Artificial Intelligence 2
Summer Semester 2024

– Lecture Notes –

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0.1 Preface

Disclaimer: This document is adapted from the notes for the course of the same name by Prof. Dr. Michael Kohlhase. It should be assumed by default that all credit goes primarily to him; whereas all mistakes should be assumed to be mine.

0.1.1 Course Concept

Objective: The course aims at giving students a solid (and often somewhat theoretically oriented) foundation of the basic concepts and practices of artificial intelligence. The course will predominantly cover symbolic AI – also sometimes called "good old-fashioned AI (GofAI)" – in the first semester and offers the very foundations of statistical approaches in the second. Indeed, a full account sub symbolic, machine learning based AI deserves its own specialization courses and needs much more mathematical prerequisites than we can assume in this course.
Context: The course "Artificial Intelligence" (AI 1 & 2) at FAU Erlangen is a two-semester course in the "Wahlpflichtbereich" (specialization phase) in semesters 5/6 of the Bachelor program "Computer Science" at FAU Erlangen. It is also available as a (somewhat remedial) course in the "Vertiefungsmodul Künstliche Intelligenz" in the Computer Science Master's program.
Prerequisites: AI-1 & 2 builds on the mandatory courses in the FAU Bachelor's program, in particular the course "Grundlagen der Logik in der Informatik" [Glo], which already covers a lot of the materials usually presented in the "knowledge and reasoning" part of an introductory AI course. The AI 1& 2 course also minimizes overlap with the course.

The course is relatively elementary, we expect that any student who attended the mandatory CS courses at FAU Erlangen can follow it.
Open to external students:

Other Bachelor programs are increasingly co-opting the course as specialization option. There is no inherent restriction to computer science students in this course. Students with other study biographies – e.g. students from other Bachelor programs our external Master's students should be able to pick up the prerequisites when needed.

0.1.2 Course Contents

Goal: To give students a solid foundation of the basic concepts and practices of the field of Artificial Intelligence. The course will be based on Russell/Norvig's book "*Artificial Intelligence; A modern Approach*" [RN09]
Artificial Intelligence I (the first semester): introduces AI as an area of study, discusses "rational agents" as a unifying conceptual paradigm for AI and covers problem solving, search, constraint propagation, logic, knowledge representation, and planning.
Artificial Intelligence II (the second semester): is more oriented towards exposing students to the basics of statistically based AI: We start out with reasoning under uncertainty, setting the foundation with Bayesian Networks and extending this to rational decision theory. Building on this we cover the basics of machine learning.

0.1.3 This Document

Format: The document mixes the slides presented in class with comments of the instructor to give students a more complete background reference.
Caveat: This document is made available for the students of this course only. It is still very much a draft and will develop over the course of the current course and in coming academic years. **Licensing:** This document is licensed under a Creative Commons license that requires attribution, allows commercial use, and allows derivative works as long as these are licensed under the same license. **Knowledge Representation Experiment:** This document is also an experiment in knowledge representation. Under the hood, it uses the sTeX package [Koh08; sTeX], a TeX/LaTeX extension for semantic markup, which allows to export the contents into

active documents that adapt to the reader and can be instrumented with services based on the explicitly represented meaning of the documents.

0.1.4 Acknowledgments

Materials: Most of the materials in this course is based on Russel/Norvik's book "Artificial Intelligence — A Modern Approach" (AIMA [RN95]). Even the slides are based on a LaTeX-based slide set, but heavily edited. The section on search algorithms is based on materials obtained from Bernhard Beckert (then Uni Koblenz), which is in turn based on AIMA. Some extensions have been inspired by an AI course by Jörg Hoffmann and Wolfgang Wahlster at Saarland University in 2016. Finally Dennis Müller suggested and supplied some extensions on AGI. Florian Rabe, Max Rapp and Katja Berčič have carefully re-read the text and pointed out problems.

All course materials have bee restructured and semantically annotated in the sTeX format, so that we can base additional semantic services on them.

AI Students: The following students have submitted corrections and suggestions to this and earlier versions of the notes: Rares Ambrus, Ioan Sucan, Yashodan Nevatia, Dennis Müller, Simon Rainer, Demian Vöhringer, Lorenz Gorse, Philipp Reger, Benedikt Lorch, Maximilian Lösch, Luca Reeb, Marius Frinken, Peter Eichinger, Oskar Herrmann, Daniel Höfer, Stephan Mattejat, Matthias Sonntag, Jan Urfei, Tanja Würsching, Adrian Kretschmer, Tobias Schmidt, Maxim Onciul, Armin Roth, Liam Corona, Tobias Völk, Lena Voigt, Yinan Shao, Michael Girstl, Matthias Vietz, Anatoliy Cherepantsev, Stefan Musevski, Matthias Lobenhofer, Philipp Kaludercic, Diwarkara Reddy, Martin Helmke, Stefan Müller, Dominik Mehlich, Paul Martini, Vishwang Dave, Arthur Miehlich, Christian Schabesberger, Vishaal Saravanan, Simon Heilig, Michelle Fribrance, Wenwen Wang, Xinyuan Tu, Lobna Eldeeb.

0.1.5 Recorded Syllabus

The recorded syllabus – a record the progress of the course in the academic year 2024– is in the course page in the ALeA system at `https://courses.voll-ki.fau.de/course-home/ai-1`. The table of contents in the AI-2 notes at `https://courses.voll-ki.fau.de` indicates the material covered to date in yellow.

The recorded syllabus of AI-2 can be found at `https://courses.voll-ki.fau.de/course-home/ai-2`. For the topics planned for this course, see subsection 0.1.2.

Contents

Chapter 1

Administrativa

We will now go through the ground rules for the course. This is a kind of a social contract between the instructor and the students. Both have to keep their side of the deal to make learning as efficient and painless as possible.

About this course...

- ▷ AI1 and AI2 are "traditionally" taught by Prof. Michael Kohlhase (since 2016, on sabbatical this semester)
- ▷ This is the first time I'm teaching AI2 as a lecturer! ☺

But I've been a member of Prof. Kohlhase's research group since 2015 (Ph.D. 2019)

⇒ I'm familiar with the course content (Lead TA 2016 – 2019)

⇒ I've adopted *and adapted* his course material. The topics are the same, *but* I changed some notations, clarified and changed some definitions, restructured some parts (Hopefully for the better!)

⇒ Feel free to check out older versions of the course material *but* don't rely on them *entirely* (especially for exam prep!)

Also: I'm working on my habilitation currently

⇒ Teaching this course is part of that

⇒ Please take the course evaluation seriously ;) (I'm still learning and it helps me improve!)

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Dates, Links, Materials

- ▷ **Lectures**: Tuesday 16:15 – 17:45 **H9**, Thursday 10:15 – 11:45 **H8**
- ▷ **Tutorials**:
  - ▷ Friday 10:15 – 11:45 *Room 11501.02.019*
  - ▷ Friday 14:15 – 15:45 *Zoom:* `https://fau.zoom.us/j/97169402146`
  - ▷ Monday 12:15 – 13:45 *Room H4*

- Tuesday 08:15 – 09:45 *Room 11302.02.134-113*

(Starting thursday in week 2 (25.04.2024))

- **studon**: `https://www.studon.fau.de/studon/goto.php?target=crs_5645530` (Used for announcements, e.g. homeworks, and homework submissions)
- **Video streams / recordings**: `https://www.fau.tv/course/id/3816`
- **Lecture notes / slides / exercises:** `https://kwarc.info/teaching/AI/` (Most importantly: `notes2.pdf` and `slides2.pdf`)
- **ALeA**: `https://courses.voll-ki.fau.de/course-home/ai-2`: Lecture notes, forum, **tuesday quizzes**, flashcards,...

Textbook: *Russel/Norvig: Artificial Intelligence, A modern Approach* [RN09]. Make sure that you read the edition ≥ 3 $\leadsto$ vastly improved over ≤ 2.

AI-2 Homework Assignments

Homework Assignments: Every thursday (starting in the second week)
Small individual problem/programming/proof tasks

⚠ Homeworks give no bonus points, but without trying you are unlikely to pass the exam.

Homework/Tutorial Discipline:

- Start early! (many assignments need more than one evening's work)
- Don't start by sitting at a blank screen (talking & study group help)
- Humans will be trying to understand the text/code/math when grading it. (For those that *do* get graded – see later)
- Go to the tutorials, discuss with your TA! (they are there for you!)

- Homeworks will be posted on `kwarc.info/teaching/AI/assignments`. (Announced on studon)
- Sign up for AI-2 under `https://www.studon.fau.de/crs4941850.html`.
- Homeworks are handed in electronically there. (plain text, program files, PDF)
- Do not sign up for the "AI-2 Übungen" on StudOn (we do not use them)

It is very well-established experience that without doing the homework assignments (or something similar) on your own, you will not master the concepts, you will not even be able to ask sensible questions, and take very little home from the course. Just sitting in the course and nodding is not enough! If you have questions please make sure you discuss them with the instructor, the teaching assistants, or your fellow students. There are three sensible venues for such discussions: online in the lecture, in the tutorials, which we discuss now, or in the course forum – see below. Finally, it is always a very good idea to form study groups with your friends.

Tutorials for Artificial Intelligence 1

Weekly tutorials starting in week two – Lead TA: Florian Rabe (KWARC Postdoc, Privat-dozent) (Room: 11.137 @ Händler building, florian.rabe@fau.de)

The tutorials:

- ▷ reinforce what was taught in class.
- ▷ allow you to ask any question you have in a protected environment.
- ▷ discuss the (solutions to) *homework assignments*

Caveat: We cannot grade all submissions :((too many students, too few TAs)
Group submission has not worked well in the past (too many freeloaders)
Likely solution: We will grade *one* exercise per week – but you should attempt all of them!

Life-saving advice: Go to your tutorial, and prepare for it by having looked at the slides and the homework assignments!

Doing your homework is probably even *more* important (and predictive of exam success) than attending the lecture!

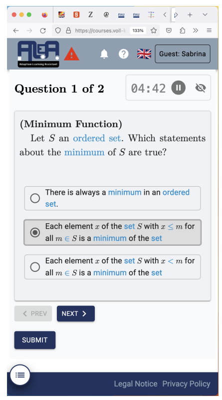
Tuesday Quizzes

Tuesday Quizzes: Every tuesday we start the lecture with a 10 min online quiz – the tuesday quiz – about the material from the previous week. (starts in week 2) **Motivations:** We do this to

- ▷ keep you prepared and working continuously. (primary)
- ▷ update the ALeA learner model (fringe benefit)
- ▷ give *bonus points* for the exam! (as an incentive)

The tuesday quiz will be given in the ALEA system

- ▷ https://courses.voll-ki.fau.de/quiz-dash/ai-2
- ▷ You have to be logged into ALEA!
- ▷ You can take the quiz on your laptop or phone, ...
- ▷ ... in the lecture or at home ...
- ▷ ... via WLAN or 4G Network. (do not overload)
- ▷ Quizzes will only be available 16:15-16:25!



Now we come to a topic that is always interesting to the students: the grading scheme.

Assessment, Grades

- ▷ **Overall (Module) Grade:**
  - ▷ Grade via the exam (Klausur) $\rightsquigarrow$ 100% of the grade.
  - ▷ Up to 10% bonus on-top for an exam with $\geq 50\%$ points. ($\leq 50\% \rightsquigarrow$ no bonus)
  - ▷ Bonus points $\widehat{=}$ percentage sum of the best 10 tuesday quizzes divided by 100.
- ▷ **Exam:** 90 minutes exam conducted in presence on paper ($\sim$ Oct. 1. 2023)
- ▷ **Retake Exam:** 90 min exam six months later ($\sim$ April 1. 2024)
- ▷ ⚠ You have to register for exams in campo in the first month of classes.
- ▷ **Note:** You can de-register from an exam on campo up to three working days before.

Due to the current AI hype, the course Artificial Intelligence is very popular and thus many degree programs at FAU have adopted it for their curricula. Sometimes the course setup that fits for the CS program does not fit the other's very well, therefore there are some special conditions. I want to state here.

⚠ Special Admin Conditions ⚠

- ▷ Some degree programs do not "import" the course Artificial Intelligence, and thus you may not be able to register for the exam via `https://campus.fau.de`.

- ▷ Just send me an e-mail and come to the exam, we will issue a "Schein".
- ▷ 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 $\rightsquigarrow$ $7.5 + 7.5 = 15$.

I can only warn of what I am aware, so if your degree program lets you jump through extra hoops, please tell me and then I can mention them here.

The ALeA System

Prerequisites

▷ **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.)

The following should therefore be seen as "*weak prerequisites*":

▷ AI-1 (in particular: PEAS, propositional logic/first-order logic (mostly the syntax), some logic programming)

▷ (very) elementary complexity theory. (big Oh and friends)

▷ rudimentary probability theory (e.g. from stochastics)

▷ basic linear algebra (vectors, matrices,...)

▷ basic real analysis (primarily:(partial) derivatives)

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.

"Strict" Prerequisites

▷ **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.

- motivation, interest, curiosity, hard work. (AI-2 is non-trivial)

Note: Grades correlate significantly with invested effort; including, but not limited to: time spent on exercises, being here, asking questions, talking to your peers,...

What you should learn here...

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

In other words: Many things you learn here are *means to an end* (e.g. understanding the underlying *ideas* behind algorithms), not the end itself. But the best way to understand these means is to first treat them as an end in themselves.

Compare two employees

"We have the following problem and we need a solution: ..."

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 15`unit`, or I will need to retrain on a bigger input layer..."

Employee 2: "...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 1000`unit`, you might need a slightly bigger potato though..."

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

Obviously, that is not to say that machine learning is not a useful tool! (It is!)

If your job is to e.g. filter customer support requests, or to recognize cats in pictures, trying to write a prolog program from scratch is probably the wrong approach: Just use a language model / image model and finetune it on a classification head.

But it is also not the only tool, and it is not always the right tool for the job – despite what some people might tell you. And even in scenarios where machine learning *can* yield decent results, it is not always the *best* tool. (Some people care about efficiency, explainability, etc ;))

Do use the opportunity to discuss the AI-2 topics with others. After all, one of the non-trivial skills you want to learn in the course is how to talk about Artificial Intelligence topics. And that takes practice, practice, and practice.

Chapter 2

Overview over AI and Topics of AI-II

We restart the new semester by reminding ourselves of (the problems, methods, and issues of) Artificial Intelligence, and what has been achived so far.

2.1 What is Artificial Intelligence?

A Video Nugget covering this section can be found at `https://fau.tv/clip/id/21701`.
The first question we have to ask ourselves is "What is Artificial Intelligence?", i.e. how can we define it. And already that poses a problem since the natural definition *like human intelligence, but artificially realized* presupposes a definition of intelligence, which is equally problematic; even Psychologists and Philosophers – the subjects nominally "in charge" of natural intelligence – have problems defining it, as witnessed by the plethora of theories e.g. found at [WHI].

What is Artificial Intelligence? Definition

- ▷ **Definition 2.1.1 (According to Wikipedia).** Artificial Intelligence (AI) is intelligence exhibited by machines
- ▷ **Definition 2.1.2 (also).** Artificial Intelligence (AI) is a sub-field of computer science that is concerned with the automation of intelligent behavior.
- ▷ **BUT:** it is already difficult to define intelligence precisely.
- ▷ **Definition 2.1.3 (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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Maybe we can get around the problems of defining "what artificial intelligence is", by just describing the necessary components of AI (and how they interact). Let's have a try to see whether that is more informative.

What is Artificial Intelligence? Components

▷ **Elaine Rich:** AI studies how we can make the computer do things that humans can still do better at the moment.

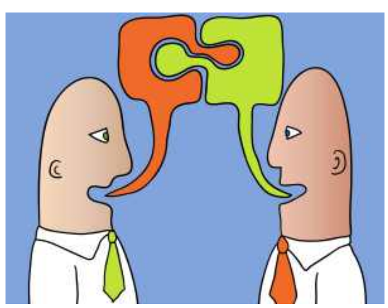
▷ This needs a combination of

the ability to learn

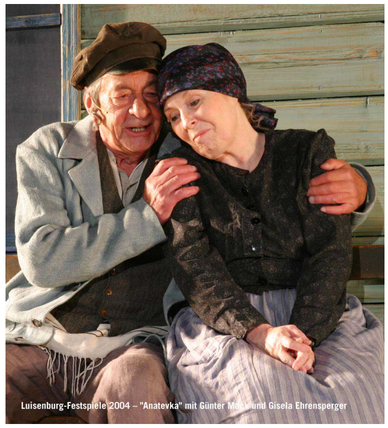
Inference

Perception

Language understanding



Emotion

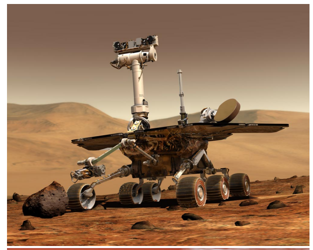


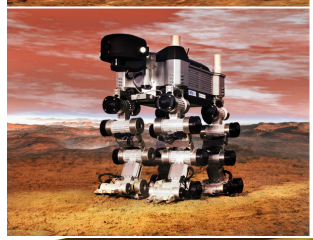
Note that list of components is controversial as well. Some say that it lumps together cognitive capacities that should be distinguished or forgets others, ... We state it here much more to get AI-2 students to think about the issues than to make it normative.

2.2 Artificial Intelligence is here today!

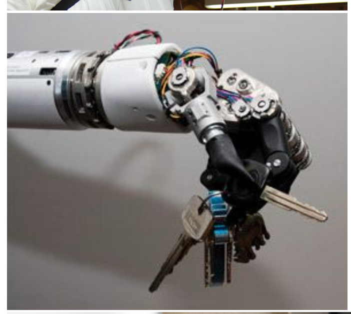
A Video Nugget covering this section can be found at `https://fau.tv/clip/id/21697`.
The components of Artificial Intelligence are quite daunting, and none of them are fully understood, much less achieved artificially. But for some tasks we can get by with much less. And indeed that is what the field of Artificial Intelligence does in practice – but keeps the lofty ideal around. This practice of "trying to achieve AI in selected and restricted domains" (cf. the discussion starting with slide **??**) has borne rich fruits: systems that meet or exceed human capabilities in such areas. Such systems are in common use in many domains of application.

Artificial Intelligence is here today!



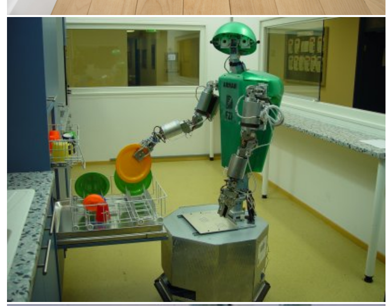


- ▷ in outer space
  - ▹ in outer space systems need autonomous control:
  - ▹ remote control impossible due to time lag



- ▷ in artificial limbs
  - ▹ the user controls the prosthesis via existing nerves, can e.g. grip a sheet of paper.

- ▷ in household appliances
  - ▹ The iRobot Roomba vacuums, mops, and sweeps in corners, . . . , parks, charges, and discharges.
  - ▹ general robotic household help is on the horizon.



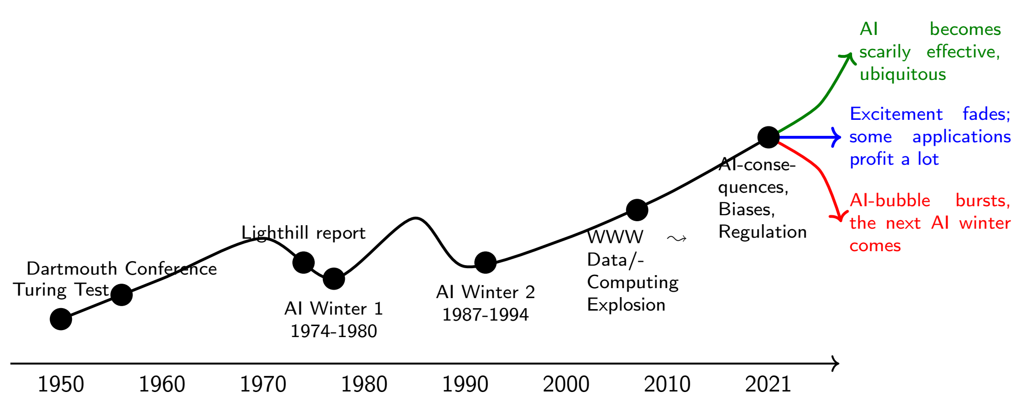
- ▷ in hospitals
  - ▹ in the USA 90% of the prostate operations are carried out by RoboDoc
  - ▹ Paro is a cuddly robot that eases solitude in nursing homes.

We will conclude this section with a note of caution.

The AI Conundrum

- ▷ **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:** AI still asks the big questions.
- ▷ **Another Consequence:** AI as a field is an incubator for many innovative technologies.
- ▷ **AI Conundrum:** Once AI solves a subfield it is called "computer science". (becomes a separate subfield of CS)
- ▷ **Example 2.2.1.** Functional/Logic Programming, automated theorem proving, Planning, machine learning, Knowledge Representation, . . .
- ▷ **Still Consequence:** AI research was alternatingly flooded with money and cut off brutally.

The current AI Hype — Part of a longer Story



2.3 Ways to Attack the AI Problem

A Video Nugget covering this section can be found at `https://fau.tv/clip/id/21717`.

There are currently three main avenues of attack to the problem of building artificially intelligent systems. The (historically) first is based on the symbolic representation of knowledge about the world and uses inference-based methods to derive new knowledge on which to base action decisions. The second uses statistical methods to deal with uncertainty about the world state and learning methods to derive new (uncertain) world assumptions to act on.

Four Main Approaches to Artificial Intelligence

- **Definition 2.3.1.** 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.
- **Definition 2.3.2.** 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.
- **Definition 2.3.3.** 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.
- **Definition 2.3.4.** 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.

As a consequence, the field of Artificial Intelligence (AI) is an engineering field at the intersection of computer science (logic, programming, applied statistics), cognitive science (psychology, neuroscience), philosophy (can machines think, what does that mean?), linguistics (natural language understanding), and mechatronics (robot hardware, sensors).
Subsymbolic AI and in particular machine learning is currently hyped to such an extent, that many people take it to be synonymous with "Artificial Intelligence". It is one of the goals of this course to show students that this is a very impoverished view.

Two ways of reaching Artificial Intelligence?

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

Deep	symbolic AI-1	not there yet cooperation?
Shallow	no-one wants this	statistical/sub symbolic AI-2
Analysis ↑ vs. Coverage →	Narrow	Wide

- **This semester** we will cover foundational aspects of symbolic AI (deep/narrow processing)

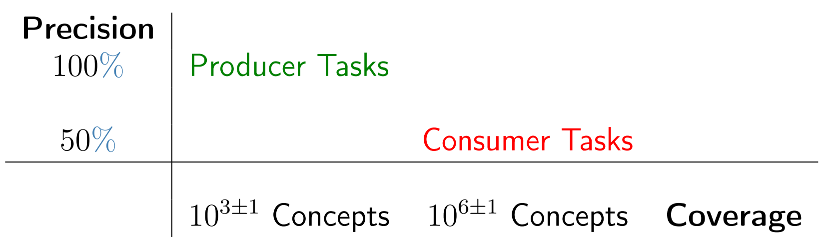
▷ **next semester** concentrate on statistical/subsymbolic AI. (shallow/wide-coverage)

We combine the topics in this way in this course, not only because this reproduces the historical development but also as the methods of statistical and subsymbolic AI share a common basis.
It is important to notice that all approaches to AI have their application domains and strong points. We will now see that exactly the two areas, where symbolic AI and statistical/subsymbolic AI have their respective fortes correspond to natural application areas.

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)



▷ **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.

An example of a producer task – indeed this is where the name comes from – is the case of a machine tool manufacturer T, which produces digitally programmed machine tools worth multiple million Euro and sells them into dozens of countries. Thus T must also comprehensive machine operation manuals, a non-trivial undertaking, since no two machines are identical and they must be translated into many languages, leading to hundreds of documents. As those manual share a lot of semantic content, their management should be supported by AI techniques. It is critical that these methods maintain a high precision, operation errors can easily lead to very costly machine damage and loss of production. On the other hand, the domain of these manuals is quite restricted. A machine tool has a couple of hundred components only that can be described by a comple of thousand attribute only.

Indeed companies like T employ high-precision AI techniques like the ones we will cover in this course successfully; they are just not so much in the public eye as the consumer tasks.

2.4 AI in the KWARC Group

The KWARC Research 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 (too tedious)
  - User support and quality control instead of "The Truth" (elusive anyway)
  - use Mathematics as a test tube (Mathematics $\widehat{=}$ Anything Formal)
  - 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

Overview: KWARC Research and Projects

<table>
<tr><td colspan="3">Applications: eMath 3.0, Active Documents, Active Learning, Semantic Spreadsheets/CAD/CAM, Change Mangagement, Global Digital Math Library, Math Search Systems, SMGloM: Semantic Multilingual Math Glossary, Serious Games, . . .</td></tr>
<tr><td>Foundations of Math:
▷ MathML, OpenMath
▷ advanced Type Theories
▷ MMT: Meta Meta Theory
▷ Logic Morphisms/Atlas
▷ Theorem Prover/CAS Interoperability
▷ Mathematical Models/Simulation</td><td>KM & Interaction:
▷ Semantic Interpretation (aka. Framing)
▷ math-literate interaction
▷ MathHub: math archives & active docs
▷ Active documents: embedded semantic services
▷ Model-based Education</td><td>Semantization:
▷ LaTeXML: LaTeX ⇝ XML
▷ sTeX: Semantic LaTeX
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▷ Context-Aware IDEs
▷ Mathematical Corpora
▷ Linguistics of Math
▷ ML for Math Semantics Extraction</td></tr>
<tr><td colspan="3">Foundations: Computational Logic, Web Technologies, OMDoc/MMT</td></tr>
</table>

Research Topics in the KWARC Group

- 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, ...

▷ We always try to find a topic at the intersection of your and our interests.

▷ We also often have positions!. (HiWi, Ph.D.: $\frac{1}{2}$, PostDoc: full)

2.5 Agents and Environments in AI2

This part of the course notes addresses inference and agent decision making in partially observable environments, i.e. where we only know probabilities instead of certainties whether propositions are true/false. We cover basic probability theory and – based on that – Bayesian Networks and simple decision making in such environments. Finally we extend this to probabilistic temporal models and their decision theory.

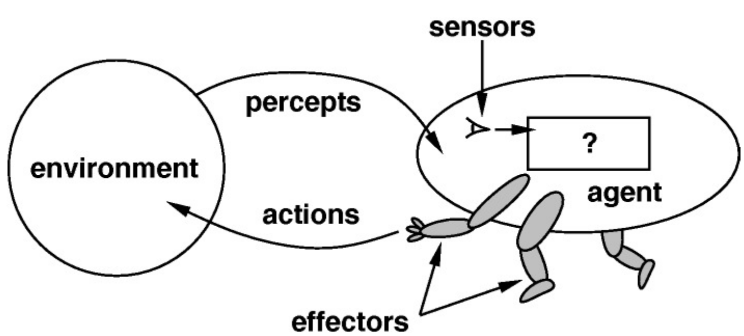
2.5.1 Recap: Rational Agents as a Conceptual Framework

A Video Nugget covering this subsection can be found at `https://fau.tv/clip/id/27585`.

Agents and Environments

▷ **Definition 2.5.1.** An agent is anything that

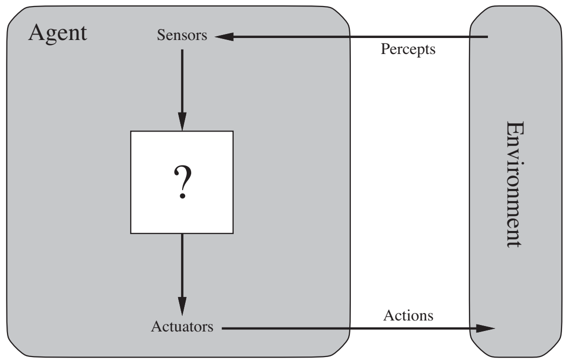
- ▷ perceives its environment via sensors (a means of sensing the environment)
- ▷ acts on it with actuators (means of changing the environment).



▷ **Example 2.5.2.** Agents include humans, robots, softbots, thermostats, etc.

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.

Rationality

- **Idea:** Try to design agents that are successful! (aka. "do the right thing")
- **Definition 2.5.3.** A performance measure is a function that evaluates a sequence of environments.
- **Example 2.5.4.** 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 2.5.5.** An agent is called rational, if it chooses whichever action maximizes the expected value of the performance measure given the percept sequence to date.
- **Question:** Why is rationality a good quality to aim for?

Possible Consequences of Rationality: Exploration, Learning, Autonomy

- **Note:** a rational agent need not be perfect
  - 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:** rational may entail exploration, learning, autonomy (depending on the environment / task)
- ▷ **Definition 2.5.6.** An agent is called autonomous, if it does not rely on the prior knowledge about the environment of the designer.
- ▷ 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.

PEAS: Describing the Task Environment

- ▷ **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 2.5.7.** 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 2.5.8 (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

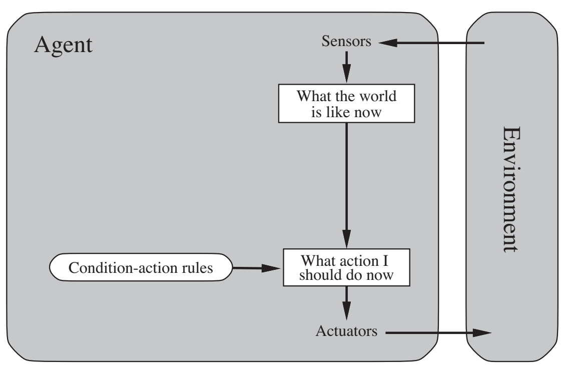
- ▷ **Observation 2.5.9.** *Agent design is largely determined by the type of environment it is intended for.*
- ▷ **Problem:** There is a vast number of possible kinds of environments in AI.
- ▷ **Solution:** Classify along a few "dimensions". (independent characteristics)
- ▷ **Definition 2.5.10.** 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 (when must we count parts of e as agents?)

Simple reflex agents

▷ **Definition 2.5.11.** A simple reflex agent is an agent a that only bases its actions on the last percept: so the agent function simplifies to $f_a : \mathcal{P} \to \mathcal{A}$.

