging, extending the network from ???





- **Problem:** When training a vanilla RNN using back-propagation through time, the long-term gradients which are back-propagated can "vanish" - tend to zero - or "explode" - tend to infinity.
- Definition 2.8. LSTMs provide a short-term memory for RNN that can last thousands of time steps. thus the name "long short-term memory". A LSTM can learn when to remember and when to forget pertinent information.
- **Example 2.9.** In NLP LSTMs can learn grammatical dependencies. An LSTM might process the sentence "Dave, as a result of his controversial claims, is now a pariah" by
 - remembering the (statistically likely) grammatical gender and number of the subject "Dave".

1102

- note that this information is pertinent for the pronoun "his" and
- note that this information is no longer important after the verb "is".



Introduce a *memory vector* c in addition to the recurrent (short-term memory) vector z

- c is essentially copied from the previous time step, but can be modified by the *forget gate f*, the *input gate i*, and the *output gate o*.
- \blacktriangleright the forget gate f decides which components of c to retain or discard
- ► the *input gate i* decides which components of the *current* input to *add* to *c* multiplicative ~> no vanishing gradients)

(additive, not

the output gate o decides which components of c to output as z



32.3 Sequence-to-Sequence Models



- Question: Machine translation (MT) is an important task in NLP, can we do it with neural networks?
- Observation: If there were a one-to-one correspondence between source words and target words MT would be a simple tagging task. But
 - ▶ the three Spanish words "caballo de mar" translate to the English "seahorse" and
 - the two Spanish words "perro grande" translate to English as "big dog".
 - in English, the subject is usually first and in Fijian last.
- ▶ Idea: For MT, generate one word at a time, but keep track of the context, so that
 - ▶ we can remember parts of the source we have not translated yet
 - we remember what we already translated so we do not repeat ourselves.

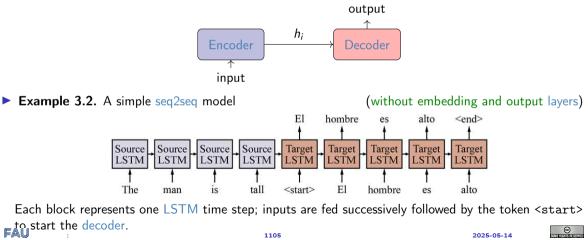
We may have to process the whole source sentence before generating the target!

Remark: This smells like we need LSTMs.



Sequence-To-Sequence Models

- Idea: Use two coupled RNNs, one for the source, and one for the target. The input for the target is the output of the last hidden layer of the source RNN.
- Definition 3.1. A sequence-to-sequence (seq2seq) model is a neural model for translating an input sequence x into an output sequence y by an encoder followed by a decoder generates y.



- Remark: Seq2seq models were a major breakthrough in NLP and MT. But they have three major shortcomings:
 - nearby context bias: RNNs remember with their hidden state, which has more information about a word in - say - step 56 than in step 5. BUT long-distance context can also be important.
 - Fixed context size: the entire information about the source sentence must be compressed into the fixed-dimensional typically 1024 vector. Larger vectors → slow training and overfitting.
- Idea: Concatenate all source RNN hidden vectors to use all of them to mitigate the nearby context bias.
- ▶ **Problem:** Huge increase of weights ~→ slow training and overfitting.



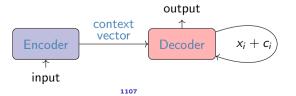
Attention

- **Bad Idea:** Concatenate all source RNN hidden vectors to use all of them to mitigate the nearby context bias.
- ▶ Better Idea: The decoder generates the target sequence one word at a time. ~> Only a small part of the source is actually relevant.

the decoder must focus on different parts of the source for every word.

