Artificial Intelligence

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Outline

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Thinking and Acting Humanly

- Assuming humans are the embodiment of intelligence, an intelligent agent should maybe act and think **like humans**;
- This is useful in defining what an intelligent agent should be able to do;
- It also inspiring for finding ways to solve these tasks automatically.

The Turing Test

- The "imitation game" proposed by Alan Turing in 1950;
- A machine has a 5 minutes long written conversation with a human interrogator;
- It passes the test if the interrogator mistakes it for a person 30% of the time;
- In the **total** Turing test, the interrogator can test the visual perception of the machine and pass objects through a hatch.
- No machine has ever passed the test (though some did in restricted settings).

Acting Rationally

- Alternatively, we can consider a machine is intelligent if it thinks and acts rationally;
- It makes correct inferences;
- It acts so as to always produce the best outcome (up to some measure of utility);
- This a pragmatic approach that does not enforce a predefined form of intelligence;
- It is more amenable to mathematical analysis.
- John Von Neumann said (cited by E. T. Jaynes):

  > *You insist that there is something a machine cannot do. If you will tell me precisely what it is that a machine cannot do, then I can always make a machine which will do just that!*

Strong and Weak AI

- Some philosophers make a difference between **weak AI** and **strong AI**;
- In weak AI, machines can act *as if* they were intelligent;
- In strong AI, machines *actually think*;
- The difference is mostly **irrelevant** to AI researchers.
- Turing's response:

  > *Instead of arguing continually over this point, it is usual to have the polite convention that everyone thinks.*

Artificial Intelligence as a Field of Research

- Artificial intelligence is a relatively recent field of research (1950's);
- It regroups lots of (very) different subfields;
- It draws upon philosophy, mathematics, economics, neuroscience, psychology, computer science, control theory, linguistics, etc.

Outline

Turing's "Computing Machinery and Intelligence" article

- Published in 1950;
- Puts the objective on making "intelligent" **digital machines**;
- Introduced many of the key concepts of AI:
  - the Turing test;
  - machine learning;
  - genetic algorithms;
  - reinforcement learning.

The Dartmouth Conference

- "A 2 month, 10 man study of artificial intelligence (...) during the summer of 1956 at Dartmouth College in Hanover, New Hampshire"
- Included Marvin Minsky, Claude Shannon, John McCarthy and many others.
- A basic theorem prover "Logic Theorist" was introduced at the occasion.
- The founding event of AI:
  - emphasises duplicating human faculties;
  - sets it apart from others research fields.

Expert Systems

- Initial successes (simple geometry prover, self-taught checkers program, LISP, perceptrons, etc.) until the late 1960's
- Disappointment and cut of funding from 1966 to 1973
- The first big industrial successes of AI is expert systems (1970s-1980s):
  - logical inference (if - then rules);
  - extensively use domain-specific knowledge;
  - Prolog;
  - dozens of installed systems in big companies.

Deep Blue

- 1997: Chess world-champion Gary Kasparov lost to IBM's Deep Blue in a 6-game match;
- Program working on dedicated hardware;
- Evaluated 200 millions moves per seconds;
- Nowadays purely software chess programs routinely perform at this level.

Autonomous Cars

- A very old problem (1920's, remote control);
- 1990's: First successes: semi-autonomous driving
- 2000's: Fully autonomous driving in deserts
- 2010's: Fully autonomous driving in cities (still with many limitations)
- Now a major topic for all the car industry.

(Image) Classification

- Programs now perform classification tasks at or above human-level;
- Examples include ImageNet Large-Scale Visual Recognition challenge;
- Error improved from 25% in 2011 to 16% in 2012 with deep neural network based approaches;
- Now at less than 5%

Alpha Go

- 2015: first victory over a Go professional without handicap;
- 2017: first victory over a top-rated player;
- Used deep neural networks for move and position evaluation;
- Used Monte Carlo tree search variants for move tree exploration.

ChatGPT

- 2017: *Transformers*: « Attention is all you need »;
- 2022: ChatGPT;
- Basé sur un *Large Language Model* : GPT3.5 puis GPT4;
- GPT = *Generative Pre-trained Transformer*;
- Architecture de décodeur avec couches d'attention;
- GPT3.5: 175 miliards de paramètres; GPT4 ?
- Apprentissage supervisé + apprentissage par renforcement.

Outline

Structure of a Rational Artificial Agent

- An agent has **sensors** and **actuators** to operate with its **environment**;
- It has some internal **memory**;
- Within the memory, possibly a **model** of the environment;
- It can use all this to find out:
  - how the environment evolves by itself;
  - the outcomes of the agents' actions;
  - the "best" action.
- A **performance evaluation** module;
- A **learning** module.

The Notion of Environment

- The environment can be many things:
  - The real-world;
  - A mathematical construct;
  - Computer programs, etc.;
- It has several key properties (in relation with the capabilities of the agent):
  - Observability;
  - Uncertainty;
  - Presence of other agents;
  - Static or dynamic;
  - Discrete or continuous;
  - Known or not.

Taking Decisions

- To find out the best action, the agent can:
  - Use only the current state (based on the sensor inputs) and:
    - a database of good decisions;
    - or a learned representation of good decisions.
  - Use a model of the environment and plan optimally over several actions;
  - Ideally a mix of the two (e. g. AlphaZero).
- These involve tradeoffs between computational power/memory and accuracy;
- The complexity of the models (for learning or planning) is part of this tradeoff.

Learning

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  - Supervised learning: use positive and negative examples.

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Optimal Strategies in Deterministic Environments
- The Simple Case
- Path Finding
- Optimal Decisions

Non-Deterministic Environments

Uncertain (Probabilistic) Environments

Accounting for other Agents

Supervised Learning

Conclusion

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Modelling successive states

- The agent should be able to evaluate the **outcomes** of its actions;
  - We need to model the different **states** the system can be in;
  - And to model how we **move** from one state to another;
- A basic model for that is the **directed graph**.

Example: A Sliding Puzzle

1	2	3
4		5
7	8	6

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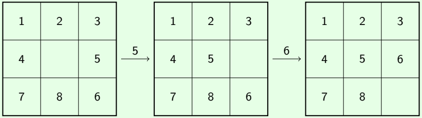

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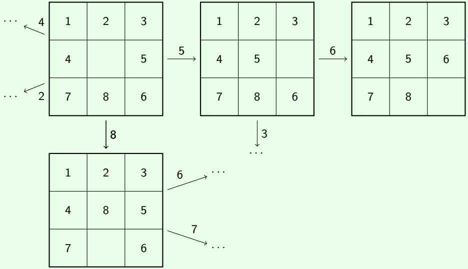

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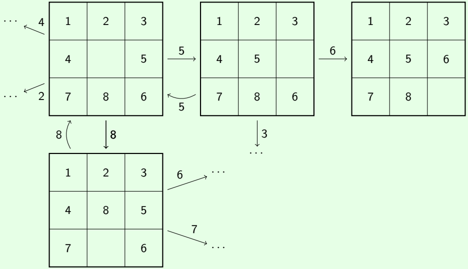

(Labeled) Directed Graphs

Definition (Directed Graph)

A **directed graph** is a pair (V, E) where:

- V is a set of **vertices**;
- $E \subseteq V \times V$ is a set of **edges**.

- There is an edge from v to v', and we write $v \to v'$, when $(v, v') \in E$;
- We can label nodes with a function $V \to \Lambda$ for some label set Λ;
- We can label edges with a function $E \to \Sigma$ for some label set Σ.

(Labeled) Directed Graphs: Exercise

Exercise

A farmer, a wolf, a goat, and a cabbage are on one side of a river that they must cross. There is a boat that can be operated only by the farmer, and with only two places. When the farmer is not there, the wolf will eat the goat, and the goat will eat the cabbage.

1. Draw a directed graph modelling this problem. You should not expand the nodes in which the “game” is won or lost;
2. Give a strategy for the farmer allowing everyone to safely cross the river.

Continuous Environments

- For some systems the environment is intrinsically **continuous**;
- We can use the previous approach by **discretising** the continuous variables:
- For instance: replace a continuous variable $x \in [0, 30]$ by a discrete variable with three different discrete values corresponding to: $0 \leq x < 10$, $10 \leq x < 20$ and $20 \leq x \leq 30$.
- Another possibility is to use more expressive formalisms: e.g. **timed automata** or **hybrid automata**.

Achieving a (distant) goal

- A **goal** for some agent, is to make the system reach some beneficial state of the system;
- To achieve this we could move **at random** but:
  - This can take a very long (even infinite!) time;
  - The agent might first reach forbidden states.
- We need to **plan** ahead and find a **strategy** to get the goal in the **model** of the system.

Strategies

Definition (Strategy)

A **strategy** is a function $f : V^* \to V$ such that for all $\sigma \in V^*, (\mathrm{last}(\sigma), f(\sigma)) \in E$.

V^* is the set of finite sequences of elements of V.
For a sequence σ, $\mathrm{last}(\sigma)$ is the last element of σ.

Definition (Positional Strategy)

A **strategy** f is **positional** (or memoryless) if: $\forall \sigma, \sigma', \mathrm{last}(\sigma) = \mathrm{last}(\sigma')$ implies $f(\sigma) = f(\sigma')$.

We can thus define positional strategies as functions $V \to V$.

Outcome

- When the agent applies a strategy, it produces sequences of vertices, the **outcome**, that represent the successive results of each action.
- In the case when the environment is fully observable, there is only one agent, and all actions are deterministic, the outcome of a strategy is a **single path**:

Definition (Outcome)

The **outcome** $\mathrm{Outcome}(v, f)$ of strategy f from vertex v is the set of vertex sequences inductively defined by:

- $v \in \mathrm{Outcome}(v, f)$;
- if $\sigma \in \mathrm{Outcome}(v, f)$ then $\sigma.v' \in \mathrm{Outcome}(v, f)$ iff $v' = f(\sigma)$.

- We will extend these definitions as we relax those hypotheses later on.

Objectives

Definition (Objective)

An **objective** is a set of vertex sequences.

Definition (Maximal sequence)

A vertex sequence is **maximal** within a sequence set X if it is either **infinite** or it is **not a prefix** of some sequence in X.

When $X = V^*$, we just say the sequence is maximal.
We denote by $\mathrm{MaxOutcome}(v, f)$ the subset of sequences of $\mathrm{Outcome}(v, f)$ that are maximal within $\mathrm{Outcome}(v, f)$

Definition (Reachability Objective)

Given a target vertex g, the reachability objective $\mathrm{Reach}(g)$ is the set of maximal sequences σ such that $g \in \sigma$.

Winning Strategies, Winning Vertices

Definition (Winning Strategy)

A strategy f is **winning** from some vertex v for some objective X if $\mathrm{MaxOutcome}(v, f) \subseteq X$.

Definition (Winning Vertex)

A vertex v is **winning** if there exists a winning strategy from v.

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Path finding

- Under the hypothesis of a fully observable, monoagent, and deterministic environment, with a reachability objective:
  - if there is a winning strategy there is a **positional** winning strategy;
  - the outcome of a strategy is a **single path**.
- Finding a winning strategy to reach some vertex therefore amounts to find this path;
- The strategy then consists in each vertex of the path in **going to the next one**.

Spanning Tree Walk

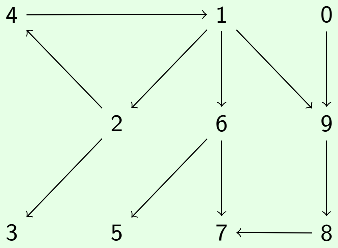
```
input:  s0     // source state
        t      // target state
output: r      // is t reachable from s0?
        pred   // state predecessors table

∀s', pred[s'] ← ⊥ // No predecessor initially
r ← false
P ← ∅ // The set of visited vertices
W ← {s0} // The set of open vertices (waiting to be explored)
while W ≠ ∅ and not r:
    s ← next(W) // take and remove the next state from W
    if s = t:
        r ← true
    else :
        P ← P ∪ {s}
        foreach successor s' of s:
            if s' ∉ P and s' ∉ W:
                pred[s'] ← s // build the path
                W ← W ∪ {s'}
```

Breadth-first Search (BFS)

- If W is a **queue**, then the order of exploration if **breadth-first**.

Example

Look for a path from 1 to 0 (impossible):



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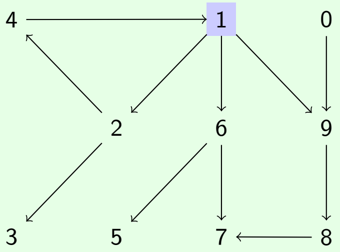

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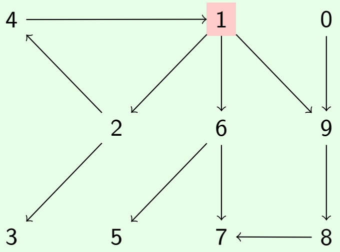

W = [2,6,9]

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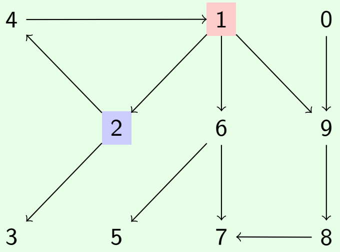

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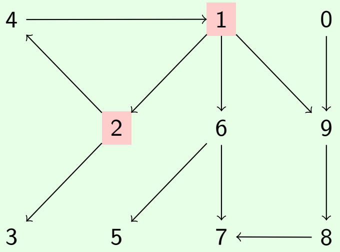

W = [6,9,4,3]

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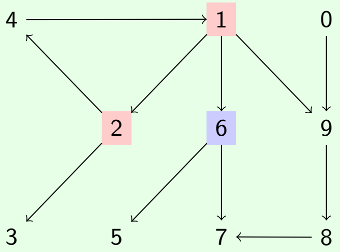

W = [9,4,3]

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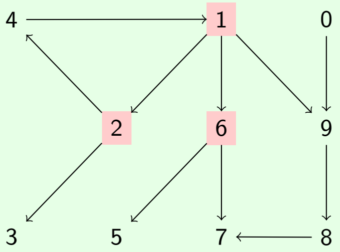

W = [9,4,3,5,7]

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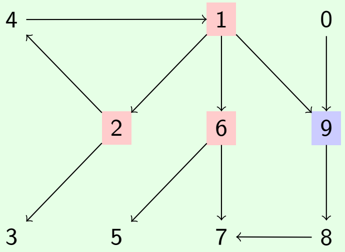

W = [4,3,5,7]

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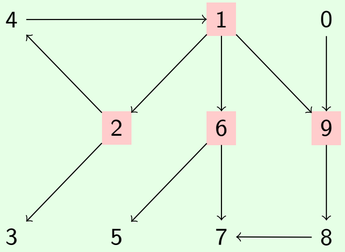

W = [4,3,5,7,8]

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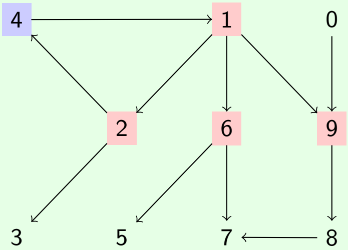

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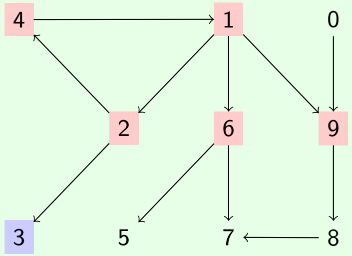

W = [5,7,8]

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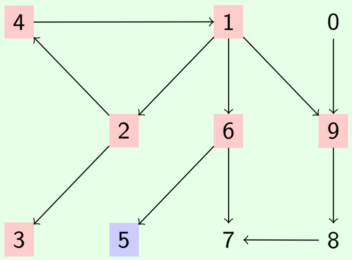

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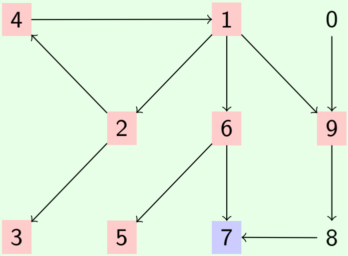

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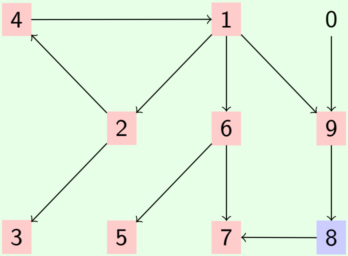

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Depth-first Search (DFS)

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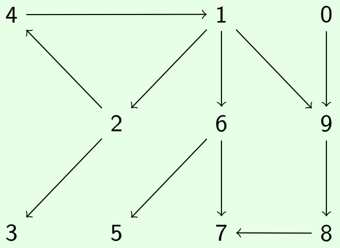

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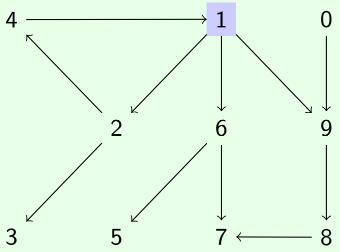

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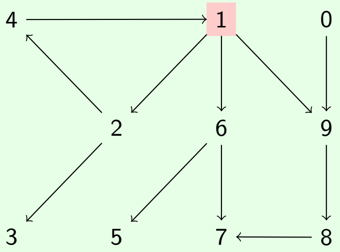

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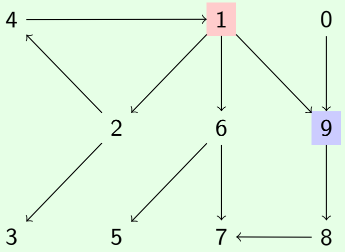

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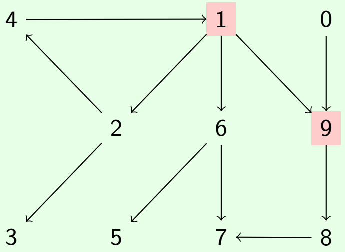

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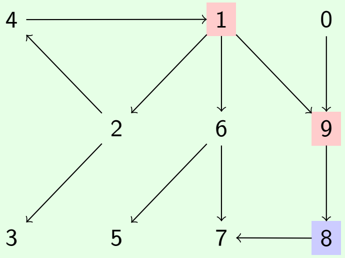

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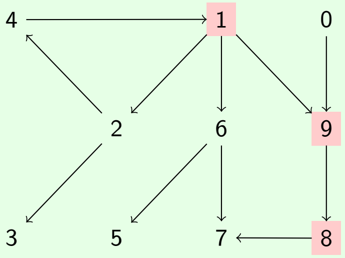

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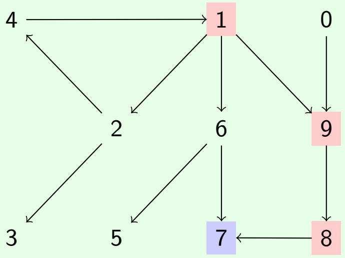

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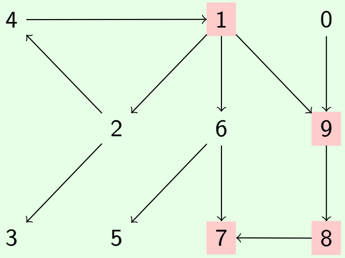
Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

Look for a path from 1 to 0 (impossible):



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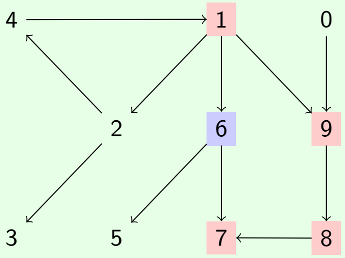

W = [2]

Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

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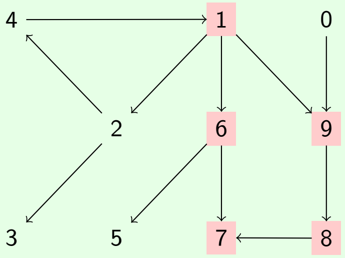


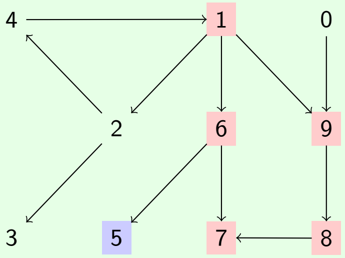
W = [5,2]

Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

Look for a path from 1 to 0 (impossible):



W = [2]

Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

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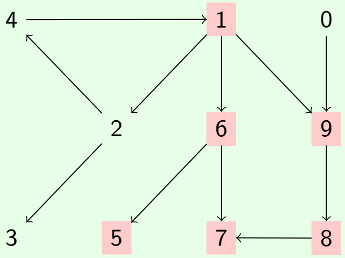

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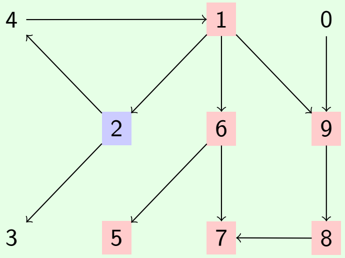

W = []

Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

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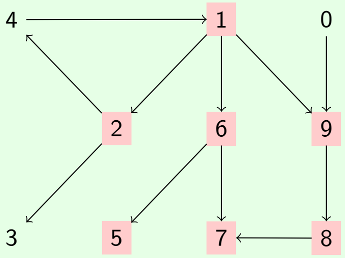


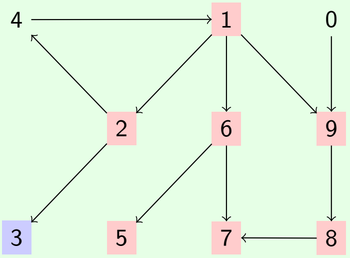
W = [3,4]

Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

Look for a path from 1 to 0 (impossible):



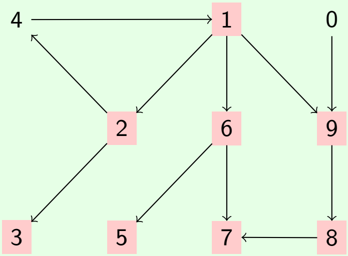
W = [4]

Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

Look for a path from 1 to 0 (impossible):



W = [4]

Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

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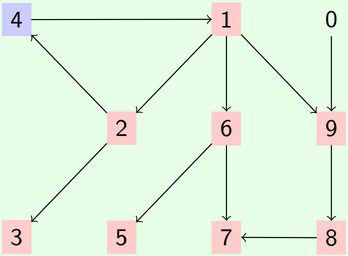


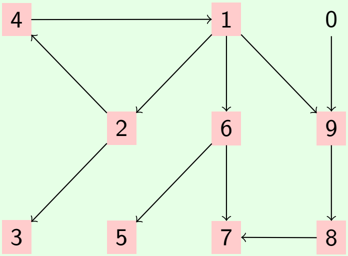
W = []

Depth-first Search (DFS)

- If W is a **stack**, then the order of exploration if **depth-first**.