▷ **Agent Schema:**



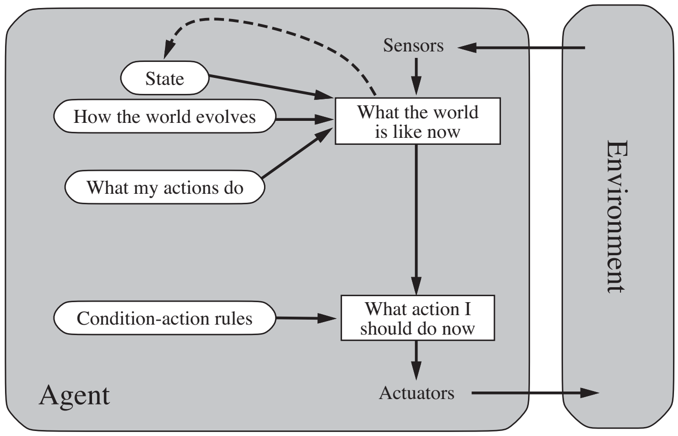
▷ **Example 2.5.12 (Agent Program).**

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:**



Model-based Reflex Agents: Definition

- **Definition 2.5.13.** A model-based agent is an agent whose actions depend on
  - a world model: a set $\mathcal{S}$ of possible states.
  - a sensor model S that given a state s and a percepts p determines a new state $S(s, p)$.
  - a transition model T, that predicts a new state $T(s, a)$ from a state s and an action a.
  - An action function f that maps (new) states to an actions.

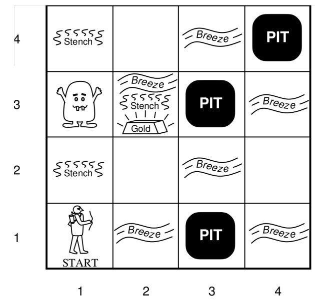
  If the world model of a model-based agent A is in state s and A has taken action a, A will transition to state $s' = T(S(p, s), a)$ and take action $a' = f(s')$.
- **Note:** As different percept sequences lead to different states, so the agent function $f_a : \mathcal{P}^* \to \mathcal{A}$ no longer depends only on the last percept.
- **Example 2.5.14 (Tail Lights Again).** Model-based agents can do the ?? if the states include a concept of tail light brightness.

2.5.2 Sources of Uncertainty

A Video Nugget covering this subsection can be found at https://fau.tv/clip/id/27582.

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."
- ▷ **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]."
- ▷ **Uncertainty about the domain behavior:**
  - ▷ "Are you *sure* the Wumpus never moves?"

Unreliable Sensors

- ▷ **Robot Localization:** Suppose we want to support localization using landmarks to narrow down the area.
- ▷ **Example 2.5.15.** *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.

2.5.3 Agent Architectures based on Belief States

We are now ready to proceed to environments which can only partially observed and where are our actions are non deterministic. Both sources of uncertainty conspire to allow us only partial knowledge about the world, so that we can only optimize "expected utility" instead of "actual utility" of our actions.

World Models for Uncertainty

- **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 2.5.16.** 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, and
  - a sensor model that updates the belief state based on sensor information
  - 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 member the world state) and the transition model is a function from states and actions to states: a transition function.

That is exactly what we have been doing until now: we have been studying methods that build on descriptions of the "actual" world, and have been concentrating on the progression from atomic to factored and ultimately structured representations. Tellingly, we spoke of "world states" instead of "belief states"; we have now justified this practice in the brave new belief-based world models by the (re-) definition of "world states" above. To fortify our intuitions, let us recap from a belief-state-model perspective.

World Models by Agent Type in AI-1

- **Search-based Agents:** In a fully observable, deterministic environment
  - goal-based agent with world state $\widehat{=}$ "current state"
  - 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 $\widehat{=}$ constraint propagation. (goal $\widehat{=}$ satisfying assignment)
- **Logic-based Agents:** In a fully observable, deterministic environment
  - model-based agent with world state $\widehat{=}$ logical formula
  - inference $\widehat{=}$ e.g. DPLL or resolution.
- **Planning Agents:** In a fully observable, deterministic, environment
  - goal-based agent with world state $\widehat{=}$ PL0, transition model $\widehat{=}$ STRIPS,
  - inference $\widehat{=}$ state/plan space search. (goal: complete plan/execution)

Let us now see what happens when we lift the restrictions of total observability and determinism.

World Models for Complex Environments

- ▷ In a fully observable, but stochastic environment,
  - ▷ the belief state must deal with a set of possible states.
  - ▷ $\leadsto$ 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. (sensor model + transition relation)

Preview: New World Models (Belief) $\leadsto$ new Agent Types

- ▷ **Probabilistic Agents:** In a partially observable environment
  - ▷ belief state $\widehat{=}$ Bayesian networks,
  - ▷ inference $\widehat{=}$ probabilistic inference.
- ▷ **Decision-Theoretic Agents:** In a partially observable, stochastic environment
  - ▷ belief state + transition model $\widehat{=}$ decision networks,
  - ▷ inference $\widehat{=}$ maximizing expected utility.
- ▷ We will study them in detail this semester.

Overview: AI2

- ▷ Basics of probability theory (probability spaces, random variables, conditional probabilities, independence,...)
- ▷ 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)

- ▷ Decision theory: Making decisions under uncertainty (Preferences, Utilities, Decision networks, Markov Decision Procedures,...)

⇒ We can choose the right action based on our world model and the likely outcomes of our actions

- ▷ Machine learning: Learning from data (Decision Trees, Classifiers, Neural Networks,...)

Part I

Reasoning with Uncertain Knowledge

This part of the course notes addresses inference and agent decision making in partially observable environments, i.e. where we only know probabilities instead of certainties whether propositions are true/false. We cover basic probability theory and – based on that – Bayesian Networks and simple decision making in such environments. Finally we extend this to probabilistic temporal models and their decision theory.

Chapter 3

Quantifying Uncertainty

3.1 Probability Theory

Probabilistic Models

- **Definition 3.1.1 (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 $\mathcal{P}(\Omega) \to [0,1]$, 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 $\omega \in \Omega$. $P(X)$ 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 3.1.2 (Dice throws).** Assume we throw a (fair) die two times. Then the sample space is $\{(i,j)|1 \leq i,j \leq 6\}$. 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

The definition is simplified in two places: Firstly, we assume that P is defined on the full power set. This is not always possible, especially if Ω is uncountable. In that case we need an additional set of "events" instead, and lots of mathematical machinery to make sure that we can safely take unions, intersections, complements etc. of these events.

Secondly, we would technically only demand that P is additive on countably many disjoint sets.

In this course we will assume that our sample space is at most countable anyway; usually even finite.

Random Variables

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 3.1.3.** The probability that the *sum* of our two dice throws is 7 is $P(\{(i,j) \in \Omega | i+j=7\}) = P(\{(6,1),(1,6),(5,2),(2,5),(4,3),(3,4)\}) = \frac{6}{36} = \frac{1}{6}$.

▷ **Definition 3.1.4 (Again, slightly simplified).** Let D be a set. A random variable is a function $X\colon \Omega \to D$. We call D (somewhat confusingly) the domain of X, denoted $\mathrm{dom}(X)$.

For $x \in D$, we define the probability of x as $P(X=x) := P(\{\omega \in \Omega | X(\omega) = x\})$.

▷ **Definition 3.1.5.** We say that a random variable X is finite domain, iff its domain $\mathrm{dom}(X)$ is finite and Boolean, iff $\mathrm{dom}(X) = \{\mathsf{T},\mathsf{F}\}$.

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

Note that a random variable, according to the formal definition, is *neither* random *nor* a variable: It is a function with clearly defined domain and codomain – and what we call the domain of the "variable" is actually its codomain... are you confused yet? ☺

This confusion is a side-effect of the *mathematical* formalism. In practice, a random variable is some indeterminate value that results from some statistical experiment – i.e. it is *random*, because the result is not predetermined, and it is a variable, because it can take on different values.

It just so happens that if we want to model this scenario *mathematically*, a function is the most natural way to do so.

Some Examples

▷ **Example 3.1.6.** Summing up our two dice throws is a random variable $S\colon \Omega \to [2,12]$ with $S((i,j)) = i+j$. The probability that they sum up to 7 is written as $P(S=7) = \frac{1}{6}$.

▷ **Example 3.1.7.** The first and second of our two dice throws are random variables $\mathrm{First}, \mathrm{Second}\colon \Omega \to [1,6]$ with $\mathrm{First}((i,j)) = i$ and $\mathrm{Second}((i,j)) = j$.

▷ *Remark 3.1.8.* Note, that the *identity* $\Omega \to \Omega$ is a random variable as well.

▷ **Example 3.1.9.** We can model toothache, cavity and gingivitis as Boolean random variables, with the underlying probability space being...?? ¯_(ツ)_/¯

▷ **Example 3.1.10.** We can model tomorrow's weather as a random variable with domain $\{\mathtt{sunny}, \mathtt{rainy}, \mathtt{foggy}, \mathtt{warm}, \mathtt{cloudy}, \mathtt{humid}, ...\}$, with the underlying probability space being...?? ¯_(ツ)_/¯

⇒ 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*.

Propositions

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 3.1.11. We can express the above as: $P(\neg(\text{First} = 3) \wedge \neg(\text{Second} = 3) \wedge (S = 7))$

Definition 3.1.12. 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. $P(X_1 \neq x_1) {:=} P(\neg(X_1 = x_1)) := P(\{\omega \in \Omega | X_1(\omega) \neq x_1\}) = 1 - P(X_1 = x_1)$.
2. $P((X_1 = x_1) \wedge (X_2 = x_2)) := P(\{\omega \in \Omega | (X_1(\omega) = x_1) \wedge (X_2(\omega) = x_2)\}) = P(\{\omega \in \Omega | X_1(\omega) = x_1\} \cap \{\omega \in \Omega | X_2(\omega) = x_2\})$.
3. $P((X_1 = x_1) \vee (X_2 = x_2)) := P(\{\omega \in \Omega | (X_1(\omega) = x_1) \vee (X_2(\omega) = x_2)\}) = P(\{\omega \in \Omega | X_1(\omega) = x_1\} \cup \{\omega \in \Omega | X_2(\omega) = x_2\})$.

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

Example 3.1.13. $P((\text{First} \neq 3) \wedge (\text{Second} \neq 3) \wedge (S = 7)) = P(\{(1,6), (6,1), (2,5), (5,2)\}) = \frac{1}{9}$

Events

Definition 3.1.14 (Again slightly simplified). Let $\langle \Omega, P \rangle$ be a probability space. An event is a subset of Ω.

Definition 3.1.15 (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 $A \vee B := \neg(\neg A \wedge \neg B)$, $\mathsf{T} := A \vee \neg A$ and $\mathsf{F} := \neg \mathsf{T}$ – 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 $P(A \vee B) = P(A) + P(B) - P(A \wedge B)$.

Problem 1.3

Show that $P(A) = P(A \wedge B) + P(A \wedge \neg B)$

Conditional Probabilities

▷ As we gather new information, our beliefs (*should*) change, and thus our probabilities!

▷ **Example 3.1.16.** Your "probability of missing the connection train" increases when you are informed that your current train has 30 minutes delay.

▷ **Example 3.1.17.** The "probability of cavity" increases when the doctor is informed that the patient has a toothache.

▷ **Example 3.1.18.** The probability that $S = 3$ is clearly higher if I know that $\mathrm{First} = 1$ than otherwise – or if I know that $\mathrm{First} = 6$!

▷ **Definition 3.1.19.** Let A and B be events where $P(B) \neq 0$. The conditional probability of A given B is defined as:

$$P(A|B){:=}\frac{P(A \wedge B)}{P(B)}$$

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

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

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")

Examples

▷ **Example 3.1.20.** If we assume $\mathrm{First} = 1$, then $P(S = 3|\mathrm{First} = 1)$ should be precisely $P(\mathrm{Second} = 2) = \frac{1}{6}$. We check:

$$P(S = 3|\mathrm{First} = 1) = \frac{P((S = 3) \wedge (\mathrm{First} = 1))}{P(\mathrm{First} = 1)} = \frac{1/36}{1/6} = \frac{1}{6}$$

▷ **Example 3.1.21.** Assume the prior probability $P(\mathrm{cavity})$ is 0.122. The probability that a patient has both a cavity and a toothache is $P(\mathrm{cavity} \wedge \mathrm{toothache}) = 0.067$. The probability that a patient has a toothache is $P(\mathrm{toothache}) = 0.15$.

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

$$P(\mathrm{cavity}|\mathrm{toothache}) = \frac{P(\mathrm{cavity} \wedge \mathrm{toothache})}{P(\mathrm{toothache})} = \frac{0.067}{0.15} = 0.45.$$

▷ **Note:** We just computed the probability of some underlying *disease* based on the presence of a *symptom*!

Or 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:

- ▷ $P(A|C) = 1 - P(\neg A|C)$.
- ▷ $P(A|C) = P(A \wedge B|C) + P(A \wedge \neg B|C)$.
- ▷ $P(A \vee B|C) = P(A|C) + P(B|C) - P(A \wedge B|C)$.

But **not on the right hand side!**

Problem 1.5

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

- ▷ $P(A|C) = 1 - P(A|\neg C)$
- ▷ $P(A|C) = P(A|B \wedge C) + P(A|B \wedge \neg C)$.
- ▷ $P(A|B \vee C) = P(A|B) + P(A|C) - P(A|B \wedge C)$.

Bayes' Rule

- ▷ **Note:** By definition, $P(A|B) = \frac{P(A \wedge B)}{P(B)}$. In practice, we often know the conditional probability already, and use it to compute the probability of the conjunction instead: $P(A \wedge B) = P(A|B) \cdot P(B) = P(B|A) \cdot P(A)$.
- ▷ **Theorem 3.1.22 (Bayes' Theorem).** *Given propositions A and B where $P(A) \neq 0$ and $P(B) \neq 0$, we have:*

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

- ▷ *Proof:*
  1. $P(A|B) = \frac{P(A \wedge B)}{P(B)} = \frac{P(B|A) \cdot P(A)}{P(B)}$

  ...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.

Bayes' Theorem - Why the Hype?

Say we have a *hypothesis* H about the world. (e.g. "The universe had a beginning")
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* $P(E|H)$) – *and*, importantly, the ability of *competing hypotheses* to predict the *same* evidence. (This is actually how scientific hypotheses should be evaluated)

$$\underbrace{P(H|E)}_{\text{posterior}} = \frac{P(E|H)\cdot P(H)}{P(E)} = \frac{\overbrace{P(E|H)}^{\text{likelihood}}\cdot\overbrace{P(H)}^{\text{prior}}}{\underbrace{P(E|H)}_{\text{likelihood}}\underbrace{P(H)}_{\text{prior}}+\underbrace{P(E|\neg H)P(\neg H)}_{\text{competition}}}$$

...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"

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 3.1.23.** Two events A and B are called independent, iff $P(A\wedge B) = P(A)\cdot P(B)$.

Two random variables X_1, X_2 are called independent, iff for all $x_1 \in \mathrm{dom}(X_1)$ and $x_2 \in \mathrm{dom}(X_2)$, the events $X_1 = x_1$ and $X_2 = x_2$ are independent.

We write $A \perp B$ or $X_1 \perp X_2$, respectively.

▷ **Theorem 3.1.24.** *Equivalently: Given events A and B with $P(B) \neq 0$, then A and B are independent iff $P(A|B) = P(A)$ (equivalently: $P(B|A) = P(B)$).*

▷ *Proof:*

1. $\Rightarrow$ By definition, $P(A|B) = \frac{P(A\wedge B)}{P(B)} = \frac{P(A)\cdot P(B)}{P(B)} = P(A)$,
2. $\Leftarrow$ Assume $P(A|B) = P(A)$. Then $P(A \wedge B) = P(A|B)\cdot P(B) = P(A)\cdot P(B)$.

▷ **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 $P(A \wedge B) = P(A)\cdot P(B)$.

In practice, this is impossible to check. Instead, we *assume* independence based on *domain knowledge*, and then *exploit* this to compute $P(A \wedge B)$.

Independence (Examples)

▷ **Example 3.1.25.**

- ▷ $\mathrm{First} = 2$ and $\mathrm{Second} = 3$ 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: $P((\mathrm{First} = a) \wedge (\mathrm{Second} = b)) = \frac{1}{36} = P(\mathrm{First} = a) \cdot P(\mathrm{Second} = b)$ ✓
- ▷ First and S are **not** independent. (The outcome of the first die affects the sum of the two dice.) Counterexample: $P((\mathrm{First} = 1) \wedge (S = 4)) = \frac{1}{36} \neq P(\mathrm{First} = 1) \cdot P(S = 4) = \frac{1}{6} \cdot \frac{1}{2} = \frac{1}{72}$
- ▷ **But:** $P((\mathrm{First} = a) \wedge (S = 7)) = \frac{1}{36} = \frac{1}{6} \cdot \frac{1}{6} = P(\mathrm{First} = a) \cdot P(S = 7)$ – so the events $\mathrm{First} = a$ and $S = 7$ *are* independent. (Why?)

▷ **Example 3.1.26.**

- ▷ Are cavity and toothache independent?

  ...since cavities can cause a toothache, that would probably be a bad design decision...
- ▷ 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 probabilty of gingivitis, even if they are not directly causally related.

Conditional Independence – Motivation

▷ 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 $P(\mathrm{cavity}) = 0.2$, $P(\mathrm{toothache}|\mathrm{cavity}) = 0.6$, $P(\mathrm{toothache}|\neg\mathrm{cavity}) = 0.1$, $P(\mathrm{catch}|\mathrm{cavity}) = 0.9$, and $P(\mathrm{catch}|\neg\mathrm{cavity}) = 0.2$.

▷ Assume the patient complains about a toothache, and our probe indeed catches in the aching tooth. What is the likelihood of having a cavity $P(\mathrm{cavity}|\mathrm{toothache} \wedge \mathrm{catch})$?

⇒ Use Bayes' rule:

$$P(\mathrm{cavity}|\mathrm{toothache} \wedge \mathrm{catch}) = \frac{P(\mathrm{toothache} \wedge \mathrm{catch}|\mathrm{cavity}) \cdot P(\mathrm{cavity})}{P(\mathrm{toothache} \wedge \mathrm{catch})}$$

▷ Note: $P(\mathrm{toothache} \wedge \mathrm{catch}) = P(\mathrm{toothache} \wedge \mathrm{catch}|\mathrm{cavity}) \cdot P(\mathrm{cavity}) + P(\mathrm{toothache} \wedge \mathrm{catch}|\neg\mathrm{cavity}) \cdot P(\neg\mathrm{cavity})$

⇒ Now we're only missing $P(\mathrm{toothache} \wedge \mathrm{catch}|\mathrm{cavity} = b)$ 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 $P(\cdot|\mathrm{cavity})$ 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.

- **Definition 3.1.27.** Given events A, B, C with $P(C) \neq 0$, then A and B are called conditionally independent given C, iff $P(A \wedge B|C) = P(A|C) \cdot P(B|C)$.

  Equivalently: iff $P(A|B \wedge C) = P(A|C)$, or $P(B|A \wedge C) = P(B|C)$.

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

- **Example 3.1.28.** Let's assume toothache and catch are conditionally independent given cavity/$\neg$cavity. Then we can finally compute:

  $$P(\text{cavity}|\text{toothache} \wedge \text{catch}) = \frac{P(\text{toothache} \wedge \text{catch}|\text{cavity}) \cdot P(\text{cavity})}{P(\text{toothache} \wedge \text{catch})}$$

  $$= \frac{P(\text{toothache}|\text{cavity}) \cdot P(\text{catch}|\text{cavity}) \cdot P(\text{cavity})}{P(\text{toothache}|\text{cavity}) \cdot P(\text{catch}|\text{cavity}) \cdot P(\text{cavity}) + P(\text{toothache}|\neg\text{cavity}) \cdot P(\text{catch}|\neg\text{cavity}) \cdot P(\neg\text{cavity})} = \frac{0.6 \cdot 0.9 \cdot 0.2}{0.6 \cdot 0.9 \cdot 0.2 + 0.1 \cdot 0.2 \cdot 0.8} = 0.87$$

Conditional Independence

- **Lemma 3.1.29.** *If A and B are conditionally independent given C, then $P(A|B \wedge C) = P(A|C)$*

  Proof:

  $$P(A|B \wedge C) = \frac{P(A \wedge B \wedge C)}{P(B \wedge C)} = \frac{P(A \wedge B|C) \cdot P(C)}{P(B \wedge C)} = \frac{P(A|C) \cdot P(B|C) \cdot P(C)}{P(B \wedge C)} = \frac{P(A|C) \cdot P(B \wedge C)}{P(B \wedge C)} = P(A|C)$$

- **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: $\text{First} = a$, $\text{Second} = b$ 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?

  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)

Summary

- ▷ 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

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*?

- ▷ **Frequentist:** The probability of an event is the limit of its relative frequency in a large number of trials.

  In other words: "In 30% of the cases where we have similar weather conditions, it rained the next day."

Objection: Okay, but what about *unique* events? "The probability of me passing the exam is 80%" – does this mean anything, if I only take the exam once? Am I comparable to "similar students"? What counts as sufficiently "similar"?

- ▷ **Bayesian:** Probabilities are *degrees of belief*. It means you **should** be 30% confident that it will rain tomorrow.

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

Pragmatics

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?

▷ [DF31]: 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.

▷ ...and, more importantly, your AI agents! ☺

3.2 Probabilistic Reasoning Techniques

Okay, now how do I implement this?

This is a computer science 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* are sparse as possible, by exploiting independence, conditional independence, ...

Probability Distributions

▷ **Definition 3.2.1.** The probability distribution for a random variable X, written $\mathbb{P}(X)$, 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 3.2.2.** $\mathbb{P}(\text{First}) = \mathbb{P}(\text{Second}) = \langle\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}\rangle$. (Both First and Second are uniformly distributed)

▷ **Example 3.2.3.** The probability distribution $\mathbb{P}(S)$ is $\langle\frac{1}{36}, \frac{1}{18}, \frac{1}{12}, \frac{1}{9}, \frac{5}{36}, \frac{1}{6}, \frac{5}{36}, \frac{1}{9}, \frac{1}{12}, \frac{1}{18}, \frac{1}{36}\rangle$. 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 3.2.4.** Probability distributions for Boolean random variables are naturally *pairs* (probabilities for T and F), e.g.:

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

▷ More generally:

Definition 3.2.5. A probability distribution is a vector $\mathbf{v}$ of values $\mathbf{v}_i \in [0,1]$ such that $\sum_i \mathbf{v}_i = 1$.

The Full Joint Probability Distribution

▷ **Definition 3.2.6.** Given random variables $X_1, \ldots, X_n$, the full joint probability distribution, denoted $\mathbb{P}(X_1, \ldots, X_n)$, is the n-dimensional array of size $|D_1 \times \ldots \times D_n|$ that lists the probabilities of all conjunctions of values of the random variables.

▷ **Example 3.2.7.** $\mathbb{P}(\text{cavity}, \text{toothache}, \text{gingivitis})$ could look something like this:

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

▷ **Example 3.2.8.** $\mathbb{P}(\text{First}, S)$

First \ S	2	3	4	5	6	7	8	9	10	11	12
1	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	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	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$	$\frac{1}{36}$

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 3.2.9.** 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: $\mathbb{P}(X_1, \ldots, X_n | Y_1, \ldots, Y_m)$.

▷ **Example 3.2.10.** $\mathbb{P}(\text{cavity}|\text{toothache})$:

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

▷ **Example 3.2.11.** $\mathbb{P}(\text{First}|S)$

First \ S	2	3	4	5	6	7	8	9	10	11	12
1	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	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	0	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	0	0	0
4	0	0	0	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	$\frac{1}{3}$	0	0
5	0	0	0	0	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	0
6	0	0	0	0	0	$\frac{1}{6}$	$\frac{1}{5}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{1}{2}$	1

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

Convention

We now "lift" multiplication and division to the level of whole probability distributions:

▷ **Definition 3.2.12.** Whenever we use $\mathbb{P}$ in an equation, we take this to mean a *system of equations*, for each value in the domains of the random variables involved.

Example 3.2.13.

▷ $\mathbb{P}(X,Y) = \mathbb{P}(X|Y) \cdot \mathbb{P}(Y)$ represents the system of equations $P(X = x \wedge Y = y) = P(X = x|Y = y) \cdot P(Y = y)$ for all x, y in the respective domains.

▷ $\mathbb{P}(X|Y) := \frac{\mathbb{P}(X,Y)}{\mathbb{P}(Y)}$ represents the system of equations $P(X = x|Y = y) := \frac{P((X=x)\wedge(Y=y))}{P(Y=y)}$

▷ Bayes' Theorem: $\mathbb{P}(X|Y) = \frac{\mathbb{P}(Y|X)\cdot\mathbb{P}(X)}{\mathbb{P}(Y)}$ represents the system of equations $P(X = x|Y = y) = \frac{P(Y=y|X=x)\cdot P(X=x)}{P(Y=y)}$

So, what's the point?

▷ Obviously, the probability distribution contains all the information about a specific random variable we need.

▷ **Observation:** The full joint probability distribution of variables $X_1, \ldots, X_n$ contains *all* the information about the random variables *and their conjunctions* we need.

▷ **Example 3.2.14.** We can read off the probability $P(\text{toothache})$ from the full joint probability distribution as $0.007 + 0.06 + 0.08 + 0.003{=}0.15$, and the probability $P(\text{toothache} \wedge \text{cavity})$ 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 $X_1, \ldots, X_n$, the full joint probability distribution has $\prod_{i=1}^{n} |\text{dom}(X_i)|$ entries! ($\mathbb{P}(\text{First}, S)$ already has 60 entries!)

⇒ The rest of this section deals with keeping things small, by *computing* probabilities instead of *storing* them all.

Probabilistic Reasoning

- **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.

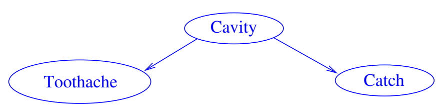
- **Note:** In practice, we are *primarily* interested in, and have access to, conditional probabilities rather than the unconditional probabilities of conjunctions of events:

  - 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*)

    $\Rightarrow$ we are interested in the conditional probability $P(\text{hypothesis}|\text{observation})$.
  - *"80% of patients with a cavity complain about a toothache"* (i.e. $P(\text{toothache}|\text{cavity})$) 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. $P(\text{cavity} \wedge \text{toothache})$).
  - Consider the probe catching in a cavity. The probe is a diagnostic tool, which is usually evaluated in terms of its *sensitivity* $P(\text{catch}|\text{cavity})$ and *specificity* $P(\neg\text{catch}|\neg\text{cavity})$. (You have probably heard these words a lot since 2020...)

Naive Bayes Models

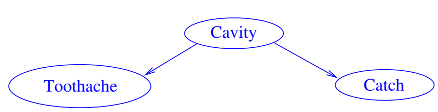
Consider again the dentistry example with random variables cavity, toothache, and catch. We assume cavity **causes** both toothache and catch, and that toothache and catch are conditionally independent given cavity:



We likely know the *sensitivity* $P(\text{catch}|\text{cavity})$ and *specificity* $P(\neg\text{catch}|\neg\text{cavity})$, which jointly give us $\mathbb{P}(\text{catch}|\text{cavity})$, and from medical studies, we should be able to determine $P(\text{cavity})$ (the *prevalence* of cavities in the population) and $\mathbb{P}(\text{toothache}|\text{cavity})$.

This kind of situation is surprisingly common, and deserves a name

Naive Bayes Models



Definition 3.2.15. 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 $\mathbb{P}(\mathrm{cavity}, \mathrm{toothache}, \mathrm{catch})$ from this information?

Recovering the Full Joint Probability Distribution

▷ **Lemma 3.2.16 (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 3.2.17 (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 3.2.18.** *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 $\mathbb{P}(C|E_1, \ldots, E_n) = \frac{\mathbb{P}(C, E_1, \ldots, E_n)}{\mathbb{P}(E_1, \ldots, E_n)}$...
...except that we don't know $\mathbb{P}(E_1, \ldots, E_n)$:-/
...except that we can compute the full joint probability distribution, so we can recover it:

Lemma 3.2.19 (Marginalization). *Given random variables $X_1, \ldots, X_n$ and $Y_1, \ldots, Y_m$, we have $\mathbb{P}(X_1, \ldots, X_n) = \sum_{y_1 \in \mathrm{dom}(Y_1), \ldots, y_m \in \mathrm{dom}(Y_m)} \mathbb{P}(X_1, \ldots, X_n, Y_1 = y_1, \ldots, Y_m = y_m)$.*

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

Example 3.2.20. Say we observed toothache $=$ T and catch $=$ T. Using marginalization, we can compute

$$P(\text{cavity}|\text{toothache} \wedge \text{catch}) = \frac{P(\text{cavity} \wedge \text{toothache} \wedge \text{catch})}{P(\text{toothache} \wedge \text{catch})}$$
$$= \frac{P(\text{cavity} \wedge \text{toothache} \wedge \text{catch})}{\sum_{c \in \{\text{cavity}, \neg\text{cavity}\}} P(c \wedge \text{toothache} \wedge \text{catch})}$$
$$= \frac{P(\text{cavity}) \cdot P(\text{toothache}|\text{cavity}) \cdot P(\text{catch}|\text{cavity})}{\sum_{c \in \{\text{cavity}, \neg\text{cavity}\}} P(c) \cdot P(\text{toothache}|c) \cdot P(\text{catch}|c)}$$

Unknowns

What if we don't know catch? (I'm not a dentist, I don't have a probe...)

We split our effects into $\{E_1, \ldots, E_n\} = \{O_1, \ldots, O_{n_O}\} \cup \{U_1, \ldots, U_{n_U}\}$ – the *observed* and *unknown* random variables.

Let $D_U := \text{dom}(U_1) \times \ldots \times \text{dom}(U_{n_u})$. Then

$$\mathbb{P}(C|O_1, \ldots, O_{n_O}) = \frac{\mathbb{P}(C, O_1, \ldots, O_{n_O})}{\mathbb{P}(O_1, \ldots, O_{n_O})}$$
$$= \frac{\sum_{u \in D_U} \mathbb{P}(C, O_1, \ldots, O_{n_O}, U_1 = u_1, \ldots, U_{n_u} = u_{n_u})}{\sum_{c \in \text{dom}(C)} \sum_{u \in D_U} \mathbb{P}(O_1, \ldots, O_{n_O}, C = c, U_1 = u_1, \ldots, U_{n_u} = u_{n_u})}$$
$$= \frac{\sum_{u \in D_U} \mathbb{P}(C) \cdot \prod_{i=1}^{n_O} \mathbb{P}(O_i|C) \cdot \prod_{j=1}^{n_U} \mathbb{P}(U_j = u_j|C)}{\sum_{c \in \text{dom}(C)} \sum_{u \in D_U} P(C = c) \cdot \prod_{i=1}^{n_O} \mathbb{P}(O_i|C = c) \cdot \prod_{j=1}^{n_U} P(U_j = u_j|C = c)}$$
$$= \frac{\mathbb{P}(C) \cdot \prod_{i=1}^{n_O} \mathbb{P}(O_i|C) \cdot (\sum_{u \in D_U} \prod_{j=1}^{n_U} \mathbb{P}(U_j = u_j|C))}{\sum_{c \in \text{dom}(C)} P(C = c) \cdot \prod_{i=1}^{n_O} \mathbb{P}(O_i|C = c) \cdot (\sum_{u \in D_U} \prod_{j=1}^{n_U} P(U_j = u_j|C = c))}$$

...oof...