- ▶ Idea: We need a neural component that does context-free summarization.
- **Definition 3.3.** An attentional seq2seq model is a seq2seq that passes along a context vector c_i in the decoder. If $h_i = RNN(h_{i-1}, x_i)$ is the standard decoder, then the decoder with attention is given by $h_i = RNN(h_{i-1}, x_i + c_i)$, where $x_i + c_i$ is the concatenation of the input x_i and context vectors c_i with

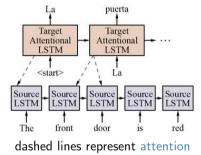
$$\begin{array}{lll} r_{ij} &=& h_{i-1} \cdot s_j & \text{raw attention score} \\ a_{ij} &=& e^{r_{ij}} / (\sum_k e^{r_{ij}}) & \text{attention probability matrix} \\ c_i &=& \sum_j a_{ij} \cdot s_j & \text{context vector} \end{array}$$

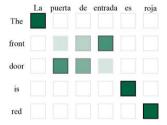


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Example 3.4. An attentional seq2seq model for English-to-Spanish translation





attention probablity matrix darker colors \rightsquigarrow higher probabilities

Remarks: The attention

- component learns no weights and supports variable-length sequences.
- is entirely latent the developer does not influence it.



- During training, a seq2seq model tries to maximize the probability of each word in the training sequence, conditioned on the source and the previous target words.
- Definition 3.5. The procedure that generates the target one word at a time and feeds it back at the next time step is called decoding.
- **Definition 3.6.** Always selecting the highest probability word is called greedy decoding.
- > Problem: This may not always maximize the probability of the whole sequence
- **Example 3.7.** Let's use a greedy decoder on "*The front door is red*".
 - The correct translation is "La puerta de entrada es roja".
 - Suppose we have generated the first word "La" for "The".
 - ► A greedy decoder might propose "*entrada*" for "*front*".
- Greedy decoding is fast, but has no mechanism for correcting mistakes.
- **Solution:** Use an optimizing search algorithm

(e.g. local beam search)



Recall: Greedy decoding is not optimal!

- Idea: Search for an optimal decoding (or at least a good one) using one of the search algorithms from ???.
- ► Local beam search is a common choice in machine translation. Concretely:
 - keep the top k hypotheses at each stage,

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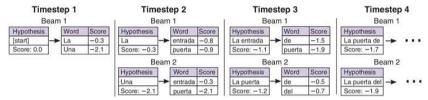
- extending each by one word using the top k choices of words,
- then chooses the best k of the resulting k^2 new hypotheses.

When all hypotheses in the beam generate the special <end> token, the algorithm outputs the highest scoring hypothesis.

► Observation: The better the seq2seq models get, the smaller we can keep beam size Today beams of b = 4 are sufficient after b = 100 a decade ago.

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Example 3.8. A local beam search with beam size b = 2



- Word scores are log-probabilities generated by the decoder softmax
- hypothesis score is the sum of the word scores.

FAU

At time step 3, the highest scoring hypothesis "*La entrada*" can only generate low-probability continuations, so it "falls off the beam". (as intended)



32.4 The Transformer Architecture



Self-Attention

- Idea: "Attention is all you need!" (see [VasShaPar:aiayn17])
- ► So far, attention was used from the encoder to the decoder.
- Self-attention extends this so that each hidden states sequence also attends to itself. (*coder to *coder)
- Idea: Just use the dot product of the input vectors
- ▶ Problem: Always high, so each hidden state will be biased towards attending to itself.
- Self-attention solves this by first projecting the input into three different representations using three different weight matrices:
 - ▶ the query vector $q_i = W_q \times_i \cong$ standard attention
 - key vector $k_i = W_k \times_i \cong$ the source in seq2seq
 - ▶ value vector $v_i = W_v \times_i$ is the context being generated

$$\begin{array}{rcl} r_{ij} &=& (\mathsf{q}_i \cdot \mathsf{k}_i) / \sqrt{d} \\ \mathsf{a}_{ij} &=& e^{r_{ij}} / (\sum_k e^{r_{ij}}) \\ c_i &=& \sum_j \mathsf{a}_{ij} \cdot \mathsf{v}_j \end{array}$$

where d is the dimension of k and q.

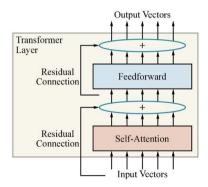


The Transformer Architecture

- Definition 4.1. The transformer architecture uses neural blocks called transformers, which are built up from multiple transformer layers.
- ► Remark: The context modeled in self-attention is agnostic to word order ~> transformers use positional embeddings to cope with that.