Example

Look for a path from 1 to 0 (impossible):



W = []

BFS Vs DFS

- BFS gives the **shortest** path (wrt. number of edges);
- DFS can easily find loops;
- DFS explores in a more **local** manner;
- DFS can be made more **memory-efficient** (at the cost of exploring **redundant** paths).

Forgetful DFS

```
function fDFS:
    input:  s     // source state
            t     // target state
            path  // Current path
    output: r     // is t reachable from s?
            path' // Path to goal

    path' ← path : s // concatenate s
    if s = t:
        r ← true
    else:
        r ← false
        foreach successor s' of s and while not r:
            if s' ∉ path':
                (r, path'') ← fDFS(s', t, path')
                if r:
                    path' ← path''
```

Forgetful DFS

Exemple

$$\begin{tikzcd}
1 \arrow[r] \arrow[dr] & 2 \arrow[r] & 4 \arrow[loop right] \\
& 3 \arrow[u] & \\
5 \arrow[uu] & &
\end{tikzcd}$$

How many nodes are visited in the worst case by BFS, DFS and "forgetful DFS", before we can conclude that 5 is not reachable?

Completeness

A search algorithm is **complete** *if whenever there exists a path to the target vertex, the algorithm always finds one.*

Exercise

Are BFS and DFS (normal and forgetful) complete?

Completeness

A search algorithm is **complete** *if whenever there exists a path to the target vertex, the algorithm always finds one.*

Exercise

Are BFS and DFS (normal and forgetful) complete? What about infinite graphs?

Iterative Deepening

- Even in finite graphs, DFS can go astray for a while if unlucky;
- To alleviate these problems, we can arbitrarily **bound** the length of the paths explored;
- If we find a path, we are done;
- Otherwise, **increase** the bound and **retry**.
- Works well because in a tree there are much more **leaves** than **internal nodes**.

Exercise

Exercise

Two person move *simultaneously* on a map in a turn-wise manner. Each turn they both move to one the neighboring city. The new turn starts when both have reached their destination. We want a (global) strategy to make them meet.

- Can we model this as a graph path-finding problem?
- If the map is completely connected, is there always a solution?
- Find a map for which one of the two persons must visit a city twice before meeting the other.

Outline

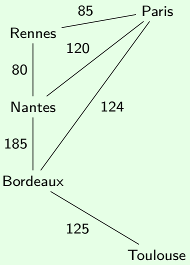
Costs

- BFS gives the **shortest** path to the goal;
- But all actions might not have the same **cost**;
- Cost may represent time, money, energy, etc.
- We may be interested in the **minimum cost** path to the goal:
  - extend the model;
  - modify the algorithms.

Weighted (Directed) Graphs

- we add an integer **weight** (or cost) to each edge with a function $\omega : E \rightarrow \mathbb{N}_{>0}$;
- the case where weights can be **non-positive** leads to more complex algorithms (e.g. Bellman-Ford).

Example: Some train travel durations in the West



What is the best option to go from Rennes to Bordeaux?

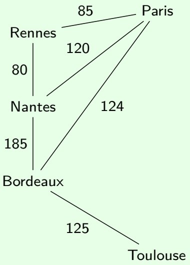
Dijkstra's Algorithm

```
input:  s0    // source state
        t     // target state
output: r     // is t reachable from s0?
        pred  // state predecessors table
        cost  // state cost table

∀s', pred[s'] ← ⊥ // No predecessor initially
cost[s0] ← 0
∀s' ≠ s0, cost[s'] ← +∞ // Initial costs
r ← false
W ← {s0} // W is a priority queue
while W ≠ ∅ and not r:
    s ← extract_min(W, cost) // take and remove the mincost state from W
    if s = t:
        r ← true
    else :
        foreach successor s' of s:
            if cost[s] + ω(s, s') < cost(s'):
                cost[s'] ← cost[s] + ω(s, s')
                pred[s'] ← s // build the path
                W ← W ∪ {s'}
```

Dijkstra's Algorithm: Example

Example: Some train travel durations in the West



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Dijkstra's Algorithm: Example

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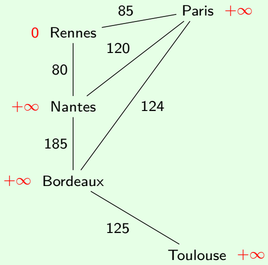

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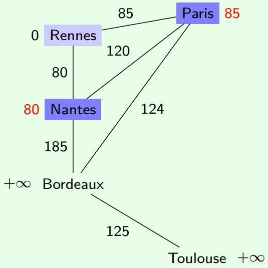

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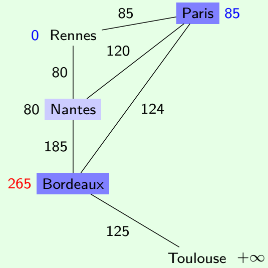

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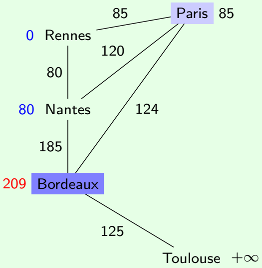

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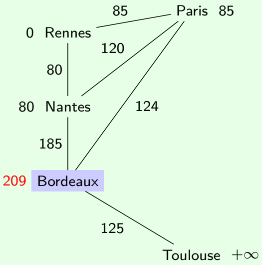

What is the best option to go from Rennes to Bordeaux?

A^*

- Dijkstra's algorithm explores first the vertex n with the minimum **path-cost** $g(n)$ but knows nothing of what remains to do (**uninformed search**);
- Suppose now we have a **heuristic** $h(n)$ that estimates the cost from n to the target;
- We assume $h(x) = 0$ for the target vertex;
- We explore nodes by selecting the one with the minimum value for

$$f(n) = g(n) + h(n)$$

A^*: Example

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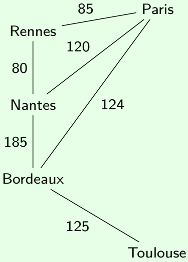

Rennes	45
Nantes	33
Paris	60
Toulouse	25
Bordeaux	0

Table: Straight flight times (min) to Bordeaux at 500 km/h

What is the best option to go from Rennes to Bordeaux?

Use straight flight times as heuristic

A^*: Example

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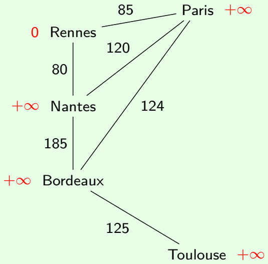

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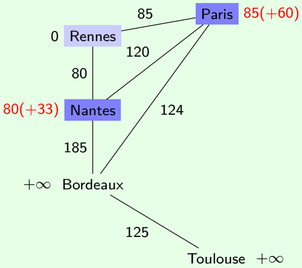

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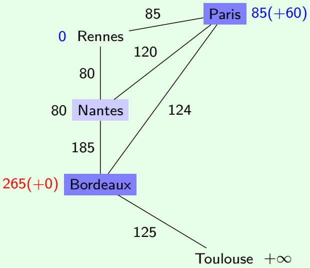

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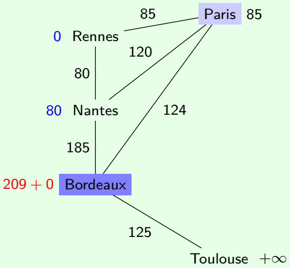

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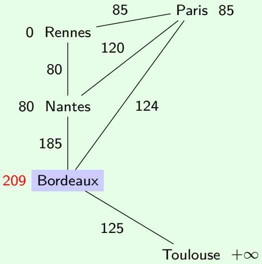

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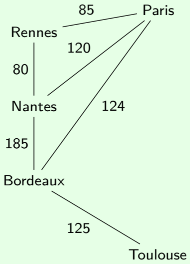

Rennes	45
Nantes	185
Paris	124
Toulouse	125
Bordeaux	0

Table: Actual duration when direct connection or straight flight times (min) to Bordeaux at 500 km/h

What is the best option to go from Rennes to Bordeaux?

Use actual direct times when available or straight flight times otherwise as heuristic

A^*: Example

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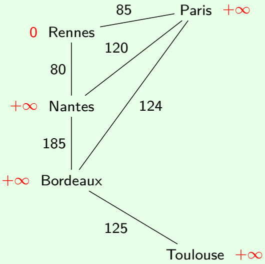

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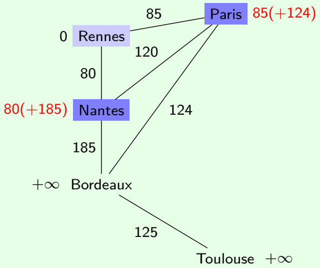

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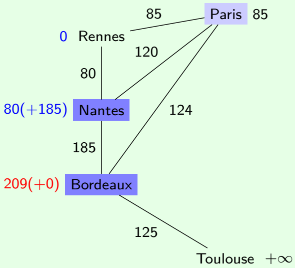

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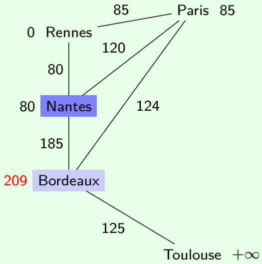

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A^*: About heursitics

- The heuristic is a **function** that takes a **state** as input;
- Its output is an **estimate** of the cost from that state to the goal;
- Its result has the **same unit** as the weight on edges;
- By adding the cost from the initial state s_0 to state s and the heuristic at s, we get an estimate of the **total cost** of going through s to reach the goal;
- Finding a (good) heuristic is part of solving the minimum cost problem with A^*.

A^*: Optimality and "good" heuristics

- A^* is guaranteed to find an **optimal** path if h is **admissible**:
  An A^* heuristic is admissible if it never overestimates the cost to the goal.
- A^* is guaranteed never to visit a vertex twice if h is **consistent**:
  An A^* heuristic h is consistent if:
  $\forall (x, y) \in E, h(x) \leq \omega(x, y) + h(y)$.
- We can obtain **admissible** heuristics by solving **relaxed** versions versions of the problem, i.e., by removing some constraints.

Exercise

1. Were the previous two heuristics admissible and consistent?
2. Prove that if h is consistent then it is admissible;
3. Give an admissible heuristic that is not consistent.

Exercises

Exercise

Bridge crossing (Levmore & Cook, 1981). We quote the version of (Rote, 2002): "Four people begin on the same side of a bridge. You must help them across tothe other side. It is night. There is one flashlight. A maximum of two people can cross at a time. Any party who crosses, either one or two people, must have the flashlight to see. The flashlight must be walked back and forth, it cannot be thrown, etc. Each person walks at a different speed. A pair must walk together at the rate of the slower person's pace, based on this information: Person 1 takes $t_1 = 1$ min to cross, and the other persons take $t_2 = 2$ min, $t_3 = 5$ min, and $t_4 = 10$ min to cross, respectively."

We want to find the fastest strategy to cross.

1. Can you intuitively find a strategy that wins in less than 20 min?
2. Give an admissible heuristic for this problem;
3. Find the fastest strategy using A^* and expanding only the relevant part of the weighted graph.

Exercises

Exercise

Knowing the straight line travel times $d(i,j)$ between cities i and j, what is an admissible heuristic for minimizing the time to meet in the previous two persons simultaneously moving (at the same speed) on a map problem? What if we want to minimise the sum of the travel times of both persons?

Exercise

Greedy Best-first Search. Suppose that instead of using $f = g + h$ to select the vertex to explore we use only h. Show that this does not always lead to an optimal path in finite graphs and that it might not be complete in infinite graphs.

Outline

Outline

Introduction

Optimal Strategies in Deterministic Environments

Non-Deterministic Environments

- (Optimal) Strategies in Non-deterministic Environments
- Partially Observable Non-deterministic Environments

Uncertain (Probabilistic) Environments

Accounting for other Agents

Supervised Learning

Conclusion

Non-determinism

- We have supposed that performing an action always has the **same outcome**;
- We now relax this assumption: performing an action may lead **non-deterministically** to (a finite number of) **different states**;
- We have no information on what state will be reached but we can **observe** it.

Non-determinism: Example

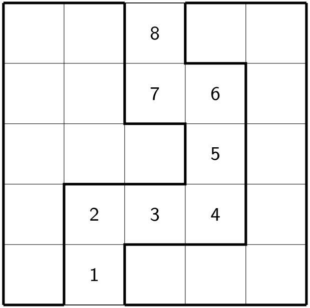
Exemple

A robot goes through a given tiled turning corridor while carrying a big pile of important stuff.

- When it turns left the pile **may**:
  - get left-unbalanced if it was balanced;
  - fall down if it was already left-unbalanced;
  - get balanced again, if it was right-unbalanced.
- The situation is symmetric when turning right.
- The robot moves the next tile in 1s or 2s if unbalanced.
- The robot can always stop and balance the pile again (4s).

Find a strategy to cross the corridor as fast as possible without the pile falling down.

Non-determinism: Example



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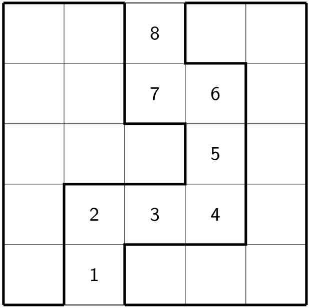
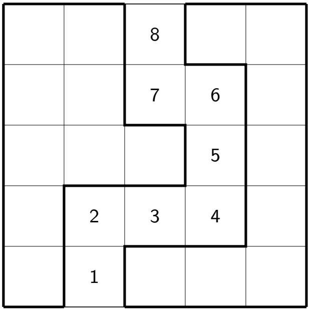
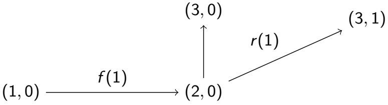


$$(1,0) \xrightarrow{f(1)} (2,0)$$

Non-determinism: Example





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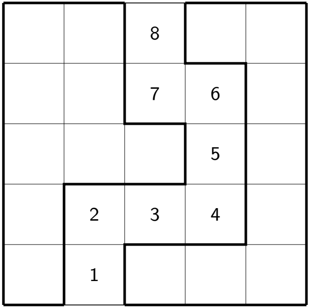
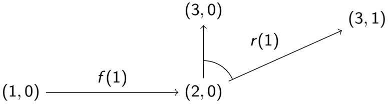
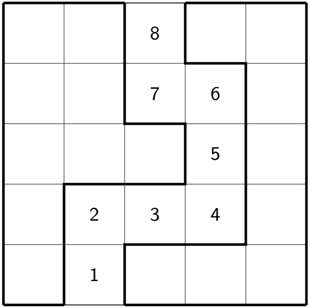
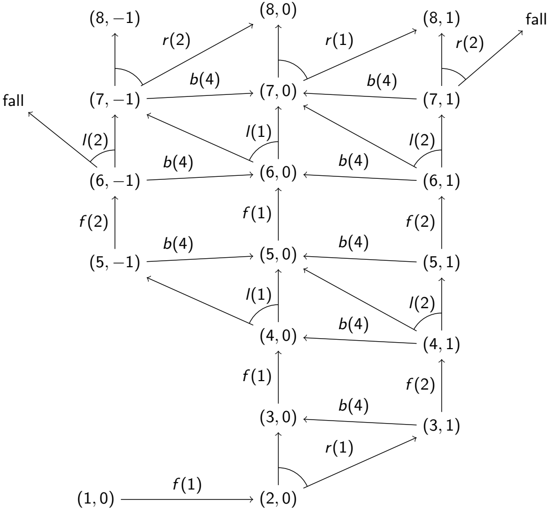




Non-determinism: Example





Hypergraphs

- We use **hyperedges** to model non-deterministic outcomes:

Definition (Hypergraph)

A (directed) *hypergraph* is a pair (V, E) where V is a set of vertices and $E \subseteq V \times 2^V \setminus \{\emptyset\}$ a set of **hyperedges**.

2^V denotes the **powerset** of V, i.e, the set of all subsets of V

- An hyperedge $(v, \{v_1, \ldots, v_n\})$ models a unique action from v that can lead non-deterministically to any of the vertices $v_1, \ldots, v_n$.
- Hypergraphs are also called an **AND-OR** graphs;
- We can define **weighted** hypergraphs as before.

Non-determinism

- Playing some action means choosing an hyperedge:

Definition (Strategy)

A **strategy** is a function $f : V^* \to 2^V$ such that for all $\sigma \in V^*, (\mathrm{last}(\sigma), f(\sigma)) \in E$.

- It may have **several outcomes** and **all** of them must be winning:

Definition (Outcome)

The **outcome** $\mathrm{Outcome}(v, f)$ of strategy f from vertex v is the set of vertex sequences inductively defined by:

- $v \in \mathrm{Outcome}(v, f)$;
- if $\sigma \in \mathrm{Outcome}(v, f)$ then $\sigma.v' \in \mathrm{Outcome}(v, f)$ iff $v' \in f(\sigma)$.

- The outcome is not a single path anymore but a **tree** allowing to deal with all **contingencies**.