Unknowns

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

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

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

Secondly, note that the *denominator* is

1. the same for any given observations $O_1, \ldots, O_{n_O}$, 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 $\mathbb{P}(C|O_1,\ldots,O_{n_O})$ to sum up to 1.

Normalization

Definition 3.2.21 (Normalization). Given a vector $w := \langle w_1,\ldots,w_k\rangle$ of numbers in $[0,1]$ where $\sum_{i=1}^{k} w_i \leq 1$.

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 3.2.22 (Inference in a Naive Bayes model). *Let $C, E_1,\ldots,E_n$ a naive Bayes model and $E_1,\ldots,E_n = O_1,\ldots,O_{n_O},U_1,\ldots,U_{n_U}$.*

Then

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

Note, that this is entirely independent of the *unknown* random variables $U_1,\ldots,U_{n_U}$!

Also, note that this is just a fancy way of saying "first, compute all the numerators, then divide all of them by their sums".

Dentistry Example

Putting things together, we get:

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

Say we have $P(\text{cavity}) = 0.1$, $P(\text{toothache}|\text{cavity}) = 0.8$, and $P(\text{toothache}|\neg\text{cavity}) = 0.05$. Then

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

$0.08 + 0.045 = 0.125$, hence

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

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 $\mathbb{P}(\mathrm{category})$, and of words per category – i.e. $\mathbb{P}(\mathrm{word}_i|\mathrm{category})$ for some (huge) list of words $(\mathrm{word}_i)_{i=1}^n$.

▷ 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

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

▷ We then choose the category with the highest probability.

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 3.2.23. *Let* $Q, E_1, \ldots, E_{n_E}, U_1, \ldots, U_{n_U}$ *be random variables and* $D := \mathrm{dom}(U_1) \times \ldots \times \mathrm{dom}(U_{n_U})$. *Then*

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

.

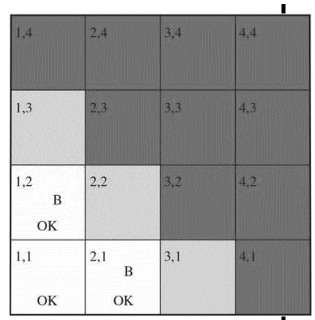
We call Q *the* ***query variable***, $E_1, \ldots, E_{n_E}$ *the* ***evidence***, *and* $U_1, \ldots, U_{n_U}$ *the* ***unknown*** *(or* ***hidden****)* ***variables***, *and computing a conditional probability this way* ***enumeration***.

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.

We will fortify our intuition about naive Bayes models with a variant of the Wumpus world we looked at **??** to understand whether logic was up to the job of guiding an agent in the Wumpus cave.

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!

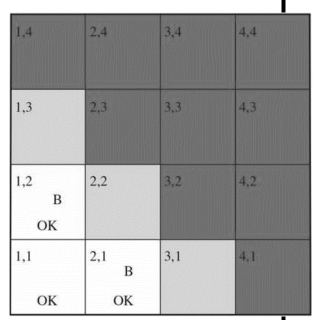
We can model this using the Boolean random variables:

▷ $P_{i,j}$ 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 $[i,j]$

⇒ let's apply our machinery!

Wumpus: Probabilistic Model



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 $\mathbb{P}(B_{1,1},B_{1,2},B_{2,1}|P_{1,1},\ldots,P_{4,4})\cdot\mathbb{P}(P_{1,1},\ldots,P_{4,4})$.
2. Note that $\mathbb{P}(B_{1,1},B_{1,2},B_{2,1}|P_{1,1},\ldots,P_{4,4})$ 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 $\mathbb{P}(P_{1,1},\ldots,P_{4,4}) = \prod_{i,j=1,1}^{4,4}\mathbb{P}(P_{i,j})$

⇒ We know all of these probabilities.

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

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!

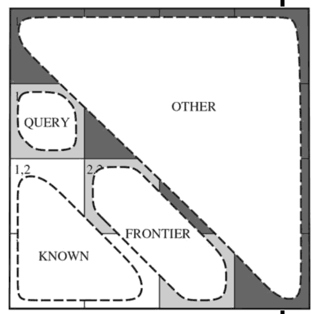
Let's do better.

▷ Let $b := \neg B_{1,1} \wedge B_{1,2} \wedge B_{2,1}$ (All the breezes we know about)

▷ Let $p := \neg P_{1,1} \wedge \neg P_{1,2} \wedge \neg P_{2,1}$. (All the pits we know about)

▷ Let $F := \{P_{3,1} \wedge P_{2,2}, \neg P_{3,1} \wedge P_{2,2}, P_{3,1} \wedge \neg P_{2,2}, P_{3,1} \wedge \neg P_{2,2}\}$ (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.)

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

Optimized Wumpus

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

$\Rightarrow$ this is just a sum over the frontier, i.e. 4 terms ☺

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 $[2,2]$!)

Cooking Recipe

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. $\mathbb{P}(b|p,f) \in \{0,1\}$)

$\Rightarrow$ the problem can be solved at all!

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

Summary

- ▷ 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 4

Probabilistic Reasoning: Bayesian Networks

4.1 Introduction

John, Mary, and My Brand-New Alarm

Example 4.1.1 (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.

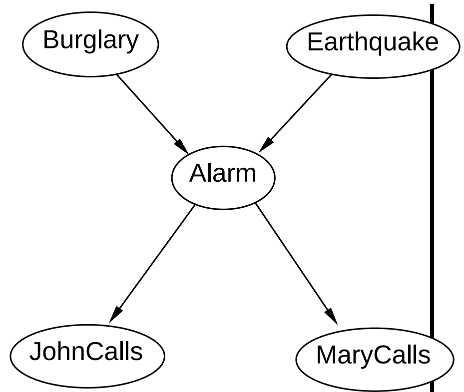
⇒ Random variables: `Burglary`, `Earthquake`, `Alarm`, `John`, `Mary`.

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`.

John, Mary, and My Alarm: Assumptions

We assume:



- We (should) know $\mathbb{P}(\mathtt{Alarm}|\mathtt{Burglary},\mathtt{Earthquake})$, $\mathbb{P}(\mathtt{John}|\mathtt{Alarm})$, and $\mathbb{P}(\mathtt{Mary}|\mathtt{Alarm})$.
- 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 $\mathbb{P}(\mathtt{Burglary}|\mathtt{John}=\mathsf{T},\mathtt{Mary}=\mathsf{T})$.

John, Mary, and My Alarm: The Distribution

$$\begin{aligned}&\mathbb{P}(\mathtt{John},\mathtt{Mary},\mathtt{Alarm},\mathtt{Burglary},\mathtt{Earthquake})\\ =&\mathbb{P}(\mathtt{John}|\mathtt{Mary},\mathtt{Alarm},\mathtt{Burglary},\mathtt{Earthquake})\cdot\mathbb{P}(\mathtt{Mary}|\mathtt{Alarm},\mathtt{Burglary},\mathtt{Earthquake})\\ &\cdot\mathbb{P}(\mathtt{Alarm}|\mathtt{Burglary},\mathtt{Earthquake})\cdot\mathbb{P}(\mathtt{Burglary}|\mathtt{Earthquake})\cdot\mathbb{P}(\mathtt{Earthquake})\\ =&\mathbb{P}(\mathtt{John}|\mathtt{Alarm})\cdot\mathbb{P}(\mathtt{Mary}|\mathtt{Alarm})\cdot\mathbb{P}(\mathtt{Alarm}|\mathtt{Burglary},\mathtt{Earthquake})\cdot\mathbb{P}(\mathtt{Burglary})\cdot\mathbb{P}(\mathtt{Earthquake})\end{aligned}$$

We plug into the equation for enumeration:

$$\mathbb{P}(\mathtt{Burglary}|\mathtt{John}=\mathsf{T},\mathtt{Mary}=\mathsf{T})=\alpha(\mathbb{P}(\mathtt{Burglary})\sum_{a\in\{\mathsf{T},\mathsf{F}\}}P(\mathtt{John}|\mathtt{Alarm}=a)\cdot P(\mathtt{Mary}|\mathtt{Alarm}=a)$$
$$\cdot\sum_{q\in\{\mathsf{T},\mathsf{F}\}}\mathbb{P}(\mathtt{Alarm}=a|\mathtt{Burglary},\mathtt{Earthquake}=q)P(\mathtt{Earthquake}=q))$$

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

Bayesian Networks: Definition

Definition 4.1.2. A Bayesian network consists of

1. a directed acyclic graph $\langle\mathcal{X},E\rangle$ of random variables $\mathcal{X}=\{X_1,\ldots,X_n\}$, and
2. a conditional probability distribution $\mathbb{P}(X_i|\mathrm{Parents}(X_i))$ 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 $\mathrm{Parents}(X_i)$.

Definition 4.1.3. Let $\langle\mathcal{X},E\rangle$ be a directed acyclic graph, $X\in\mathcal{X}$, and E^* the reflexive transitive closure of E. The non-descendents of X are the elements of the set $\mathrm{NonDesc}(X):=\{Y|(X,Y)\notin E^*\}\backslash\mathrm{Parents}(X)$.

Note that the roots of the graph are conditionally independent given the empty set; i.e. they are independent.

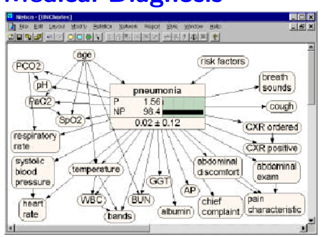
Theorem 4.1.4. *The full joint probability distribution of a Bayesian network $\langle\mathcal{X}, E\rangle$ is given by*

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

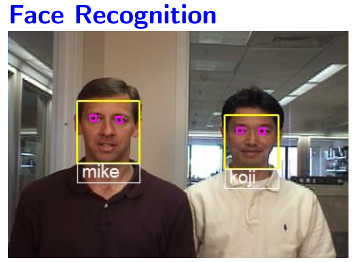
Some Applications

▷ A ubiquitous problem: Observe "symptoms", need to infer "causes".

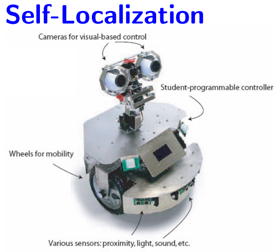
Medical Diagnosis



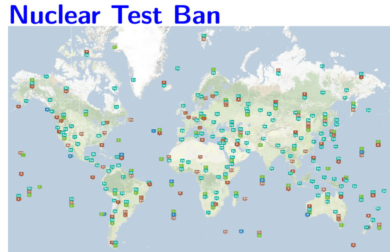
Face Recognition



Self-Localization



Nuclear Test Ban



4.2 Constructing Bayesian Networks

Compactness of Bayesian Networks

▷ **Definition 4.2.1.** Given random variables $X_1,\ldots,X_n$ with finite domains $D_1,\ldots,D_n$, the size of $\mathcal{B} := \langle\{X_1,\ldots,X_n\}, E\rangle$ is defined as

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

▷ **Note:** $\mathrm{size}(\mathcal{B})$ $\widehat{=}$ The total number of entries in the conditional probability distributions.

▷ **Note:** Smaller BN $\rightsquigarrow$ need to assess less probabilities, more efficient inference.

▷ **Observation 4.2.2.** *Explicit full joint probability distribution has size* $\prod_{i=1}^{n} |D_i|$.

▷ **Observation 4.2.3.** *If* $|\text{Parents}(X_i)| \leq k$ *for every* X_i, *and* $D_{\max}$ *is the largest random variable domain, then* $\text{size}(\mathcal{B}) \leq n|D_{\max}|^{k+1}$.

▷ **Example 4.2.4.** For $|D_{\max}| = 2$, $n = 20$, $k = 4$ we have $2^{20} = 1048576$ probabilities, but a Bayesian network of size $\leq 20 \cdot 2^5 = 640 \ldots$!

▷ In the *worst case*, $\text{size}(\mathcal{B}) = n \cdot \prod_{i=1}^{n} |D_i|$, 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.

Keeping Networks Small

To keep our Bayesian networks small, we can:

1. **Reduce the number of edges:** ⇒ Order the variables to allow for exploiting conditional independence (causes before effects), or
2. **represent the conditional probability distributions efficiently:**
   (a) For Boolean random variables X, we only need to store $\mathbb{P}(X = \mathsf{T}|\text{Parents}(X))$ $(\mathbb{P}(X = \mathsf{F}|\text{Parents}(X)) = 1 - \mathbb{P}(X = \mathsf{T}|\text{Parents}(X)))$ (Cuts the number of entries in half!)
   (b) 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 $X_1, \ldots, X_n$, consider the following (impractical, but illustrative) pseudo-algorithm for constructing a Bayesian network:

▷ **Definition 4.2.5 (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** $i := 1, \ldots, n$ **do**
   a. Choose a minimal set $\text{Parents}(X_i) \subseteq \{X_1, \ldots, X_{i-1}\}$ 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 $\text{Parents}(X_i)$ depends on what "$\{X_1, \ldots, X_{i-1}\}$" 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.

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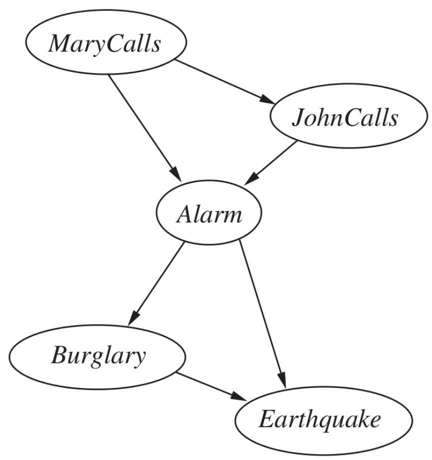
John and Mary Depend on the Variable Order!

▷ **Example 4.2.6.** `Mary`, `John`, `Alarm`, `Burglary`, `Earthquake`.



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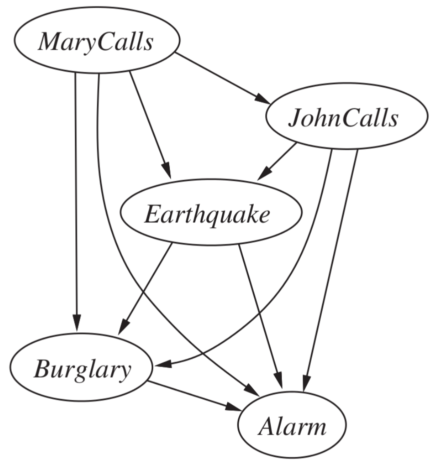
Note: For **??** we try to determine whether – given different value assignments to potential parents – the probability of X_i being true differs? If yes, we include these parents. In the particular case:

1. M to J yes because the common cause may be the alarm.
2. M, J to A yes because they may have heard alarm.
3. A to B yes because if A then higher chance of B.
4. However, M/J to B no because M/J only react to the alarm so if we have the value of A then values of M/J don't provide more information about B.
5. A to E yes because if A then higher chance of E.
6. B to E yes because, if A and not B then chances of E are higher than if A and B.

John and Mary Depend on the Variable Order! Ctd.

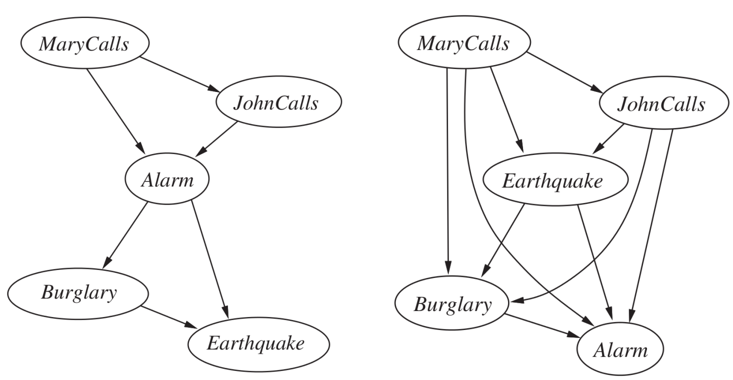
▷ **Example 4.2.7.** `Mary`, `John`, `Earthquake`, `Burglary`, `Alarm`.



Again: Given different value assignments to potential parents, does the probability of X_i being true differ? If yes, include these parents.

1. M to J as before.
2. M, J to E as probability of E is higher if M/J is true.
3. Same for B; E to B because, given M and J are true, if E is true as well then prob of B is lower than if E is false.
4. $M/J/B/E$ to A because if $M/J/B/E$ is true (even when changing the value of just one of these) then probability of A is higher.

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`!

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

Representing Conditional Distributions: Deterministic Nodes

Definition 4.2.8. A node X in a Bayesian network is called deterministic, if its value is completely determined by the values of $\mathrm{Parents}(X)$.

Example 4.2.9. The *sum of two dice throws* S is entirely determined by the values of the two dice $First$ and $Second$.

Example 4.2.10. In the *Wumpus* example, the *breezes* are entirely determined by the *pits*

⇒ *Deterministic* nodes model direct, *causal* relationships.

⇒ If X is deterministic, then $P(X|\mathrm{Parents}(X)) \in \{0, 1\}$

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

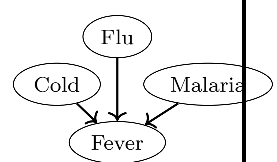
Representing Conditional Distributions: Noisy Nodes

Sometimes, values of nodes are "almost deterministic":

Example 4.2.11 (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.



⇒ We can model the inhibitions by individual inhibition factors q_d.

Definition 4.2.12. The conditional probability distribution of a noisy disjunction node X with $\mathrm{Parents}(X) = X_1, \ldots, X_n$ in a Bayesian network is given by $P(X|X_1, \ldots, X_n) = 1 - \prod_{\{j|X_j = \mathsf{T}\}} q_j$, where the q_i are the inhibition factors of $X_i \in \mathrm{Parents}(X)$, defined as $q_i := P(\neg X|\neg X_1, \ldots, \neg X_{i-1}, X_i, \neg X_{i+1}, \ldots, \neg X_n)$

⇒ Instead of a distribution with 2^k parameters, we only need k parameters!

Representing Conditional Distributions: Noisy Nodes

▷ **Example 4.2.13.** Assume the following inhibition factors for Example 4.2.11:

$$\begin{aligned} q_{\mathrm{cold}} &= P(\neg\mathrm{fever}|\mathrm{cold}, \neg\mathrm{flu}, \neg\mathrm{malaria}) = 0.6 \\ q_{\mathrm{flu}} &= P(\neg\mathrm{fever}|\neg\mathrm{cold}, \mathrm{flu}, \neg\mathrm{malaria}) = 0.2 \\ q_{\mathrm{malaria}} &= P(\neg\mathrm{fever}|\neg\mathrm{cold}, \neg\mathrm{flu}, \mathrm{malaria}) = 0.1 \end{aligned}$$

If we model Fever as a noisy disjunction node, then the general rule $P(X_i|\mathrm{Parents}(X_i)) =$

$\prod_{\{j|X_j=\mathsf{T}\}} q_j$ for the CPT gives the following table:

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

Representing Conditional Distributions: Summary

- ▷ 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 $\mathcal{O}(k)$ parameters instead of $\mathcal{O}(2^k)$ for the full conditional probability table. This can make assessment (and learning) tractable.
- ▷ **Example 4.2.14.** The CPCS network [Pra+94] 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.

4.3 Inference in Bayesian Networks

Probabilistic Inference Tasks in Bayesian Networks

Remember:

Definition 4.3.1 (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: $\mathbb{P}(X_1, \ldots, X_n) = \prod_{i=1}^{n} \mathbb{P}(X_i | \text{Parents}(X_i))$

And we know about enumeration:

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

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

Enumeration: The Alarm-Example

Remember our example: $\mathbb{P}(\texttt{Burglary}|\texttt{John}, \texttt{Mary})$
(hidden variables: $\texttt{Alarm}, \texttt{Earthquake}$)

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

⇒ These are 5 factors in 4 summands ($b_a, b_e \in \{\mathsf{T}, \mathsf{F}\}$) over two cases ($\texttt{Burglary} \in \{\mathsf{T}, \mathsf{F}\}$),
⇒ 38 arithmetic operations (+3 for α)

General worst case: $\mathcal{O}(n2^n)$

Let's do better!

Enumeration: First Improvement

Some abbreviations: $j := \texttt{John}, m := \texttt{Mary}, a := \texttt{Alarm}, e := \texttt{Earthquake}, b := \texttt{Burglary}$,

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

Let's "optimize":

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

⇒ 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)

Second Improvement: Variable Elimination 1

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

$$=\alpha(P(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e = b_e) \cdot (\sum_{a_e \in \{\mathsf{T},\mathsf{F}\}} P(a = a_e|e = b_e, b) \cdot \mathbb{P}(j|a = a_e) \cdot \underbrace{(\sum_{a_m \in \{\mathsf{T},\mathsf{F}\}} P(m = a_m|a = a_e))}_{=1})))$$

⇒ $\mathbb{P}(\texttt{John}|\texttt{Burglary} = \mathsf{T})$ does not depend on $\texttt{Mary}$ (duh...)

More generally:

Lemma 4.3.2. *Given a query* $\mathbb{P}(Q_1, \ldots, Q_{n_Q}|E_1 = e_1, \ldots, E_{n_E} = e_{n_E})$*, we can ignore (and remove) all hidden leafs of the Bayesian network.*

...doing so yields new leafs, which we can then ignore again, etc., until:

Lemma 4.3.3. *Given a query* $\mathbb{P}(Q_1, \ldots, Q_{n_Q}|E_1 = e_1, \ldots, E_{n_E} = e_{n_E})$*, we can ignore (and remove) all hidden variables that are not ancestors of any of the* $Q_1, \ldots, Q_{n_Q}$ *or* $E_1, \ldots, E_{n_E}$*.*

Enumeration: First Algorithm

Assume the $X_1, \ldots, X_n$ are topologically sorted (causes before effects)

function ENUMERATE-QUERY(Q,$\langle E_1 = e_1, \ldots, E_{n_E} = e_{n_E}\rangle$)
  $P := \langle\rangle$ /* $= \mathbb{P}(Q|E_i = e_i)$ */
  $X_1, \ldots, X_n :=$ variables filtered according to ??, topologically sorted
  for all $q \in \mathbf{dom}(Q)$ **do**
    $P_i :=$ENUMALL($\langle X_1, \ldots, X_n\rangle$,$\langle E_1 = e_1, \ldots, E_{n_E} = e_{n_E}, Q = q\rangle$)
  return $\alpha(P)$

function ENUMALL($\langle Y_1, \ldots, Y_{n_Y}\rangle$,$\langle A_1 = a_1, \ldots, A_{n_A} = a_{n_A}\rangle$)
  /* *By construction*, $\text{Parents}(Y_1) \subset \{A_1, \ldots, A_{n_A}\}$ */
  if $n_y = 0$ **then return** 1.0
  else if $Y_1 = A_j$ **then return** $P(A_j = a_j|\text{Parents}(A_j))\cdot$ENUMALL($\langle Y_2, \ldots, Y_{n_Y}\rangle$,$\langle A_1 = a_1, \ldots, A_{n_A} = a_{n_A}\rangle$)
  else return $\sum_{y \in \mathbf{dom}(Y_1)} P(Y_1 = y|\text{Parents}(Y_1))\cdot$ENUMALL($\langle Y_2, \ldots, Y_{n_Y}\rangle$,$\langle A_1 = a_1, \ldots, A_{n_A} = a_{n_A}, Y_1 = y\rangle$)

General worst case: $\mathcal{O}(2^n)$ – better, but still not great

Enumeration: Example

Variable order: b, e, a, j, m

$$\triangleright\ P_0 := P(b) \cdot \left[+ \begin{array}{l} P(e) \cdot \left[+ \begin{array}{l} P(a|b,e) \cdot P(j|a) \cdot P(m|a) \cdot 1.0 \\ P(\neg a|b,e) \cdot P(j|\neg a) \cdot P(m|\neg a) \cdot 1.0 \end{array}\right. \\ P(\neg e) \cdot \left[+ \begin{array}{l} P(a|b,\neg e) \cdot P(j|a) \cdot P(m|a) \cdot 1.0 \\ P(\neg a|b,\neg e) \cdot P(j|\neg a) \cdot P(m|\neg a) \cdot 1.0 \end{array}\right. \end{array}\right.$$

$$\triangleright\ P_1 := P(\neg b) \cdot \left[+ \begin{array}{l} P(e) \cdot \left[+ \begin{array}{l} P(a|\neg b,e) \cdot P(j|a) \cdot P(m|a) \cdot 1.0 \\ P(\neg a|\neg b,e) \cdot P(j|\neg a) \cdot P(m|\neg a) \cdot 1.0 \end{array}\right. \\ P(\neg e) \cdot \left[+ \begin{array}{l} P(a|\neg b,\neg e) \cdot P(j|a) \cdot P(m|a) \cdot 1.0 \\ P(\neg a|\neg b,\neg e) \cdot P(j|\neg a) \cdot P(m|\neg a) \cdot 1.0 \end{array}\right. \end{array}\right.$$

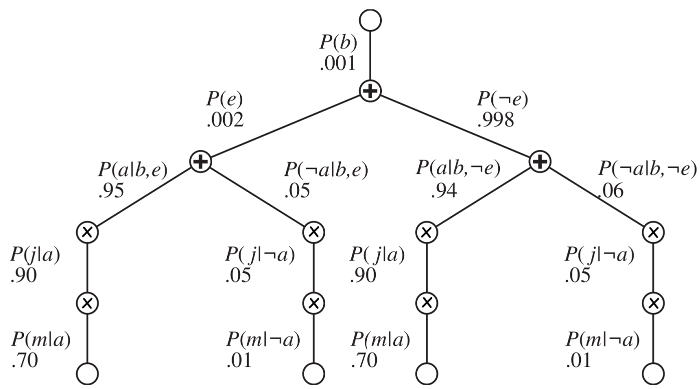
$$\Leftarrow \langle \frac{P_0}{P_0+P_1}, \frac{P_1}{P_0+P_1} \rangle$$

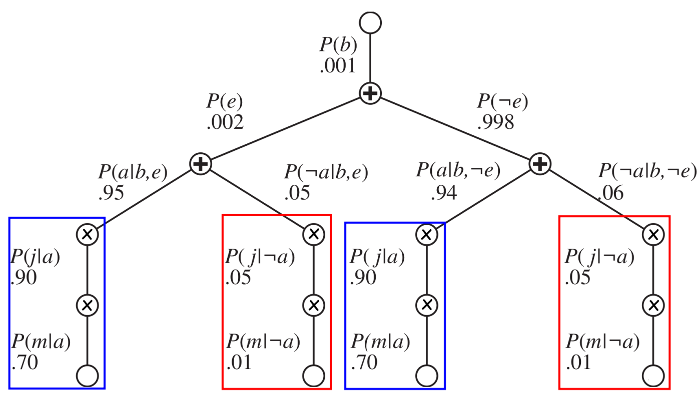
$$\mathbb{P}(b|j = \mathsf{T}, m = \mathsf{T}) = \alpha(\mathbb{P}(b) \cdot (\sum_{b_e \in \{\mathsf{T},\mathsf{F}\}} P(e = b_e) \cdot (\sum_{b_a \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(a = b_a|e = b_e, b) \cdot P(j|a = b_a) \cdot P(m|a = b_a))))$$

The Evaluation of $P(b|j, m)$ as a "Search Tree"

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

Note: Enumerate-Query corresponds to depth-first traversal of an arithmetic expression-tree:





Variable Elimination 2

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

The last two factors $P(j|a=b_a), P(m|a=b_a)$ 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":

$$\alpha(\underbrace{\mathbb{P}(b)}_{\mathbf{f}_7(b)}\cdot\underbrace{(\sum_{b_e\in\{\mathsf{T},\mathsf{F}\}} \underbrace{P(e=b_e)}_{\mathbf{f}_5(e)}\cdot\underbrace{(\sum_{b_a\in\{\mathsf{T},\mathsf{F}\}} \underbrace{\mathbb{P}(a=b_a|e=b_e,b)}_{\mathbf{f}_3(a,b,e)}\cdot\underbrace{P(j|a=b_a)}_{\mathbf{f}_2(a)}\cdot\underbrace{P(m|a=b_a)}_{\mathbf{f}_1(a)}))}_{\mathbf{f}_4(b,e)}}_{\mathbf{f}_6(b)})$$

Variable Elimination: Example

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

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

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" $\mathbf{f}(a){:=}\mathbf{f}_1(a) := \langle P(m|a), P(m|\neg a)\rangle$.
- ▷ j works analogously, $\mathbf{f}_2(a) := \langle P(j|a), P(j|\neg a)\rangle$. We "multiply" with the existing factor, yielding $\mathbf{f}(a) := \langle \mathbf{f}_1(a) \cdot \mathbf{f}_2(a), \mathbf{f}_1(\neg a) \cdot \mathbf{f}_2(\neg a)\rangle {=} \langle P(m|a) \cdot P(j|a), P(m|\neg a) \cdot P(j|\neg a)\rangle$
- ▷ a is a hidden variable with dependencies e (hidden) and b (query).
  1. We introduce a new "factor" $\mathbf{f}_3(a, e, b)$, a $2 \times 2 \times 2$ table with the relevant conditional probabilities $\mathbb{P}(a|e, b)$.
  2. We multiply each entry of $\mathbf{f}_3$ with the relevant entries of the existing factor $\mathbf{f}$, yielding $\mathbf{f}(a, e, b)$.
  3. We "sum out" the resulting factor over a, yielding a new factor $\mathbf{f}(e, b) = \mathbf{f}(a, e, b) + \mathbf{f}(\neg a, e, b)$.
- ▷ ...

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

The Complexity of Exact Inference

- ▷ **Definition 4.3.4.** 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 4.3.5 (Good News).** *On singly connected Bayesian networks, variable elimination runs in polynomial time.*
- ▷ Is our BN for Mary & John a polytree? (Yes.)
- ▷ **Theorem 4.3.6 (Bad News).** *For multiply connected Bayesian networks, probabilistic inference is $\#\mathbf{P}$-hard.* *($\#\mathbf{P}$ is harder than $\mathbf{NP}$, i.e. $\mathbf{NP} \subseteq \#\mathbf{P}$)*
- ▷ **So?:** Life goes on ... In the hard cases, if need be we can throw exactitude to the winds and approximate.
- ▷ **Example 4.3.7.** Sampling techniques as in MCTS.

4.4 Conclusion

A Video Nugget covering this section can be found at `https://fau.tv/clip/id/29228`.

Summary

- ▷ 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 $\#\mathbf{P}$-hard. Approximate probabilistic inference methods exist.

Topics We Didn't Cover Here

- ▷ **Inference by sampling**: A whole zoo of methods for doing this exists.
- ▷ **Clustering**: Pre-combining subsets of variables to reduce the running time of inference.
- ▷ **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).
- ▷ **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.