Example 4.2.

A single-layer transformer consists of self-attention, a feed-forward network, and residual connections to cope with the vanishing gradient problem.

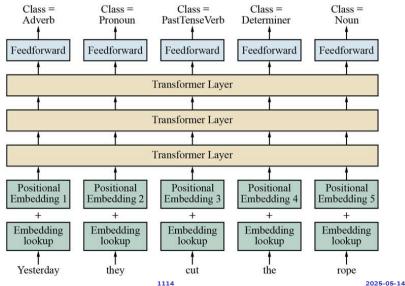


In practice transformers consist of 6-7 transformer layers.



A Transformer for POS tagging

Example 4.3. A transformers for POS tagging:





32.5 Large Language Models

Pretraining and Transfer Learning

- Getting enough data to build a robust model can be a challenge.
- In NLP we often work with unlabeled data
 - \blacktriangleright syntactic/semantic labeling is much more difficult \rightsquigarrow costly than image labeling.
 - the Internet has lots of texts

(adds $\sim 10^{11}$ words/day)

- ▶ Idea: Why not let other's do this work and re-use their training efforts.
- Definition 5.1. In pretraining we use
 - ▶ a large amount of shared general-domain language data to train an initial version of an NLP model.
 - a smaller amount of domain-specific data (perhaps labeled) to finetune it to the vocabulary, idioms, syntactic structures, and other linguistic phenomena that are specific to the new domain.
- Pretraining is a form of transfer learning:
- Definition 5.2. In Transfer learning (TL), knowledge learned from a task is re-used in order to boost performance on a related task.
- Idea: Take a pretrained neural network, replace the last layer(s), and then train those on your own corpus.
- Observation: Simple but surprisingly efficient!



Large Language Models

Definition 5.3. A Large Language Model (LLM) is a generic pretrained neural network, providing embeddings for sentences or entire documents for NLP tasks. In practice, they (usually) combine the following components:

- Tokenization: Splitting text into tokens
- embeddings for these tokens,
- positional embeddings of tokens
- a transformer architecture, trained on
- > a masked token prediction task.
- LLMs can be used for a variety of tasks.
- classification (e.g., sentiment analysis, POS-tagging),
- translation (bwetween languages, styles, etc.),
- generation (e.g., text completion, summarization, chatbots),

(characters, words, punctuation,...) (e.g., Word2vec – or we let the transformer learn them)

(encodes where in a sentence a token is)

...

0

So far: we have encoded text either as sequences of characters (non-semantic) or as sequences of words (semantic, but virtually unlimited vocabulary, OOV-problems).

Idea: Find a middle ground: Learn an optimal vocabulary of tokens from data and split text into a sequence of tokens.

Definition 5.4. The Byte Pair Encoding (BPE) algorithm learns a vocabulary of tokens of given size N > 256 from a corpus C, by doing the following:

- Let $\ell = 256$ and set $BPE(\langle b \rangle) = b$ for every byte $0 \le b \le 255$.
- While ℓ < N, find the most common pair of tokens (a, b) and let BPE(⟨a, b⟩) = ℓ + 1 (and increase ℓ by 1).</p>
- ▶ Repeat until $\ell = N$.

 \sim we obtain a one-hot encoding of tokens of size *N*, where the most common sequences of bytes are represented by a single token. By retaining $BPE(\langle b \rangle) = b$, we avoid OOV problems. \sim We can then train a word embedding on the resulting tokens

Alternative techniques include *WordPiece* and *SentencePiece*.



https://huggingface.co/spaces/Xenova/the-tokenizer-playground





Definition 5.5. Let $\langle w_1, \ldots, w_n \rangle$ be a sequence of tokens. A positional encoding $PE_i(w_i)$ is a vector that retains the position of w_i in the sequence *alongside* the word embedding of w_i . We want positional encodings to satisfy the following properties:

1.
$$\operatorname{PE}_i(w) \neq \operatorname{PE}_j(w)$$
 for $i \neq j$,

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2. PE should retain *distances*: if $i_1 - i_2 = j_1 - j_2$, then given the embeddings for w_1, w_2 , we should be able to linearly transform $\langle \text{PE}_{i_1}(w_1), \text{PE}_{i_2}(w_2) \rangle$ into $\langle \text{PE}_{j_1}(w_1), \text{PE}_{j_2}(w_2) \rangle$.