Solving Non-determinism

```
input:  s0     // source state
        G      // target state set
output: r      // is G reachable from s0?
        strat  // strategy

∀s′, strat[s′] ← ⊥ // No strategy initially
r ← false
∀s′ ∈ G, R[s′] ← true, ∀s′ ∉ G, R[s′] ← false
W ← G // The set of open vertices (waiting to be explored)
while W ≠ ∅ and not R[s0]:
    s′ ← next(W) // take and remove the next state from W
    foreach s such that not R[s] and ∃(s, K) ∈ E with s′ ∈ K:
        R[s] ← ⋁_{(s,K′)∈E} ( ⋀_{s′′∈K′} R[s′′])
        if R[s]:
            W ← W ∪ {s}
            strat[s] ← K′, s.t. ⋀_{s′′∈K′} R[s′′]

r ← R[s0]
```

- $\vee$ is a notation for the **logical or** between two booleans: e.g. true $\vee$ false $=$ true;
- $\wedge$ is a notation for the **logical and** between two booleans: e.g. true $\wedge$ false $=$ false;
- $\bigvee_{b \in B} b$, with $B = \{b_1, b_2, \ldots, b_n\}$ and each b_i a boolean variable is the **logical or** between all the b_i: $\bigvee_{b \in B} b = b_1 \vee b_2 \vee \cdots \vee b_n$
- Similarly, $\bigwedge_{b \in B} = b_1 \wedge b_2 \wedge \cdots \wedge b_n$ is the **logical and** between all the b_i.

Non-determinism: Exercise

Exercise: Moving Robot

Apply the previous algorithm to find a strategy for the robot to safely reach tile 8 (disregarding costs).

Optimal Decisions in Non-deterministic Environments

- To deal with costs, we can extend Dijkstra's and A* algorithms (A*LD, AO*);
- For instance Knuth extension of Dijkstra's algorithm:
  - initially goals have cost 0 and others $+\infty$;
  - always visit the vertex with the smallest cost first.
  - move backwards (hence start with goals);
  - compute costs instead of booleans, using max instead of $\wedge$ and min instead of $\vee$.

Exercise

Apply this algorithm to find an *optimal* strategy for the robot.

- We can also use other functions than max (e.g. $+$).

Outline

Partial Observability

- The agent often **perceives** the environment through a **limited number** of **sensors**;
- It might however have a more complete internal representation (model) of the environment;
- It then uses its percepts to **estimate** its current state and act accordingly;
- The evolution of the system is perceived through an **observation function** mapping states to a finite set of **observations** $\mathcal{O}$.

Partially Observable Non-deterministic Environments

- We model the environment with an hypergraph with edges labeled by actions from a finite set Σ. We also call Σ the labelling function.

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- The observation function has type $V \to \mathcal{O}$;
- Let $\mathcal{R}$ be the set of **runs**, *i.e.*, sequences $v_1 a_1 v_2 a_2 \dots v_n$, with $v_i \in V$ and $a_i \in \Sigma$:

Definition (Strategy)

A **strategy** is a function $f : \mathcal{O}(\mathcal{R}) \to \Sigma$ such that for all $\sigma, \sigma' \in V^*$ such that $\mathcal{O}(\sigma) = \mathcal{O}(\sigma')$, there is a an hyperedge labeled by $f(\sigma)$ from $\mathrm{last}(\sigma)$ iff there is one from $\mathrm{last}(\sigma')$.

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Finding a Strategy

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Prove that we may need a non-positional strategy to win in such a setting.

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- At each step we need to do some **state estimation** (aka **filtering**);
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- We then reduce the problem of finding a strategy to a fully observable graph problem.

Building Belief States

- We build **sets of vertices**;

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$$V'_a = \bigcup_{v \in V'} \Big(\bigcup_{(v,X) \in E \text{ s.t. } \Sigma((v,X))=a} X \Big)$$

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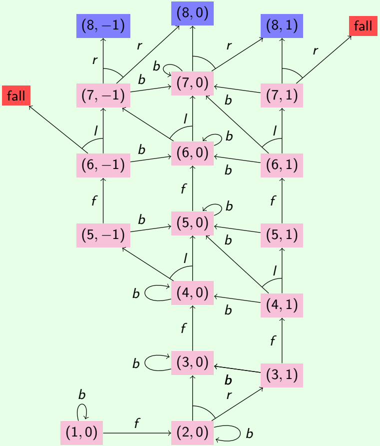
- We build a **finite** belief hypergraph by considering:
  - Belief states as vertices;
  - There is an hyperedge labeled by a between V' and all the $V'_{a,o}$ for all observations o that can occur.

Example

Back to the balancing robot

- We ignore costs;
- We add explicit b loops on balanced states;
- Suppose the pile is so high the robot cannot see where it is and whether the pile is unbalanced or not;
- We have only three observations:
  - we are in 8,
  - we are not in 8 and all is well,
  - the pile has fallen down.



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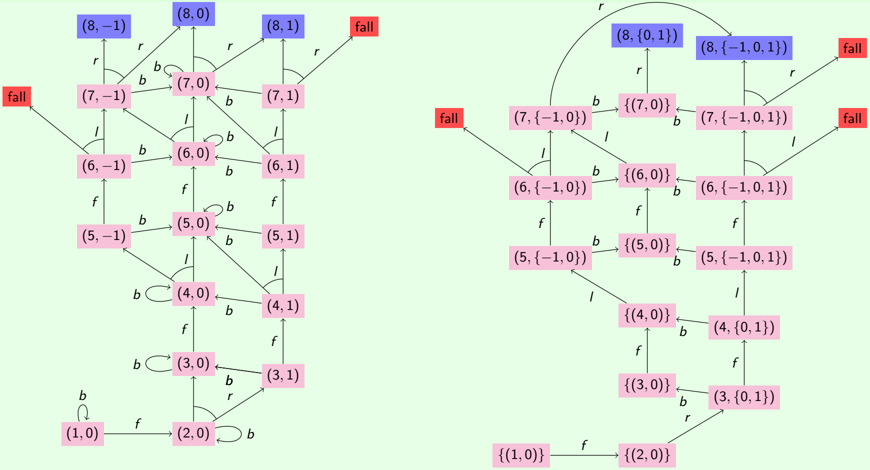

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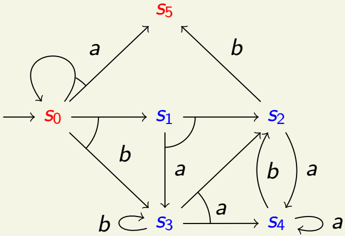
- For each run on observations $\omega = o_1 a_1 \dots o_n$, there is by construction a **unique** vertex sequence σ_ω in the belief hypergraph;
- The winning strategy is therefore $f(\omega) = F(\text{last}(\sigma_\omega))$.

Exercises

Exercise



Does there exist a winning strategy to go from s_0 to s_5? *Explain by building the corresponding **belief graph**.*

Exercises

Back to the balancing robot

1. What is the minimum number of balancing moves necessary in a winning strategy?
2. What is the minimal size of the memory necessary for a winning strategy? (number of past pairs (observation, action) memorised)
3. Give (a minimal number of) observations to add to have a memoryless winning strategy.

Exercises

The blind bartender (Martin Gardner, 1979)

4 glasses are places on the corners of a square tray. Some are upright, some are upside-down. There are two players: a blindfolded bartender (B), and an antagonist (A). The bartender faces one side of the tray, cannot observe the board and wins if the glasses are all up or all down. At each round, B announces which glasses (1 or 2) to turn, then A turns the tray by a multiple of 90 degrees, and finally A turns the glasses at the positions originally announced by B (or equivalently B turns them with boxing gloves on).

1. Using symmetries, down to how many different configurations can we reduce the problem?
2. Using symmetries, how many different moves can we distinguish on those configurations?
3. Model this problem using an hypergraph with partial observability;
4. Can the bartender win? If so give a winning strategy.

Outline

Quantifying Uncertainty

- We often have some information on the relative possibility of the occurrence of uncertain outcomes;
- This can be modeled using **probabilities**;
- A rational agent then chooses actions maximizing its **utility**.

Utility of Morgenstern and Von Neumann (1944)

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- That value is defined up to any **affine transformation**: $U'(R) = aU(R) + b$ also works.
- A rational agent can decide between outcomes by choosing the one that **maximises utility** (principle of maximal expected utility, or MEU).

Exercise: Allais' Paradox

- Choose between the following two lotteries:

A :

Gain	$0M€$	$1M€$	$5M€$
Prob.	0	1	0

B :

Gain	$0M€$	$1M€$	$5M€$
Prob.	0.01	0.89	0.1

- and between those two:

C :

Gain	$0M€$	$1M€$	$5M€$
Prob.	0.89	0.11	0

D :

Gain	$0M€$	$1M€$	$5M€$
Prob.	0.9	0	0.1

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Prob.	0.9	0	0.1

Exercise

Prove that $B \preceq A$ and $C \preceq D$ cannot be represented by a Von Neumann and Morgenstern utility function. You may want to start by assuming the utility of 0€ is 0, the utility of 5M€ is 1, and the utility of 1M€ is somewhere in between.

Outline

Markov Decision Processes

- We now consider **sequences** of decisions;

Markov Decision Processes

- We now consider **sequences** of decisions;
- We extend hypergraphs to introduce probabilities for possible outcomes:

Definition (Markov Decision Process (MDP))

An MDP is a tuple $(S, s_0, A, P, R, \gamma)$ where:

- S is a finite set of states;
- s_0 is the initial state;
- A is a finite set of actions;
- $P : S \times A \to \text{Dist}(S)$ is the transition function;
- $R : S \times A \times S \to \mathbb{R}$ is the reward function;

Markov Decision Processes

Back to the balancing robot

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- We put reward 1 on states $(8, *)$;
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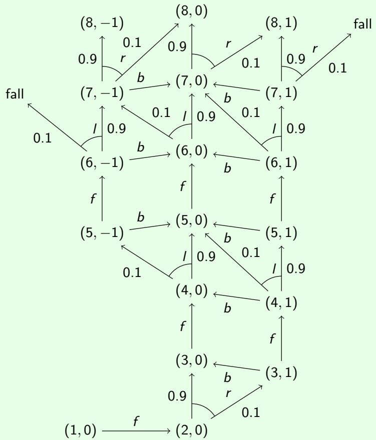

Markov Decision Processes

Exercise

Which of the following games can be modelled as MDPs?

- Roulette;
- Russian roulette;
- Blackjack
- Backgammon;
- Slot machines (one-armed bandit).

Sequential Decisions: Strategies

Definition (Strategy in an MDP)

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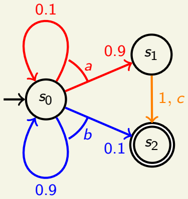

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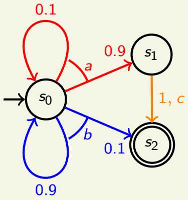


If only two successive moves are allowed (finite horizon), what is the optimal strategy to reach s_2?

- They are if we consider an **infinite horizon**.

Winning and Rewards

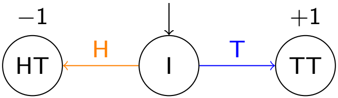
- The notion of winning strategy is not as useful as before:
- We have no definite **goal state**;
- We are more interested in **maximising the rewards** obtained.

Example: Let's play matching pennies

Matching pennies

Matching pennies is a two-player game. Let S and D be the two players. Initially, each player has a penny. They independently and secretly choose heads or tails and reveal their choices simultaneously. If both faces match, S takes both coins, otherwise D takes them.

Consider the point of view of S. Assume we know that D always plays tails. What is the best strategy and how much is the associated gain?



$$
\begin{aligned}
&U(HT) = -1, U(TT) = 1,\\
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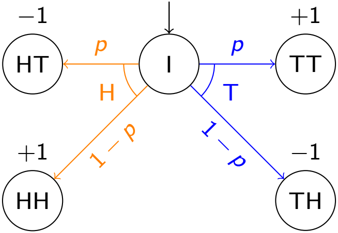
&U(T) = U(TT) = 1\\
&U(I) = 0 + \max\big(U(H), U(T)\big) = 1
\end{aligned}
$$

Example: Let's play matching pennies

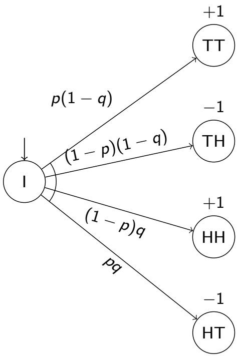
- Assume now we know that D always plays tails with probability p. What is the best **deterministic** strategy?



$$U(HT) = -1, U(HH) = 1, U(TT) = 1, U(TH) = -1$$
$$U(H) = pU(HT) + (1-p)U(HH)$$
$$U(T) = pU(TT) + (1-p)U(TH)$$
$$U(I) = 0 + \max\left(U(H), U(T)\right) = \max\left(1-2p, 2p-1\right)$$

Example: Let's play matching pennies

- Assume still we know that D always play tails with probability p. What is the best **probabilistic** strategy?
- Assume we play heads with probability q.



$$
\begin{aligned}
U(I) &= p(1-q) + q(1-p) - pq - (1-p)(1-q) \\
&= 2(p+q-2pq) - 1 \\
\frac{\partial U(I)}{\partial q} &= 2(1-2p)
\end{aligned}
$$

- when $p < 0.5$, $U(I)$ increases with q so $q = 1$ is the optimal.
- when $p > 0.5$, $U(I)$ decreases with q so $q = 0$ is the optimal.
- when $p = 0.5$, $U(I)$ is constant, so any strategy is fine.

Theorem

For any (finite) MDP, there exists a ***deterministic*** *strategy that maximizes the expected gain over an infinite horizon.*

Example: Let's play matching pennies

- Assume D's strategy is to play tails with probability 0.2 and S's strategy is to always play heads.
- Now if D knows these two strategies (a.k.a. the **strategy profile**), she would certainly want to change her strategy.

Definition (Nash equilibrium)

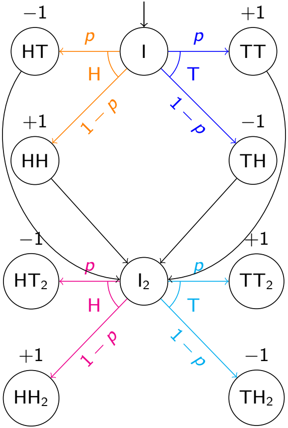
A strategy profile is a **Nash equilibrium** if none of the players has an incentive to unilaterally change their strategy.

Exercise

Does there exist a Nash equilibrium in *matching pennies*?

Example: Let's play matching pennies

- Assume D's strategy is to play tails with probability p and we play 2 rounds. What is the best strategy?



$$
\begin{aligned}
U(I_2) &= \max\left(1-2p, 2p-1\right)\\
U(HT) &= U(TH) = -1 + U(I_2)\\
U(TT) &= U(HH) = 1 + U(I_2)\\
U(I) &= \max\big(p(-1+U(I_2)) + (1-p)(1+U(I_2)),\\
&\qquad\quad p(1+U(I_2)) + (1-p)(-1+U(I_2))\big)\\
&= \max\left(U(I_2) + (1-2p), U(I_2) + (2p-1)\right)\\
&= 2\max\left(1-2p, 2p-1\right)
\end{aligned}
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Suppose that we have chosen rewards to match preferences between states. Consider the length of sequences:

- length 1 (one state): the utility is clearly the reward of that state.

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    - $\gamma < 1$ implies getting a reward sooner increases utility.

Utility of Sequences of States

- Infinite sequences:
  - if $\gamma < 1$, the utility is finite (we assume that here) and bounded by:

$$\sum_{i=0}^{\infty} \gamma^i R_{\max} = \frac{R_{\max}}{1-\gamma}$$

  - otherwise, one can also use averages on the number of states.

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- From some state s, the states that will be visited are random variables: S_t is the state visited after t transitions (*at time t*).
- The utility of a state, for a given strategy, is the expected utility of the sequence we obtain:

  To simplify the notation, we assume the rewards depend only on the state

$$U^{\pi}(s) = E\Big[\sum_{t=0}^{\infty} \gamma^{t} R(S_t)\Big]$$

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- Until we have $\max_s |U_{i+1}(s) - U_i(s)| < \frac{\epsilon(1-\gamma)}{\gamma}$.

Convergence of Value Iteration

- Let B be the **Bellman update**, i.e., the function s.t. $U_{i+1} = B(U_i)$;
- B is a **contraction** by a factor of γ for the **max norm** $||U|| = \max |U(s)|$:

$$||B(U) - B(U')|| \leq \gamma ||U - U'||$$

- So, if $\gamma < 1$, it has a **unique** fixed point U^* (i.e. such that $B(U^*) = U^*$);
- In particular, for U^*, and any i:

$$||B(U_i) - U^*|| \leq \gamma ||U_i - U^*||$$

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- We can also prove that if $||U_{i+1} - U_i|| < \epsilon\frac{1-\gamma}{\gamma}$ then $||U_{i+1} - U^*|| < \epsilon$.

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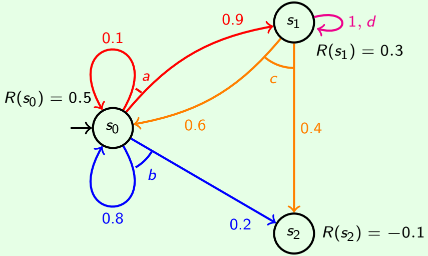
- Let π_i be the strategy defined using U_i.
- It might not be optimal, even after the utilities have been computed up to ϵ.
- But if $||U_i - U^*|| < \epsilon$, we can prove that $||U^{\pi_i} - U^*|| < \epsilon\frac{\gamma}{1-\gamma}$

Value Iteration: Example

Exemple



Assume $\gamma = 1$

	s_0	s_1	s_2
U_0	0	0	0
U_1	$0.5 + \gamma \max(0.1 * 0 + 0.9 * 0, 0.8 * 0 + 0.2 * 0) = \mathbf{0.5}$	$0.3 + \gamma \max(0.6 * 0 + 0.4 * 0, 1 * 0) = \mathbf{0.3}$	-0.1
U_2	$0.5 + \gamma \max(0.1 * 0.5 + 0.9 * 0.3, \mathbf{0.8} * \mathbf{0.5} - \mathbf{0.2} * \mathbf{0.1}) = \mathbf{0.88}$	$0.3 + \gamma \max(0.6 * 0.5 - 0.4 * 0.1, \mathbf{1} * \mathbf{0.3}) = \mathbf{0.6}$	-0.1
U_3	$0.5 + \gamma \max(0.1 * 0.88 + 0.9 * 0.6, \mathbf{0.8} * \mathbf{0.88} - \mathbf{0.2} * \mathbf{0.1}) = \mathbf{1.184}$	$0.3 + \gamma \max(0.6 * 0.88 - 0.4 * 0.1, \mathbf{1} * \mathbf{0.6}) = \mathbf{0.9}$	-0.1
U_4	...	...	...

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- This can be done in $\mathcal{O}(n^3)$ with standard linear algebra techniques.

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- We can use a with a fixed number of iterations (we do not need exact utility values).
- It is also possible to only update the utility for subsets of the state set: e.g. or states likely to be reached, or predecessors of those that have been modified in the previous iteration.

Outline

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- Once we have the model, we can learn utilities for π using **value iteration**.

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- and finally:

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- When we know utilities for all states, we can use the MEU principle to improve the strategy, like in **policy iteration**;

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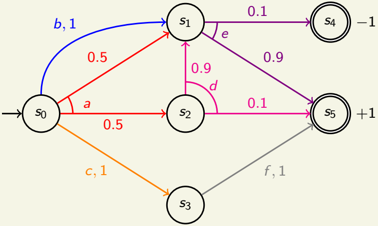

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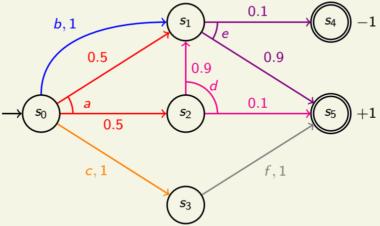

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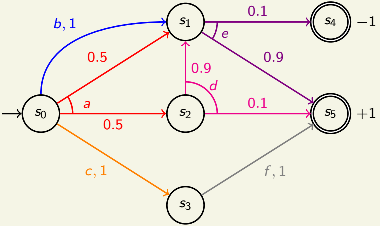

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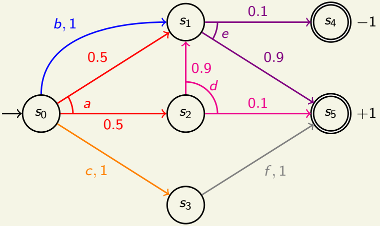

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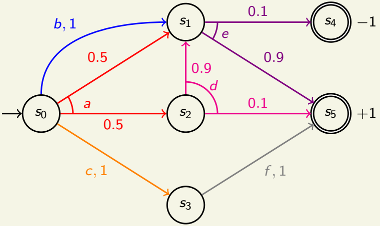

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- We need to explore **beyond** π and be sure to visit **all states** often enough.