Reading:

- *Chapter 14: Probabilistic Reasoning* of [RN03].
  - Section 14.1 roughly corresponds to my "What is a Bayesian Network?".
  - Section 14.2 roughly corresponds to my "What is the Meaning of a Bayesian Network?" and "Constructing Bayesian Networks".The main change I made here is to *define* the semantics of the BN in terms of the conditional independence relations, which I find clearer than RN's definition that uses the reconstructed full joint probability distribution instead.
  - Section 14.4 roughly corresponds to my "Inference in Bayesian Networks". RN give full details on variable elimination, which makes for nice ongoing reading.

- Section 14.3 discusses how CPTs are specified in practice.
- Section 14.5 covers approximate sampling-based inference.
- Section 14.6 briefly discusses relational and first-order BNs.
- Section 14.7 briefly discusses other approaches to reasoning about uncertainty.

All of this is nice as additional background reading.

Chapter 5

Making Simple Decisions Rationally

5.1 Introduction

A Video Nugget covering this section can be found at `https://fau.tv/clip/id/30338`.

Overview

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

For that we need to answer two questions:

Questions:

- ▷ Given a world model and a set of *actions*, what will the likely consequences of each action be?
- ▷ How "good" are these consequences?

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 $u\colon \mathbf{dom}(X) \to \mathbb{R}$) indicating their desirability.
- ▷ Choose the action that maximizes the *expected value* of u

Definition 5.1.1. Decision theory investigates decision problems, i.e. how a model-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. $u\colon S \to \mathbb{R}$.

Decision Theory

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

Definition 5.1.2. Given a probability model $\langle\Omega, P\rangle$ and a random variable $X\colon\Omega\to D$ 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 $E(X|e_1,\ldots,e_n){:=}\sum_{x\in D}P(X=x|e_1,\ldots,e_n)\cdot x$.

Putting things together:

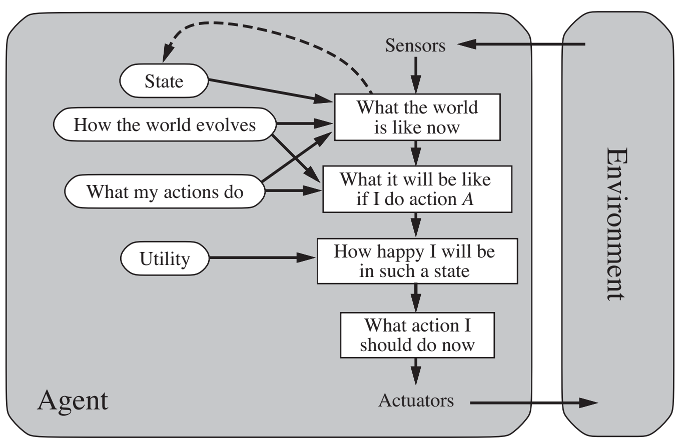
Definition 5.1.3. Let $A\colon\Omega\to D$ a random variable (where D is a set of actions) $X_i\colon\Omega\to D_i$ random variables (the state), and $u\colon D_1\times\ldots\times D_n\to\mathbb{R}$ a utility function. Then the expected utility of the action $a\in D$ is the expected value of u (interpreted as a random variable) given $A=a$; i.e.

$$\mathrm{EU}(a) := \sum_{\langle x_1,\ldots,x_n\rangle\in D_1\times\ldots\times D_n} P(X_1=x_1,\ldots,X_n=x_n|A=a)\cdot u(x_1,\ldots,x_n)$$

Utility-based Agents

▷ **Definition 5.1.4.** 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:**



Maximizing Expected Utility (Ideas)

Definition 5.1.5 (MEU principle for Rationality). We call an action rational if it maximizes expected (MEU). An utility-based agent is called rational, iff it always chooses a rational action.

Hooray: This solves all of AI. (in principle)

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 5.1.6. A simple 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 5.1.7 (AI1). Heuristics in tree search (greedy search, A^*) and game-play (minimax, alpha-beta pruning) maximize "expected" utility.

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

$\mathrm{EU}(a) = U(T(S(s,e),a))$, 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!

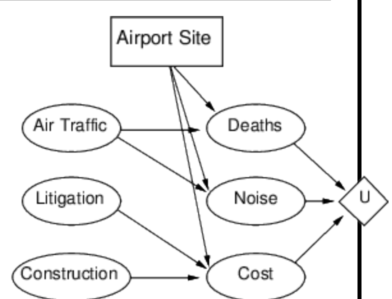
5.2 Decision Networks

A Video Nugget covering this section can be found at `https://fau.tv/clip/id/30345`.
Now that we understand multi-attribute utilitysutility function, we can complete our design of a utility-based agent, which we now recapitulate as a refresher. As we already use Bayesian networks for the belief state of an utility-based agent, integrating utilities and possible actions into the network suggests itself naturally. This leads to the notion of a decision network.

Decision networks

Definition 5.2.1. A decision network is a Bayesian network with two additional kinds of nodes:

- ▷ action nodes, representing a set of possible actions, and (square nodes)
- ▷ A single utility node (also called value node). (diamond node)



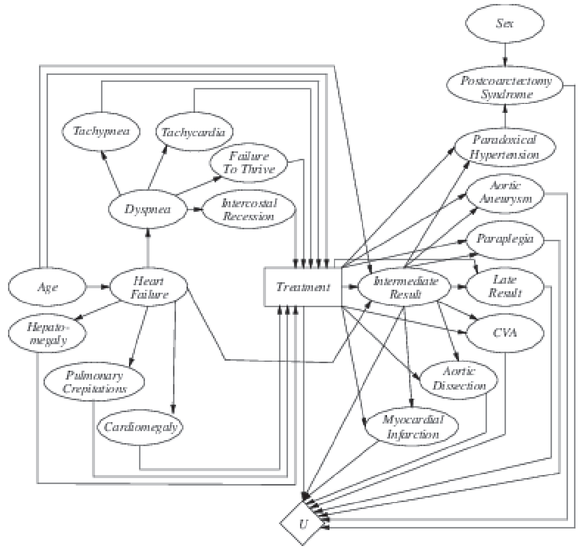
General Algorithm: Given evidence $E_j = e_j$, and action nodes $A_1, \ldots, A_k$, compute the expected utility of each action, given the evidence, i.e. return the sequence of actions

$$\operatorname{argmax}\, a_1,\ldots,a_k \overbrace{\sum_{\langle x_1,\ldots,x_n\rangle} \underbrace{P(X_i = x_i | A_1 = a_1,\ldots,A_k = a_k, E_j = e_j)}_{\text{usual Bayesian Network inference}} \cdot U(X_i = x_i)}^{=\text{expected utility of } a_1,\ldots,a_k}$$

Note the sheer amount of summands in the sum above in the general case! (⇒ We will simplify where possible later)

Decision Networks: Example

▷ **Example 5.2.2 (A Decision-Network for Aortic Coarctation).** from [Luc96]



5.3 Preferences and Utilities

Preferences in Deterministic Environments

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

Example 5.3.1. 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 5.3.2. *Give me your cell-phone or I will give you a bloody nose.* $\rightsquigarrow$
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 5.3.3. Given states A and B (we call them prizes) an agent can express preferences of the form

- $A \succ B$ A prefered over B
- $A \sim B$ indifference between A and B
- $A \succeq B$ B not prefered over A

i.e. Given a set $\mathcal{S}$ (of states), we define binary relations $\succ$ and $\sim$ on $\mathcal{S}$.

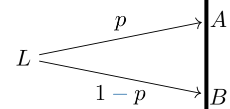
Preferences in Non-Deterministic Environments

Problem: In nondeterministic environments we do not have full information about the states we choose between.

Example 5.3.4 (Airline Food). *Do you want chicken or pasta*(but we cannot see through the tin foil)

Definition 5.3.5.

Let $\mathcal{S}$ a set of states. We call a random variable X with domain $\{A_1, \ldots, A_n\} \subseteq \mathcal{S}$ 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 $\mathcal{S}$ to be *closed under lotteries*, i.e. lotteries themselves are also states. That allows us to consider lotteries such as $[p,A;1-p,[q,B;1-q,C]]$.

Rational Preferences

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

Definition 5.3.6. We call a set $\succ$ of preferences rational, iff the following constraints hold:

Orderability	$A \succ B \vee B \succ A \vee A \sim B$
Transitivity	$A \succ B \wedge B \succ C \Rightarrow A \succ C$
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.

The rationality constraints can be understood as follows:

Orderability: $A \succ B \vee B \succ A \vee A \sim B$ Given any two prizes or lotteries, a rational agent must either prefer one to the other or else rate the two as equally preferable. That is, the agent cannot avoid deciding. Refusing to bet is like refusing to allow time to pass.

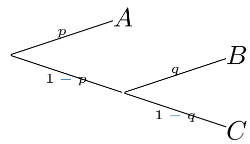
Transitivity: $A \succ B \wedge B \succ C \Rightarrow A \succ C$

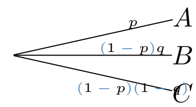
Continuity: $A \succ B \succ C \Rightarrow (\exists p.[p,A;1-p,C] \sim B)$ If some lottery B is between A and C in preference, then there is some probability p for which the rational agent will be indifferent between getting B for sure and the lottery that yields A with probability p and C with probability $1-p$.

Substitutability: $A \sim B \Rightarrow [p,A;1-p,C] \sim [p,B;1-p,C]$ If an agent is indifferent between two lotteries A and B, then the agent is indifferent between two more complex lotteries that are the same except that B is substituted for A in one of them. This holds regardless of the probabilities and the other outcome(s) in the lotteries.

Monotonicity: $A \succ B \Rightarrow (p > q) \Leftrightarrow [p,A;1-p,B] \succ [q,A;1-q,B]$ Suppose two lotteries have the same two possible outcomes, A and B. If an agent prefers A to B, then the agent must prefer the lottery that has a higher probability for A (and vice versa).

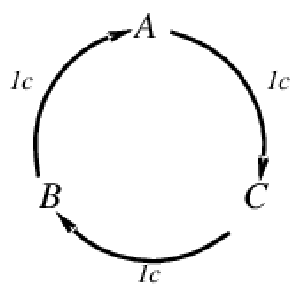
Decomposability: $[p,A;1-p,[q,B;1-q,C]] \sim [p,A;((1-p)q),B;((1-p)(1-q)),C]$ Compound lotteries can be reduced to simpler ones using the laws of probability. This has been called the "no fun in gambling" rule because it says that two consecutive lotteries can be compressed into a single equivalent lottery: the following two are equivalent:





Rational preferences contd.

- Violating the rationality constraints from **??** leads to self-evident irrationality.
- **Example 5.3.7.** 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



5.4 Utilities

Ramseys Theorem and Value Functions

- **Theorem 5.4.1.** *(Ramsey, 1931; von Neumann and Morgenstern, 1944)*

  Given a rational set of preferences there exists a real valued function U *such that* $U(A) \geq U(B)$, *iff* $A \succeq B$ *and* $U([p_1,S_1\,;\ldots;p_n,S_n]) = \sum_i p_i U(S_i)$
- This is an existence theorem, uniqueness not guaranteed.
- **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 5.4.2.** 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!)

Utilities

- **Intuition:** Utilities map states to real numbers.
- **Question:** Which numbers exactly?
- **Definition 5.4.3 (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" $u_\bot$ with probability $1-p$

  adjust lottery probability p until $A{\sim}L_p$. Then $U(A)=p$.
- **Example 5.4.4.** Choose $u_\top \mathrel{\widehat{=}}$ current state, $u_\bot \mathrel{\widehat{=}}$ instant death

pay \$30$\sim L$ $\xrightarrow{0.999999}$ continue as before

pay \$30$\sim L$ $\xrightarrow[0.000001]{}$ instant death

Popular Utility Functions

- **Definition 5.4.5.** Normalized utilities: $u_\top = 1$, $u_\bot = 0$.

  (Not very meaningful, but at least it's independent of the specific problem...)
- **Obviously**: *Money* (Very intuitive, often easy to determine, but actually not well-suited as a utility function (see later))
- **Definition 5.4.6.** 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...

  Better:
- **Definition 5.4.7.** QALYs: quality adjusted life years

  QALYs are useful for medical decisions involving substantial risk.

Comparing Utilities

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!)

But their behavior suggests a lower price:

- Driving in a car for $370\mathrm{km}$ incurs a risk of one micromort;
- Over the life of your car – say, $150,000\mathrm{km}$ 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.

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!)

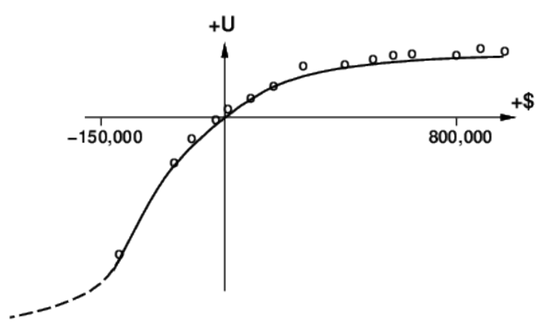
Money vs. Utility

▷ Money does *not* behave as a utility function should.

▷ Given a lottery L with expected monetary value $\mathrm{EMV}(L)$, usually $U(L) < U(\mathrm{EMV}(L))$, 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 positive numbers.

5.5 Multi-Attribute Utility

Video Nuggets covering this section can be found at https://fau.tv/clip/id/30343 and https://fau.tv/clip/id/30344.

In this section we will make the ideas introduced above more practical. The discussion above conceived utility functions as functions on atomic states, which were good enough for introducing the theory. But when we build decision models for utility-based agent we want to characterize states by attributes that are already random variables in the Bayesian network we use to represent the belief state. For factored states, the utility function can be expressed as a multivariate function on attribute values.

Utility Functions on Attributes

Recap: So far we understand how to obtain utility functions $u\colon S \to \mathbb{R}$ 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 5.5.1. Let $X_1, \ldots, X_n$ be random variables with domains $D_1, \ldots, D_n$. Then we call a function $u \colon D_1 \times \ldots \times D_n \to \mathbb{R}$ a (multi-attribute) utility function on attributes $X_1, \ldots, X_n$.

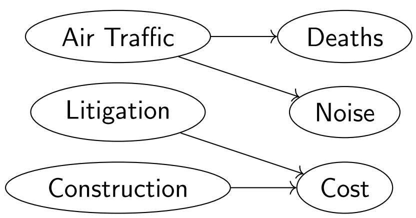
Note: In the general (worst) case, a multi-attribute utility function on n random variables with domain sizes k each requires k^n parameters to represent.

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 5.5.2 (Assessing an Airport Site).**



▷ Attributes: Deaths, Noise, Cost.

▷ **Question**: What is $U(\text{Deaths}, \text{Noise}, \text{Cost})$ for a projected airport?

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

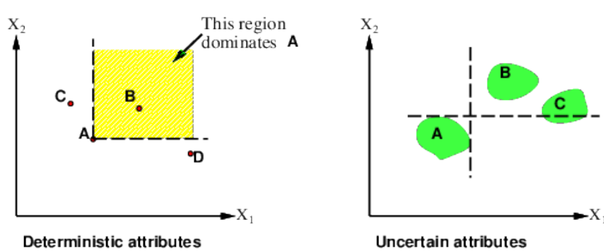
▷ **Idea 1:** Identify conditions under which decisions can be made without complete identification of $U(X_1, \ldots, X_n)$.

▷ **Idea 2:** Identify various types of *independence* in preferences and derive consequent canonical forms for $U(X_1, \ldots, X_n)$.

Strict Dominance

First Assumption: U is often *monotone* in each argument. (wlog. growing)

Definition 5.5.3. *(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,



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.

Stochastic Dominance

Definition 5.5.4. 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 $P(X_1 \geq t) \geq P(X_2 \geq t)$, and for some t, we have $P(X_1 \geq t) > P(X_2 \geq t)$.

Observation 5.5.5. *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.

Observation: Stochastic dominance can often be determined without exact distributions using *qualitative* reasoning.

Example 5.5.6 (Construction cost increases with distance). If airport location S_1 is closer to the city than $S_2 \leadsto S_1$ stochastically dominates S_2 on cost.q

We have seen how we can do inference with attribute-based utility functions, let us consider the computational implications. We observe that we have just replaced one evil – exponentially many states (in terms of the attributes) – by another – exponentially many parameters of the utility functions.

Wo we do what we always do in AI-2: we look for structure in the domain, do more theory to be able to turn such structures into computationally improved representations.

Preference structure: Deterministic

- **Recall:** In deterministic environments an agent has a value function.
- **Definition 5.5.7.** 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 5.5.8.** E.g., $\langle \mathrm{Noise}, \mathrm{Cost}, \mathrm{Safety}\rangle$: are preferentially independent
  $\langle$20,000 suffer, 4.6 G\$, 0.06 deaths/mpm$\rangle$ vs. $\langle$70,000 suffer, 4.2 G\$, 0.06 deaths/mpm$\rangle$
- **Theorem 5.5.9 (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 5.5.10 (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. (often a good approximation)
- **Example 5.5.11.** The value function for the airport decision might be

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

Preference structure: Stochastic

Definition 5.5.12. $\mathbf{X}$ is utility independent of $\mathbf{Y}$ iff preferences over lotteries in $\mathbf{X}$ do not depend on particular values in $\mathbf{Y}$

Definition 5.5.13. A set $\mathbf{X}$ is mutually utility independent (MUI), iff each subset is utility independent of its complement.

Theorem 5.5.14. *For a MUI set of attributes $\mathcal{X}$, there is a multiplicative utility function of the form:* [Kee74]

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

⇒ *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.

Decision networks - Improvements

Ways to improve inference in decision networks:

- ▷ Exploit "inner structure" of the utility function to simplify the computation,
- ▷ eliminate dominated actions,
- ▷ label 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)

5.6 The Value of Information

Video Nuggets covering this section can be found at `https://fau.tv/clip/id/30346` and `https://fau.tv/clip/id/30347`.
So far we have tacitly been concentrating on actions that directly affect the environment. We will now come to a type of action we have hypothesized in the beginning of the course, but have completely ignored up to now: information gathering actions.

What if we do not have all information we need?

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 5.6.1 (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 5.6.2. Information value theory is concerned with agent making decisions on information gathering rationally.

Value of Information by Example

Idea: Compute the expected *gain in utility* from acquring information.
Example 5.6.3 (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 $\frac{k}{n}$€.
- 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 5.6.4 (Oil Drilling Rights contd.).

- Survey may say *oil in block 3 with probability* $\frac{1}{n}$ $\rightsquigarrow$ we buy block 3 for $\frac{k}{n}$€ and make a profit of $(k-\frac{k}{n})$€.
- 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 $\frac{k}{n-1}-\frac{k}{n}$€.
- 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 $\frac{k}{n}$€ for the information. (as much as block 3 is worth!)

General formula (VPI)

Definition 5.6.5. 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.: $\alpha=\underset{a\in A}{\operatorname{argmax}}\ \mathrm{EU}(a|E_i=e_i)$ and $\alpha_f=\underset{a\in A}{\operatorname{argmax}}\ \mathrm{EU}(a|E_i=e_i,F=f)$

The value of perfect information (VPI) on F given evidence $E_i=e_i$ is defined as

$$\mathrm{VPI}_{E_i=e_i}(F):=(\sum_{f\in\mathbf{dom}(F)}P(F=f|E_i=e_i)\cdot\mathrm{EU}(\alpha_f|E_i=e_i,F=f))-\mathrm{EU}(\alpha|E_i=e_i)$$

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.

Properties of VPI

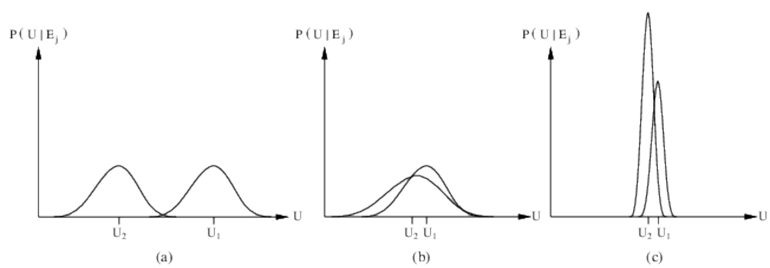
- **Observation 5.6.6 (VPI is Non-negative).**
  $\mathrm{VPI}_E(F) \geq 0$ *for all* j *and* E *(in expectation, not post hoc)*
- **Observation 5.6.7 (VPI is Non-additive).**
  $\mathrm{VPI}_E(F, G) \neq \mathrm{VPI}_E(F) + \mathrm{VPI}_E(G)$ *(consider, e.g., obtaining F twice)*
- **Observation 5.6.8 (VPI is Order-independent).**

$$\mathrm{VPI}_E(F, G) = \mathrm{VPI}_E(F) + \mathrm{VPI}_{E,F}(G) = \mathrm{VPI}_E(G) + \mathrm{VPI}_{E,G}(F)$$

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

Qualitative behavior of VPI

- **Question:** Say we have three distributions for $P(U|E_j)$



  Qualitatively: What is the value of information (VPI) in these three cases?
- **Answers:** reserved for the plenary sessions $\leadsto$ be there!

We will now use information value theory to specialize our utility-based agent from above.

A simple Information-Gathering Agent

- **Definition 5.6.9.** A simple information gathering agent. (gathers info before acting)

function Information—Gathering—Agent (percept) **returns** an action
  persistent: D, a decision network
  integrate percept into D

$j := \underset{k}{\mathrm{argmax}}\ \mathrm{VPI}_E(E_k)/Cost(E_k)$
if $\mathrm{VPI}_E(E_j) > Cost(E_j)$ **return** Request(E_j)
else return the best action from D

The next percept after 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 (Not discussed in this lecture)

Summary

- ▷ 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.

Chapter 6

Temporal Probability Models

6.1 Modeling Time and Uncertainty

Stochastic Processes

The world changes in *stochastically predictable ways*.

Example 6.1.1.

- ▷ 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,
- ▷ 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 6.1.2. 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 $\mathbf{dom}(X_t) = D$ 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 6.1.3. Given a stochastic process X_t over S and $a, b \in S$ with $a \preceq b$, we write $\mathbf{X}_{a:b}$ for the sequence $X_a, X_{a+1}, \ldots, X_{b-1}, X_b$ and $E_{a:b}^{=e}$ for $E_a = e_a, \ldots, E_b = e_b$.

Stochastic Processes (Running Example)

Example 6.1.4 (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 $\mathtt{Rain}_0, \mathtt{Rain}_1, \mathtt{Rain}_2, \ldots$ of hidden variables, and
- ▷ a related stochastic process $\mathtt{Umbrella}_0, \mathtt{Umbrella}_1, \mathtt{Umbrella}_2, \ldots$ of evidence variables.

...and a combined stochastic process $\langle \mathtt{Rain}_0, \mathtt{Umbrella}_0 \rangle, \langle \mathtt{Rain}_1, \mathtt{Umbrella}_1 \rangle, \ldots$

Note that $\mathtt{Umbrella}_t$ only depends on $\mathtt{Rain}_t$, not on e.g. $\mathtt{Umbrella}_{t-1}$ (except indirectly through $\mathtt{Rain}_t$ / $\mathtt{Rain}_{t-1}$).

Definition 6.1.5. We call a stochastic process of *hidden* variables a state variable.

Markov Processes

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

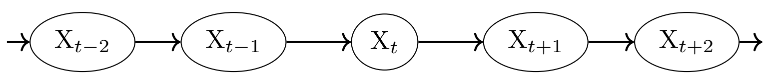
Definition 6.1.6. Let $(X_t)_{t \in S}$ a stochastic process. X has the (nth order) Markov property iff X_t only depends on a bounded subset of $\mathbf{X}_{0:t-1}$ – i.e. for all $t \in S$ we have $\mathbb{P}(X_t | X_0, \ldots X_{t-1}) = \mathbb{P}(X_t | X_{t-n}, \ldots X_{t-1})$ for some $n \in S$.

A stochastic process with the Markov property for some n is called a (nth order) Markov process.

Important special cases:

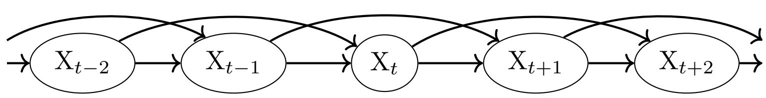
Definition 6.1.7.

▷ First-order Markov property: $\mathbb{P}(\mathbf{X}_t | \mathbf{X}_{0:t-1}) = \mathbb{P}(\mathbf{X}_t | \mathbf{X}_{t-1})$



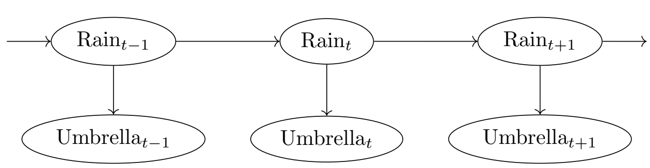
A first order Markov process is called a Markov chain.

▷ Second-order Markov property: $\mathbb{P}(\mathbf{X}_t | \mathbf{X}_{0:t-1}) = \mathbb{P}(\mathbf{X}_t | \mathbf{X}_{t-2}, \mathbf{X}_{t-1})$



Markov Process Example: The Umbrella

Example 6.1.8 (Umbrellas continued). We model the situation in a Bayesian network:



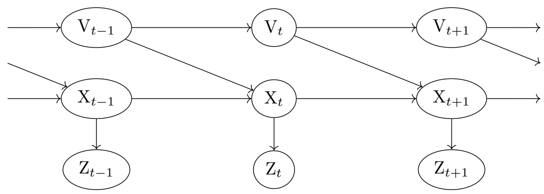
Problem: This network does not actually have the First-order Markov property...

Possible fixes: We have two ways to fix this:

1. Increase the order of the Markov process. (more dependencies $\Rightarrow$ more complex inference)
2. Add more state variables, e.g., Temp_t, $\mathrm{Pressure}_t$. (more information sources)

Markov Process Example: Robot Motion

Example 6.1.9 (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.

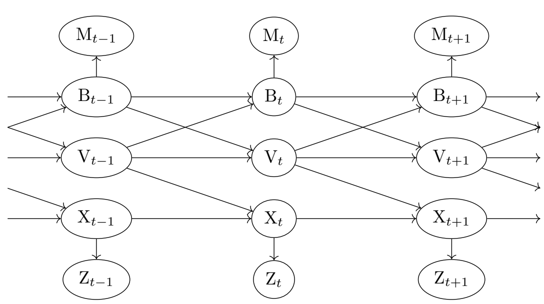
Example 6.1.10 (Battery Powered Robot). If the robot has a *battery*, the Markov property is violated!

- ▷ 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 6.1.11 (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 6.1.12. Given a stochastic process with state variables X_t and evidence variables E_t, then $\mathbb{P}(X_t|\mathbf{X}_{0:t})$ is a transition model and $\mathbb{P}(E_t|\mathbf{X}_{0:t},\mathbf{E}_{1:t-1})$ a sensor model in the sense of a model-based agent.

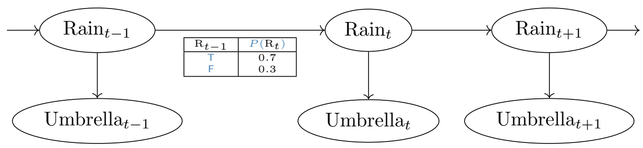
Note that we assume that the X_t do not depend on the E_t.

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

Problem: Even with the Markov property the transition model is infinite. ($t \in \mathbb{N}$)

Definition 6.1.13. 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 6.1.14 (Umbrellas are stationary). $\mathbb{P}(\mathtt{Rain}_t|\mathtt{Rain}_{t-1})$ 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 AI-2.

Markov Sensor Models

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

Problem: The evidence variables E_t could depend on any of the variables $\mathbf{X}_{0:t},\mathbf{E}_{1:t-1}$...

Definition 6.1.15. We say that a sensor model has the sensor Markov property, iff $\mathbb{P}(E_t|\mathbf{X}_{0:t},\mathbf{E}_{1:t-1}) = \mathbb{P}(E_t|X_t)$ – i.e., the sensor model depends only on the current state.

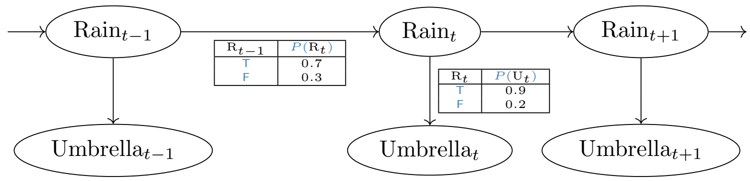
Assumptions on Sensor Models: We usually assume the sensor Markov property and make it stationary as well: $\mathbb{P}(E_t|X_t)$ is fixed for all t.

Definition 6.1.16 (Note).

- ▷ If a Markov chain X is stationary and discrete, we can represent the transition model as a matrix $\mathbf{T}_{ij} := P(X_t = j|X_{t-1} = i)$.
- ▷ 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 $\mathbf{O}_t$ with $\mathbf{O}_{tii} := P(E_t = e_t|X_t = i)$.
- ▷ A pair $\langle X, E\rangle$ 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)

Umbrellas, the full Story

Example 6.1.17 (Umbrellas, Transition & Sensor Models).



This is a hidden Markov model

Observation 6.1.18. *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*

$$\mathbb{P}(\mathbf{X}_{0:t}, \mathbf{E}_{1:t}) = \mathbb{P}(X_0) \cdot \prod_{i=1}^{t} \mathbb{P}(X_i | X_{i-1}) \cdot \mathbb{P}(E_i | X_i)$$

6.2 Inference: Filtering, Prediction, and Smoothing

Inference tasks

Definition 6.2.1. 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) $\mathbb{P}(X_t | E_{1:t}^{=e})$: Given the sequence of observations up until time t, compute the likely state of the world at *current* time t.
- ▷ Prediction (or state estimation) $\mathbb{P}(X_{t+k} | E_{1:t}^{=e})$ 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 $\underset{\mathbf{x}_{1:t}}{\operatorname{argmax}} (P(X_{1:t}^{=x} | E_{1:t}^{=e}))$: 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.

Filtering (Computing the Belief State given Evidence)

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 $\mathbb{P}(X_{t-1})$.

⇒ We want a function $\mathbb{P}(X_t|E_{1:t}^{=e}) = F(e_t, \underbrace{\mathbb{P}(X_{t-1}|E_{1:t-1}^{=e})}_{F(e_{t-1},\ldots)})$

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

Filtering Derivation

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

Reminder: In a stationary HMM, we have the matrices $\mathbf{T}_{ij} = P(X_t = j|X_{t-1} = i)$ and $\mathbf{O}_{tii} = P(E_t = e_t|X_t = i)$.