 \sim no entirely separate embeddings for w_1, w_2 depending on positions \sim learning from short sentences generalizes (ideally) to longer ones

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Idea: Let $PE_t(w) = E(w) + p_t$, for some suitable p_t (where E(w) is the word embedding for token w). $\sim p_t$ has the same dimensionality as our embedding E.

Idea: Use a combination of sine and cosine functions with different frequencies for each dimension of the embedding.

Attention is all you need: For a vocabulary size d, we define

$$p_{t_i} := \begin{cases} \sin(\frac{t}{c^{2k/d}}) & \text{if } i = 2k\\ \cos(\frac{t}{c^{2k/d}}) & \text{if } i = 2k+1 \end{cases}$$

for some constant c.

 \rightsquigarrow works for arbitrary sequence lengths and vocabulary sizes.

(10000 in the paper)



Three strategies for training LLMs:

- Masked Token Prediction: Given a sentence (e.g. "The river rose five feet"), randomly replace tokens by a special mask token (e.g. "The river [MASK] five feet"). The LLM should predict the masked tokens (e.g. "rose").
- Discrimination: Train a small masked token prediction model M. Given a masked sentence, let M generated possible completions. Train the actual model to distinguish between tokens generated by M and the original tokens. (Google Electra et al; well suited for generic tasks)
- Next Token Prediction: Given the (beginning of) a sentence, predict the next token in the sequence. (GPT et al; well suited for generative tasks)
- \sim All techniques turn an unlabelled corpus into a supervised learning task.



Deep learning methods are currently dominant in NLP!

- Data-driven methods are easier to develop and maintain than symbolic ones
- also perform better models crafted by humans
- But problems remain;
 - DL methods work best on immense amounts of data.
 - LLM contain knowledge, but integration with symbolic methods elusive.

(think ChatGPT)

(with reasonable effort)

(small languages?)



Deep learning methods are currently dominant in NLP!

- > Data-driven methods are easier to develop and maintain than symbolic ones
- also perform better models crafted by humans
- But problems remain;

Fau

- DL methods work best on immense amounts of data.
- LLM contain knowledge, but integration with symbolic methods elusive.
- DL4NLP methods do very well, but only after processing orders of magnitude more data than humans do for learning language.
- This suggests that there is of scope for new insights from all areas.

(think ChatGPT)

(with reasonable effort)

2025-05-14

(small languages?)



$\begin{array}{c} \mbox{Chapter 33} \\ \mbox{What did we learn in Al $1/2$?} \end{array}$

Topics of AI-1 (Winter Semester)

- Getting Started
 - What is artificial intelligence?
 - Logic programming in Prolog
 - Intelligent Agents
- Problem Solving
 - Problem Solving and search
 - Adversarial search (Game playing)
 - constraint satisfaction problems
- Knowledge and Reasoning
 - Formal Logic as the mathematics of Meaning
 - Propositional logic and satisfiability
 - First-order logic and theorem proving
 - Logic programming
 - Description logics and semantic web
- Planning

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- Planning Frameworks
- Planning Algorithms
- Planning and Acting in the real world

(situating ourselves) (An influential paradigm) (a unifying framework)

(Black Box World States and Actions) (A nice application of search) (Factored World States)

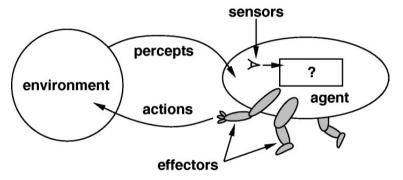
> (Atomic Propositions) (Quantification) (Logic + Search→ Programming)

> > 2025-05-14



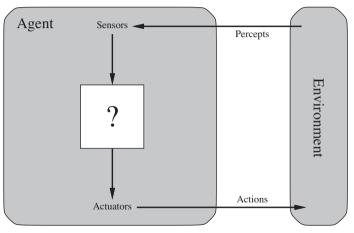
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Agents interact with the environment