Exploration and Exploitation

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- We can use a variety of such schemes, including UCB1, ϵ-greedy policies, and softmax-based policies.

Exploration and Exploitation: ϵ-greedy policies

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- When updating the policy using the MEU principle, we always transform it into an ϵ-greedy policy.

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- When T tends towards 0, the policy is nearly **deterministic**;
- When T tends towards $+\infty$, the policy is nearly **uniformly random**.

Off-policy learning

- The utility estimation schemes above do **on-policy** learning: evaluate the policy by playing it;
- To ensure exploration, we modify slightly the obtained MEU policies;
- We hope the result stays close to the original;
- It is sometimes desirable to completely separate the policies for exploration and exploitation;
- Learn a policy while exploring according to another: **off-policy** learning.

Off-policy Monte-Carlo: Importance sampling

- We want to estimate:

$$U^\pi(s) = E\Big[\sum_{t=0}^{\infty} \gamma^t R(S_t)\Big]$$

- This is the limit of the expectation on finite runs of length n when $n \to +\infty$:
  $P^\pi(\rho)$ is the probability of run ρ under policy π, and $R(\rho)$ its total reward

$$\sum_{|\rho|=n} P^\pi(\rho) R(\rho)$$

- Now assume we explore using a different policy π'. What we estimate with Monte-Carlo is:

$$\sum_{|\rho|=n} P^{\pi'}(\rho) R(\rho)$$

- So we need to correct this by multiplying the rewards by the importance-sampling ratios $\frac{P^\pi(\rho)}{P^{\pi'}(\rho)}$
- Note that the ratios depend only on the policies, not the MDP, as transition probabilities cancel out.

Off-policy Monte-Carlo: Importance sampling

- We can as before estimate the expectation with an average over runs obtained randomly: **ordinary importance sampling** (OIS)
- Or we can divide the sum of the rewards by the sum of the importance sampling ratios of the runs (instead of their number): **weighted importance sampling** (WIS)
- For any number of runs n:
  - OIS is unbiased: its expectation is the desired value
  - the variance of OIS is unbounded
  - WIS is biased but the bias goes to 0 with $n \to +\infty$;
  - the variance of OIS is bounded, and converges to 0 with $n \to +\infty$ when $R(\rho)$ is bounded.
- In practice, WIS is strongly preferred.

Off-policy TD: Q-learning

- In SARSA, the utility of the destination state is estimated according to the action that will be chosen there according to the current policy: $Q(s', a')$;
- But a' is not necessarily the best action to do in s';
- With the current knowledge this is $\text{argmax}_b Q(s', b)$;
- **Q-learning** uses this observation to compute the Q functions not for π but for the optimal strategy:

$$\boxed{Q_n^\pi(s, a) = (1 - \alpha_n) Q_{n-1}^\pi(s, a) + \alpha_n \left(R(s) + \gamma \max_b Q_{n-1}^\pi(s', b)\right)}$$

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- Models usually decrease the number of trials needed for a given accuracy;
- Models for approximating the utility function allow for better **generalisation** and a **smaller memory footprint**;
- Other techniques exist, in particular **policy search** in which we optimise directly the policy function expressed as a differentiable parameterised function.

Outline

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- We now focus on **Hidden Markov Chains** (no choice of actions).

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- Recall that we have for each observation $o \in \mathcal{O}$: $P(o|s)$ is the probability of observing o when in state s.

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- **Most likely explanation**: What is the most likely sequence of states up to now?

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Probability Notations: Probability vectors

- Probability vector of X: $\mathbb{P}(X)$
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- We also denote $P(x)$ by $\mathbb{P}(x)$ for individual values x.

Probability Reminder: Simple Rules

- Product rule:

$$P(x, y) = P(x|y)P(y) \text{ and } \mathbb{P}(X, Y) = \mathbb{P}(X|Y)\mathbb{P}(Y)$$

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Exercise

I flip a coin. If tails, then I grade all exams with 12 + roll of a fair dice and if heads, by 5 + dice.

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- Note that Markov assumptions are conditional independence assumptions.

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- Simple rule (direct from the product rule):

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Exercise

Pigritia (Pg) is a fairly common affliction that occurs with a 1/1000 rate. A person afflicted by Pg, usually also exhibits a *palmar hypertrichosis* syndrom (PHS).

- The rate of false positive is 5% (the patient may also have *lycanthropia* in 5% of the cases);
- The rate of false negative is 1% (rarely, a sick person who always sleeps with clenched fists may prevent the development of the hypertrichosis).

What is the probability that a person with PHS also has Pg?

Back to HMCs: Example

Attention estimation

- Students are attending an IA class with laptops open before them;
- They can be in two states: listening (l) and web surfing (w);
- Suppose all students are initially listening;
- The professor can witness three possible events: smiling (s), looking at the laptop screen (c), and looking at the professor or blackboard (p);
- When listening at some instant, students tend to continue listening at the next at 70% chance;
- When surfing at some instant, students tend to continue surfing at the next at 80% chance;
- When listening, students smile at 10% (jokes of the professor), look at their screen at 30% for additional info, or look up at 60%;
- When surfing, students smile at 30% (lolcats), look at their screen at 60% (social networking notification), or look up at 10% (am I busted?);

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- We could enumerate all the corresponding sequences and sum the probabilities (exponential number);
- We can do better with an iterative algorithm called **forward algorithm**.

The forward algorithm

- We compute $\mathbb{P}(X_t, o_{1:t})$ by summing out X_{t-1} from $\mathbb{P}(X_t, X_{t-1}, o_{1:t})$:

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- By the transition and sensor Markov assumptions:

$$\mathbb{P}(X_t, o_{1:t}) = \mathbb{P}(o_t | X_t) \sum_{x_{t-1}} \mathbb{P}(X_t | x_{t-1}) P(x_{t-1}, o_{1:t-1})$$

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- This gives an iterative algorithm initialised with $\mathbb{P}(X_0)$, the initial distribution on hidden states.

The forward algorithm: Matrix expression

- The transitions probabilities can be written as matrix T such that $T_{ij} = P(X_t = j|X_{t-1} = i)$;
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- We write the probabilities of $P(o_t | x_i)$ on the i-th diagonal entry of a diagonal matrix O_t;
- Let $\ell_{1:t} = P(X_t, o_{1:t})$. Then:

$$\boxed{\ell_{1:0} = \mathbb{P}(X_0) \text{ and } \ell_{1:t} = O_t T^{\mathsf{T}} \ell_{1:t-1}}$$

The forward algorithm: Exercise

Attention estimation

- Students are attending an IA class with laptops open before them;
- They can be in two states: listening (l) and web surfing (w);
- Suppose all students are initially listening;
- The professor can witness three possible events: smiling (s), looking at the laptop screen (c), and looking at the professor or blackboard (p);
- When listening at some instant, students tend to continue listening at the next at 70% chance;
- When surfing at some instant, students tend to continue surfing at the next at 80% chance;
- When listening, students smile at 10% (jokes of the professor), look at their screen at 30% for additional info, or look up at 60%;
- When surfing, students smile at 30% (lolcats), look at their screen at 60% (social networking notification), or look up at 10% (am I busted?);

Exercise

Write the matrices and compute the probabilities: $P(l_3, s_1, c_2, p_3)$ and $P(w_3, s_1, c_2, p_3)$.

Observation likelihood

- We can compute $P(o_{1:t})$ by summing X_t out of $\mathbb{P}(X_t, o_{1:t})$:

$$P(o_{1:t}) = \sum_{x_t} P(x_t, o_{1:t})$$

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$$\boxed{P(o_{1:t}) = \mathbf{1}^\top \ell_{1:t}}$$

Attention estimation

What are the likelihoods of the sequences (1) s, c, p, (2) p, p, p and (3) c, c, c?

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- We just need to **normalise** the vector $\ell_{1:t}$ so that it sums to 1.

Filtering

Exercise: Attention estimation

Compute for the previous problem the distribution formed by $P(l_3|s_1, c_2, p_3)$ and $P(w_3|s_1, c_2, p_3)$.

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Compute for the previous problem the distribution formed by $P(l_3|s_1, c_2, p_3)$ and $P(w_3|s_1, c_2, p_3)$.

Exercise: Localisation

A robot moves on a 5-tiles **circular** track with tiles painted black (b) or white (w). The robot only has a color sensor and is initially at an unknown position (with uniform probability). The robot moves at each step left with probability 0.3 and right, with probability 0.7:

Find the most likely position of the robot after observations w_1, b_2, w_3.

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- We could compute similarly n-step predictions.

$$\boxed{\mathbb{P}(X_{t+n}|o_{1:t}) = (T^{\mathsf{T}})^n\mathbf{f}_{1:t}}$$

Prediction: Exercise

Exercise: Attention estimation

After observing s_1, c_2, p_3 what is the probability that a student will be listening at time 4? What about times 13, 1003, and 1000003 ?

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- Given X_k, $o_{1:k}$ and $o_{k+1:t}$ are independent (sensor assumption):

$$\mathbb{P}(X_k|o_{1:t}) = \frac{1}{P(o_{k+1:t}|o_{1:k})}\mathbb{P}(X_k, o_{1:k})\mathbb{P}(o_{k+1:t}|X_k)$$

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- And finally:

$$\mathbb{P}(X_k|o_{1:t}) = \frac{1}{P(o_{1:t})}\mathbf{f}_{1:k}\mathbb{P}(o_{k+1:t}|X_k)$$

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$$\boxed{\mathbf{b}_{i:t} = TO_i\mathbf{b}_{i+1:t}}$$

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- Recall that for smoothing we have:

$$\mathbb{P}(X_k|o_{1:t}) = \frac{1}{P(o_{k+1:t}|o_{1:k})}\mathbb{P}(X_k|o_{1:k})\mathbb{P}(o_{k+1:t}|X_k)$$

- Then, with $\circ$ the Hadamard product, *i. e.*, pointwise:

$$\mathbb{P}(X_k|o_{1:t}) = \frac{1}{P(o_{1:t})}\mathbf{f}_{1:k} \circ \mathbf{b}_{k+1:t}$$

- And since $\mathbb{P}(X_k|o_{1:t})$ represents a distribution, we can just normalize the vector as before, and actually use $\ell_{1:k}$ instead of $\mathbf{f}_{1:k}$:

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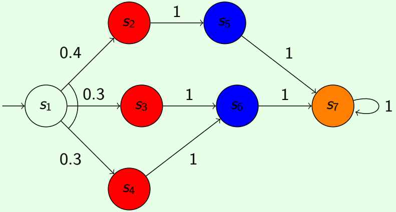
Exercise: Attention estimation & Localisation

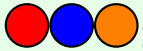
1. What is the smoothed estimate of a student listening at time 3 when observing s, c, p, s, c, p?
2. From where has the robot started in the B/W circular track, knowing we have observed w, b, w?

Smoothing: Exercise

Exercise: Sequence

Consider the following Hidden MC, in which the initial distribution is $[1, 0, 0, 0, 0, 0, 0]$:



Given the observation sequence :

1. What are the most likely states at times $3, 2$ and 1?
2. What is the most likely sequence producing the observation?

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- We want to compute the most probable sequence of hidden states given the observations:

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- By the Markov property on transitions, if we fix x_t,the most probable sequence is made of:
  1. a single transition from x_{t-1} to x_t;
  2. the most likely path to x_{t-1} given $o_{1:t-1}$
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- As before note that $P(x_{1:t}|o_{1:t})$ is just the normalisation of $P(x_{1:t}, o_{1:t})$ and the positive normalisation coefficient $P(o_{1:t})$ does not change the max.

Viterbi algorithm

- Noting $\mathbf{m}_{1:t+1} = \max_{x_{1:t}} \mathbb{P}(x_{1:t}, X_{t+1}, o_{1:t+1})$ and by the chain rule

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- Remember which state realises the max at each step to get the actual sequence.

Viterbi algorithm

input: T, O // transition and observation matrices: $O_{ij} = P(o_j|s_i)$

S_1 // initial distribution on states

X // vector of observations: obs at time i is $o_{X[i]}$

output: Y // most likely sequence: hidden state at time i is $s_{Y[i]}$

$n \leftarrow length(X)$ // number of observations

$\forall j, m[j] \leftarrow O_{jX[1]} S_1[j]$ // initial distribution of states given first observation

$\forall i, j, pred[i, j] \leftarrow \perp$ // best predecessor of state j after observation i

for i in $[2..n]$:

  foreach state s_j:

    $m'[j] \leftarrow \max_k \{O_{jX[i]} T_{kj} m[k]\}$

    $pred[i, j] \leftarrow \text{argmax}_k \{O_{jX[i]} T_{kj} m[k]\}$

  $m \leftarrow m'$

// Build the path

$Y[n] \leftarrow \text{argmax}_k m[k]$

for i in $\{n - 1, \ldots, 1\}$:

  $Y[i] \leftarrow pred[i + 1, Y[i + 1]]$

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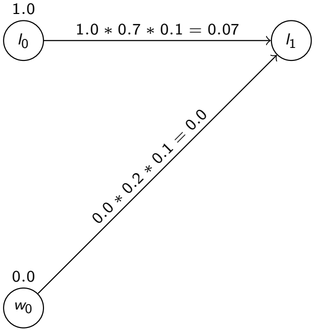

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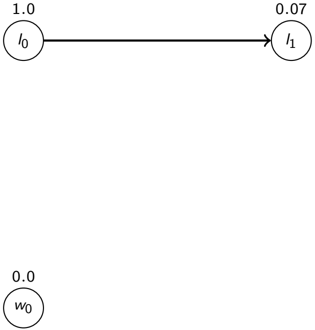

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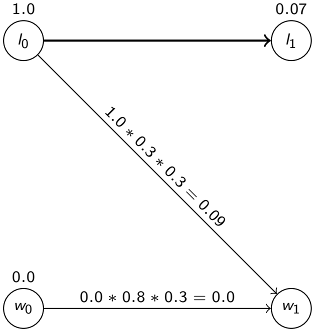

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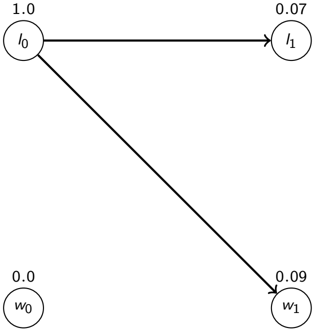

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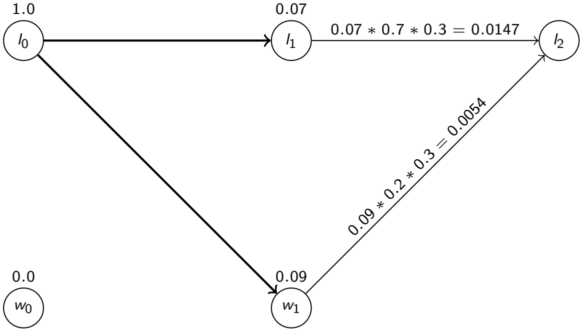

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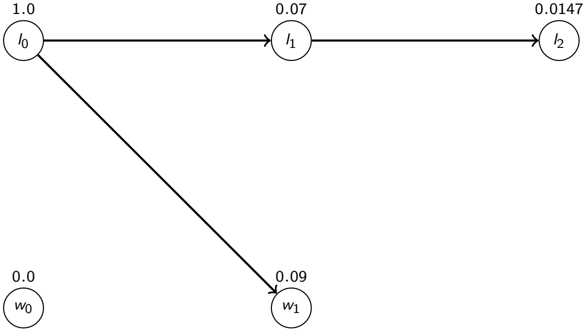

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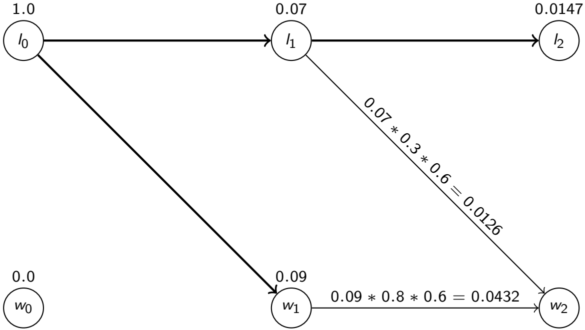

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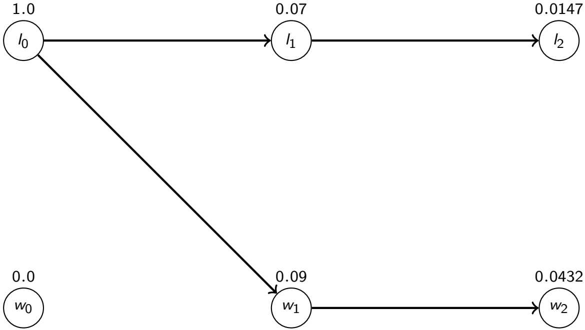

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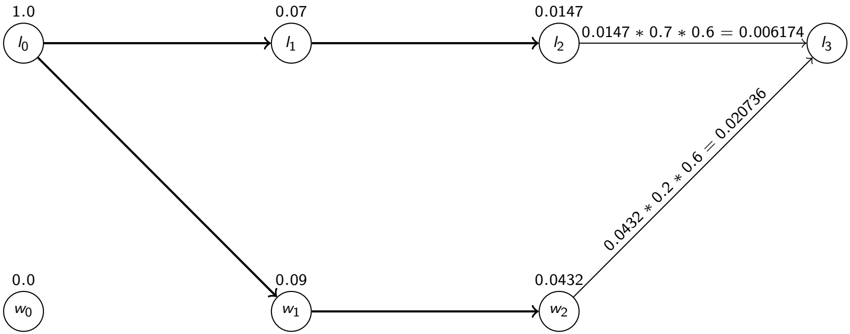

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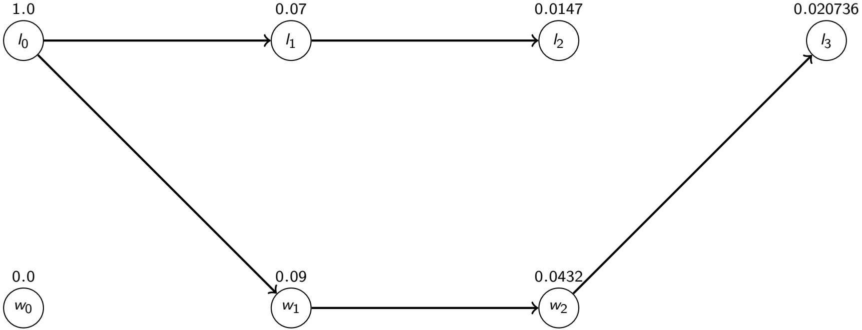

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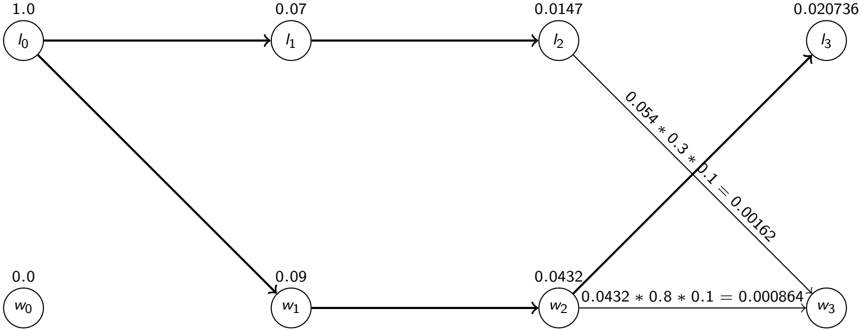

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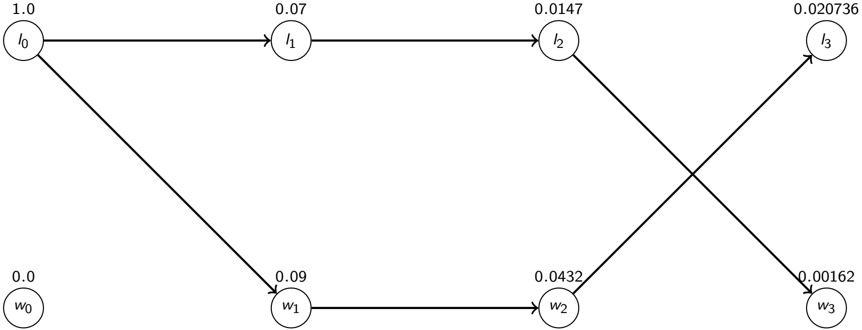

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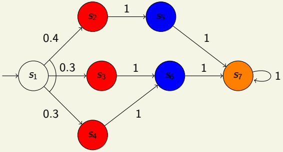
Apply Viterbi algorithm to find the correct explanation of  in:



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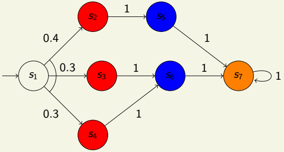

Small keyboard decoding

Given the frequencies of single letters and digrams (sequences of two letters), and considering that when hitting a key on the keyboard there is a 5% chance of hitting one the surrounding keys instead (uniformly distributed among those keys), write an HMC permitting to find the most likely intended key sequence given a sequence with typing errors.