Then interpreting $\mathbb{P}(X_{t-1}|E_{1:t-1}^{=e})$ as a vector, the above corresponds exactly to the matrix multiplication $\alpha(\mathbf{O}_t \cdot \mathbf{T}^T \cdot \mathbb{P}(X_{t-1}|E_{1:t-1}^{=e}))$

Definition 6.2.2. We call the inner part of the above expression the forward algorithm, i.e. $\mathbb{P}(X_t|E_{1:t}^{=e}) = \alpha(\mathrm{FORWARD}(e_t, \mathbb{P}(X_{t-1}|E_{1:t-1}^{=e}))) =: \mathbf{f}_{1:t}$.

Filtering the Umbrellas

Example 6.2.3. Let's assume:

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

▷ $P(\mathtt{R}_{t+1}|\mathtt{R}_t) = 0.6$, $P(\neg\mathtt{R}_{t+1}|\neg\mathtt{R}_t) = 0.8$, $P(\mathtt{U}_t|\mathtt{R}_t) = 0.9$ and $P(\neg\mathtt{U}_t|\neg\mathtt{R}_t) = 0.85$

⇒ $\mathbf{T} = \begin{pmatrix} 0.6 & 0.4 \\ 0.2 & 0.8 \end{pmatrix}$

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

⇒ $\mathbf{O}_1 = \mathbf{O}_2 = \begin{pmatrix} 0.9 & 0 \\ 0 & 0.15 \end{pmatrix}$ and $\mathbf{O}_3 = \begin{pmatrix} 0.1 & 0 \\ 0 & 0.85 \end{pmatrix}$.

Then:

▷ $\mathbf{f}_{1:1} := \mathbb{P}(\mathtt{R}_1|\mathtt{U}_1 = \mathsf{T}) = \alpha(\mathbb{P}(\mathtt{U}_1 = \mathsf{T}|\mathtt{R}_1) \cdot (\sum_{b\in\{\mathsf{T},\mathsf{F}\}} \mathbb{P}(\mathtt{R}_1|\mathtt{R}_0 = b) \cdot P(\mathtt{R}_0 = b)))$

$= \alpha(\langle 0.9, 0.15\rangle \cdot (\langle 0.6, 0.4\rangle \cdot 0.5 + \langle 0.2, 0.8\rangle \cdot 0.5)) = \alpha(\langle 0.36, 0.09\rangle) = \langle 0.8, 0.2\rangle$

▷ Using matrices: $\alpha(\mathbf{O}_1 \cdot \mathbf{T}^T \cdot \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}) = \alpha(\begin{pmatrix} 0.9 & 0 \\ 0 & 0.15 \end{pmatrix} \cdot \begin{pmatrix} 0.6 & 0.2 \\ 0.4 & 0.8 \end{pmatrix} \cdot \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix})$

$=\alpha(\begin{pmatrix} 0.9 \cdot 0.6 & 0.9 \cdot 0.2 \\ 0.15 \cdot 0.4 & 0.15 \cdot 0.8 \end{pmatrix} \cdot \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix}) = \alpha(\begin{pmatrix} 0.9 \cdot 0.6 \cdot 0.5 + 0.9 \cdot 0.2 \cdot 0.5 \\ 0.15 \cdot 0.4 \cdot 0.5 + 0.15 \cdot 0.8 \cdot 0.5 \end{pmatrix}) = \alpha(\begin{pmatrix} 0.36 \\ 0.09 \end{pmatrix})$

Filtering the Umbrellas (Continued)

Example 6.2.4. $\mathbf{f}_{1:1} := \mathbb{P}(\mathtt{R}_1|\mathtt{U}_1 = \mathsf{T}) = \langle 0.8, 0.2\rangle$

▷ $\mathbf{f}_{1:2} := \mathbb{P}(\mathtt{R}_2|\mathtt{U}_2 = \mathsf{T}, \mathtt{U}_1 = \mathsf{T}) = \alpha(\mathbf{O}_2 \cdot \mathbf{T}^T \cdot \mathbf{f}_{1:1}) = \alpha(\mathbb{P}(\mathtt{U}_2 = \mathsf{T}|\mathtt{R}_2) \cdot (\sum_{b \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(\mathtt{R}_2|\mathtt{R}_1 = b) \cdot \mathbf{f}_{1:1}(b)))$

$=\alpha(\langle 0.9, 0.15\rangle \cdot (\langle 0.6, 0.4\rangle \cdot 0.8 + \langle 0.2, 0.8\rangle \cdot 0.2)) = \alpha(\langle 0.468, 0.072\rangle) = \langle 0.87, 0.13\rangle$

▷ $\mathbf{f}_{1:3} := \mathbb{P}(\mathtt{R}_3|\mathtt{U}_3 = \mathsf{F}, \mathtt{U}_2 = \mathsf{T}, \mathtt{U}_1 = \mathsf{T}) = \alpha(\mathbf{O}_3 \cdot \mathbf{T}^T \cdot \mathbf{f}_{1:2})$

$=\alpha(\mathbb{P}(\mathtt{U}_3 = \mathsf{F}|\mathtt{R}_3) \cdot (\sum_{b \in \{\mathsf{T},\mathsf{F}\}} \mathbb{P}(\mathtt{R}_3|\mathtt{R}_2 = b) \cdot \mathbf{f}_{1:2}(b)))$

$=\alpha(\langle 0.1, 0.85\rangle \cdot (\langle 0.6, 0.4\rangle \cdot 0.87 + \langle 0.2, 0.8\rangle \cdot 0.13)) = \alpha(\langle 0.0547, 0.3853\rangle) = \langle 0.12, 0.88\rangle$

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 6.2.5. *By the same reasoning as filtering:*

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

Observation 6.2.6. *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 $S = \mathbf{T}^T \cdot S$)

⇒ the impact of the evidence vanishes.

⇒ The stationary distribution only depends on the transition model.

⇒ 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.*

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

Smoothing

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 $t - k$.

$$\begin{aligned}
\mathbb{P}(X_{t-k}|E_{1:t}^{=e}) &= \mathbb{P}(X_{t-k}|E_{t-(k-1):t}^{=e}, E_{1:t-k}^{=e}) && \text{(Divide the evidence)}\\
&= \alpha(\mathbb{P}(E_{t-(k-1):t}^{=e}|X_{t-k}, E_{1:t-k}^{=e}) \cdot \mathbb{P}(X_{t-k}|E_{1:t-k}^{=e})) && \text{(Bayes Rule)}\\
&= \alpha(\underbrace{\mathbb{P}(E_{t-(k-1):t}^{=e}|X_{t-k})}_{=:\mathbf{b}_{t-(k-1):t}} \cdot \underbrace{\mathbb{P}(X_{t-k}|E_{1:t-k}^{=e})}_{=\mathbf{f}_{1:t-k}}) && \text{(cond. independence)}\\
&= \alpha(\mathbf{f}_{1:t-k} \times \mathbf{b}_{t-(k-1):t})
\end{aligned}$$

(where $\times$ denotes component-wise multiplication)

Smoothing (continued)

Definition 6.2.7 (Backward message). $\mathbf{b}_{t-k:t} = \mathbb{P}(E_{t-k:t}^{=e}|X_{t-(k+1)})$

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

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

Definition 6.2.8. We call the associated algorithm the backward algorithm, i.e. $\mathbb{P}(X_{t-k}|E_{1:t}^{=e}) = \alpha(\underbrace{\mathrm{FORWARD}(e_{t-k}, \mathbf{f}_{1:t-(k+1)})}_{\mathbf{f}_{1:t-k}} \times \underbrace{\mathrm{BACKWARD}(e_{t-(k-1)}, \mathbf{b}_{t-(k-2):t})}_{\mathbf{b}_{t-(k-1):t}})$.

As a starting point for the recursion, we let $\mathbf{b}_{t+1:t}$ the uniform vector with 1 in every component.

Smoothing example

Example 6.2.9 (Smoothing Umbrellas). Reminder: We assumed $\mathbb{P}(\mathtt{R}_0) = \langle 0.5, 0.5\rangle$, $P(\mathtt{R}_{t+1}|\mathtt{R}_t) = 0.6$, $P(\neg\mathtt{R}_{t+1}|\neg\mathtt{R}_t) = 0.8$, $P(\mathtt{U}_t|\mathtt{R}_t) = 0.9$, $P(\neg\mathtt{U}_t|\neg\mathtt{R}_t) = 0.85$

$\Rightarrow \mathbf{T} = \begin{pmatrix} 0.6 & 0.4 \\ 0.2 & 0.8 \end{pmatrix}$, $\mathbf{O}_1 = \mathbf{O}_2 = \begin{pmatrix} 0.9 & 0 \\ 0 & 0.15 \end{pmatrix}$ and $\mathbf{O}_3 = \begin{pmatrix} 0.1 & 0 \\ 0 & 0.85 \end{pmatrix}$. (The director carries an umbrella on days 1 and 2, and *not* on day 3)

$\mathbf{f}_{1:1} = \langle 0.8, 0.2\rangle$, $\mathbf{f}_{1:2} = \langle 0.87, 0.13\rangle$ and $\mathbf{f}_{1:3} = \langle 0.12, 0.88\rangle$

Let's compute

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

- ▷ We need to compute $\mathbf{b}_{2:3}$ and $\mathbf{b}_{3:3}$:
- ▷ $\mathbf{b}_{3:3} = \mathbf{T} \cdot \mathbf{O}_3 \cdot \mathbf{b}_{4:3} = \begin{pmatrix} 0.6 & 0.4 \\ 0.2 & 0.8 \end{pmatrix} \cdot \begin{pmatrix} 0.1 & 0 \\ 0 & 0.85 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.4 \\ 0.7 \end{pmatrix}$

▷ $\mathbf{b}_{2:3} = \mathbf{T} \cdot \mathbf{O}_2 \cdot \mathbf{b}_{3:3} = \begin{pmatrix} 0.6 & 0.4 \\ 0.2 & 0.8 \end{pmatrix} \cdot \begin{pmatrix} 0.9 & 0 \\ 0 & 0.15 \end{pmatrix} \cdot \begin{pmatrix} 0.4 \\ 0.7 \end{pmatrix} = \begin{pmatrix} 0.258 \\ 0.156 \end{pmatrix}$

$\Rightarrow \alpha(\begin{pmatrix} 0.8 \\ 0.2 \end{pmatrix} \times \begin{pmatrix} 0.258 \\ 0.156 \end{pmatrix}) = \alpha(\begin{pmatrix} 0.2064 \\ 0.0312 \end{pmatrix}) = \begin{pmatrix} 0.87 \\ 0.13 \end{pmatrix}$

⇒ Given the evidence $\mathtt{U}_2, \neg\mathtt{U}_3$, the posterior probability for $\mathtt{R}_1$ went up from 0.8 to 0.87!

Forward/Backward Algorithm for Smoothing

Definition 6.2.10. Forward backward algorithm: returns the sequence of posterior distributions $\mathbb{P}(X_1)\ldots\mathbb{P}(X_t)$ given evidence $e_1, \ldots, e_t$:

```
function FORWARD-BACKWARD(⟨e_1, ..., e_t⟩, P(X_0))
    f := ⟨P(X_0)⟩
    b := ⟨1, 1, ...⟩
    S := ⟨P(X_0)⟩
    for i = 1, ..., t do
        f_i := FORWARD(f_{i-1}, e_i)          /* filtering */
    for i = t, ..., 1 do
        S_i := α(f_i × b)                     /* smoothing */
        b := BACKWARD(b, e_i)
    return S
```

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

Country dance algorithm

Idea: If $\mathbf{T}$ and $\mathbf{O}_i$ are invertible, we can avoid storing all forward messages in the smoothing algorithm by running filtering backwards:

$$\mathbf{f}_{1:i+1} = \alpha(\mathbf{O}_{i+1} \cdot \mathbf{T}^T \cdot \mathbf{f}_{1:i})$$

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

⇒ we can trade space complexity for time complexity:

▷ In the first for-loop, we only compute the final $\mathbf{f}_{1:t}$ (No need to store the intermediate results)

▷ In the second for-loop, we compute both $\mathbf{f}_{1:i}$ and $\mathbf{b}_{t-i:t}$ (Only one copy of $\mathbf{f}_{1:i}$, $\mathbf{b}_{t-i:t}$ is stored)

⇒ 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”)

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. $\max_{x_1,\ldots,x_t}(P(X_{1:t}^{=x}|E_{1:t}^{=e}))$?

Example 6.2.11. Given the sequence $\mathtt{U}_1, \mathtt{U}_2, \neg\mathtt{U}_3, \mathtt{U}_4, \mathtt{U}_5$, the most likely state for $\mathtt{R}_3$ 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 $x_t \in \mathbf{dom}(X)$ and $0 \leq i \leq t$, 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.

$\Rightarrow$ we want to know $\max_{x_1,\ldots,x_{t-1}} \mathbb{P}(X_{1:t-1}^{=x}, X_t|E_{1:t}^{=e})$, and then pick the x_t with the maximal value.

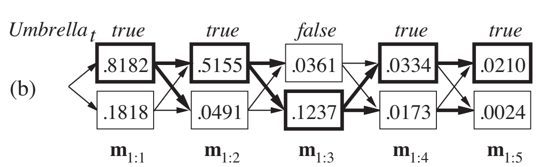
Most Likely Explanation (continued)

By the same reasoning as for filtering:

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

$\mathbf{m}_{1:t}(i)$ 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 6.2.12. For the sequence $[\mathsf{T}, \mathsf{T}, \mathsf{F}, \mathsf{T}, \mathsf{T}]$:



bold arrows: best predecessor measured by "best preceding sequence probability × transition probability"

The Viterbi Algorithm

Definition 6.2.13. The Viterbi algorithm now proceeds as follows:

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

Observation 6.2.14. *Viterbi has linear time complexity and linear space complexity (needs to keep the most likely sequence leading to each state).*

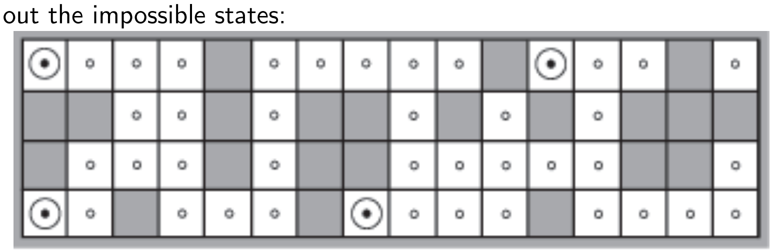
6.3 Hidden Markov Models – Extended Example

Example: Robot Localization using Common Sense

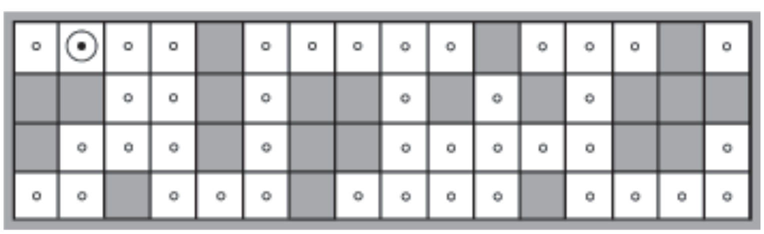
Example 6.3.1 (Robot Localization in a Maze). A robot has four sonar sensors that tell it about obstacles in four directions: N, S, W, E.

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:



a) Possible robot locations after $\mathrm{e}_1 = \mathrm{N\ S\ W}$



b) Possible robot locations after $\mathrm{e}_1 = \mathrm{N\ S\ W}$ and $\mathrm{e}_2 = \mathrm{N\ S}$

Remark 6.3.2. This only works for perfect sensors. (else no impossible states)

What if our sensors are imperfect?

HMM Example: Robot Localization (Modeling)

Example 6.3.3 (HMM-based Robot Localization). We have the following setup:

- ▷ A hidden Random variable X_t for robot location (domain: 42 empty squares)
- ▷ Let $N(i)$ be the set of neighboring fields of the field $X_i = x_i$
- ▷ The Transition matrix for the move action ($\mathbf{T}$ has $42^2 = 1764$ entries)

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

- ▷ We do not know where the robot starts: $P(X_0) = \frac{1}{n}$ (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

$$P(E_t = e_t | X_t = i) = \mathbf{O}_{tii} = (1-\epsilon)^{4-d_{it}} \cdot \epsilon^{d_{it}}$$

(We assume the sensors are independent)

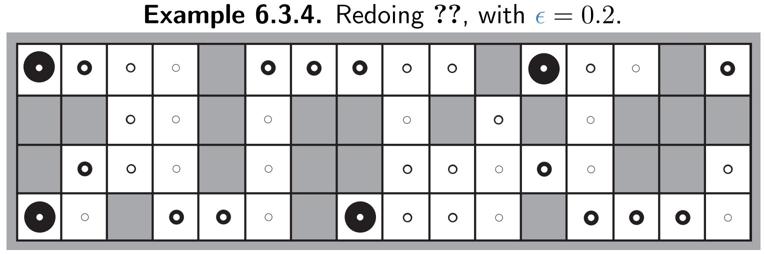
For example, the probability that the sensor on a square with obstacles in north and south would produce N S E is $(1-\epsilon)^3 \cdot \epsilon^1$.

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.

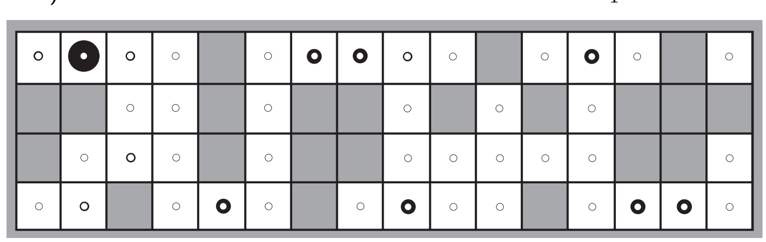
HMM Example: Robot Localization

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

Example 6.3.4. Redoing ??, with $\epsilon = 0.2$.



a) Posterior distribution over robot location after $\mathrm{E}_1 = \mathrm{N\ S\ W}$



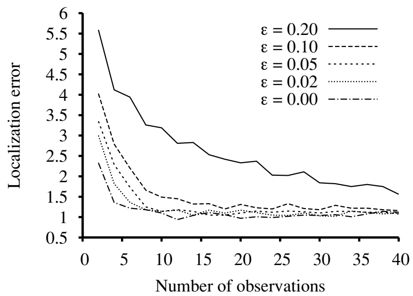
b) Posterior distribution over robot location after $\mathrm{E}_1 = \mathrm{N\ S\ W}$ and $\mathrm{E}_2 = \mathrm{N\ S}$

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

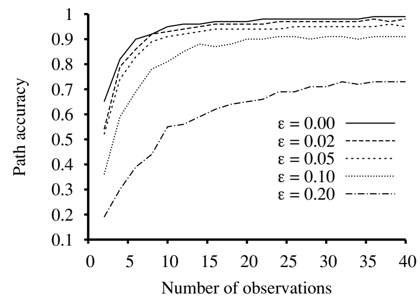
HMM Example: Further Inference Applications

Idea: We can use smoothing: $\mathbf{b}_{k+1:t} = \mathbf{T}\mathbf{O}_{k+1}\mathbf{b}_{k+2:t}$ to find out where it started and the Viterbi algorithm to find the most likely path it took.

Example 6.3.5. Performance of HMM localization vs. observation length (various error rates ϵ)



Localization error (Manhattan distance from true location)



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

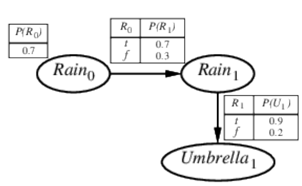
6.4 Dynamic Bayesian Networks

A Video Nugget covering this section can be found at `https://fau.tv/clip/id/30355`.

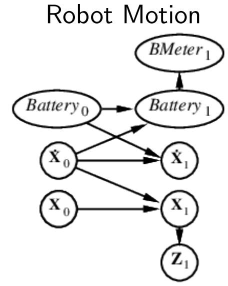
Dynamic Bayesian networks

- **Definition 6.4.1.** A Bayesian network $\mathcal{D}$ is called dynamic (a DBN), iff its random variables are indexed by a time structure. We assume that $\mathcal{D}$ is
  - time sliced, i.e. that the time slices $\mathcal{D}_t$ – 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 $\mathcal{D}_{t-1}$.
- $\mathbf{X}_t$, $\mathbf{E}_t$ contain arbitrarily many variables in a replicated Bayesian network.
- **Example 6.4.2.**

Umbrellas



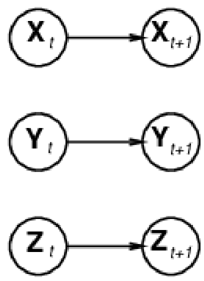
Robot Motion

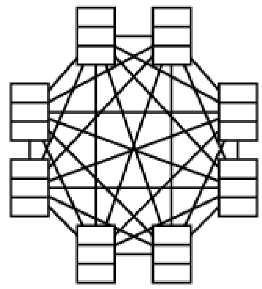


DBNs vs. HMMs

▷ **Observation 6.4.3.**

- ▷ *Every HMM is a single-variable DBN.* *(trivially)*
- ▷ *Every DBN can be turned into an HMM.* *(combine variables into tuple ⇒ lose information about dependencies)*
- ▷ *DBNs have sparse dependencies ⇝ exponentially fewer parameters;*

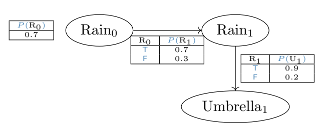


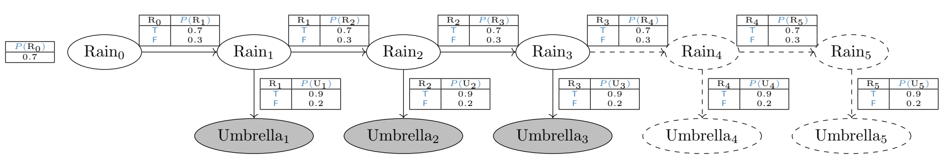


▷ **Example 6.4.4 (Sparse Dependencies).** With 20 Boolean state variables, three parents each, a DBN has $20 \cdot 2^3 = 160$ parameters, the corresponding HMM has $2^{20} \cdot 2^{20} \approx 10^{12}$.

Exact inference in DBNs

▷ **Definition 6.4.5 (Naive method).** Unroll the network and run any exact algorithm.





▷ **Problem:** Inference cost for each update grows with t.

▷ **Definition 6.4.6.** Rollup filtering: add slice $t+1$, "sum out" slice t using variable elimination.

▷ **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 $\mathcal{O}(d^{2n})$

Summary

- ▷ Temporal probability models use state and evidence variables replicated over time.
- ▷ Markov property and stationarity assumption, so we need both
  - ▷ a transition model and $\mathbf{P}(\mathbf{X}_t|\mathbf{X}_{t-1})$
  - ▷ a sensor model $\mathbf{P}(\mathbf{E}_t|\mathbf{X}_t)$.
- ▷ Tasks are filtering, prediction, smoothing, most likely sequence; (all done recursively with constant cost per time step)
- ▷ Hidden Markov models have a single discrete state variable; (used for speech recognition)
- ▷ DBNs subsume HMMs, exact update intractable.

Chapter 7

Making Complex Decisions

We will now pick up the thread from chapter 5 but using temporal models instead of simply probabilistic ones. We will first look at a sequential decision theory in the special case, where the environment is stochastic, but fully observable (Markov decision processes) and then lift that to obtain POMDPs and present an agent design based on that.

Outline

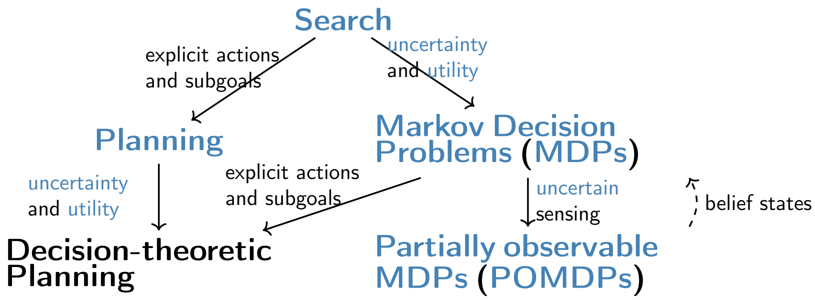
We will now combine the ideas of stochastic process with that of acting based on maximizing expected utility:

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

7.1 Sequential Decision Problems

Sequential Decision Problems

- ▷ **Definition 7.1.1.** In sequential decision problems, the agent's utility depends on a sequence of decisions (or their result states).
- ▷ **Definition 7.1.2.** 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 ⇝ 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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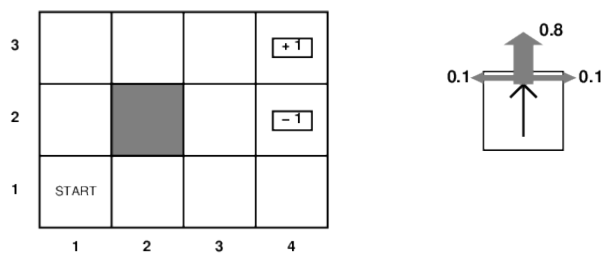
We will fortify our intuition by an example. It is specifically chosen to be very simple, but to exhibit all the peculiarities of Markov decision problems, which we will generalize from this example.

Markov Decision Problem: Running Example

▷ **Example 7.1.3 (Running Example: The 4x3 World).** A (fully observable) 4×3 environment with non-deterministic actions:



- ▷ States $s \in \mathcal{S}$, actions $a \in \mathrm{Act}(s)$.
- ▷ Transition model: $P(s'|s,a) \mathrel{\widehat{=}}$ 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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Perhaps what is more interesting than the components of an MDP is that is *not* a component: a belief and/or sensor model. Recall that MDPs are for fully observable environments.

Markov Decision Process

▷ **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 7.1.4.** A Markov decision process (MDP) $\langle \mathcal{S}, \mathrm{Act}, \mathcal{T}, s_0, R \rangle$ consists of

- ▷ a set of $\mathcal{S}$ of states (with initial state $s_0 \in \mathcal{S}$),

- for every state s, a sets of actions $\mathrm{Act}(s)$.
- a transition model $\mathcal{T}(s,a) = \mathbb{P}(\mathcal{S}|s,a)$, and
- a reward function $R\colon \mathcal{S} \to \mathbb{R}$; 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

$\Rightarrow$ need to take future actions and future states into account

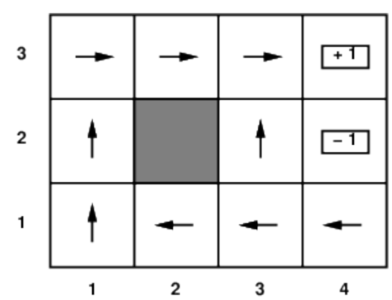
Solving MDPs

▷ 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 7.1.5.** A policy π for an MDP is a function mapping each state s to an action $a \in \mathrm{Act}(s)$.

An optimal policy is a policy that maximizes the expected total rewards. (for some notion of "total"...)

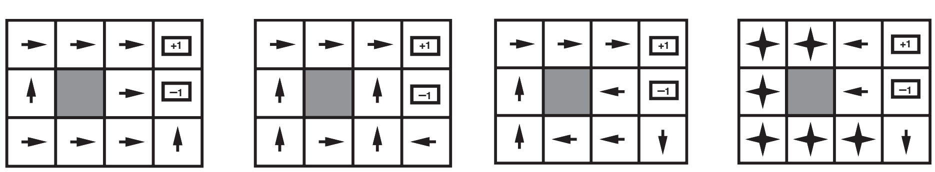
▷ **Example 7.1.6.** Optimal policy when state penalty $R(s)$ is 0.04:



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

Risk and Reward

▷ **Example 7.1.7.** Optimal policy depends on the reward function $R(s)$.



$R(s) < -1.6284$ $\quad -0.4278 < R(s) < -0.0850$ $\quad -0.0221 < R(s) < 0$ $\quad R(s) > 0$

▷ **Question:** Explain what you see in a qualitative manner!

▷ **Answer:** reserved for the plenary sessions ⇝ be there!

7.2 Utilities over Time

In this section we address the problem that even if the transition models are stationary, the utilities may not be. In fact we generally have to take the utilities of state sequences into account in sequential decision problems. If we can derive a notion of the utility of a (single) state from that, we may be able to reuse the machinery we introduced above, so that is exactly what we will attempt.

Utility of state sequences

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 7.2.1.** 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 7.2.2. *For stationary preferences, there are only two ways to combine rewards over time.*

- ▷ *additive rewards:* $U([s_0, s_1, s_2, \ldots]) = R(s_0) + R(s_1) + R(s_2) + \cdots$
- ▷ *discounted rewards:* $U([s_0, s_1, s_2, \ldots]) = R(s_0) + \gamma R(s_1) + \gamma^2 R(s_2) + \cdots$ *where* $0 \leq \gamma \leq 1$ *is called discount factor.*

⇒ we can reduce utilities over time to rewards on individual states

Utilities of State Sequences

Problem: Infinite lifetimes ⇝ additive rewards may become infinite.

Possible Solutions:

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

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

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

2. If there are absorbing states: for any policy π agent eventually "dies" with probability 1 ⇝ expected utility of every state is finite.

3. Discounting: assuming $\gamma < 1$, $R(s) \leq R_{\max}$,

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

Smaller $\gamma \rightsquigarrow$ shorter horizon.

We will only consider discounted rewards in this course

Why discounted rewards?

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.

Utility of States

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

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

Definition 7.2.3. Given a policy π and a starting state s_0, let $S^{\pi}_{s_0}$ 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 $\pi^*_{s_0} := \underset{\pi}{\operatorname{argmax}}\, U^{\pi}(s_0)$.

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

Utility of States (continued)

Observation 7.2.4. *$\pi^*_{s_0}$ 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.

⚠ Observation 7.2.4 does not hold for finite horizon policies!

Definition 7.2.5. We call $\pi^* := \pi^*_s$ for some s the optimal policy.

Definition 7.2.6. The utility $U(s)$ of a state s is $U^{\pi^*}(s)$.

Remark: $R(s) \hat{=}$ "immediate reward", whereas $U \hat{=}$ "long-term reward".

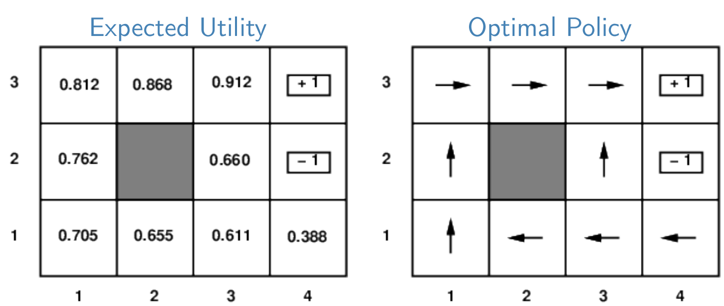
Given the utilities of the states, choosing the best action is just MEU: maximize the expected utility of the immediate successor states

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

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

Utility of States (continued)

▷ **Example 7.2.7 (Running Example Continued).**



▷ **Question:** Why do we go left in $(3,1)$ and not up? (follow the utility)

7.3 Value/Policy Iteration

A Video Nugget covering this section can be found at `https://fau.tv/clip/id/30359`.