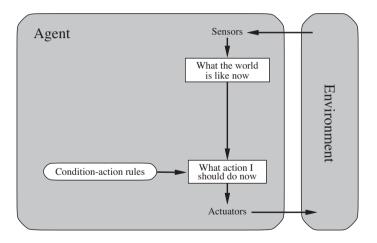


General agent schema



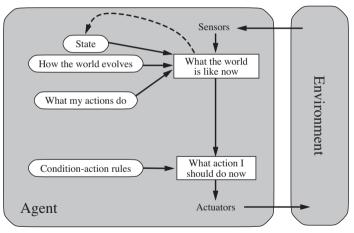
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Reflex Agents



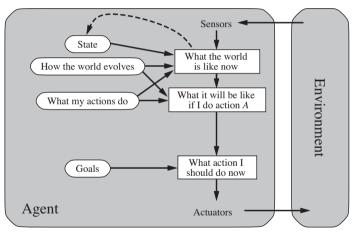


Reflex Agents with State



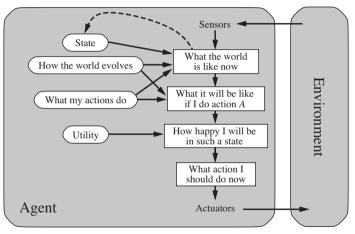
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► Goal-Based Agents



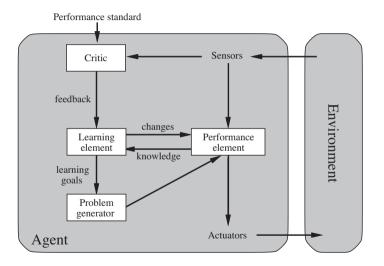
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Utility-Based Agent





Learning Agents





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Idea: Try to design agents that are successful

Definition 0.1. An agent is called rational, if it chooses whichever action maximizes the expected value of the performance measure given the percept sequence to date. This is called the MEU principle.

Note: A rational agent need not be perfect

	only	needs	to	maximize	expected	value
--	------	-------	----	----------	----------	-------

- need not predict e.g. very unlikely but catastrophic events in the future
- percepts may not supply all relevant information
 - if we cannot perceive things we do not need to react to them.
 - but we may need to try to find out about hidden dangers
- action outcomes may not be as expected
 - but we may need to take action to ensure that they do (more often)
- Rational \sim exploration, learning, autonomy

(rational \neq omniscient)

(do the right thing)

```
(Rational \neq clairvoyant)
```

```
(exploration)
(rational \neq successful)
(learning)
```



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- Problem Solving
 - Framework: Problem Solving and Search
 - Variant: Game playing (Adversarial search)

(Black Box States, Transitions, Heuristics) (basic tree/graph walking) (minimax + $\alpha\beta$ -Pruning)



- Problem Solving
 - Framework: Problem Solving and Search
 - Variant: Game playing (Adversarial search)
- Constraint Satisfaction Problems
 - States as partial variable assignments, transitions as assignment
 - Heuristics informed by current restrictions, constraint graph
 - Inference as constraint propagation

(Black Box States, Transitions, Heuristics)

(basic tree/graph walking) (minimax + $\alpha\beta$ -Pruning)

(heuristic search over partial assignments)

(transferring possible values across arcs)



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- Describing world states by formal language
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 - First-order logic and ATP
 - Digression: Logic programming
 - Description logics as moderately expressive, but decidable logics

(Black Box States, Transitions, Heuristics)

(basic tree/graph walking) (minimax + $\alpha\beta$ -Pruning)

(heuristic search over partial assignments)

(transferring possible values across arcs)

(and drawing inferences)

(deciding entailment efficiently) (reasoning about infinite domains) (logic + search)



- Problem Solving
 - Framework: Problem Solving and Search
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 - Digression: Logic programming
 - Description logics as moderately expressive, but decidable logics
- Planning: Problem Solving using white-box world/action descriptions
 - Framework: describing world states in logic as sets of propositions and actions by preconditions and add/delete lists
 - ► Algorithms: e.g heuristic search by problem relaxations

(basic tree/graph walking) (minimax + $\alpha\beta$ -Pruning)

(heuristic search over partial assignments)

(transferring possible values across arcs)