Learning HMCs: The EM algorithm

- From sequences of observations, we can learn a corresponding HMC;
- The hidden states and observations must be known in advance: we learn the coefficients of the transition and observation matrices, and the initial distribution on hidden states;
- We use the Baum-Welch algorithm, a special case of the **Expectation-Maximisation** (EM) algorithm.

Learning HMCs: The EM algorithm

- Let $\theta = (T, O, X_0)$ be the parameters we want to learn;
- Given an observation sequence $o_{1:t}$, we want to maximise its probability (likelihood);
- That is we search:
$$\theta^* = \text{argmax}_\theta P_\theta(o_{1:t})$$
- Since we do not known the corresponding sequence $x_{1:t}$ of hidden states, this is:
$$\theta^* = \text{argmax}_\theta \sum_{x_{1:t}} P_\theta(o_{1:t}, x_{1:t})$$
- This requires enumerating all the possible values of the sequence $x_{1:t}$ however, which is intractable;
- Instead we **maximise** the **expectation** (for random sequences $x_{1:t}$, given $o_{1:t}$) of the (log-)likelihood, and proceed iteratively:
$$\begin{cases} \theta^0 \text{ chosen arbitrarily} \\ \theta^{n+1} = \text{argmax}_{\theta^n} \sum_{x_{1:t}} \log\left(P_{\theta^n}(o_{1:t}, x_{1:t})\right) P_{\theta^n}(x_{1:t}|o_{1:t}) \end{cases}$$
- This converges to a local optimum.

Learning HMCs: The Baum-Welch algorithm

- In the special case of HMCs, we can prove that θ^{n+1} can be computed using:
  - $\gamma_i(k) = P_{\theta^n}(x_k = s_i | o_{1:t})$.
    This is just **smoothing**.
  - $\zeta_{ij}(k) = P_{\theta^n}(x_k = s_i, x_{k+1} = s_j | o_{1:t})$.
    This is the normalisation of matrix $\mathbf{f}_k \circ (\mathbf{b}_{k+1} \circ O_{:t+1})^\mathsf{T} \circ T$
    $O_{:t+1}$ is the $t+1$-th column of O
- And:
  - $X_0^{n+1} = \gamma(1)$
  - $T_{ij}^{n+1} = \frac{\sum_{k=1}^{t-1} \zeta_{ij}(k)}{\sum_{k=1}^{t} \gamma_i(k)}$: the expected total number of transitions between s_i and s_j divided by the expected total number of transitions from state s_i;
  - $O_{ij}^{n+1} = \frac{\sum_{k=1, o_k=j}^{t} \gamma_i(k)}{\sum_{k=1}^{t} \gamma_i(k)}$: the expected total number of times we observed o_j when in state s_i divided by the expected total number of times we were in state s_i.

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- If the matrices T and O are invertible, we can do some (space) optimisations to the backward computation;
- The setting of HMCs can be generalised into **Dynamic Bayesian Networks** (DBNs);
- Another instance of DBNs using (linear) gaussian distributions is the **Kalman filter**;
- HMCs/ DBNs can be learnt using the **Expectation-Maximisation** (EM) algorithm.

Outline

Multiagent systems

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- We (continue to) model this as games on graphs: there are now several players.

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- if $\sigma \in \text{Outcome}(s, \pi_1, \pi_2)$ then $\sigma.s' \in \text{Outcome}(s, \pi_1, \pi_2)$ iff there exist an action a and a state s' such that $s \xrightarrow{a} s'$ and $a \in \pi_1(\sigma)$ or $a \in \pi_2(\sigma)$.

Utility of States

- Since the game is zero-sum we assume that if Player 1 tries to **maximise** the rewards, then Player 2 tries to **minimise** them;
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- Given strategies π_1 and π_2 for both players, the utility of state s for Player 1 is then:

$$U^{\pi_1,\pi_2}(s) = R(s) + \gamma \min\Big(\sum_{s' \in S} P(s'|\pi_1(s), s) U^{\pi_1,\pi_2}(s'), \sum_{s' \in S} P(s'|\pi_2(s), s) U^{\pi_1,\pi_2}(s')\Big)$$

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- From the previous equation, we can easily adapt **value iteration** and **policy iteration** to find optimal strategies.

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  - if s belongs to Player 1:

$$U^{\pi_1^*,\pi_2^*}(s) = R(s) + \gamma \max_{a \in A_1} \sum_{s' \in S} P(s'|a,s) U^{\pi_1^*,\pi_2^*}(s')$$

Turn-based Games

- A game played on a graph is **turn-based** if for any state s all the outgoing actions belong to a single player
  We do not require alternation
- We then say that s itself belongs to that player;
- This allows to simplify the previous equation:
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  - if s belongs to Player 2:

$$U^{\pi_1^*,\pi_2^*}(s) = R(s) + \gamma \min_{a \in A_2} \sum_{s' \in S} P(s'|a,s) U^{\pi_1^*,\pi_2^*}(s')$$

Turn-based Games

Exercise

1. Prove that, in a turn-based game on a regular graph (with no probabilities, and no non-determinism), finding a strategy (if its exists) for Player 1 to reach some state whatever Player 2 does is equivalent to finding a strategy in an “and-or” graph (aka hypergraph).
2. Same question for general zero-sum 2-player reachability games on (regular) graphs (i.e., removing the turn-based assumption).
3. Deduce from 2 an algorithm to solve (find if winning and extract the strategy) directly general zero-sum 2-player reachability games on (regular) graphs.

Turn-based Games

Subtraction game

1. Model the subtraction game (simpler variant of the game of Nim), where starting from 6, each player subtracts a number between 1 and 3. The result must be strictly positive and the first player unable to move loses (and the other wins). We start with Player 1. Apply the previous algorithm to confirm that Player 1 has a winning strategy.
2. Idem when both players decide concurrently how much to subtract and we subtract the sum. If the result is non-positive then Player 1 wins if it is even (or zero) and Player 2 if it is odd.

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- There are two natural ideas to cope with the complexity:
  - arbitrarily **limit the length** of paths;
  - only **explore some** of the paths.

Outline

Limiting the depth

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  - Obtained by expert knowledge;
  - Or by learning (e.g. reinforcement learning).

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- The value of $U(s)$ computed should be more precise than $\tilde{U}(s)$ thanks to the L-steps **look-ahead**;
- If there are no probabilities then EXPECTIMINIMAX is called **Minimax** (historically introduced before).

Minimax (turn-based)

```
input:  s          // source state
        maximizer  // player to play: true if Player 1 (maximiser)
        d          // depth (distance to L)
output: U          // utility of s

if d = 0 or s is terminal: // Leaf of the tree
    U ← evaluate(s)
else:
    if maximizer: // Player 1 is playing
        v ← −∞
        foreach child s′ of s:
            v ← max(v, MINIMAX(s′, not maximizer, d − 1))
    else: // Player 2 is playing
        v ← +∞
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    U ← v
```

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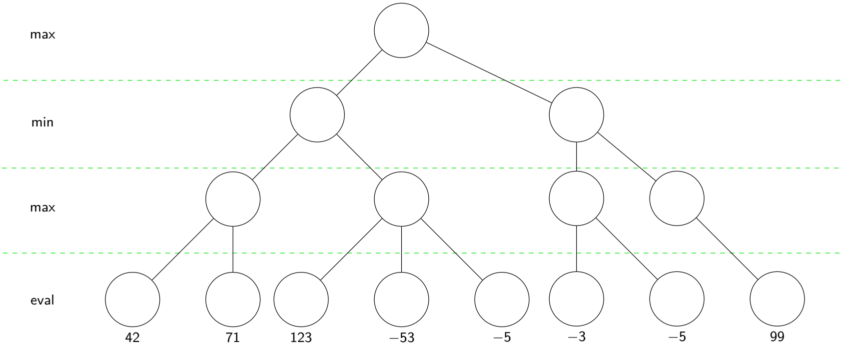

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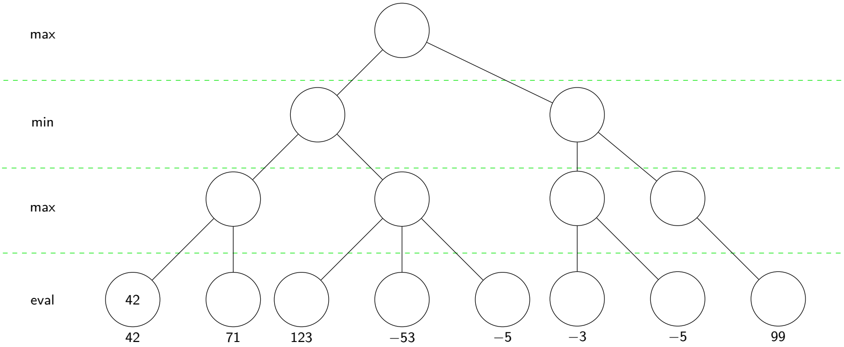

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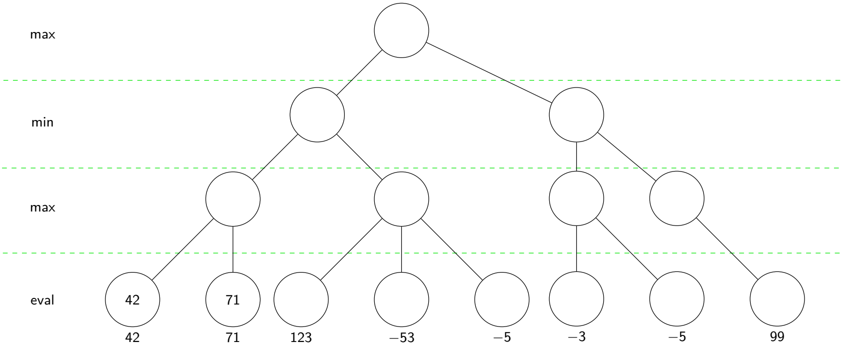

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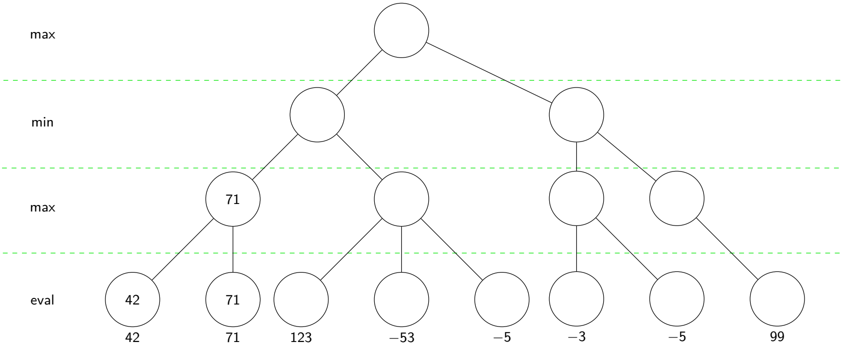

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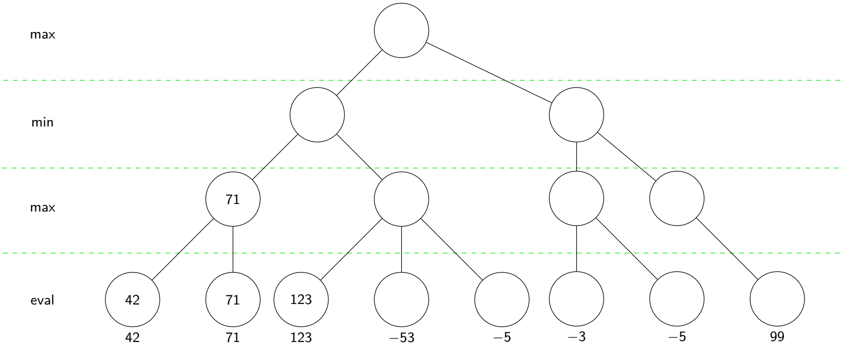

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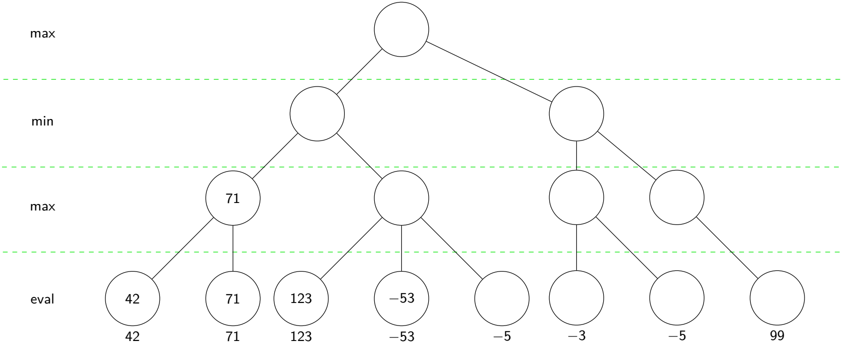

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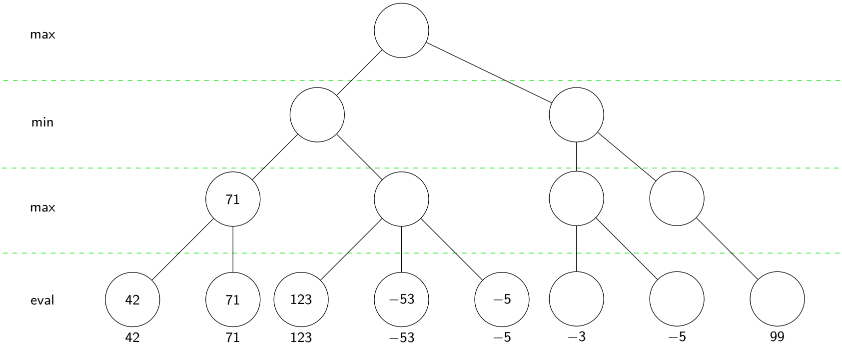

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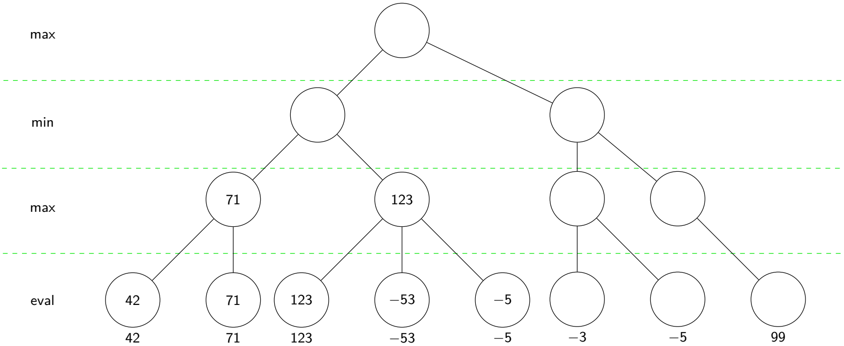

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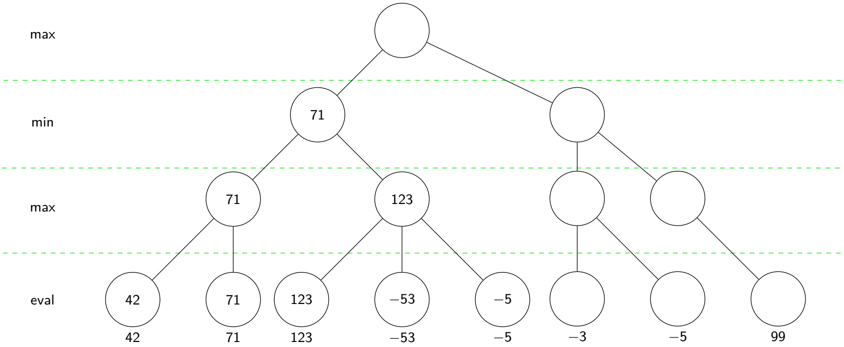

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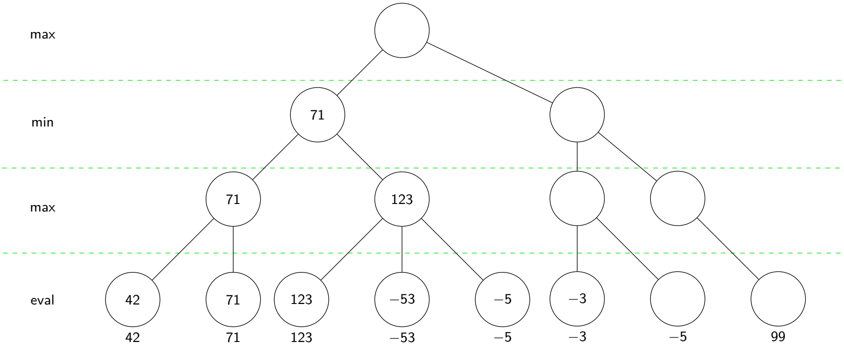

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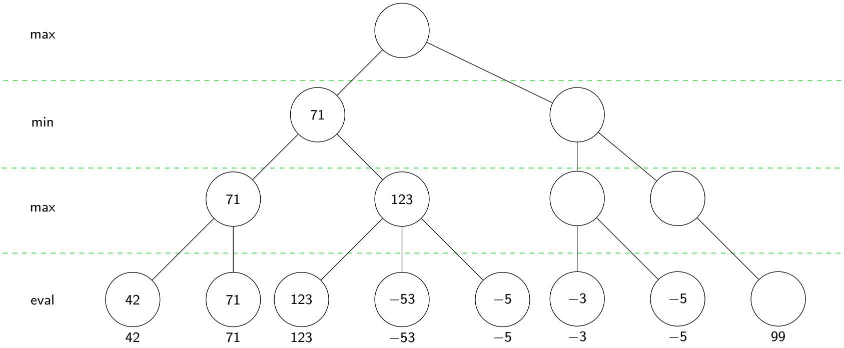

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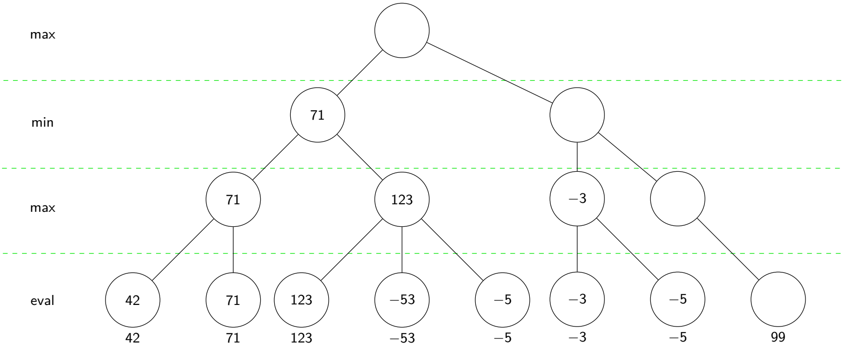