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 7.3.1 (Bellman equation (1957)).**

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

We call this equation the Bellman equation

▷ **Example 7.3.2.** $U(1,1) = -0.04$

$+\ \gamma\ \max\{0.8U(1,2) + 0.1U(2,1) + 0.1U(1,1),$	*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 $\rightsquigarrow$ n nonlinear (max isn't) equations in n unknowns.
$\rightsquigarrow$ cannot use linear algebra techniques for solving them.

Value Iteration Algorithm

▷ **Idea:** We use a simple iteration scheme to find a fixpoint:

1. start with arbitrary utility values,
2. update to make them locally consistent with the Bellman equation,
3. everywhere locally consistent $\rightsquigarrow$ global optimality.

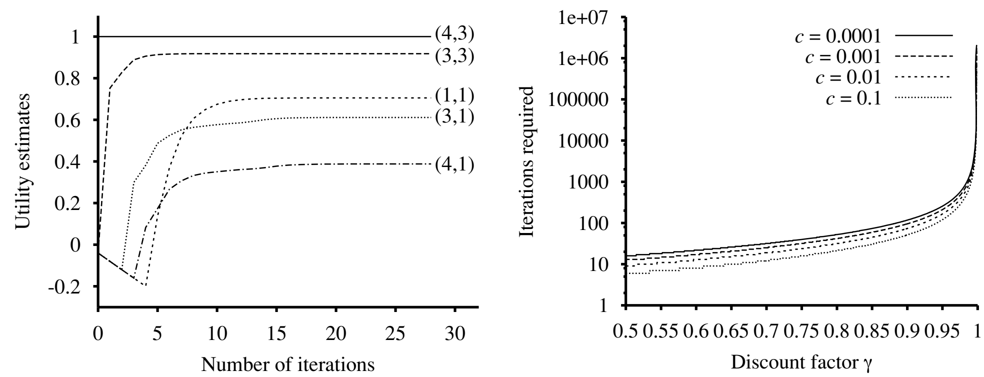
▷ **Definition 7.3.3.** The value iteration algorithm for utilitysutility function is given by

```
function VALUE−ITERATION (mdp,ϵ) 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 γ
       ϵ, the maximum error allowed in the utility of any state
  local variables: U, U′, vectors of utilities for states in S, initially zero
          δ, the maximum change in the utility of any state in an iteration
  repeat
     U := U′; δ := 0
     for each state s in S do
       U′[s] := R(s) + γ · max_{a∈A(s)} (∑_{s′} U[s′] · P(s′|s,a))
       if |U′[s] − U[s]| > δ then δ := |U′[s] − U[s]|
     until δ < ϵ(1 − γ)/γ
     return U
```

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

Value Iteration Algorithm (Example)

▷ **Example 7.3.4 (Iteration on 4x3).**



(where $\varepsilon = c \cdot R_{max}$)

Convergence

▷ **Definition 7.3.5.** The maximum norm is defined as $\|U\| = \max_s |U(s)|$, 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 7.3.6.** *For any two approximations U^t and V^t*

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

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

▷ **Theorem 7.3.7.** *If $\left\|U^{t+1} - U^t\right\| < \epsilon$, then $\left\|U^{t+1} - U\right\| < 2\epsilon\gamma/1 - \gamma$*
(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!

So we see that iteration with Bellman updates will always converge towards the utility of a state, even without knowing the optimal policy. That gives us a first way of dealing with sequential decision problems: we compute utility functions based on states and then use the standard MEU machinery. We have seen above that optimal policies and state utilities are essentially interchangeable: we can compute one from the other. This leads to another approach to computing state utilities: policy iteration, which we will discuss now.

Policy Iteration

▷ **Recap:** Value iteration computes utilities ⇝ optimal policy by MEU.

▷ This even works if the utility estimate is inaccurate. (⇜ policy loss small)

▷ **Idea:** Search for optimal policy and utility values simultaneously [How60]: Iterate

- ▷ policy evaluation: given policy π_i, calculate $U_i = U^{\pi_i}$, the utility of each state were π_i to be executed.
- ▷ policy improvement: calculate a new MEU policy π_{i+1} using 1 lookahead

Terminate if policy improvement yields no change in computed utilities.

▷ **Observation 7.3.8.** *Upon termination U_i is a fixpoint of Bellman update $\rightsquigarrow$ Solution to Bellman equation $\rightsquigarrow$ π_i is an optimal policy.*

▷ **Observation 7.3.9.** *Policy improvement improves policy and policy space is finite $\rightsquigarrow$ termination.*

Policy Iteration Algorithm

▷ **Definition 7.3.10.** 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
    π a policy indexed by state, initially random,
  repeat
    U := POLICY−EVALUATION(π,U,mdp)
    unchanged? := **true**
    foreach state s **in** X **do**
      if $\max_{a\in A(s)} (\sum_{s'} P(s'|s,a)\cdot U(s')) > \sum_{s'} P(s'|s,\pi[s'])\cdot U(s')$ **then do**
        $\pi[s] := \operatorname{argmax}_{b\in A(s)} (\sum_{s'} P(s'|s,b)\cdot U(s'))$
        unchanged? := **false**
  until unchanged?
  return π

Policy Evaluation

▷ **Problem:** How to implement the POLICY−EVALUATION algorithm?

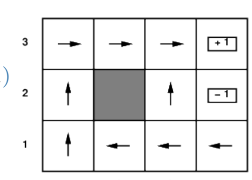
▷ **Solution:** To compute utilities given a fixed π: For all s we have

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

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

▷ **Example 7.3.11 (Simplified Bellman Equations for π).**

$$\begin{aligned}
U_i(1,1) &= -0.04 + 0.8U_i(1,2) + 0.1U_i(1,1) + 0.1U_i(2,1)\\
U_i(1,2) &= -0.04 + 0.8U_i(1,3) + 0.1U_i(1,2)\\
&\vdots
\end{aligned}$$



▷ **Observation 7.3.12.** *n simultaneous linear equations in n unknowns, solve in $\mathcal{O}(n^3)$ with standard linear algebra methods.*

Modified Policy Iteration

▷ Value iteration requires many iterations, but each one is cheap.

▷ Policy iteration often converges in few iterations, but each is expensive.

▷ **Idea:** 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.

7.4 Partially Observable MDPs

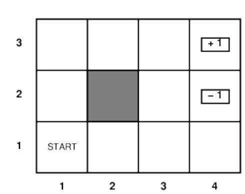
We will now lift the last restriction we made in the decision problems for our agents: in the definition of Markov decision processes we assumed that the environment was fully observable. As we have seen Observation 25.2.6 (Utilities over Time) in the AI lecture notes this entails that the optimal policy only depends on the current state.

Partial Observability

▷ **Definition 7.4.1.** 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: $O(s, e) = P(e|s)$.

▷ **Example 7.4.2 (Noisy 4x3 World).**

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



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

▷ **Theorem 7.4.3 (Astrom 1965).** *The optimal policy in a POMDP is a function $\pi(b)$ 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.

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

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

We write $b' = \mathrm{FORWARD}(b,a,e)$ 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 7.4.4.** 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 $\mathrm{FORWARD}(b,a,e)$ and repeat.

▷ **Intuition:** POMDP decision cycle is search in belief state space.

Partial Observability contd.

▷ **Recap:** The POMDP decision cycle is search in belief state space.

▷ **Observation 7.4.5.** *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 7.4.6.** The belief state of the 4x3 world is a 11 dimensional continuous space. (11 states)

▷ **Theorem 7.4.7.** *Solving POMDPs is very hard!* *(actually, **PSPACE** hard)*

▷ **In particular,** none of the algorithms we have learned applies. (discreteness assumption)

▷ The real world is a POMDP (with initially unknown transition model T and sensor model O)

Reducing POMDPs to Belief-State MDPs

▷ **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 $b' = \mathrm{FORWARD}(b, a, e)$. (deterministic update to the belief state)
- ▷ but we don't, since b' depends on e. (let's calculate $P(e|a,b)$)

▷ **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:

$$\begin{aligned} P(e|a,b) &= \sum_{s'} P(e|a,s',b) \cdot P(s'|a,b) \\ &= \sum_{s'} P(e|s') \cdot P(s'|a,b) \\ &= \sum_{s'} P(e|s') \cdot (\sum_{s} P(s'|s,a), b(s)) \end{aligned}$$

Write the probability of reaching b' from b, given action a, as $P(b'|b,a)$, then

$$\begin{aligned} P(b'|b,a) &= P(b'|a,b) = \sum_{e} P(b'|e,a,b) \cdot P(e|a,b) \\ &= \sum_{e} P(b'|e,a,b) \cdot (\sum_{s'} P(e|s') \cdot (\sum_{s} P(s'|s,a), b(s))) \end{aligned}$$

where $P(b'|e,a,b)$ is 1 if $b' = \mathrm{FORWARD}(b,a,e)$ 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 7.4.8.** *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 $\rightsquigarrow$ 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: $\pi^* \widehat{=}$ 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 7.4.9. 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 $\sum_s b(s) \cdot \alpha_p(s) \widehat{=} b{\cdot}\alpha_p$ as vectors.
  - the expected utility of a fixed conditional plan varies linearly with b
  - $\rightsquigarrow$ the "*best* conditional plan to execute" corresponds to a hyperplane in belief state space.
- **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:

$$U(b) = U^{\pi^*}(b) = \max_b \left(b{\cdot}\alpha_p\right)$$

  - 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.
- **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

▷ **Example 7.4.10.** 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.

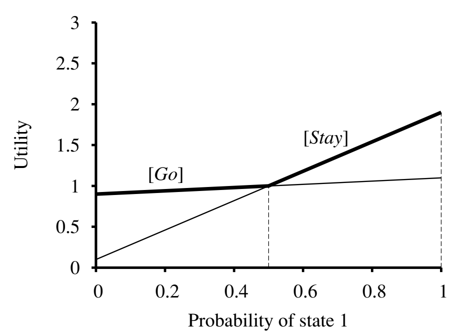
Obviously, the agent should "Stay" when it thinks it's in state S_1 and "Go" when it thinks it's in state S_0.

▷ 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:

$$\begin{aligned} \alpha_{([Stay])}(S_0) &= 0.9R(S_0) + 0.1R(S_1) = 0.1 \\ \alpha_{([stay])}(S_1) &= 0.9R(S_1) + 0.1R(S_0) = 0.9 \\ \alpha_{([go])}(S_0) &= 0.9R(S_1) + 0.1R(S_0) = 0.9 \\ \alpha_{([go])}(S_1) &= 0.9R(S_0) + 0.1R(S_1) = 0.1 \end{aligned}$$

▷ Let us visualize the hyperplanes $b{\cdot}\alpha_{([Stay])}$ and $b{\cdot}\alpha_{([Go])}$.



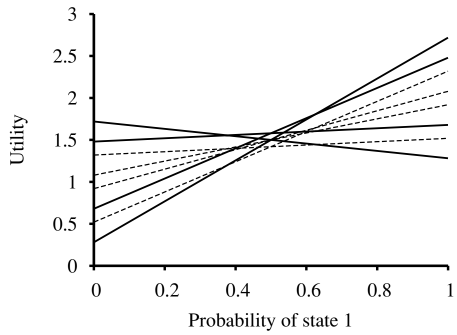
- ▷ The maximum represents the utility function for the finite-horizon problem that allows just one action
- ▷ in each "piece" the optimal action is the first action of the corresponding plan.
- ▷ Here the optimal one-step policy is to "Stay" when $b(1) > 0.5$ and "Go" otherwise.

▷ compute the utilities for conditional plans of depth 2 by considering

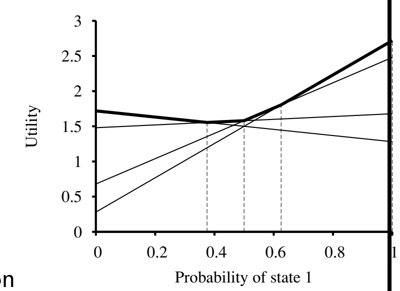
- ▷ each possible first action,
- ▷ each possible subsequent percept, and then
- ▷ each way of choosing a depth-1 plan to execute for each percept:

There are eight of depth 2:

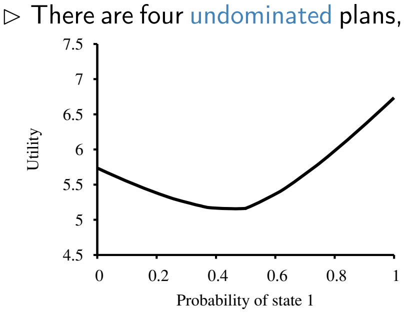
$$[Stay, \text{if } P = 0 \text{ then } Stay \text{ else } Stay \text{ fi}], [Stay, \text{if } P = 0 \text{ then } Stay \text{ else } Go \text{ fi}], \ldots$$



Four of them (dashed lines) are suboptimal for the whole belief space
We call them dominated (they can be ignored)



▷ There are four undominated plans, each optimal in their region



▷ **Idea:** Repeat for depth 3 and so on.

▷ **Theorem 7.4.11 (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*

$$\alpha_p(s) = R(s) + \gamma(\sum_{s'} P(s'|s,a)(\sum_e P(e|s') \cdot \alpha_{p.e}(s')))$$

▷ This recursion naturally gives us a value iteration algorithm,

A Value Iteration Algorithm for POMDPs

Definition 7.4.12. The POMDP value iteration algorithm for POMDPs is given by recursively updating

$$\alpha_p(s) = R(s) + \gamma(\sum_{s'} P(s'|s,a)(\sum_e P(e|s') \cdot \alpha_{p.e}(s')))$$

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.
- Even for the example with $d = 8$, we have 2255 (144 undominated)
- 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!

7.5 Online Agents with POMDPs

In the last section we have seen that even though we can in principle compute utilities of states – and thus use the MEU principle – to make decisions in sequential decision problems, all methods based on the "lifting idea" are hopelessly inefficient.

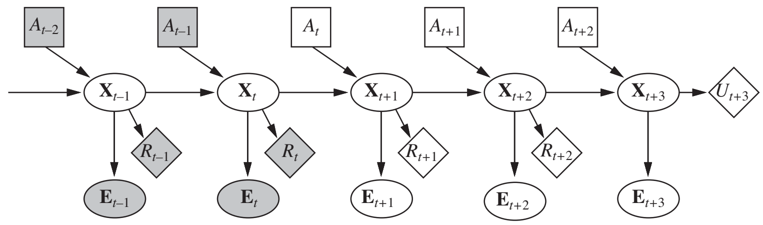
This section describes a different, approximate method for solving POMDPs, one based on look-ahead search. **A Video Nugget** covering this section can be found at `https://fau.tv/clip/id/30361`.

DDN: Decision Networks for POMDPs

- **Idea:** Let's try to use the computationally efficient representations (dynamic Bayesian networks and decision networks) for POMDPs.
- **Definition 7.5.1.** 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
  $\rightsquigarrow$ 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: $\mathbb{P}(\mathrm{X}_{t+1}|\mathrm{X}_t, A_t)$; sensor model: $\mathbb{P}(\mathrm{E}_t|\mathrm{X}_t)$.
- Reward functions R_t and utility U_t of state S_t.
- Variables with known values are gray, rewards for $t = 0, \ldots, t+2$, but utility for $t+3$($\widehat{=}$ discounted sum of rest)

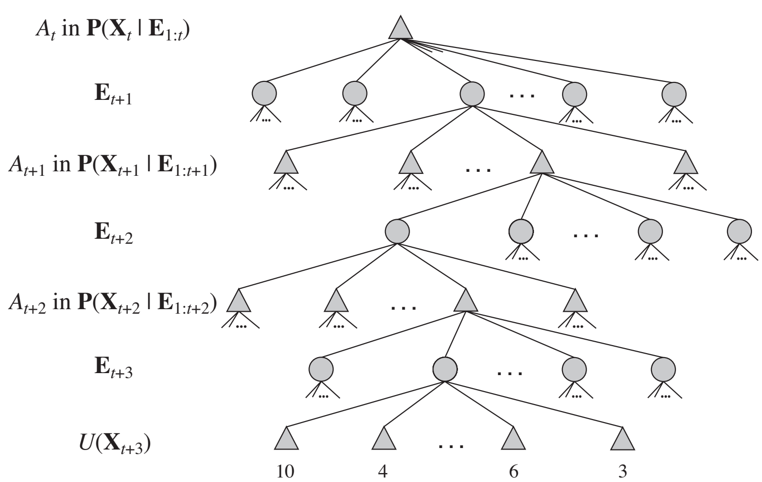
▷ **Problem:** How do we compute with that?

▷ **Answer:** All POMDP algorithms can be adapted to DDNs! (only need CPTs)

Lookahead: Searching over the Possible Action Sequences

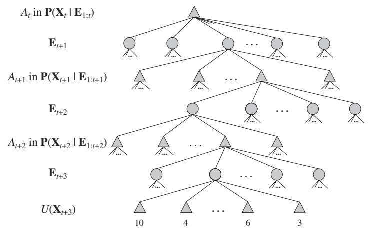
▷ **Idea:** Search over the tree of possible action sequences (like in game-play)

▷ Part of the lookahead solution of the DDN above (three steps lookahead)



- circle $\widehat{=}$ chance nodes (the environment decides)
- triangle $\widehat{=}$ belief state (each action decision is taken there)

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 $\mathbf{E}_{t+1:t+i}$ (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 $\mathcal{O}(|A|^d \cdot |\mathbf{E}|^d)$($|A| \hat{=}$ number of actions, $|\mathbf{E}| \hat{=}$ 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.

Summary

- ▷ Decision theoretic agents for sequential environments
- ▷ Building on temporal, probabilistic models/inference (dynamic Bayesian networks)
- ▷ MDPs for fully observable case.
- ▷ Value/Policy Iteration for MDPs $\leadsto$ optimal policies.
- ▷ POMDPs for partially observable case.
- ▷ POMDPs$\hat{=}$ MDP on belief state space.
- ▷ The world is a POMDP with (initially) unknown transition and sensor models.

Part II

Machine Learning

This part introduces the foundations of machine learning methods in AI. We discuss the problem learning from observations in general, study inference-based techniques, and then go into elementary statistical methods for learning.

The current hype topics of deep learning, reinforcement learning, and large language models are only very superficially covered, leaving them to specialized lectures.

Chapter 8

Learning from Observations

In this chapter we introduce the concepts, methods, and limitations of inductive learning, i.e. learning from a set of given examples.

Outline

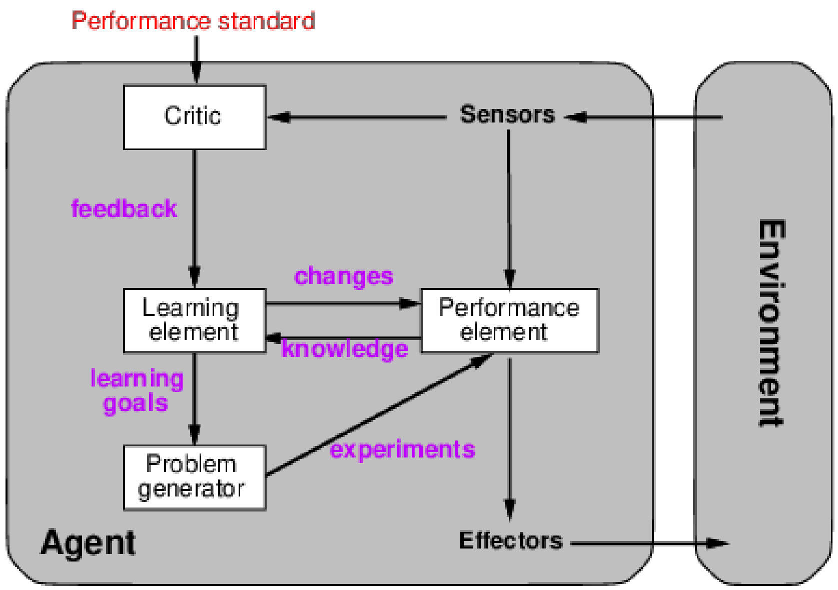
- ▷ Learning agents
- ▷ Inductive learning
- ▷ Decision tree learning
- ▷ Measuring learning performance
- ▷ Computational Learning Theory
- ▷ Linear regression and classification
- ▷ Neural Networks
- ▷ Support Vector Machines

8.1 Forms of Learning

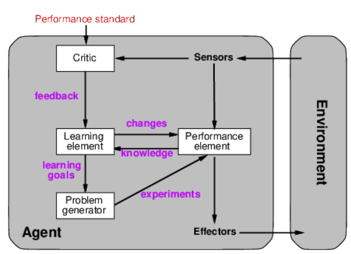
Learning (why is this a good idea)

- ▷ 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



Recap: Learning Agents (continued)



- **Definition 8.1.1.** Performance element is what we called "agent" up to now.
- **Definition 8.1.2.** Critic/learning element/problem generator do the "improving".
- **Definition 8.1.3.** 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 8.1.4.** Learning element may use knowledge already acquired in the performance element.
- **Definition 8.1.5.** Learning may require experimentation actions an agent might not normally consider such as dropping rocks from the Tower of Pisa.

Ways of Learning

- ▷ Supervised learning: There's an unknown function $f\colon A \to B$ 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 $f\colon A \to B$ for some predetermined B. (Primarily *clustering/dimensionality reduction*)
- ▷ Reinforcement learning: The agent receives a reward for each action performed. The goal is to iteratively adapt the action function to maximize the total reward. (Useful in e.g. game play)

8.2 Supervised Learning

Supervised learning a.k.a. inductive learning (a.k.a. Science)

Definition 8.2.1. A supervised (or inductive) learning problem consists of the following data:

- ▷ A set of hypotheses $\mathcal{H}$ consisting of functions $A \to B$,
- ▷ a set of examples $T \subseteq A \times B$ called the training set, such that for every $a \in A$, there is at most one $b \in B$ with $\langle a, b\rangle \in T$, ($\Rightarrow$ T is a function on some subset of A)

We assume there is an *unknown* function $f\colon A \to B$ called the target function with $T \subseteq f$.

Definition 8.2.2. 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).

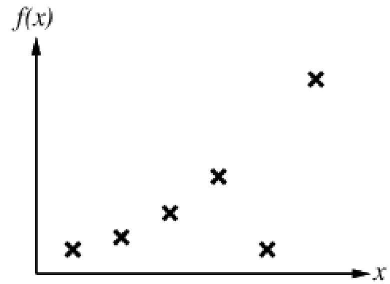
Definition 8.2.3. We call a supervised learning problem with target function $A \to B$ a classification problem if B is finite, and call the members of B classes.

We call it a regression problem if $B = \mathbb{R}$.

Inductive Learning Method

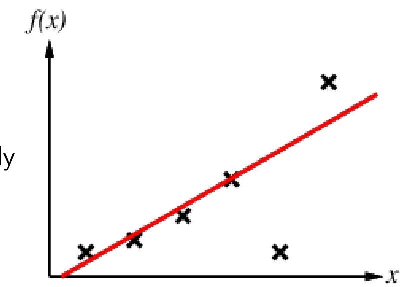
- ▷ **Idea:** Construct/adjust hypothesis $h \in \mathcal{H}$ to agree with a training set T.
- ▷ **Definition 8.2.4.** We call h consistent with f (on a set $T \subseteq \mathbf{dom}(f)$), if it agrees with f (on all examples in T).
- ▷ **Example 8.2.5 (Curve Fitting).**

Training Set



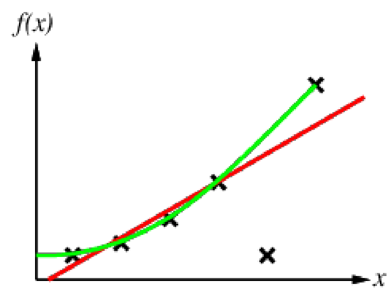
Linear Hypothesis

partially, approximatively consistent



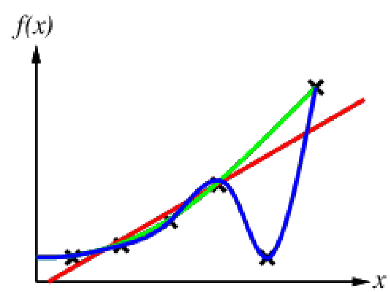
Quadratic Hypothesis

partially consistent



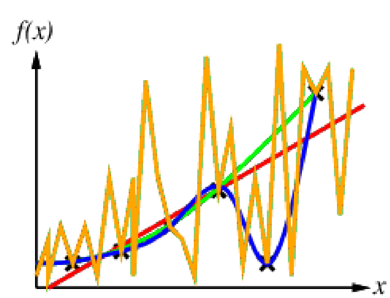
Degree-4 Hypothesis

consistent



High-degree Hypothesis

consistent



▷ **Ockham's-razor:** maximize a combination of consistency and simplicity.

Choosing the Hypothesis Space

▷ **Observation:** Whether we can find a consistent hypothesis for a given training set depends on the chosen hypothesis space.

▷ **Definition 8.2.6.** We say that an supervised learning problem is realizable, iff there is a hypothesis $h \in \mathcal{H}$ consistent with the training set 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.

Independent and Identically Distributed

▷ **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 8.2.7.** A sequence of $E_1, \ldots, E_n$ of random variables is independent and identically distributed (short IID), iff they are

- ▷ independent, i.e. $\mathbf{P}(E_j|E_{(j-1)}, E_{(j-2)}, \ldots) = \mathbf{P}(E_j)$ and
- ▷ identically distributed, i.e. $\mathbf{P}(E_i) = \mathbf{P}(E_j)$ for all i and j.

▷ **Example 8.2.8.** 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.

8.3 Learning Decision Trees

Attribute-based Representations

▷ **Definition 8.3.1.** In attribute-based representations, examples are described by

- ▷ attributes: (simple) functions on input samples, (think pre classifiers on examples)
- ▷ their value, and (classify by attributes)
- ▷ classifications. (Boolean, discrete, continuous, etc.)

▷ **Example 8.3.2 (In a Restaurant).** Situations where I will/won't wait for a table:

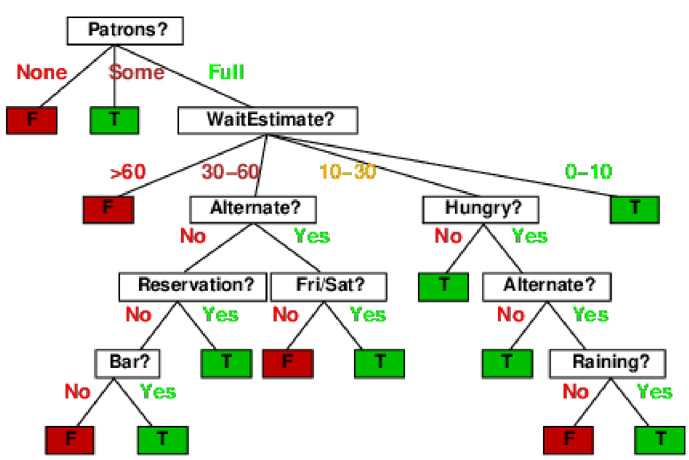
Example	*Attributes*										*Target*
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	WillWait
X_1	T	F	F	T	Some	\$\$\$	F	T	French	0–10	T
X_2	T	F	F	T	Full	\$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	\$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	\$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	\$\$\$	F	T	French	>60	F
X_6	F	T	F	T	Some	\$\$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	\$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	\$\$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	\$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	\$\$\$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	\$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	\$	F	F	Burger	30–60	T

▷ **Definition 8.3.3.** 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 8.3.4 (Restaurant continued).** Here is the "true" tree for deciding whether to wait:



We evaluate the tree by going down the tree from the top, and always take the branch whose attribute matches the situation; we will eventually end up with a Boolean value; the result. Using the attribute values from X_3 in Example 8.3.2 to descend through the tree in Example 8.3.4 we indeed end up with the result "true". Note that

1. some of the original set of attributes X_3 are irrelevant.
2. the training set in Example 8.3.2 is realizable – i.e. the target is definable in hypothesis class of decision trees.

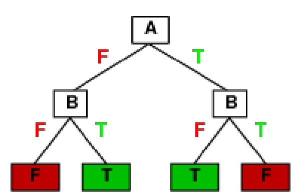
Decision Trees (Definition)

- **Definition 8.3.5.** 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 8.3.6.** 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 $A_1 \times \ldots \times A_n \to C$, where A_i are the domains of the attributes and C is the set of classifications.