(and drawing inferences)

(deciding entailment efficiently) (reasoning about infinite domains) (logic + search)

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Topics of AI-2 (Summer Semester)

Uncertain Knowledge and Reasoning

- Uncertainty
- Probabilistic reasoning
- Making Decisions in Episodic Environments
- Problem Solving in Sequential Environments
- Foundations of machine learning
 - Learning from Observations
 - Knowledge in Learning
 - Statistical Learning Methods
- Communication
 - Natural Language Processing
 - Natural Language for Communication

(If there is time)

2025-05-14



- Problem Solving under uncertainty (non-observable environment, stochastic states)
 Framework: Probabilistic Inference: Conditional Probabilities/Independence
 - Intuition: Reasoning in Belief Space instead of State Space!
 - Implementation: Bayesian Networks
 - **Extension**: Utilities and Decision Theory

(exploit conditional independence) (for static/episodic environments)



Implementation: Dynamic Bayesian Networks

Problem Solving under uncertainty (non-observable environment, stochastic states)
 Framework: Probabilistic Inference: Conditional Probabilities/Independence
 Intuition: Reasoning in Belief Space instead of State Space!
 Implementation: Bayesian Networks (exploit conditional independence)
 Extension: Utilities and Decision Theory (for static/episodic environments)
 Problem Solving in Sequential Worlds:
 Framework: Markov Processes, transition models
 Extension: MDPs, POMDPs (+ utilities/decisions)



Problem Solving under uncertainty	(non-observable environment, stochastic states)
Framework: Probabilistic Inference: Conditional Proba	abilities/Independence
Intuition: Reasoning in Belief Space instead of State S	Space!
Implementation: Bayesian Networks	(exploit conditional independence)
Extension: Utilities and Decision Theory	(for static/episodic environments)
Problem Solving in Sequential Worlds:	
Framework: Markov Processes, transition models	
Extension: MDPs, POMDPs	(+ utilities/decisions)
Implementation: Dynamic Bayesian Networks	
Machine learning: adding optimization in changing e	environments (unsupervised)
Framework: Learning from Observations	(positive/negative examples)
Intuitions: finding consistent/optimal hypotheses in a	hypothesis space
Problems: consistency, expressivity, under/overfitting,	
Extensions	
knowledge in learning	(based on logical methods)
 statistical learning (optimizin 	ng the probability distribution over hypspace, learning BNs)

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Problem Solving under uncertainty	(non-observab	e environment, stochastic states)
Framework: Probabilistic Inference: Condi	tional Probabilities/Independ	lence
Intuition: Reasoning in Belief Space instea	d of State Space!	
Implementation: Bayesian Networks	•	(exploit conditional independence)
Extension: Utilities and Decision Theory		(for static/episodic environments)
 Problem Solving in Sequential Worlds: 		(for static, episodic environments)
Framework: Markov Processes, transition	models	
Extension: MDPs, POMDPs		(+ utilities/decisions)
Implementation: Dynamic Bayesian Netwo	orks	
► Machine learning: adding optimization in	(unsupervised)	
Framework: Learning from Observations	(positive/negative examples)	
Intuitions: finding consistent/optimal hypo	otheses in a hypothesis space	
Problems: consistency, expressivity, under/		
Extensions	3, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,	
knowledge in learning		(based on logical methods)
statistical learning	(optimizing the probability d	istribution over hypspace, learning BNs)
Communication		
Phenomena of natural language		(NL is interesting/complex)
symbolic/statistical NLP		(historic/as a backup)
Deep Learning for NLP		(the current hype/solution)

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Deep Learning for NLP

Topics of AI-3 – A Course not taught at FAU \odot

- Machine Learning
 - Theory and Practice of Deep Learning
 - More Reinforcement Learning
- Communicating, Perceiving, and Acting
 - More NLP, dialogue, speech acts, …
 - Natural Language Semantics/Pragmatics
 - Perception
 - Robotics
 - Emotions, Sentiment Analysis
- ► The Good News: All is not lost
 - There are tons of specialized courses at FAU
 - Russell/Norvig's AIMA [RusNor:AIMA09] cover some of them as well!

(more as we speak)