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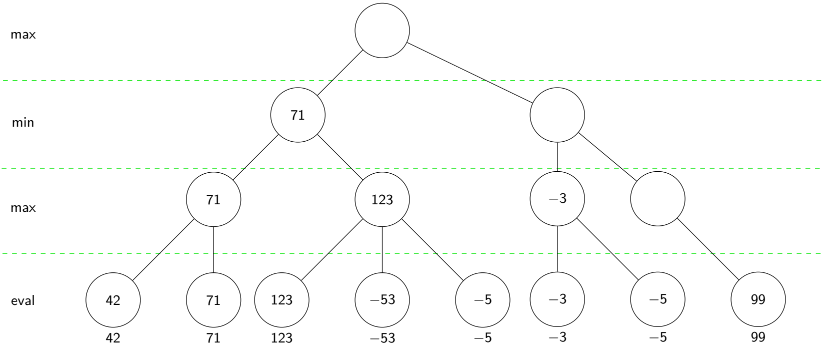

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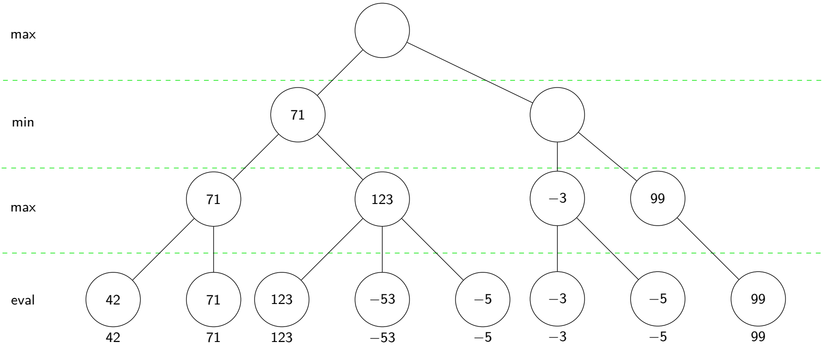

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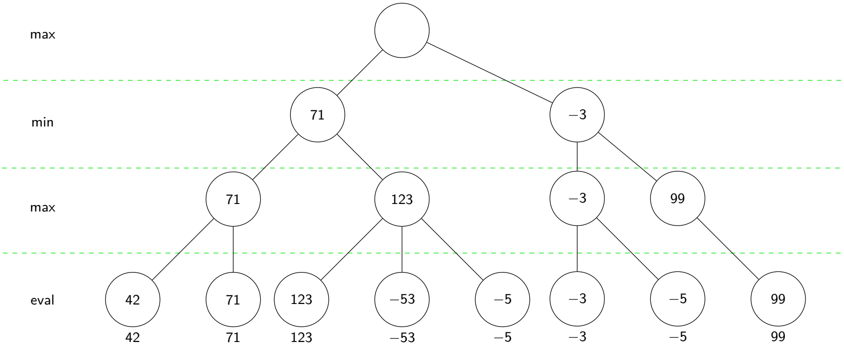

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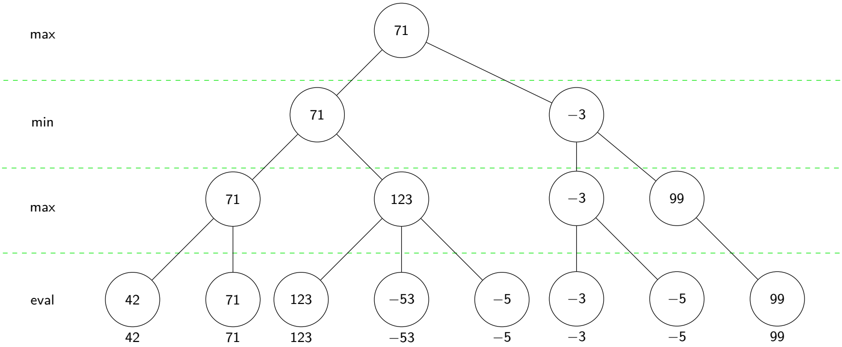


Minimax: Choosing the best move

- It is possible to modify the previous algorithm to also return the best move;
- Or, more flexible, we can select the best move wiht another function, play_minimax :

```
input:  s          // source state, supposed non terminal
        maximizer  // joueur : true for maximiser, false for minimiser
        d          // depth (distance to L)
output: m          // best move

   if maximizer: // Player 1 plays
        m ← argmax_{s -a-> s'} MINIMAX(s', not maximizer, d − 1)
   else : // Player 2 moves
        m ← argmin_{s -a-> s'} MINIMAX(s', not maximizer, d − 1)
```

- We could also choose using a probability distribution on possible moves generated from the MINIMAX scores.

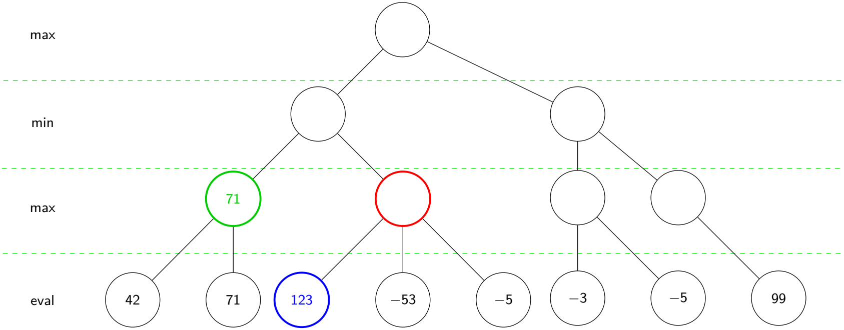
Negamax

- We can have Player 2 maximise too by using the fact that $\min(a, b) = -\max(-a, -b)$

```
input:  s // source state
        p // player to play: +1 for Player 1, -1 for Player 2
        d // depth (distance to L)
output: U // utility of s

if d = 0 or s is terminal: // Leaf of the tree
    U ← evaluate(s)
else:
    v ← −∞
    foreach child s′ of s:
        v ← max(v, p ∗ NEGAMAX(s′, −p, d − 1))
    U ← p ∗ v
```

Alpha-beta Pruning



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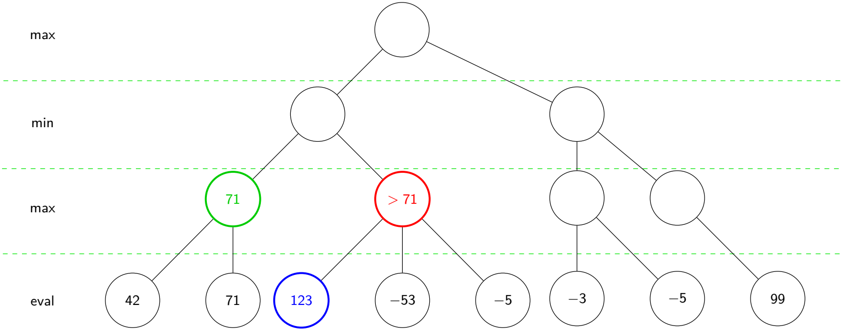

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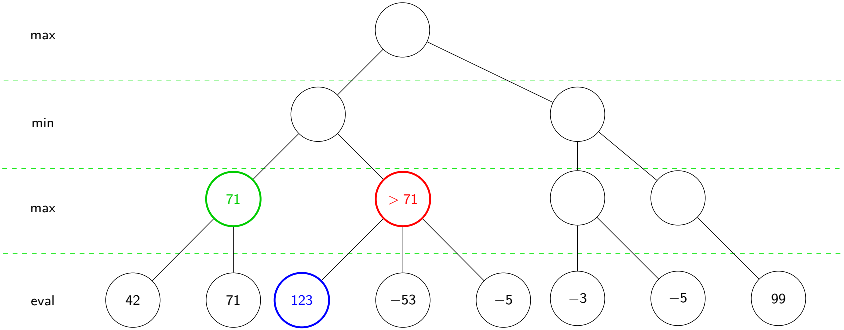

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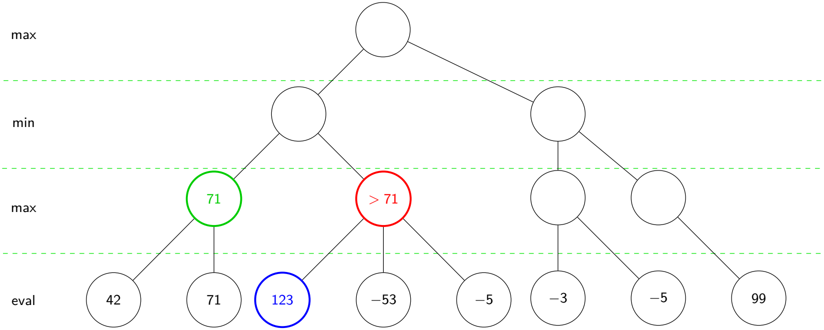

- After exploring ◯, we know the value of ◯ is **at least** 123;
- Since the parent of ◯ is minimising, ◯ will never be chosen over ◯;
- So it is **futile** to continue explore its successors: β **cut-off**;
- The same situation may arise with a child of a max node with a utility provably worse than another one: α **cut-off.**

AlphaBeta

```
input:  s          // source state
        maximizer  // player to play: true if Player 1 (maximiser)
        d          // depth (distance to L)
        α          // utility lower-bound (start with −∞)
        β          // utility upper-bound (start with +∞)
output: U          // utility of s

if d = 0 or s is terminal: // Leaf of the tree
    U ← evaluate(s)
else:
    if maximizer: // Player 1 is playing
        v ← −∞
        foreach child s′ of s while α ≤ β:
            v ← max(v, AlphaBeta(s′, not maximizer, d − 1, α, β))
            α ← max(α, v)
    else: // Player 2 is playing
        v ← +∞
        foreach child s′ of s while α ≤ β:
            v ← min(v, AlphaBeta(s′, not maximizer, d − 1, α, β))
            β ← min(β, v)
    U ← v
```

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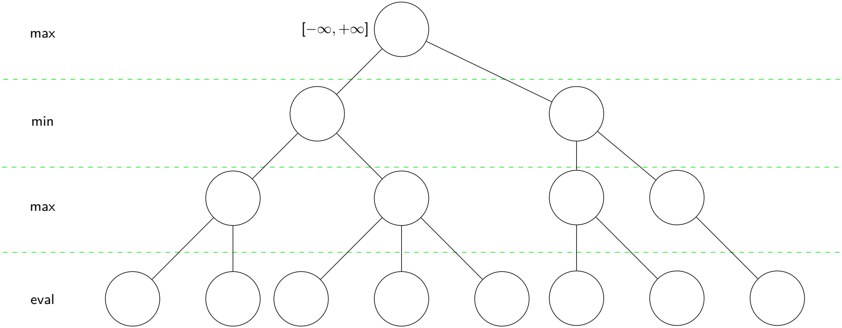

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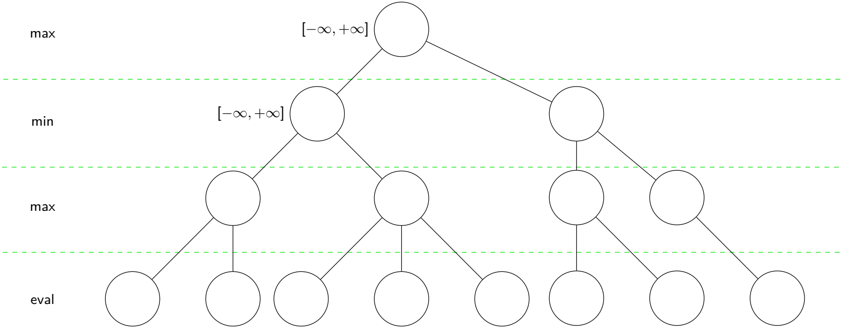

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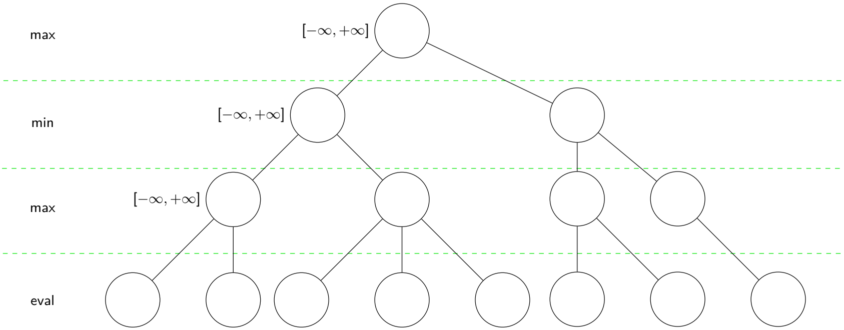

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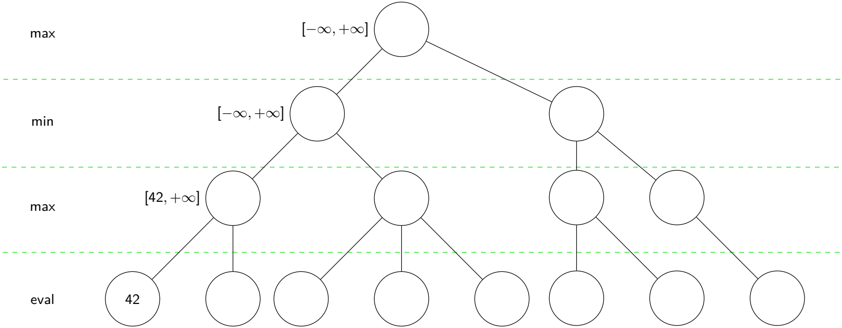

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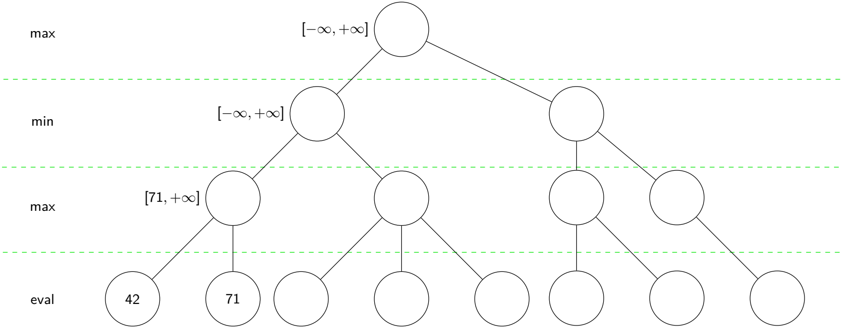

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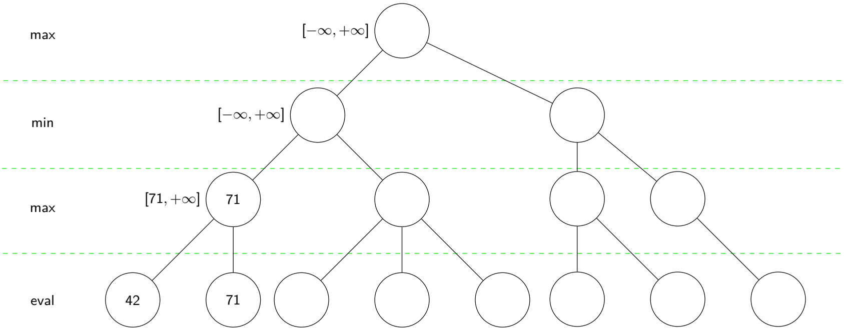

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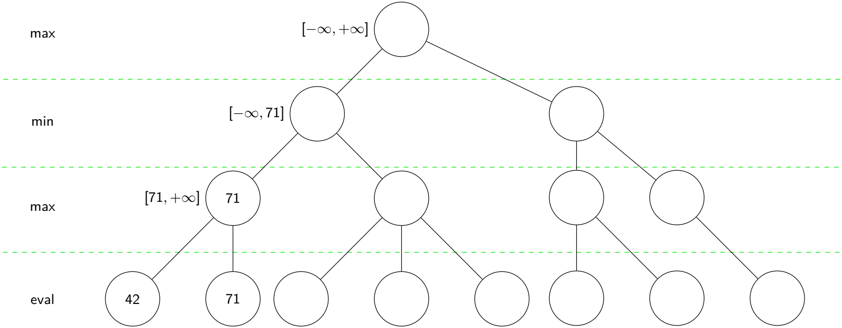

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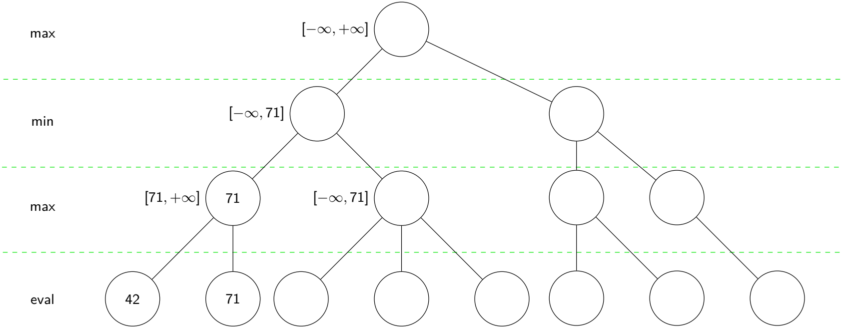

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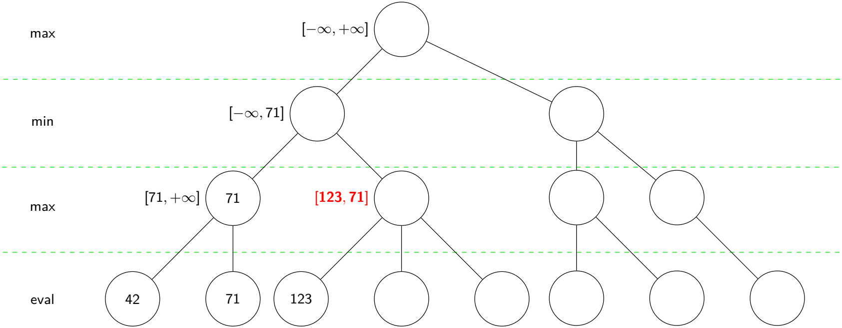

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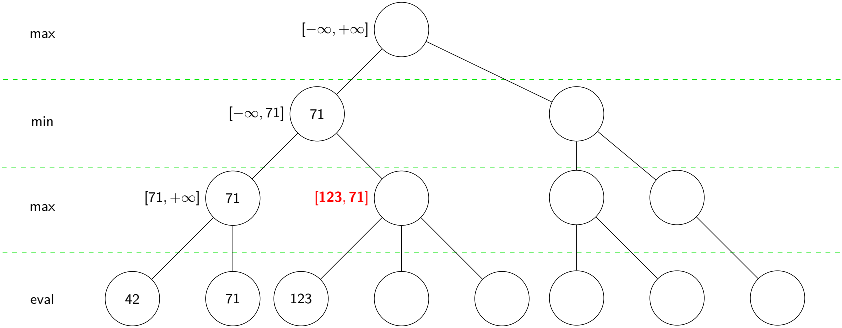

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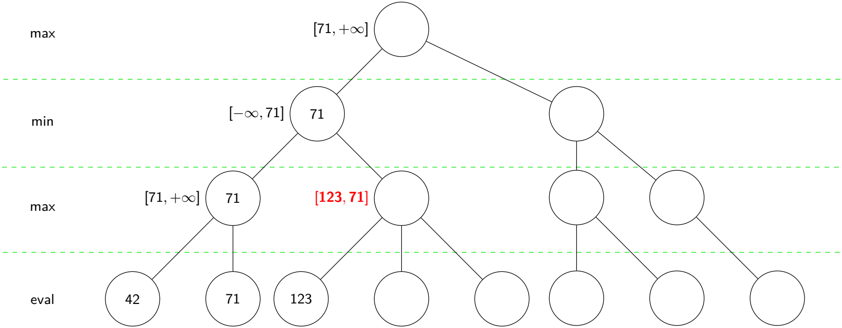