Expressiveness

- Decision trees can express any function of the input attributes $\Rightarrow \mathcal{H} = A_1 \times \ldots \times A_n$
- **Example 8.3.7.** For Boolean functions, a path from the root to a leaf corresponds to a row in a truth table:

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



$\Rightarrow$ 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.
- **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 8.3.8.** 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_i of best do
         examples_i := {elements of examples with best = v_i}
         subtree := DTL(examples_i, attributes \ best, m)
         add a branch to tree with label v_i and subtree subtree
    return tree
```

MODE($examples$)= most frequent value in $example$.

Note: We have three base cases:

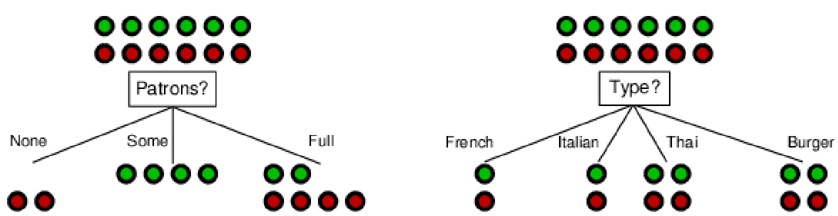
1. empty examples ⇜ arises for empty branches of non Boolean parent attribute.
2. uniform example classifications ⇜ this is "normal" leaf.
3. $attributes$ empty ⇜ target is not deterministic in input $attributes$.

The recursive step steps pick an attribute and then subdivides the examples.

Choosing an Attribute

▷ **Idea:** A good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative".

▷ **Example 8.3.9.**



Attribute "Patrons?" is a better choice, it gives gives information about the classification.

▷ Can we make this more formal? ⇝ Use information theory! (up next)

8.4 Using Information Theory

Video Nuggets covering this section can be found at `https://fau.tv/clip/id/20373` and `https://fau.tv/clip/id/30374`.

Information Entropy

Intuition: Information answers questions – the less I know initially, the more Information is contained in an answer.

Definition 8.4.1. Let $\langle p_1, \ldots, p_n \rangle$ the distribution of a random variable P. The information (also called entropy) of P is

$$I(\langle p_1, \ldots, p_n \rangle) := \sum_{i=1}^{n} -p_i \cdot \log_2(p_i)$$

Note: For $p_i = 0$, we consider $p_i \cdot \log_2(p_i) = 0$ ($\log_2(0)$ is undefined)

The unit of information is a bit, where $1\text{b} := I(\langle \frac{1}{2}, \frac{1}{2} \rangle) = 1$

Example 8.4.2 (Information of a Coin Toss).

- ▷ For a fair coin toss we have $I(\langle \frac{1}{2}, \frac{1}{2} \rangle) = -\frac{1}{2}\log_2(\frac{1}{2}) - \frac{1}{2}\log_2(\frac{1}{2}) = 1\text{b}$.
- ▷ With a loaded coin (99% heads) we have $I(\langle \frac{1}{100}, \frac{99}{100} \rangle) = 0.08\text{b}$.

$Rightarrow$ Information goes to 0 as head probability goes to 1.

"How likely is the outcome actually going to tell me something informative?"

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 $\mathbf{P}(C) = \langle \frac{p}{p+n}, \frac{n}{p+n} \rangle$, and need $I(\mathbf{P}(C))$ bits to correctly classify a new example.

Example 8.4.3. For 12 restaurant examples and $p = n = 6$, we need $I(\mathbf{P}(\text{WillWait})) = I(\langle \frac{6}{12}, \frac{6}{12} \rangle) = 1\text{b}$ 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 8.4.4. If we know $\text{Pat} = \text{Full}$, we only need $I(\mathbf{P}(\text{WillWait}|\text{Pat} = \text{Full})) = I(\langle \frac{4}{6}, \frac{2}{6} \rangle) \approx 0.9$ bits of information.

Note: The expected number of bits needed after an attribute test on A is

$$\sum_a P(A = a) \cdot I(\mathbf{P}(C|A = a))$$

Definition 8.4.5. The information gain from an attribute test A is

$$\text{Gain}(A) := I(\mathbf{P}(C)) - \sum_a P(A = a) \cdot I(\mathbf{P}(C|A = a))$$

Information Gain (continued)

- ▷ **Definition 8.4.6.** Assume we know the results of some attribute tests $b := B_1 = b_1 \wedge \ldots \wedge$

$B_n = b_n$. Then the conditional information gain from an attribute test A is

$$\mathrm{Gain}(A|b) := I(\mathbf{P}(C|b)) - \sum_a P(A=a|b) \cdot I(\mathbf{P}(C|a,b))$$

▷ **Example 8.4.7.** If the classification C is Boolean and we have p positive and n negative examples, the information gain is

$$\mathrm{Gain}(A) = I(\langle \frac{p}{p+n}, \frac{n}{p+n} \rangle) - \sum_a \frac{p_a+n_a}{p+n} I(\langle \frac{p_a}{p_a+n_a}, \frac{n_a}{p_a+n_a} \rangle)$$

where p_a and n_a are the positive and negative examples with $A = a$.

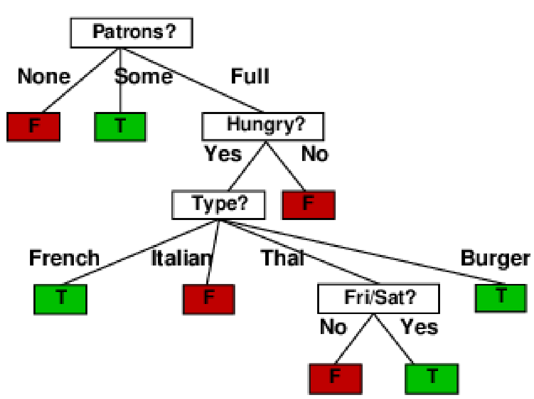
▷ **Example 8.4.8.**

$$\begin{aligned}
\mathrm{Gain}(Patrons?) &= 1 - (\frac{2}{12} I(\langle 0,1 \rangle) + \frac{4}{12} I(\langle 1,0 \rangle) + \frac{6}{12} I(\langle \frac{2}{6}, \frac{4}{6} \rangle)) \\
&\approx 0.541\mathrm{b} \\
\mathrm{Gain}(Type) &= 1 - (\frac{2}{12} I(\langle \frac{1}{2}, \frac{1}{2} \rangle) + \frac{2}{12} I(\langle \frac{1}{2}, \frac{1}{2} \rangle) + \frac{4}{12} I(\langle \frac{2}{4}, \frac{2}{4} \rangle) + \frac{4}{12} I(\langle \frac{2}{4}, \frac{2}{4} \rangle)) \\
&\approx 0\mathrm{b}
\end{aligned}$$

▷ **Idea:** Choose the attribute that maximizes information gain.

Restaurant Example contd.

▷ **Example 8.4.9.** 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.

8.5 Evaluating and Choosing the Best Hypothesis

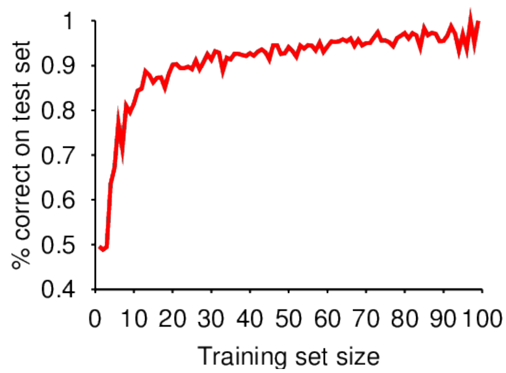
Performance measurement

▷ **Question:** How do we know that $h \approx f$? (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 8.5.1.** The learning curve $\hat{=}$ percentage correct on test set as a function of training set size.

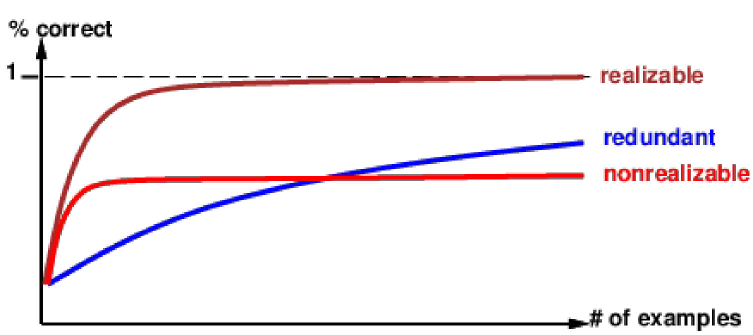
▷ **Example 8.5.2.** Restaurant data; graph averaged over 20 trials



Performance measurement contd.

▷ **Observation 8.5.3.** *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)*



Generalization and Overfitting

- **Observation:** Sometimes a learned hypothesis is more specific than the experiments warrant.
- **Definition 8.5.4.** 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.

Decision Tree Pruning

- **Idea:** Combat overfitting by "generalizing" decision trees $\rightsquigarrow$ prune "irrelevant" nodes.
- **Definition 8.5.5.** 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 8.5.6.** 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) $\widehat{p}_k = p \cdot \frac{p_k+n_k}{p+n}$ and $\widehat{n}_k = n \cdot \frac{p_k+n_k}{p+n}$.
- A convenient measure of the total deviation is (sum of squared errors)

$$\Delta = \sum_{k=1}^{d} \frac{(p_k - \widehat{p}_k)^2}{\widehat{p}_k} + \frac{(n_k - \widehat{n}_k)^2}{\widehat{n}_k}$$

▷ **Lemma 8.5.7 (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 8.5.8.** Decision tree pruning with Pearson's χ^2 with $d-1$ degrees of freedom for Δ is called χ^2 pruning. (χ^2 values from stats library.)

▷ **Example 8.5.9.** The *type* attribute has four values, so three degrees of freedom, so $\Delta = 7.82$ would reject the null hypothesis at the 5% level.

Error Rates and Cross-Validation

▷ **Recall:** We want to learn a hypothesis that fits the future data best.

▷ **Definition 8.5.10.** Given an inductive learning problem with a set of examples $T \subseteq AB$, we define the error rate of a hypothesis $h \in \mathcal{H}$ as the fraction of errors:

$$\frac{|\{\langle x,y\rangle \in T \,|\, h(x) \neq y\}|}{|T|}$$

▷ **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 8.5.11.** 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. (no peeking at test set allowed)

Error Rates and Cross-Validation

▷ **Question:** What is a good ratio between training set and test set size?

- ▷ small training set $\leadsto$ poor hypothesis.
- ▷ small test set $\leadsto$ poor estimate of the accuracy.

▷ **Definition 8.5.12.** 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.

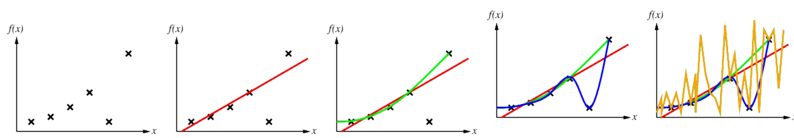
▷ $k=5$ and $k=10$ are popular $\leadsto$ good accuracy at k times computation time.

▷ **Definition 8.5.13.** If $k = |\mathbf{dom}(f)|$, then k fold cross validation is called leave one out cross validation (LOOCV).

Model Selection

▷ **Definition 8.5.14.** The model selection problem is to determine – given data – a good hypothesis space.

▷ **Example 8.5.15.** What is the best polynomial degree to fit the data



▷ **Observation 8.5.16.** *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 8.5.17.** The model selection algorithm (MSA) jointly optimizes model selection and optimization by partitioning and cross-validation:

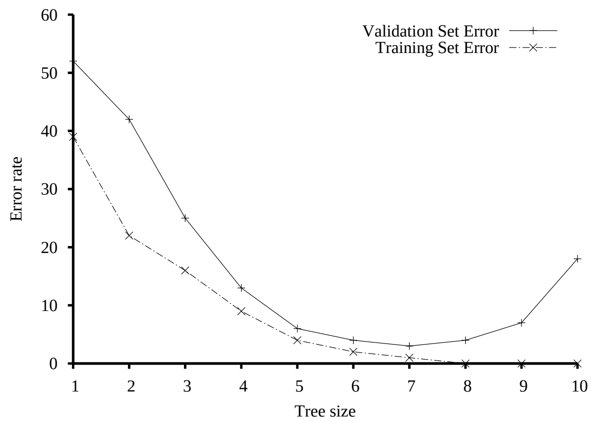
```
function CROSS−VALIDATION−WRAPPER(Learner,k,examples) returns a hypothesis
  local variables: errT, an array, indexed by size, storing training−set error rates
                   errV, an array, indexed by size, storing validation−set error rates
  for size = 1 to ∞ do
   errT[size], errV[size] := 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 := 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 8.5.18 (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)

From Error Rates to Loss Functions

▷ **So far** we have been minimizing error rates. (better than maximizing ☺)

▷ **Example 8.5.19 (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". (not only minimize error rates)

▷ machine learning traditionally deals with utilities in form of "loss functions".

▷ **Definition 8.5.20.** The loss function L is defined by setting $L(x,y,\widehat{y})$ to be the amount of utility lost by prediction $h(x)=\widehat{y}$ instead of $f(x)=y$. If L is independent of x, we often use $L(y,\widehat{y})$.

▷ **Example 8.5.21.** $L(spam,ham)=1$, while $L(ham,spam)=10$.

Generalization Loss

▷ **Note:** $L(y,y)=0$. (no loss if you are exactly correct)

▷ **Definition 8.5.22 (Popular general loss functions).**

absolute value loss	$L_1(y,\widehat{y}){:=}\lvert y-\widehat{y}\rvert$	small errors are good
squared error loss	$L_2(y,\widehat{y}){:=}(y-\widehat{y})^2$	dito, but differentiable
0/1 loss	$L_{0/1}(y,\widehat{y}){:=}0$, if $y=\widehat{y}$, else 1	error rate

▷ **Idea:** Maximize expected utility by choosing hypothesis h that minimizes expected loss over all $(x,y) \in f$.

▷ **Definition 8.5.23.** 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

$$\mathrm{GenLoss}_L(h){:=}\sum_{(x,y)\in\mathcal{E}} L(y,h(x))\cdot P(x,y)$$

and the best hypothesis $h^* := \underset{h\in\mathcal{H}}{\operatorname{argmin}}\ \mathrm{GenLoss}_L(h)$.

Empirical Loss

▷ **Problem:** $\mathbb{P}(X,Y)$ is unknown $\leadsto$ learner can only estimate generalization loss:

▷ **Definition 8.5.24.** Let L be a loss function and E a set of examples with $|E| = N$, then we call

$$\mathrm{EmpLoss}_{L,E}(h){:=}\frac{1}{N}\Big(\sum_{(x,y)\in E} L(y,h(x))\Big)$$

the empirical loss and $\widehat{h}^* := \underset{h\in\mathcal{H}}{\operatorname{argmin}}\ \mathrm{EmpLoss}_{L,E}(h)$ the estimated best hypothesis.

▷ There are four reasons why $\widehat{h}^*$ may differ from f:

1. Realizablility: then we have to settle for an approximation $\widehat{h}^*$ of f.
2. Variance: different subsets of f give different $\widehat{h}^*\leadsto$ 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.

Regularization

▷ **Idea:** Directly use empirical loss to solve model selection. (finding a good $\mathcal{H}$)

Minimize the weighted sum of empirical loss and hypothesis complexity. (to avoid overfitting).

▷ **Definition 8.5.25.** Let $\lambda \in \mathbb{R}$, $h \in \mathcal{H}$, and E a set of examples, then we call

$$\mathrm{Cost}_{L,E}(h){:=}\mathrm{EmpLoss}_{L,E}(h)+\lambda\mathrm{Complexity}(h)$$

the total cost of h on E.

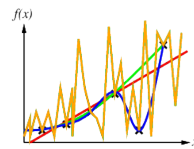
▷ **Definition 8.5.26.** The process of finding a total cost minimizing hypothesis

$$\widehat{h}^* := \underset{h \in \mathcal{H}}{\operatorname{argmin}} \operatorname{Cost}_{L,E}(h)$$

is called regularization; $\mathrm{Complexity}$ is called the regularization function or hypothesis complexity.

▷ **Example 8.5.27 (Regularization for Polynomials).**

A good regularization function for polynomials is the sum of squares of exponents. $\rightsquigarrow$ keep away from wriggly curves!



Minimal Description Length

▷ **Remark:** In regularization, empirical loss and hypothesis complexity are not measured in the same scale $\rightsquigarrow$ λ mediates between scales.

▷ **Idea:** Measure both in the same scale $\rightsquigarrow$ use information content, i.e. in bits.

▷ **Definition 8.5.28.** 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:
   - ▹ correctly predicted example $\rightsquigarrow$ $0\mathrm{b}$
   - ▹ incorrectly predicted example $\rightsquigarrow$ 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?

The Scale of Machine Learning

▷ 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. (millions of examples)

- ▹ 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.

8.6 Computational Learning Theory

Video Nuggets covering this section can be found at `https://fau.tv/clip/id/30377` and `https://fau.tv/clip/id/30378`.

A (General) Theory of Learning?

▷ **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.

PAC Learning

▷ **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.
- ▹ $\rightsquigarrow$ h is probably approximately correct.

▷ **Definition 8.6.1.** 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 $\mathcal{E}$ of possible examples is IID
⇝ we have a fixed distribution $\mathbf{P}(E) = \mathbf{P}(X, Y)$ on examples.

▷ **Simplifying Assumptions:** f is a function (deterministic) and $f \in \mathcal{H}$.

PAC Learning

▷ Start with PAC theorems for Boolean functions, for which $L_{0/1}$ is appropriate.

▷ **Definition 8.6.2.** The error rate $\mathrm{error}(h)$ of a hypothesis h is the probability that h misclassifies a new example.

$$\mathrm{error}(h) := \mathrm{GenLoss}_{L_{0/1}}(h) = \sum_{(x,y)\in\mathcal{E}} L_{0/1}(y, h(x)) \cdot P(x, y)$$

▷ **Intuition:** $\mathrm{error}(h)$ is the probability that h misclassifies a new example.

▷ This is the same quantity as measured in the learning curves above.

▷ **Definition 8.6.3.** A hypothesis h is called approximatively correct, iff $\mathrm{error}(h) \leq \epsilon$ for some small $\epsilon > 0$.

We write $\mathcal{H}_b := \{h \in \mathcal{H} \,|\, \mathrm{error}(h) > \epsilon\}$ for the "seriously bad" hypotheses.

Sample Complexity

▷ Let's compute the probability that $h_b \in \mathcal{H}_b$ is consistent with the first N examples.

▷ We know $\mathrm{error}(h_b) > \epsilon$
⇝ $P(h_b$ agrees with N examples$) \leq (1-\epsilon)^N$. (independence)
⇝ $P(\mathcal{H}_b$ contains consistent hyp.$) \leq |\mathcal{H}_b| \cdot (1-\epsilon)^N \leq |\mathcal{H}| \cdot (1-\epsilon)^N$. ($\mathcal{H}_b \subseteq \mathcal{H}$)
⇝ to bound this by a small δ, show the algorithm $N \geq \frac{1}{\epsilon} \cdot (\log_2(\frac{1}{\delta}) + \log_2(|\mathcal{H}|))$ examples.

▷ **Definition 8.6.4.** The number of required examples as a function of ϵ and δ is called the sample complexity of $\mathcal{H}$.

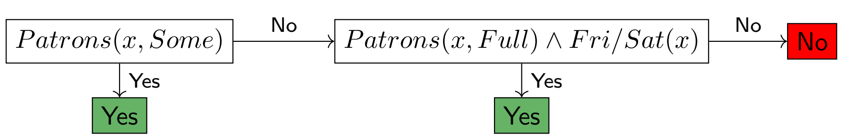
▷ **Example 8.6.5.** If $\mathcal{H}$ is the set of n-ary Boolean functions, then $|\mathcal{H}| = 2^{2^n}$.
⇝ sample complexity grows with $\mathcal{O}(\log_2(2^{2^n})) = \mathcal{O}(2^n)$.
There are 2^n possible examples,
⇝ PAC learning for Boolean functions needs to see (nearly) all examples.

Escaping Sample Complexity

- **Problem:** PAC learning for Boolean functions needs to see (nearly) all examples.
  - $\mathcal{H}$ 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 $\mathcal{H}$ in some way (but we may lose realizability)
- **Three Ways out of this Dilemma:**
  1. bring prior knowledge into the problem. (??)
  2. prefer simple hypotheses. (e.g. decision tree pruning)
  3. focus on "learnable subsets" of $\mathcal{H}$. (next)

PAC Learning: Decision Lists

- **Idea:** Apply PAC learning to a "learnable hypothesis space".
- **Definition 8.6.6.** 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 8.6.7 (A decision list for the Restaurant Problem).**



- **Lemma 8.6.8.** *Given arbitrary size conditions, decision lists can represent arbitrary Boolean functions.*
- This directly defeats our purpose of finding a "learnable subset" of $\mathcal{H}$.

Decision Lists: Learnable Subsets (Size-Restricted Cases)

- **Definition 8.6.9.** The set of decision lists where tests are of conjunctions of at most k literals is denoted by $k\mathbf{-DL}$.

▷ **Example 8.6.10.** The decision list from Example 8.6.7 is in $2\mathbf{-DL}$.

▷ **Observation 8.6.11.** *$k\mathbf{-DL}$ contains $k\mathbf{-DT}$, the set of decision trees of depth at most k.*

▷ **Definition 8.6.12.** We denote the set of $k\mathbf{-DL}$ decision lists with at most n Boolean attributes with $k\mathbf{-DL}(n)$. The set of conjunctions of at most k literals over n attributes is written as $\mathrm{Conj}(k, n)$.

▷ Decision lists are constructed of optional yes/no tests, so there are at most $3^{|\mathrm{Conj}(k,n)|}$ distinct sets of component tests. Each of these sets of tests can be in any order, so $|k\mathbf{-DL}(n)| \leq 3^{|\mathrm{Conj}(k,n)|} \cdot |\mathrm{Conj}(k, n)|!$

Decision Lists: Learnable Subsets (Sample Complexity)

▷ The number of conjunctions of k literals from n attributes is given by

$$|\mathrm{Conj}(k, n)| = \sum_{i=1}^{k} \binom{2n}{i}$$

thus $|\mathrm{Conj}(k, n)| = \mathcal{O}(n^k)$. Hence, we obtain (after some work)

$$|k\mathbf{-DL}(n)| = 2^{\mathcal{O}(n^k \log_2(n^k))}$$

▷ Plug this into the equation for the sample complexity: $N \geq \frac{1}{\epsilon} \cdot (\log_2(\frac{1}{\delta}) + \log_2(|\mathcal{H}|))$ to obtain

$$N \geq \frac{1}{\epsilon} \cdot (\log_2(\frac{1}{\delta}) + \log_2(\mathcal{O}(n^k \log_2(n^k))))$$

▷ **Intuitively:** Any algorithm that returns a consistent decision list will PAC learn a $k\mathbf{-DL}$ function in a reasonable number of examples, for small k.

Decision Lists Learning

▷ **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.

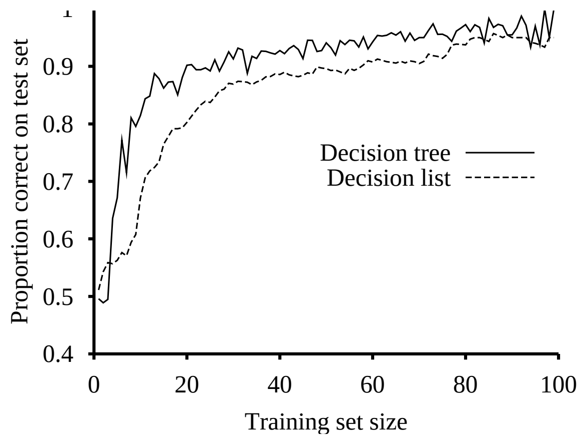
▷ **Definition 8.6.13.** The following algorithm performs decision list learning

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($E\backslash E_t$)

Decision Lists Learning in Comparison

▷ **Learning curves:** for DLL (and DTL for comparison)



▷ **Upshot:** The simpler DLL works quite well!

8.7 Regression and Classification with Linear Models

Univariate Linear Regression

▷ **Definition 8.7.1.** A univariate or unary function is a function with one argument.

▷ **Recall:** A mapping f between vector spaces is called linear, iff it preserves plus and scalar multiplication, i.e. $f(\alpha \cdot v_1 + v_2) = \alpha \cdot f(v_1) + f(v_2)$.

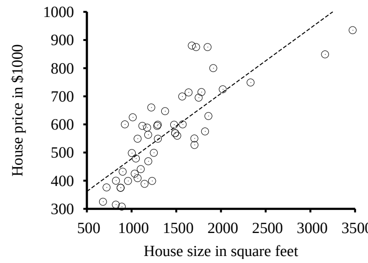
▷ **Observation 8.7.2.** *A univariate, linear function $f\colon \mathbb{R} \to \mathbb{R}$ is of the form $f(x) = \mathbf{w}_1 x + \mathbf{w}_0$ for some $\mathbf{w}_i \in \mathbb{R}$.*

▷ **Definition 8.7.3.** Given a vector $\mathbf{w} := (\mathbf{w}_0,\mathbf{w}_1)$, we define $h_{\mathbf{w}}(x) := \mathbf{w}_1 x + \mathbf{w}_0$.

▷ **Definition 8.7.4.** Given a set of examples $E \subseteq \mathbb{R}\times\mathbb{R}$, the task of finding $h_{\mathbf{w}}$ that best fits E is called linear regression.

▷ **Example 8.7.5.**

Examples of house price vs. square feet in houses sold in Berkeley in July 2009.
Also: linear function hypothesis that minimizes squared error loss $y = 0.232x + 246$.



Univariate Linear Regression by Loss Minimization

▷ **Idea:** Minimize squared error loss over $\{(x_i,y_i)|i \leq N\}$ (used already by Gauss)

$$\mathrm{Loss}(h_{\mathbf{w}}) = \sum_{j=1}^{N} L_2(y_j, h_{\mathbf{w}}(x_j)) = \sum_{j=1}^{N} (y_j - h_{\mathbf{w}}(x_j))^2 = \sum_{j=1}^{N} (y_j - (\mathbf{w}_1 x_j + \mathbf{w}_0))^2$$

Task: find $\mathbf{w}^* := \underset{\mathbf{w}}{\mathrm{argmin}}\, \mathrm{Loss}(h_{\mathbf{w}})$.

▷ **Recall:** $\sum_{j=1}^{N} (y_j - (\mathbf{w}_1 x_j + \mathbf{w}_0))^2$ is minimized, when the partial derivatives wrt. the $\mathbf{w}_i$ are zero, i.e. when

$$\frac{\partial}{\partial \mathbf{w}_0}\left(\sum_{j=1}^{N} (y_j - (\mathbf{w}_1 x_j + \mathbf{w}_0))^2\right) = 0 \quad \text{and} \quad \frac{\partial}{\partial \mathbf{w}_1}\left(\sum_{j=1}^{N} (y_j - (\mathbf{w}_1 x_j + \mathbf{w}_0))^2\right) = 0$$

▷ **Observation:** These equations have a unique solution:

$$\mathbf{w}_1 = \frac{N(\sum_j x_j y_j) - (\sum_j x_j)(\sum_j y_j)}{N(\sum_j {x_j}^2) - (\sum_j x_j)^2} \qquad \mathbf{w}_0 = \frac{(\sum_j y_j) - \mathbf{w}_1(\sum_j x_j)}{N}$$

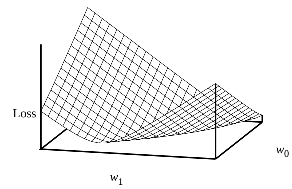
▷ **Remark:** Closed-form solutions only exist for linear regression, for other (differentiable) hypothesis spaces use gradient descent methods for adjusting/learning weights.

A Picture of the Weight Space

▷ **Remark:** Many forms of learning involve adjusting weights to minimize loss.

▷ **Definition 8.7.6.** 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 $\mathbb{R}^2$.
$\rightsquigarrow$ graph the loss function over $\mathbb{R}^2$.
Note: it is convex.



▷ **Observation 8.7.7.** *The squared error loss function is convex for any linear regression problem* $\rightsquigarrow$ *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 8.7.8.** 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,$\mathbf{w}$,α) **returns** a **local** minimum of F
  inputs: a differentiable **function** F and initial weights $\mathbf{w}$.
  loop until $\mathbf{w}$ converges **do**
    for each $\mathbf{w}_i$ **do**
      $\mathbf{w}_i \longleftarrow \mathbf{w}_i - \alpha\frac{\partial}{\partial \mathbf{w}_i}(F(\mathbf{w}))$
    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.

Gradient-Descent for Loss

▷ Let's try gradient descent for Loss.

▷ Work out the partial derivatives for one example (x,y):

$$\frac{\partial \mathrm{Loss}(\mathbf{w})}{\partial \mathbf{w}_i} = \frac{\partial (y - h_{\mathbf{w}}(x))^2}{\partial \mathbf{w}_i} = 2(y - h_{\mathbf{w}}(x))\frac{\partial (y - (\mathbf{w}_1 x + \mathbf{w}_0))}{\partial \mathbf{w}_i}$$

and thus
$$\frac{\partial \mathrm{Loss}(\mathbf{w})}{\partial \mathbf{w}_0} = -2(y - h_{\mathbf{w}}(x)) \qquad \frac{\partial \mathrm{Loss}(\mathbf{w})}{\partial \mathbf{w}_1} = -2(y - h_{\mathbf{w}}(x))x$$

Plug this into the gradient descent updates:

$$\mathbf{w}_0 \longleftarrow \mathbf{w}_0 - \alpha - 2(y - h_{\mathbf{w}}(x)) \qquad \mathbf{w}_1 \longleftarrow \mathbf{w}_1 - \alpha - 2(y - h_{\mathbf{w}}(x))x$$

Gradient-Descent for Loss (continued)

- Analogously for n training examples (x_j,y_j):
- **Definition 8.7.9.**

$$\mathbf{w}_0 \longleftarrow \mathbf{w}_0 - \alpha(\sum_j -2(y_j - h_{\mathbf{w}}(x_j))) \quad \mathbf{w}_1 \longleftarrow \mathbf{w}_1 - \alpha(\sum_j -2(y_j - h_{\mathbf{w}}(x_n))x_n)$$

  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)

Multivariate Linear Regression

- **Definition 8.7.10.** 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

$$h_{sw}(\vec{x}_j) = \mathbf{w}_0 + \mathbf{w}_1 x_{j,1} + \ldots + \mathbf{w}_n x_{j,n} = \mathbf{w}_0 + \sum_i \mathbf{w}_i x_{j,i}$$

- **Trick:** Invent $x_{j,0} := 1$ and use matrix notation:

$$h_{sw}(\vec{x}_j) = \vec{w} \cdot \vec{x}_j = \vec{w}^t \vec{x}_j = \sum_i \mathbf{w}_i x_{j,i}$$

- **Definition 8.7.11.** The best vector of weights, $\mathbf{w}^*$, minimizes squared-error loss over the examples: $\mathbf{w}^* := \underset{\mathbf{w}}{\operatorname{argmin}} \, (\sum_j L_2(y_j)(\mathbf{w} \cdot \vec{x}_j))$.
- Gradient descent will reach the (unique) minimum of the loss function; the update equation for each weight $\mathbf{w}_i$ is

$$\mathbf{w}_i \longleftarrow \mathbf{w}_i - \alpha(\sum_j x_{j,i}(y_j - h_{\mathbf{w}}(\vec{x}_j)))$$

Multivariate Linear Regression (Analytic Solutions)

▷ We can also solve analytically for the $\mathbf{w}^*$ that minimizes loss.

▷ Let $\vec{y}$ be the vector of outputs for the training examples, and $\mathbf{X}$ be the data matrix, i.e., the matrix of inputs with one n-dimensional example per row.

Then the solution $\mathbf{w}^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\vec{y}$ minimizes the squared error.

Multivariate Linear Regression (Regularization)

▷ **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 8.7.12.** $\mathrm{Complexity}(h_{\mathbf{w}}) = L_q(\mathbf{w}) = \sum_i |\mathbf{w}_i|^q$

▷ **Caveat:** Do not confuse this with the loss functions L_1 and L_2.

▷ **Problem:** Which q should be pick? (L_1 and L_2 minimize sum of absolute values/squares)

▷ **Answer:** It depends on the application.

▷ **Remark:** L_1-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 [RN03, Section 18.6.2])

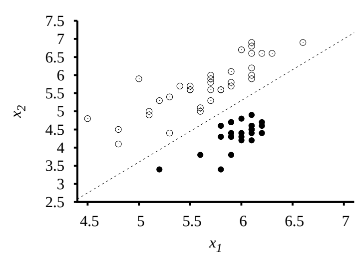
Linear Classifiers with a hard Threshold

▷ **Idea:** The result of linear regression can be used for classification.

▷ **Example 8.7.13 (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: $h_{\mathbf{w}^*}$ as a decision boundary $x_2 = 17x_1 - 4.9$.



▷ **Definition 8.7.14.** 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 8.7.15 (Nuclear Tests continued).** The linear separator for Example 8.7.13is 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 $h_{\mathbf{w}}(\mathrm{x}) = 1$ if $\mathbf{w}\cdot\mathrm{x} > 0$ and 0 otherwise.