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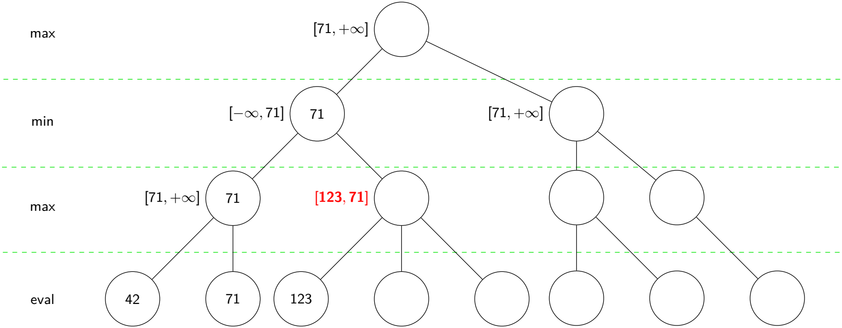

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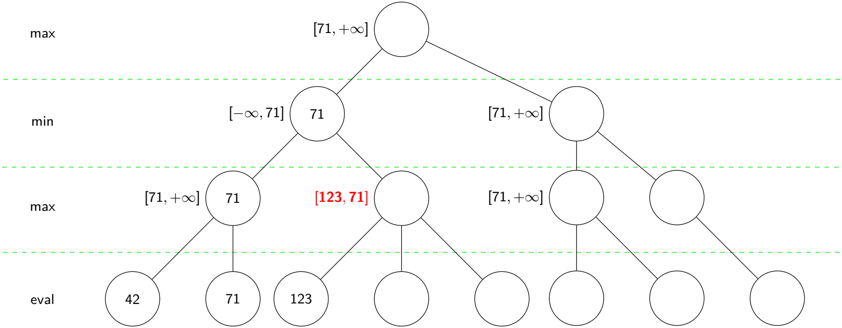

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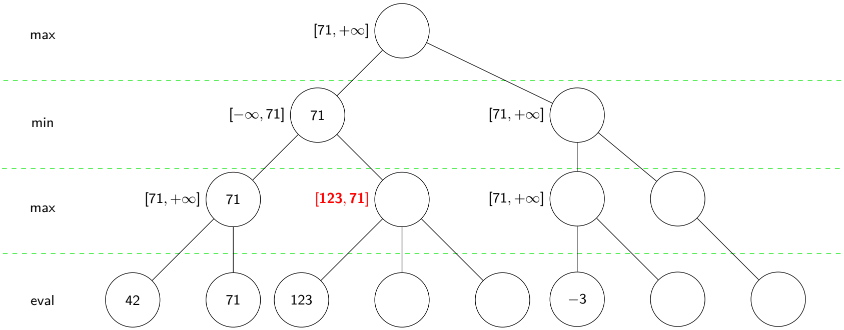

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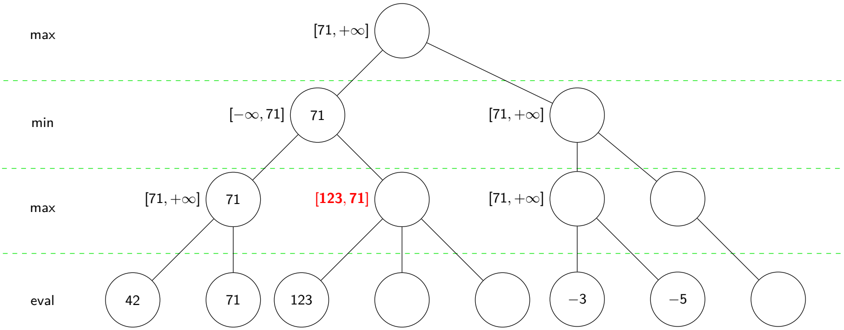

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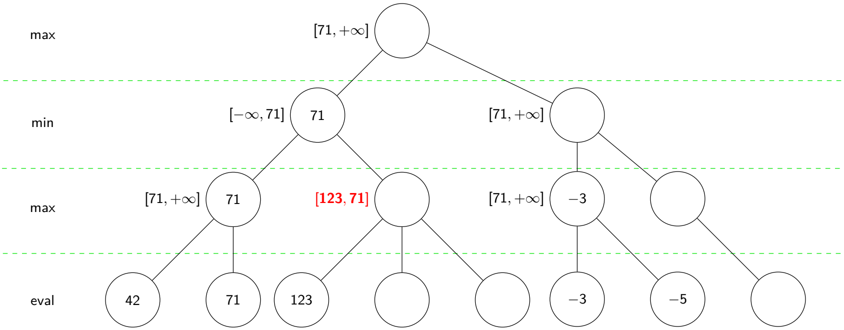

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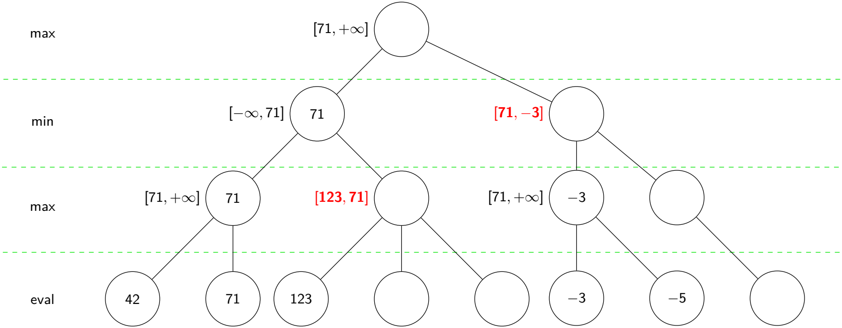

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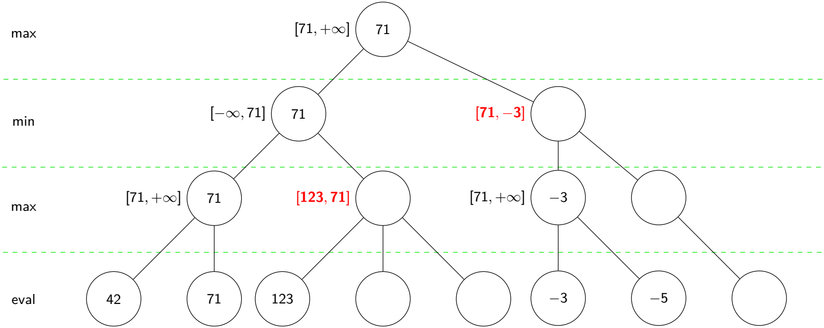

Alpha-beta Pruning

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Apply again the ALPHABETA algorithm on the previous example but consider that we always start with right-most child.

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- With alpha-beta pruning, we can explore exponentially less nodes;
- But move ordering is crucial: the **best moves** for each player should be tried **first**;
- Finding a good move ordering can be done by shallower searches, notably using **iterative deepening**.

Outline

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- We explore lots of paths that would never be chosen by a **rational strategy**.

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- $\sqrt{\frac{2\ln(n)}{n_j}}$ is an **upper bound** of the size of the **confidence interval** for the average reward, such that the true expected reward has very high probability to fall inside;
- The less a machine is played the higher this value.

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  2. otherwise **recursively** go down into the tree by selecting the child using UCB1:

     maximise $p * \left(\frac{r_j}{n_j} + p * \sqrt{\frac{2\ln(n)}{n_j}}\right)$.

     n_j is the number of times we have performed a playout from node j and n is the sum of the n_j for all the nodes j we compare.

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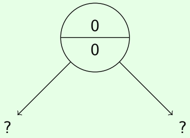

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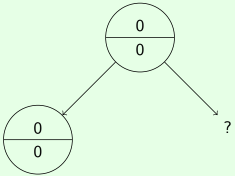

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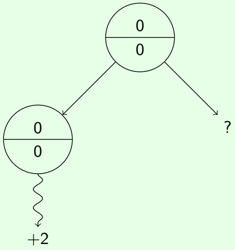

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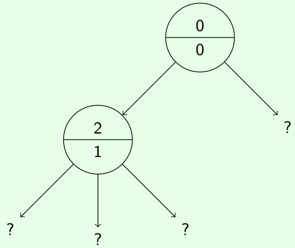

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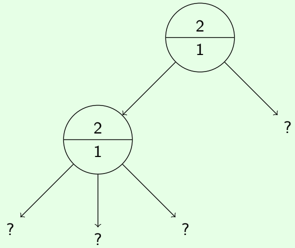

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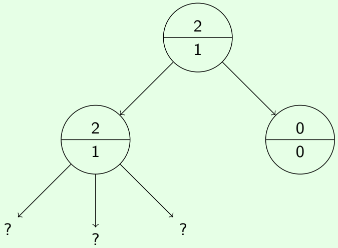

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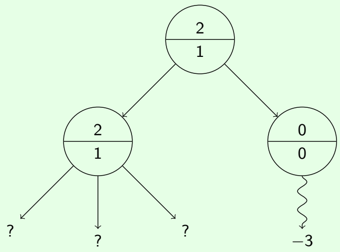

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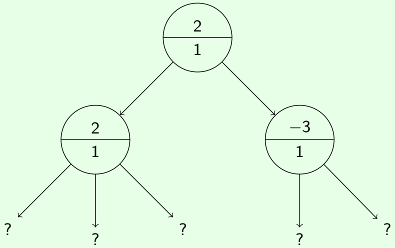

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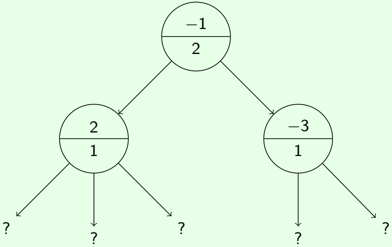

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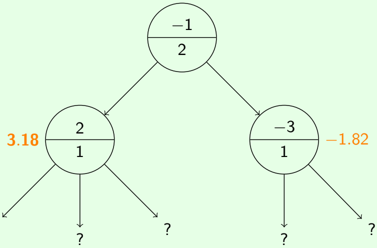

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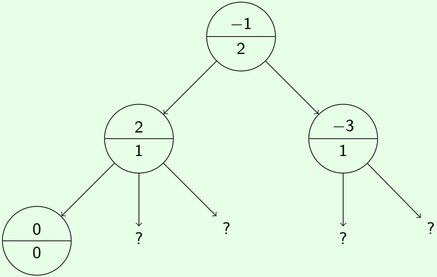

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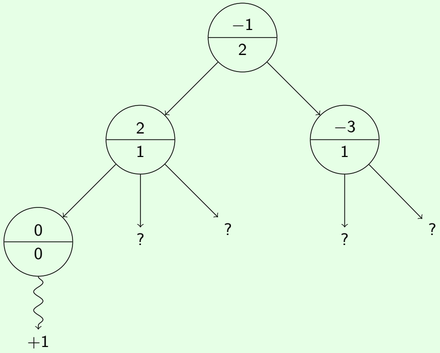

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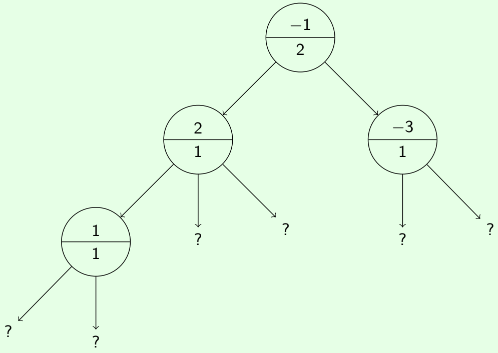

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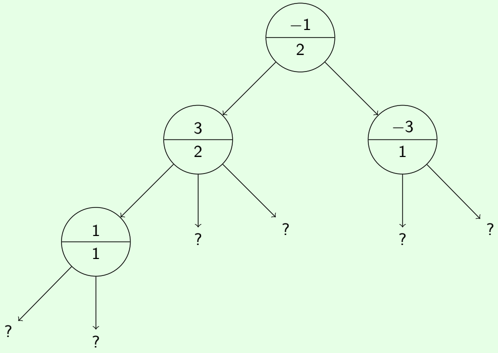

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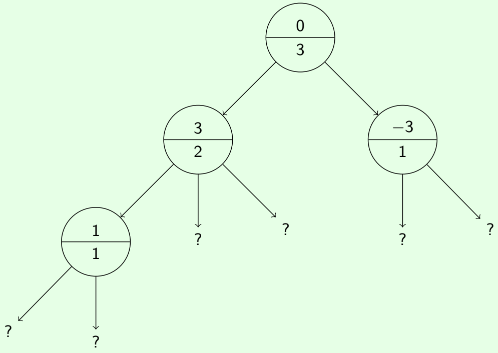

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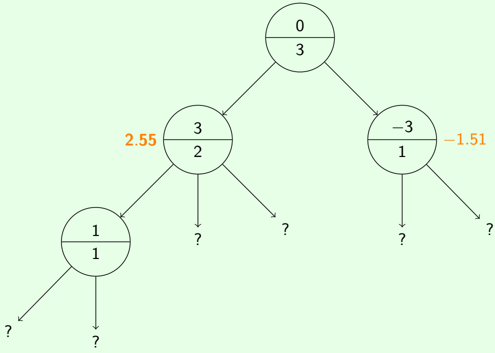

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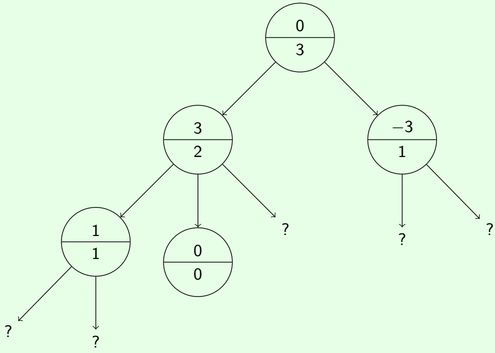

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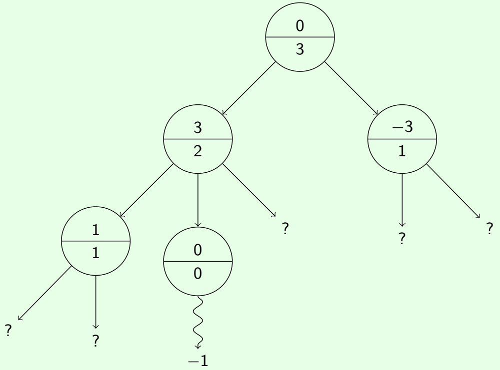

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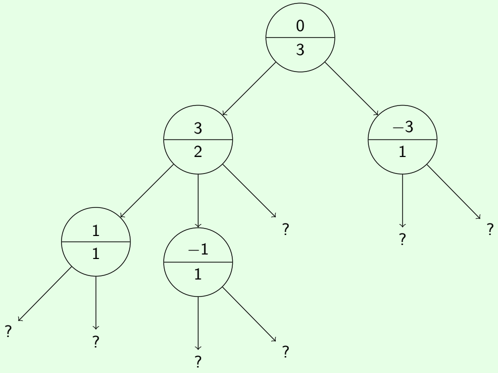

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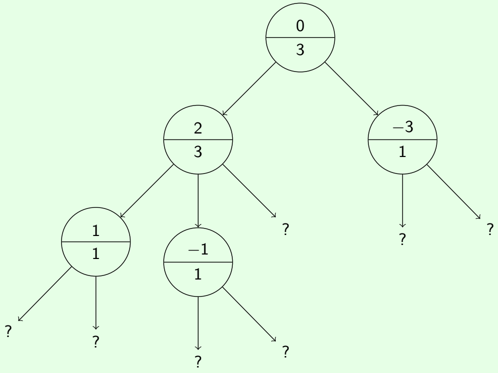

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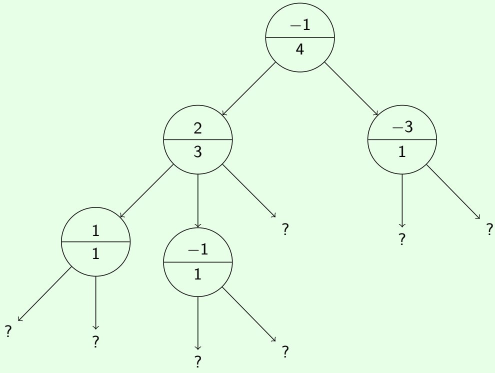

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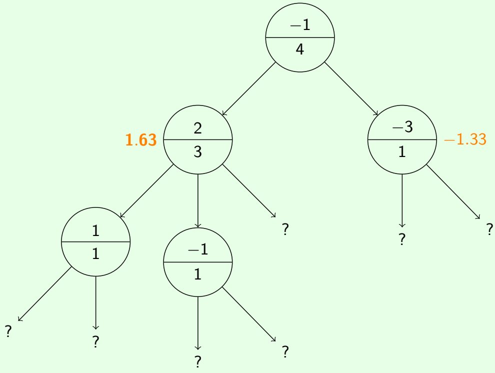

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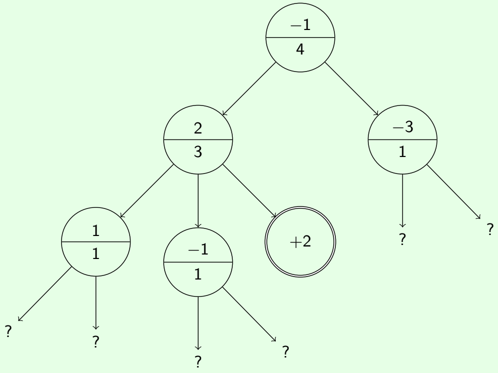

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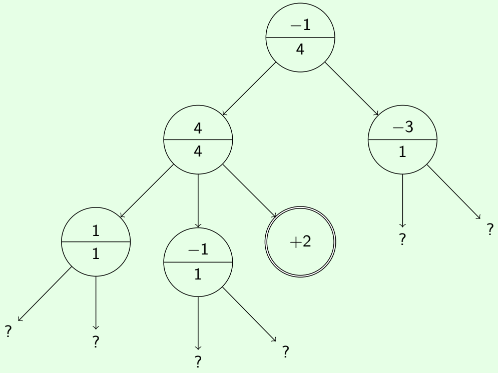

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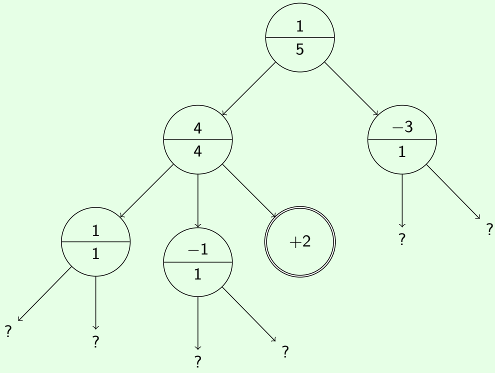

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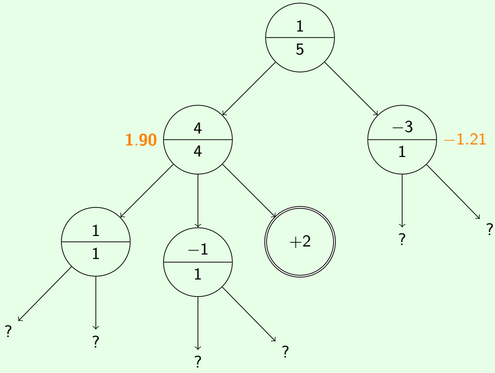

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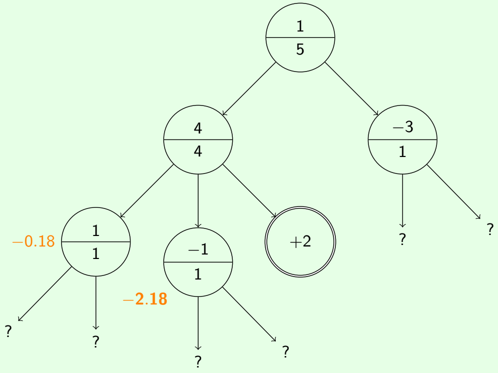

UCT

- At the limit, UCT **converges** to MINIMAX;
- The convergence is faster if we sample with a bias towards the **best moves** of each player;
- What a good move candidate might be from a given position can be **learnt**;
- UCT can be combined with depth-limiting;
- AlphaGo uses MCTS with a depth-limit and artificial neural networks for static position evaluation and finding potential good moves.

Outline

Supervised Learning

- Given **input-output pairs** $(\vec{x_1}, y_1), \ldots, (\vec{x_n}, y_n)$, generated by an **unknown** function f $(\forall i, y_i = f(\vec{x_i}))$, **supervised** (or inductive) learning consists in finding a function h that **approximates** f;

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- **Classification** is supervised learning when the output of f is **finite**;
- Otherwise, it is **regression**.

Supervised Learning: Example

Software update decision

Consider the problem of deciding whether to apply now a software update or not. The attributes are:

1. **sec**: Is it a security update? (yes / no);
2. **reboot**: Does it require a reboot? (yes / no);
3. **in use**: Does it affect something I currently use? (yes / no);
4. **problems**: Does it update a software with which I currently have problems? (no / small problems / big problems);
5. **uptime**: Current duration without any reboot;
6. **crit**: Urgency / criticality of the work I am currently doing. (low / medium / high);
7. **size**: Size / duration of the update. (small / big);
8. **tod**: Time of the day (work / break);

Supervised Learning: Example

Example Data

in_use	reboot	problems	uptime	tod	crit	size	decision
no	no	big	0	work	high	small	yes
no	no	no	30	break	med	small	no
no	no	small	62	work	low	big	yes
no	no	big	21	work	low	big	yes
no	no	big	221	work	low	big	no
no	yes	small	234	work	med	small	no
no	yes	small	1234	break	med	small	yes
yes	yes	big	42	break	low	small	yes
yes	no	no	78	break	high	big	no
yes	no	small	444	break	low	big	yes
yes	yes	small	1024	work	high	big	no
yes	yes	small	10	work	med	small	yes
yes	no	small	24	work	med	big	no

Hypothesis space

- Searching our approximation h over the set of all functions is not feasible;
- We choose a priori an **hypothesis space** (or model):
  - Decision trees;
  - Hyperplanes;
  - Artificial neural networks;
  - ...
- **Hypotheses** h are learnt within an hypothesis space by minimising some **loss function**.

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- **Ockham's razor** dictates to prefer simplicity.

Hyperparameters

- Within a given hypothesis space, we may need to further fix the value of **hyperparameters**:
  - degree of a polynomial model;
  - number of layers in a neural network;
  - number of neurons per layer;
  - ...
- Hyperparameters can also be learnt.

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  - Fix the hyperparameter values and merge the validation data back in the training data;
  - Learn the final model using all the training data. Evaluate using the test data.

k-fold cross-validation

1. Extract a test set;
2. Partition the rest of the data into k subsets S_i of equal size;
3. For each i, use S_i as validation set, and all the other sets as a single training set;
4. Choose hyperparameters that minimise the **average** error rate over the k rounds of training-evaluation;
5. Assess generalisation of the model using the test set.

Failure of the learning process

- The obtained classifier might not be the exact function because of:
  1. unrealisability / underfitting;
  2. overfitting;
  3. variance in the data;
  4. noise in the data;
  5. computational intractability of the hypothesis space.

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  - $L_{0/1}(y, \hat{y}) = 0$ if $y = \hat{y}$ else 1 for classification.

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- But since we do not know the associated probabilities, we minimise **empirical loss** on the example set E:

$$\hat{L}_E(h) = \frac{1}{N} \sum_{(\vec{x},y)\in E} L(y, h(\vec{x}))$$

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- We then try to find the best value for λ as another **hyperparameter**.

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- If their errors are jointly independent, we can decrease the error a lot by, e.g., a majority vote for classification;
- It can also be used to combine simpler hypothesis with an "and": e.g. combine several hyperplane separators to obtain a convex polyhedron.

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- Each of those new training sets (called **bootstrap samples**) are used to produce an hypothesis.

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- These subsets are determined randomly for each hypothesis;
- The number of features selected can also be random, but is often the same across hypotheses.

Outline

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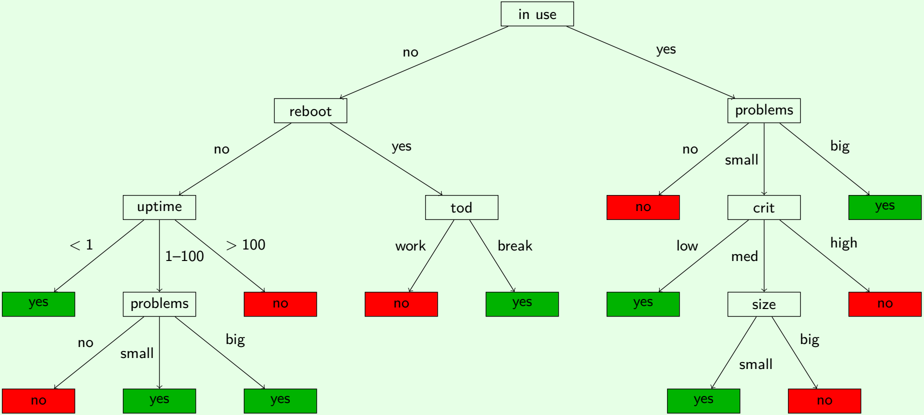
- We focus on the case where the output is finite (classification), and the possible value ranges of the attributes are given.

Decision Trees

Software update decision



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Exercise

1. Write a decision tree for the **majority function** over three boolean variables (say yes iff two or more variables say yes).
2. How does the size of the tree grow with the (odd) number of variables?

Learning Decision Trees

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- Ideally, we want, from a set of examples (values of attributes + corresponding value of the unknown function), to find the **smallest** decision tree representing it.
- This is not possible in general using brute force (e.g. 2^{2^n} trees for a boolean function on n boolean attributes);
- We rely on **heuristics**, giving small (but not the smallest) trees.

Learning Decision Trees: the Greedy Algorithm (ID3)

- Testing an attribute with k values separates the data in k subsets:

in_use	reboot	problems	uptime	tod	crit	size	decision
no	no	big	0	work	high	small	yes
no	no	no	30	break	med	small	no
no	no	small	62	work	low	big	yes
no	no	big	21	work	low	big	yes
no	no	big	221	work	low	big	no
no	yes	small	234	work	med	small	no
no	yes	small	1234	break	med	small	yes
yes	yes	big	42	break	low	small	yes
yes	no	no	78	break	high	big	no
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- If a subset contains only yes outputs or only no outputs we can select that output as the result.

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- To find the most discriminating attributes, we rely on **information theory**.

Finding Important Attributes: Entropy

- The **entropy** of a random variable V, with possible values v_k, is:

$$H(V) = -\sum_k P(v_k) \log_2 \left(P(v_k)\right)$$

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- For a random boolean variable that is true with probability q, the entropy is:

$$B(q) = -\big(q\log_2(q) + (1-q)\log_2(1-q)\big)$$

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- Since we want to be as certain as possible of the value of the output after choosing A, we want to **minimise** this value.

Finding Important Attributes: Information Gain (Ratio)

- Minimising $R(A)$ corresponds to **maximising** the **information gain** of A, defined as:

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- The **information gain ratio** corrects the bias of information gain:

$$IGR(A) = \frac{IG(A)}{IV(A)}$$

Finding Important Attributes: Information Gain (Ratio)

Exercise

problems	size	decision
big	small	yes
no	small	no
small	big	yes
big	big	yes
big	big	no
small	small	no
small	small	yes
big	small	yes
no	big	no
small	big	yes
small	big	no
small	small	yes
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Compute the information gain ratio for attributes *size* and *problems*.

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- Decision tree **pruning** is a technique to address this problem.

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- We use the classic framework of the χ^2 **statistical test**.

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- Finally, we use the following indicator, to measure the difference between the observed number p_k of examples with attribute value x_k and positive output and the number predicted by the theory $(n+p)P(e = \text{true}, A = x_k)$ estimated as $\hat{p}_k = (n+p)\hat{\pi}_k = p\frac{n_k+p_k}{n+p}$ (and similarly for negative examples: $\hat{n}_k$):

$$\chi^2_{obs} = \sum_k \frac{(p_k - \hat{p}_k)^2}{\hat{p}_k} + \frac{(n_k - \hat{n}_k)^2}{\hat{n}_k}$$

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Exercise

Suppose we want to learn the XOR function on two binary inputs x_1 and x_2. Assume that, as a training set we have exactly *a* examples for each combination of the inputs.

1. Compute the resulting decision tree, using the greedy algorithm (without pruning);
2. Can any of the bottom-most non-leaf nodes be pruned?
3. What does the pruning test give for the root of the tree?

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- This usually greatly improves the accuracy of decision trees, while remaining quite fast and fairly explainable.

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- We can use linear regression in the leaves to obtain **regression trees**.

Outline

Linear Regression

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$$y = w_0 + w_1 x_1 + \cdots + w_n x_n$$

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- This means minimising the L_2 loss over the N given examples:

$$Loss(h_{\vec{w}}) = \frac{1}{2}\sum_{k=1}^{N} L_2(y_k, h_{\vec{w}}(\vec{x}_k)) = \frac{1}{2}\sum_{k=1}^{N}(y_k - h_{\vec{w}}(\vec{x}_k))^2$$

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- We can find the global minimum (the function is convex) by writing that all **partial derivatives are zero**.

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- Two interesting subcases are $q = 1$ and $q = 2$;
- L_1 tends to produce **sparse** hypotheses by setting weights to 0;
- But it may be less appropriate than L_2 if the choice of the features is a bit arbitrary (e.g. coordinates in a rotationally invariant problem).

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  2. start from an arbitrary point in the parameters space;
  3. repeat until convergence: find the local gradient $\frac{\partial Loss}{\partial w_i}$ and apply:

$$w_i \leftarrow w_i - \alpha \frac{\partial Loss}{\partial w_i}(\vec{w})$$

Exercise

Instantiate this update rule for a single data point $\vec{x}$ at a point $\vec{w}$, without any regularisation.

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- We can also **randomly** select one of the examples at each iteration: **stochastic gradient descent**;
- It is usually faster but convergence is not guaranteed, unless we make α decrease at each iteration with

$$\sum_{t=1}^{\infty} \alpha(t) = \infty \text{ and } \sum_{t=1}^{\infty} \alpha(t)^2 < \infty$$

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- It has values between 0 and 1, so we decide by rounding to the nearest value.

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- We can then compute the gradient update for the **least square** (L_2) loss:
  Using $\mathcal{L}'(z) = \mathcal{L}(z)(1 - \mathcal{L}(z))$

$$w_i \leftarrow w_i + \alpha(y - h_{\vec{w}}(\vec{x}))h_{\vec{w}}(\vec{x})(1 - h_{\vec{w}}(\vec{x}))x_i$$

Linear Classification: Cross-entropy loss

- Instead of minimising the L_2 loss function, we can take advantage of the fact that expected answers are 0 or 1;
- The **cross-entropy** loss function is:

$$L(\vec{w}) = -\frac{1}{n}\sum_{i=1}^{n}\Big(y_i \ln\left(h_{\vec{w}}(\vec{x_i})\right) + (1-y_i)\ln\left(1-h_{\vec{w}}(\vec{x_i})\right)\Big)$$

- When $y=1$, for one example $(\vec{x},y)$, we have $L(\vec{w}) = \ln(h_{\vec{w}}(\vec{x}))$, decreasing to 0 when $h_{\vec{w}}(\vec{x})$ goes to 1 and symetrically for $y=0$.
- Also, still for one example $(\vec{x},y)$:

$$\frac{\partial L(\vec{w})}{\partial w_0} = (h_{\vec{w}}(\vec{x}) - y)$$

- And for all $i \neq 0$:

$$\frac{\partial L(\vec{w})}{\partial w_i} = (h_{\vec{w}}(\vec{x}) - y)x_i$$

Linear Classification: Logistic regression

- **Logistic regression** is the (binary) **classification** algorithm obtained by:
  - minimising the cross-entropy loss;
  - on a linear model with a logistic threshold:

$$h_{\vec{w}}(\vec{x}) = \frac{1}{1 + e^{-\vec{w}\cdot\vec{x}}}$$

- Minimisation is typically done using gradient descent:

$$\forall i, w_i \leftarrow w_i + \alpha(y - h_{\vec{w}}(\vec{x}))x_i, \text{ with } x_0 = 1$$

Linear Classification: Exercise

Learning boolean functions

1. Use the perceptron learning rule, with $\alpha = 1$, and starting from $w_0 = 0, w_1 = 0, w_2 = 1$, to compute a linear classifier for the binary OR logical function. You will successively apply each of the following examples, one at a time:

x_1	x_2	$x_1 \vee x_2$
0	0	0
0	1	1
1	0	1
1	1	1
0	0	0

2. Could we learn the majority function similarly? If yes, what weights would define the separation hyperplane?
3. Could we learn the binary XOR similarly?

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  - **Combine** several linear classifiers.

Outline

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- An **artificial neural network** connects many artificial neurons together.

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- **Perceptron networks** are ANN with a single layer of neurons: outputs depend directly on inputs;
- They correspond to a collection of unrelated linear classifiers on the same inputs.
- Since OR and NOT are linearly separable, all boolean functions are representable by chaining several perceptron units together.

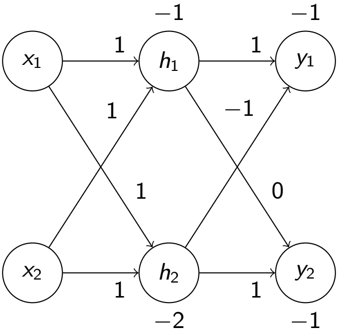
A simple ANN for the addition

Exercise

We consider two boolean inputs $x1$ and $x2$. Using hard threshold functions,

1. Give the weights for a linear classifier computing $x1$ AND $x2$;
2. Give the weights for a linear classifier computing $x1$ AND NOT $x2$;
3. Using the output of OR and AND as inputs to AND NOT, give a 2-layer neural network computing $x1$ XOR $x2$;
4. Add a neuron to compute an addition with carry.

A simple ANN for the addition



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- Neurons with outputs fed into other neurons are called **hidden** and are often arranged in **hidden layers**.

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- z_j^{ℓ} denotes the weighted input of j-th neuron in layer ℓ and a_j^{ℓ} its output (or activation):

$$z_j^{\ell} = \sum_k w_{jk}^{\ell} a_k^{\ell-1} + b_j^{\ell} \text{ and } a_j^{\ell} = g(z_j^{\ell})$$

Forward Response: Matrix Form

- $z^\ell = [z_j^\ell]_j$ and $a^\ell = [a_j^\ell]_j$ are the column vectors of (resp.) weighted input and activation of layer ℓ;
- $w^\ell = [w_{jk}^\ell]_{jk}$ is the matrix of weights between layer ℓ and $\ell - 1$;
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- Then, for $\ell \geq 1$:

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Exercise

1. Write the weight and bias matrices for the previous addition network;
2. Check on a few inputs that the result is the one expected.

Learning in Multilayer ANN

- When computing the answer of the network for a particular input, we go forward;
- Learning means (iteratively) updating the weights to optimise some loss function:
    1. Compute the answer of the network up to the output layer;
    2. Compute the error at the output layer;
    3. **Back-propagate** the error down to the first hidden layer;
    4. Compute the gradient wrt. each weight based on the error;
    5. Update the weights based on the gradient.

Output Layer Error

- We assume the loss function is **additive** across the component of the vector of outputs of the network: this is e.g. the case for the L_2 loss:

$$L_2(\vec{w}, \vec{b}) = \frac{1}{2}||\vec{y} - \vec{h}_{\vec{w},\vec{b}}(\vec{x})||_2^2 = \frac{1}{2}\sum_k (y_k - a_k^L)^2$$

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- It will be more convenient to consider the **modified error**:

$$\Delta_j^L = \frac{\partial Loss}{\partial z_j^L} = g'(z_j^L)\frac{\partial Loss}{\partial a_j^L}$$

Updating the Weights

- For the output layer, at some point $(\vec{w}, \vec{b})$:

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- Then the previous computation holds and:

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- And finally:

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Backpropagation: Exercise

Exercise

For the previous addition network, but with logistic activation functions, and starting from null biases and matrices

$$w^1 = \begin{bmatrix} 0.9 & 1.1 \\ 0.8 & 0.9 \end{bmatrix} \text{ and } w^2 = \begin{bmatrix} 1.2 & -1.1 \\ 0 & 0.9 \end{bmatrix}$$

compute the modified errors and the new values of the weights and biases for input $[1\ 1]^T$ and expected answer $[0\ 1]^T$. Use $\alpha = 0.1$ and an L_2 loss function.

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- Once an epoch is over, we can start another one, and so one until convergence.

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  Even if the output is not at all correct!

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- It is generally a better choice than L_2 loss if the the output layer has logistic neurons.

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- As with all other methods, **increasing the size** of the training set, possibly artificially, reduces overfitting.

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- L_2 regularisation: add, for $\frac{\lambda\alpha}{n} \in [0,1]$, the term ($n$ is the total number of examples):

$$R_2(\vec{w}) = \frac{\lambda}{2n}\Big(\sum_{j,k,\ell}(w_{jk}^{\ell})^2 + \sum_{j,\ell}(b_j^{\ell})^2\Big)$$

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- It reduces **overfitting**;

Regularisation in ANN: Dropout

- At the start of each batch of the SGD, **delete** each hidden neuron with probability p, and train normally;
- At then end of the training multiply all weights of the n hidden neurons by p;
- This simulates the training of 2^n nets at once, with an expected value of their results;
- It reduces **overfitting**;
- And it makes each training stage faster (less neurons).

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- Its main problem is the propagation of gradient along the many layers is **unstable**.

Exploding and Vanishing Gradients

- Suppose we have a network with n hidden layers, each with one neuron:
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  - Regularisation;
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  - Specific architectures: e.g. **convolutional** networks.

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- Fully connected layers work as seen before.

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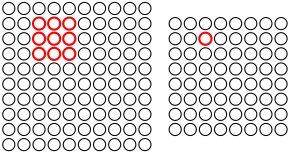
- As the square window moves on the image, with a given **stride**, we obtain as many convolution neurons:



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- Several such **feature maps** can be put in parallel, each with its own shared weights.

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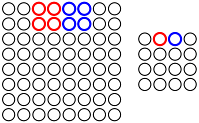

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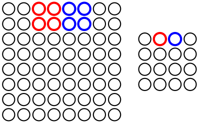

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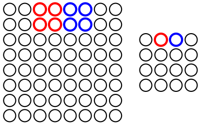

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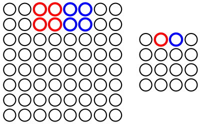

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- Commmon aggregation operations are **max** and **average**.

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- Pooling layers have no modifiable parameters and can be implemented as part of the convolutional layers to which they correspond.

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- Models that can learn incrementally can be more efficient (neural networks, linear functions, etc.)

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- Except for linear models with a fixed policy, convergence is **not theoretically guaranteed**.

Outline

Conclusion

- Rather than designing **intelligent** agents, it is easier to design **rational** agents;
- In order to do so artificial intelligence borrows heavily to mathematics, economics, computer science, control theory, signal processing, etc.
- Rational agents should **learn** from their environment and **plan** their actions to **optimise** some objective function;
- Relying on **models** for the environment usually makes this more effective;
- Useful models must cope with uncertainty, partial observation, non-determinism, and account for other agents.

Going further

Concepts we have not addressed include:

- Represent and reason on accumulated knowledge using:
  - logic;
  - Bayesian networks;
- More on supervised learning:
  - SVMs;
  - Non parameterised models (k-means...);
  - Bayesian learning.
- Unsupervised learning (clustering...)

References

- Stuart Russel and Peter Norvig, *Artificial Intelligence: A Modern Approach (3rd edition)*, Prentice-Hall, 2010.
- Richard S. Sutton and Andrew G. Barto, *Reinforcement Learning: An introduction*, MIT Press, 1998.
- The many Wikipedia pages on the topics addressed here: `http://www.wikipedia.org`
- `http://neuralnetworksanddeeplearning.com/`
- Saul X. Levmore and Elizabeth Early Cook. *Super Strategies for Puzzles and Games*. Doubleday, Garden City, NY, 1981.
- Günter Rote. *Crossing the bridge at night*. Bulletin of the European Association for Theoretical Computer Science. Vol. 78. pp. 241–246. 2002.