Linear Classifiers with a hard Threshold (Perceptron Rule)

▷ So $h_{\mathbf{w}}(\mathrm{x}) = 1$ if $\mathbf{w}\cdot\mathrm{x} > 0$ and 0 otherwise is well-defined, how to choose $\mathbf{w}$?

▷ Think of $h_{\mathbf{w}}(\mathrm{x}) = \mathcal{T}(\mathbf{w}\cdot\mathrm{x})$, where $\mathcal{T}(z) = 1$, if $z > 0$ and $\mathcal{T}(z) = 0$ otherwise. We call $\mathcal{T}$ 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 $\frac{\partial\mathcal{T}}{\partial z} = 0$ and solving.
- ▷ Gradient-descent methods in weight-space do not work either.

▷ We can learn weights by iterating over the following rule:

▷ **Definition 8.7.16.** Given an example (x,y), the perceptron learning rule is

$$\mathbf{w}_i \longleftarrow \mathbf{w}_i + \alpha\cdot(y - h_{\mathbf{w}}(\mathrm{x}))\cdot x_i$$

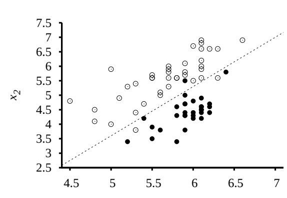
▷ as we are considering 0/1 classification, there are three possibilities:

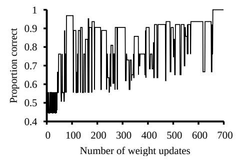
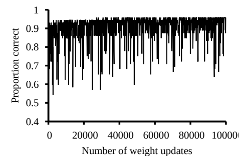
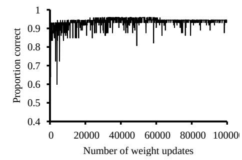
1. If $y = h_{\mathbf{w}}(\mathrm{x})$, then $\mathbf{w}_i$ remains unchanged.
2. If $y = 1$ and $h_{\mathbf{w}}(\mathrm{x}) = 0$, then $\mathbf{w}_i$ is in/decreased if x_i is positive/negative. (we want to make $\mathbf{w}\cdot\mathrm{x}$ bigger so that $\mathcal{T}(\mathbf{w}\cdot\mathrm{x}) = 1$)
3. If $y = 0$ and $h_{\mathbf{w}}(\mathrm{x}) = 1$, then $\mathbf{w}_i$ is de/increased if x_i is positive/negative. (we want to make $\mathbf{w}\cdot\mathrm{x}$ smaller so that $\mathcal{T}(\mathbf{w}\cdot\mathrm{x}) = 0$)

Learning Curves for Linear Classifiers (Perceptron Rule)

▷ **Example 8.7.17.**

Learning curves (plots of total training set accuracy vs. number of iterations) for the perceptron rule on the earthquake/explosions data.



original data	noisy, non-separable data	learning rate decay $\alpha(t) = 1000/(1000+t)$
		
messy convergence 700 iterations	convergence failure 100,000 iterations	slow convergence 100,000 iterations

▷ **Theorem 8.7.18.** *Finding the minimal-error hypothesis is NP hard, but possible with learning rate decay.*

Linear Classification with Logistic Regression

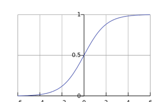
▷ **So far:** Passing the output of a linear function through a threshold function $\mathcal{T}$ yields a linear classifier.

▷ **Problem:** The hard nature of $\mathcal{T}$ brings problems:

- ▹ $\mathcal{T}$ is not differentiable nor continuous $\rightsquigarrow$ learning via perceptron rule becomes unpredictable.
- ▹ $\mathcal{T}$ is "overly precise" near the boundary $\leftrightsquigarrow$ need more graded judgments.

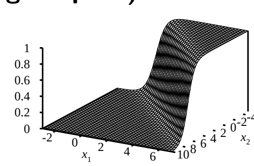
▷ **Idea:** Soften the threshold, approximate it with a differentiable function.

We use the standard logistic function $l(x) = \frac{1}{1+e^{-x}}$
So we have $h_{\mathbf{w}}(\mathbf{x}) = l(\mathbf{w}\cdot\mathbf{x}) = \frac{1}{1+e^{-(\mathbf{w}\cdot\mathbf{x})}}$



▷ **Example 8.7.19 (Logistic Regression Hypothesis in Weight Space).**

Plot of a logistic regression hypothesis for the earthquake/explosion data.
The value at $(\mathbf{w}_0,\mathbf{w}_1)$ is the probability of belonging to the class labeled 1.



We speak of the cliff in the classifier intuitively.

Logistic Regression

▷ **Definition 8.7.20.** The process of weight fitting in $h_{\mathbf{w}}(\mathbf{x}) = \frac{1}{1+e^{-(\mathbf{w}\cdot\mathbf{x})}}$ 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: (via chain rule)

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}_i}(L_2(\mathbf{w})) &= \frac{\partial}{\partial \mathbf{w}_i}(y - h_{\mathbf{w}}(\mathrm{x})^2) \\ &= 2 \cdot h_{\mathbf{w}}(\mathrm{x}) \cdot \frac{\partial}{\partial \mathbf{w}_i}(y - h_{\mathbf{w}}(\mathrm{x})) \\ &= -2 \cdot h_{\mathbf{w}}(\mathrm{x}) \cdot l'(\mathbf{w}\cdot\mathrm{x}) \cdot \frac{\partial}{\partial \mathbf{w}_i}(\mathbf{w}\cdot\mathrm{x}) \\ &= -2 \cdot h_{\mathbf{w}}(\mathrm{x}) \cdot l'(\mathbf{w}\cdot\mathrm{x}) \cdot x_i\end{aligned}$$

Logistic Regression (continued)

▷ The derivative of the logistic function satisfies $l'(z) = l(z)(1 - l(z))$, thus

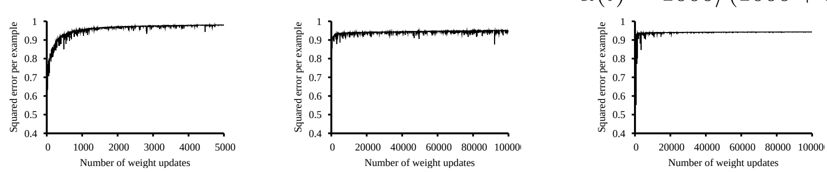
$$l'(\mathbf{w}\cdot\mathrm{x}) = l(\mathbf{w}\cdot\mathrm{x})(1 - l(\mathbf{w}\cdot\mathrm{x})) = h_{\mathbf{w}}(\mathrm{x})(1 - h_{\mathbf{w}}(\mathrm{x}))$$

▷ **Definition 8.7.21.** The rule for logistic update (weight update for minimizing the loss) is

$$\mathbf{w}_i \longleftarrow \mathbf{w}_i + \alpha \cdot (y - h_{\mathbf{w}}(\mathrm{x})) \cdot h_{\mathbf{w}}(\mathrm{x}) \cdot (1 - h_{\mathbf{w}}(\mathrm{x})) \cdot x_i$$

▷ **Example 8.7.22 (Redoing the Learning Curves).**

original data	noisy, non-separable data	learning rate decay $\alpha(t) = 1000/(1000+t)$



messy convergence 5000 iterations	convergence failure 100,000 iterations	slow convergence 100,000 iterations

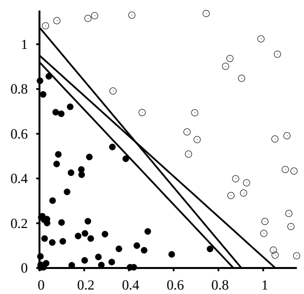
▷ **Upshot:** Logistic update seems to perform better than perceptron update.

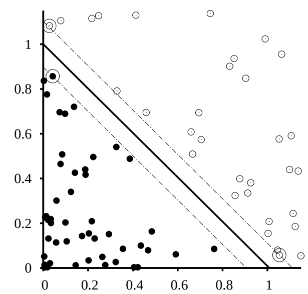
8.8 Support Vector Machines

Support Vector Machines

Definition 8.8.1. 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 8.8.2. 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).

Support Vector Machines (contd.)

Definition 8.8.3. 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.

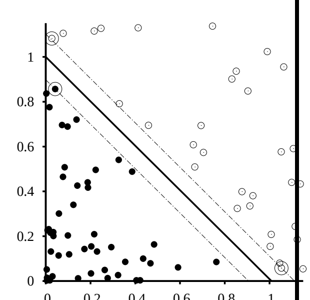
Setting:

- ▷ We have a training set $E = \{\langle x_1, y_1\rangle, \ldots, \langle x_n, y_n\rangle\}$ 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 $\{x | (\mathbf{w} \cdot x) + b = 0\}$ for some vector $\mathbf{w}$ and scalar b. ($\mathbf{w}$ 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 $\{\mathbf{x} | (\mathbf{w} \cdot \mathbf{x}) + b + 1 = 0\}$ (lower boundary) and $\{\mathbf{x} | (\mathbf{w} \cdot \mathbf{x}) + b - 1 = 0\}$ (upper boundary).
⇒ The distance between them is $\frac{2}{\|\mathbf{w}\|_2}$.
Constraints: To maximize the margin, minimize $\|\mathbf{w}\|_2$ while keeping x_i out of the margin:
$(\mathbf{w} \cdot x_i) + b \geq 1$ for $y_i = 1$ and $(\mathbf{w} \cdot x_i) + b \leq -1$ for $y_i = -1$
$\leadsto y_i((\mathbf{w} \cdot x_i) - b) \geq 1$ for $1 \leq i \leq n$.
$\leadsto$ This is an optimization problem.



Theorem 8.8.4 (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 $\mathbf{w} = \sum_j \alpha_j x_j$ *and* $b = \mathbf{w} \cdot x_i - y_i$ *for any* x_i *where* $\alpha_i \neq 0$.

Proof sketch: By the duality principle for optimization problems

Finding the Maximum Margin Separator (Separable Case)

$$\alpha = \underset{\alpha}{\operatorname{argmax}} \left(\sum_j \alpha_j - \frac{1}{2}\left(\sum_{j,k} \alpha_j \alpha_k y_j y_k (x_j \cdot x_k)\right)\right), \text{where } \alpha_j \geq 0, \quad \sum_j \alpha_j y_j = 0$$

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 $\rightsquigarrow$ the single global maximum can found efficiently,
- ▷ Data enter the expression only in the form of dot products of point pairs $\rightsquigarrow$ once the optimal α_i have been calculated, we have $h(\mathbf{x}) = \operatorname{sign}(\sum_j \alpha_j y_j (\mathbf{x} \cdot \mathbf{x}_j) - b)$
- ▷ There are good software packages for solving such quadratic programming optimizations

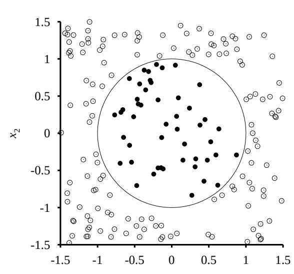
Support Vector Machines (Kernel Trick)

What if the data is not linearly separable?

Idea: Transform the data into a *feature space* where they are.

Definition 8.8.5. A feature for data in $\mathbb{R}^p$ is a function $\mathbb{R}^p \to \mathbb{R}^q$.

Example 8.8.6 (Projecting Up a Non-Separable Data Set).
The true decision boundary is $x_1{}^2 + x_2{}^2 \leq 1$.



$\rightsquigarrow$ use the feature "distance from center"

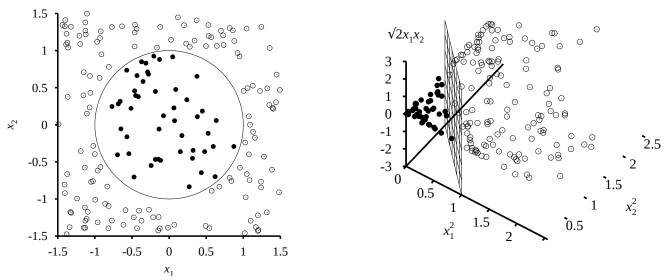
Support Vector Machines (Kernel Trick continued)

Idea: Replace $x_i{\cdot}x_j$ by some other product on the feature space in the SVM equation

Definition 8.8.7. A kernel function is a function $K\colon \mathbb{R}^p{\times}\mathbb{R}^p \to \mathbb{R}$ 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 8.8.8. If we encode the distance from the center as the feature $F(\mathrm{x}) = \langle {x_1}^2, {x_2}^2, \sqrt{2}x_1x_2\rangle$ 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

$$\underset{\alpha}{\mathrm{argmax}}\,(\sum_j \alpha_j - \frac{1}{2}(\sum_{j,k} \alpha_j\alpha_k y_j y_k K(\mathrm{x}_j, \mathrm{x}_k)))$$

where K is a kernel function

Definition 8.8.9. Let $X = \{x_1, \ldots, x_n\}$. A symmetric function $K\colon X{\times}X \to \mathbb{R}$ is called positive definite iff the matrix $K_{i,j} = K(x_i, x_j)$ is a positive definite matrix.

Theorem 8.8.10 (Mercer's Theorem). *Every positive definite function K on X is a kernel function on X for some feature F.*

Definition 8.8.11. The function $K(\mathrm{x}_j, \mathrm{x}_k) = (1 + (\mathrm{x}_j{\cdot}\mathrm{x}_j))^d$ is a kernel function corresponding to a feature space whose dimension is exponential in d. It is called the polynomial kernel.

8.9 Artificial Neural Networks

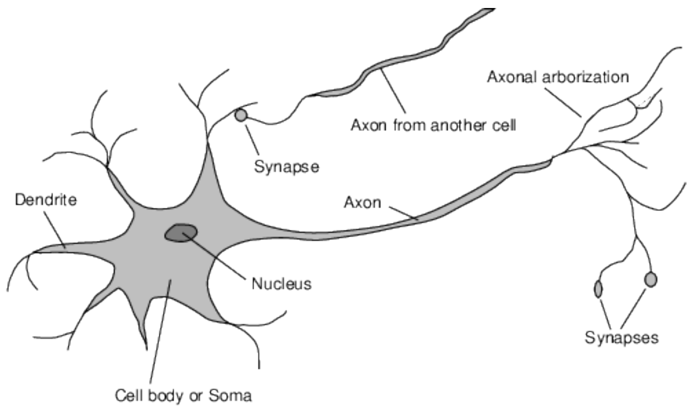
Outline

- ▷ Brains
- ▷ Neural networks
- ▷ Perceptrons

- ▷ Multilayer perceptrons
- ▷ Applications of neural networks

Brains

▷ **Axiom 8.9.1 (Neuroscience Hypothesis).** *Mental activity consists consists primarily of electrochemical activity in networks of brain cells called neurons.*



▷ **Definition 8.9.2.** The animal brain is a biological neural network

- ▹ with 10^{11} neurons of > 20 types, 10^{14} synapses, $(1\mathrm{ms}) - (10\mathrm{ms})$ cycle time.
- ▹ Signals are noisy "spike trains" of electrical potential.

Neural Networks as an approach to Artificial Intelligence

▷ One approach to Artificial Intelligence is to model and simulate brains. (and hope that AI comes along naturally)

▷ **Definition 8.9.3.** The AI sub field 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 8.9.4. An artificial neural network is a directed graph such that every edge $a_i \to a_j$

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 $f(w_{1,j}, \ldots, w_{n,j}, x_1, \ldots, x_n) \in \mathbb{R}$.

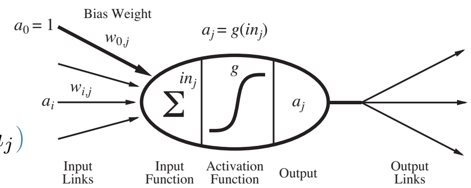
We call the output of a node's function its activation, the matrix $\mathbf{w}_{i,j}$ the weight matrix, the nodes units and the edges links.

In 1943 McCulloch and Pitts proposed a simple model for a neuron/brain:

Definition 8.9.5. A McCulloch-Pitts unit first computes a weighted sum of all inputs and then applies an activation function g to it.

$$\mathrm{in}_i = \sum_j \mathbf{w}_{j,i} a_j$$

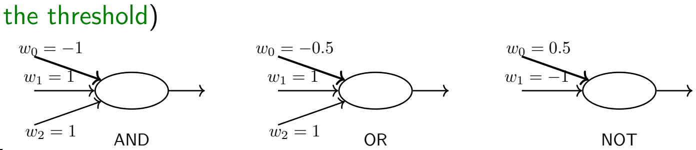
$$a_i \leftarrow g(\mathrm{in}_i) = g(\sum_j \mathbf{w}_{j,i} a_j)$$



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.

Implementing Logical Functions as Units

- ▷ 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 8.9.6 (McCulloch and Pitts).** *Every Boolean function can be implemented as McCulloch-Pitts networks.*
- ▷ *Proof:* by construction
  1. Recall that $a_i \longleftarrow g(\sum_j \mathbf{w}_{j,i} a_j)$. Let $g(r) = 1$ iff $r > 0$, else 0.
  2. As for linear regression we use $a_0 = 1 \leadsto \mathbf{w}_{0,i}$ as a bias weight (or intercept) (determines the threshold)
  3. 

  4. Any Boolean function can be implemented as a DAG of McCulloch-Pitts units.

Network Structures: Feed-Forward Networks

- ▷ We have models for neurons $\leadsto$ connect them to neural networks.
- ▷ **Definition 8.9.7.** 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 8.9.8.** Feed-forward networks are usually organized in layers: a n layer network has a partition $\{L_0, \ldots, L_n\}$ of the nodes, such that edges only connect nodes from subsequent layer.

  L_0 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.

Network Structures: Recurrent Networks

▷ **Definition 8.9.9.** A neural network is called recurrent (a RNNs), iff it has cycles.

  ▷ Hopfield networks have symmetric weights ($\mathbf{w}_{i,j} = \mathbf{w}_{j,i}$) $g(x) = \mathrm{sign}(x)$, $a_i = \pm 1$; (holographic associative memory)

  ▷ Boltzmann machines use stochastic activation functions.

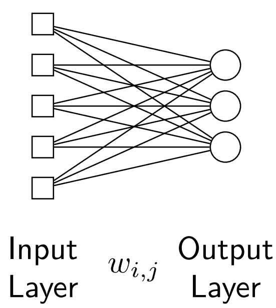
▷ Recurrent neural networks have cycles with delay $\leadsto$ have internal state (like flip-flops), can oscillate etc.

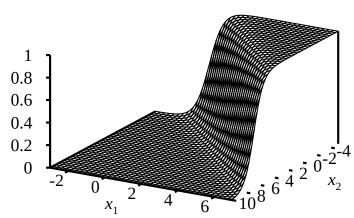
Recurrent neural networks follow largely the same principles as feed-forward networks, so we will not go into details here.

Single-layer Perceptrons

▷ **Definition 8.9.10.** A perceptron network is a feed-forward network of perceptron units. A single layer perceptron network is called a perceptron.

▷ **Example 8.9.11.**





▷ All input units are directly connected to output units.

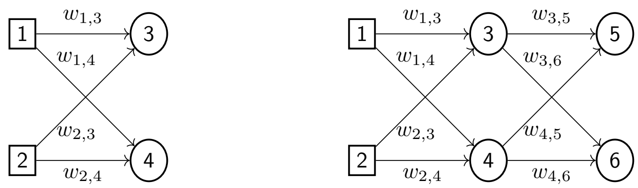
▷ Output units all operate separately, no shared weights $\leadsto$ treat as the combination of n perceptron units.

▷ Adjusting weights moves the location, orientation, and steepness of cliff.

Feed-forward Neural Networks (Example)

▷ Feed-forward network $\widehat{=}$ a parameterized family of nonlinear functions:

▷ **Example 8.9.12.** We show two feed-forward networks:



a) single layer (perceptron network) b) 2 layer feed-forward network

$$\begin{aligned} a_5 &= g(\mathbf{w}_{3,5} \cdot a_3 + \mathbf{w}_{4,5} \cdot a_4) \\ &= g(\mathbf{w}_{3,5} \cdot g(\mathbf{w}_{1,3} \cdot a_1 + \mathbf{w}_{2,3}a_2) + \mathbf{w}_{4,5} \cdot g(\mathbf{w}_{1,4} \cdot a_1 + \mathbf{w}_{2,4}a_2)) \end{aligned}$$

▷ **Idea:** Adjusting weights changes the function: do learning this way!

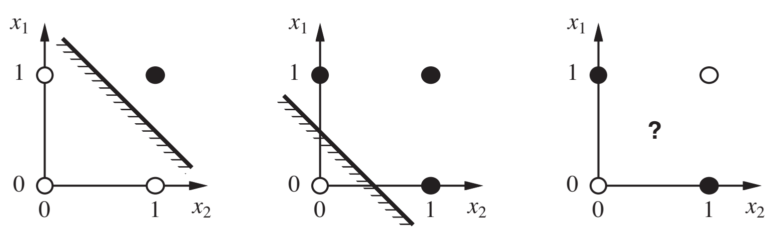
Expressiveness of Perceptrons

▷ Consider a perceptron with g = step function (Rosenblatt, 1957, 1960)

▷ Can represent AND, OR, NOT, majority, etc., but not XOR (and thus no adders)

▷ Represents a linear separator in input space:

$$\sum_j \mathbf{w}_j x_j > 0 \quad \text{or} \quad \mathbf{W}, \mathrm{x}\cdot > 0$$



(a) x_1 **and** x_2 (b) x_1 **or** x_2 (c) x_1 **xor** x_2

▷ Minsky & Papert (1969) pricked the first neural network balloon!

Perceptron Learning

For learning, we update the weights using gradient descent based on the generalization loss function.

Let e.g. $L(\mathbf{w}) = (y - h_{\mathbf{w}}(x))^2$ (the squared error loss).

We compute the gradient:

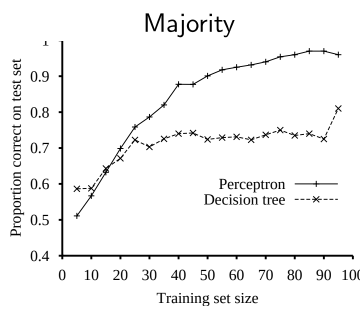
$$\begin{aligned}\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}_{j,k}} &= 2\cdot(y_k - h_{\mathbf{w}}(x)_k)\cdot\frac{\partial(y-h_{\mathbf{w}}(x))}{\partial \mathbf{w}_{j,k}} = 2\cdot(y_k - h_{\mathbf{w}}(x)_k)\cdot\frac{\partial}{\partial \mathbf{w}_{j,k}}(y - g(\sum_{j=0}^{n}\mathbf{w}_{j,k}x_j))\\ &= -2\cdot(y_k - h_{\mathbf{w}}(x)_k)\cdot g'(\mathrm{in}_k)\cdot x_j\end{aligned}$$

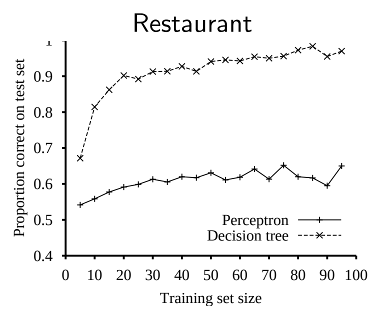
$\leadsto$ Replacing the constant factor -2 by a learning rate parameter α we get the update rule:

$$\mathbf{w}_{j,k} \leftarrow \mathbf{w}_{j,k} + \alpha\cdot(y_k - h_{\mathbf{w}}(x)_k)\cdot g'(\mathrm{in}_k)\cdot x_j$$

Perceptron learning contd.

The perceptron learning rule converges to a consistent function – *for any linearly separable data set*



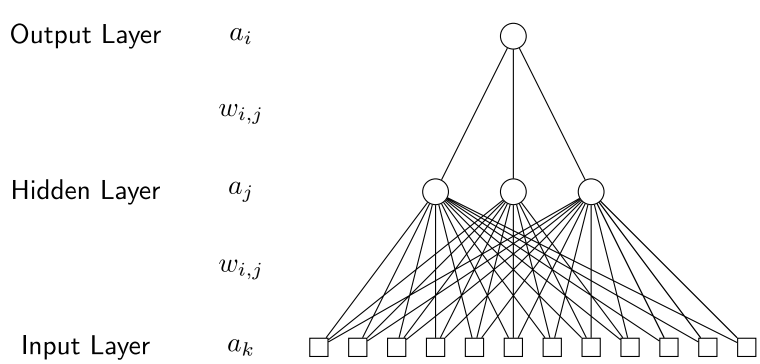


Perceptron learns the majority function easily, where DTL is hopeless.

Conversely, DTL learns the restaurant function easily, where a perceptron is hopeless. (not representable)

Multilayer perceptrons

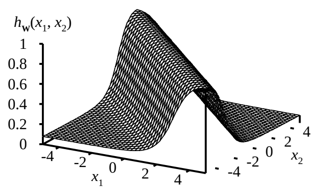
▷ **Definition 8.9.13.** In multi layer perceptron (MLPs), layers are usually fully connected; numbers of hidden units typically chosen by hand.

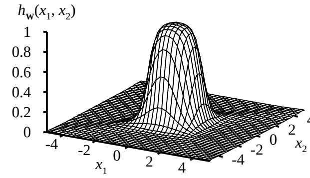


▷ **Definition 8.9.14.** Some MLPs have residual connections, i.e. connections that skip layers.

Expressiveness of MLPs

▷ 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.

$\leadsto$ We can use the perceptron learning rule to update the weights of the output layer; e.g. for a squared error loss function: $\mathbf{w}_{j,k} \leftarrow \mathbf{w}_{j,k} + \alpha \cdot (y_k - h_{\mathbf{w}}(\mathbf{x})_k) \cdot g'(\mathrm{in}_k) \cdot a_j$

What about the hidden layers?

Idea: The hidden node j is "responsible" for some fraction of the error proportional to the weight $\mathbf{w}_{j,k}$.

$\leadsto$ Back-propagate the error $\Delta_k = (y_k - h_{\mathbf{w}}(\mathbf{x})_k) \cdot g'(\mathrm{in}_j)$ from node k in the output layer to the hidden node j.

Let's justify this:

$$\begin{aligned}
\frac{\partial L(\mathbf{w})_k}{\partial \mathbf{w}_{i,j}} &= -2 \cdot \underbrace{(y_k - h_{\mathbf{w}}(\mathbf{x})_k) \cdot g'(\mathrm{in}_k)}_{=:\Delta_k} \cdot \frac{\partial \mathrm{in}_k}{\partial \mathbf{w}_{i,j}} \quad \text{(as before)} \\
&= -2 \cdot \Delta_k \cdot \frac{\partial(\sum_\ell \mathbf{w}_{\ell,k} a_\ell)}{\partial \mathbf{w}_{i,j}} = -2 \cdot \Delta_k \cdot \mathbf{w}_{j,k} \cdot \frac{\partial a_j}{\partial \mathbf{w}_{i,j}} = -2 \cdot \Delta_k \cdot \mathbf{w}_{j,k} \cdot \frac{\partial g(\mathrm{in}_j)}{\partial \mathbf{w}_{i,j}} \\
&= -2 \cdot \underbrace{\Delta_k \cdot \mathbf{w}_{j,k} \cdot g'(\mathrm{in}_j)}_{=:\Delta_{j,k}} \cdot a_i
\end{aligned}$$

Learning in Multilayer Networks (Hidden Layers)

$$\frac{\partial L(\mathbf{w})_k}{\partial \mathbf{w}_{i,j}} = -2 \cdot \underbrace{\Delta_k \cdot \mathbf{w}_{j,k} \cdot g'(\mathrm{in}_j)}_{=:\Delta_{j,k}} \cdot a_i$$

Idea: The total "error" of the hidden node j is the sum of all the connected nodes k in the next layer

Definition 8.9.15. The back-propagation rule for hidden nodes of a multilayer perceptron is $\Delta_j \leftarrow g'(\mathrm{in}_j) \cdot (\sum_i \mathbf{w}_{j,i}\Delta_i)$ And the update rule for weights in a hidden layer is $\mathbf{w}_{k,j} \leftarrow \mathbf{w}_{k,j} + \alpha \cdot a_k \cdot \Delta_j$

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:
   (a) Propagate the Δ values back to the previous (hidden) layer.
   (b) Update the weights between the two layers.

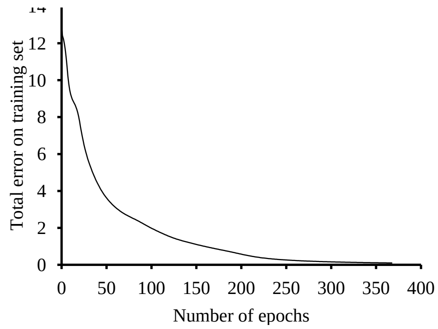
Backprogagation Learning Algorithm

▷ **Definition 8.9.16.** 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,j}, activation function g
  local variables: Δ, a vector of errors, indexed by network node
  foreach weight w_{i,j} 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 l do
            in_j := ∑_i w_{i,j} a_i
            a_j := g(in_j)
      /* Propagate deltas backward from output layer to input layer */
      foreach node j in the output layer do Δ[j] := g'(in_j) · (y_j − a_j)
      for l = L − 1 to 1 do
        foreach node i in layer l do Δ[i] := g'(in_i) · (∑_j w_{i,j} Δ[j])
      /* Update every weight in network using deltas */
      foreach weight w_{i,j} in network do w_{i,j} := w_{i,j} + α · a_i · Δ[j]
  until some stopping criterion is satisfied
  return network
```

Back-Propagation – Properties

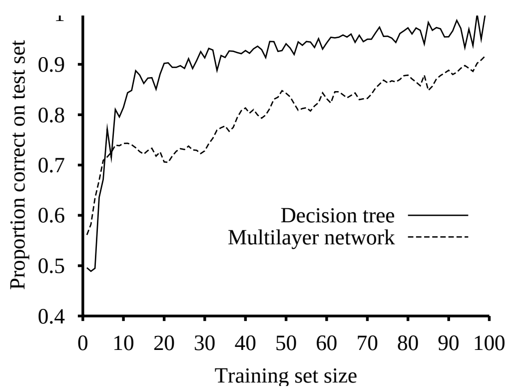
- Sum gradient updates for all examples in some "batch" and apply gradient descent.
- Learning curve for 100 restaurant examples: finds exact fit.



- **Typical problems:** slow convergence, local minima.

Back-Propagation – Properties (contd.)

- **Example 8.9.17.** 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.

Handwritten digit recognition

- ▷ 400–300–10 unit MLP = 1.6% error
- ▷ LeNet: 768–192–30–10 unit MLP = 0.9% error
- ▷ Current best (kernel machines, vision algorithms) ≈ 0.6% error

XKCD on Machine Learning

- ▷ **A Skepticists View:** see `https://xkcd.com/1838/`

Summary of Inductive Learning

- ▷ 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.

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