

EiKI Summary

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1 What is AI?

In general, there is no set definition of what artificial intelligence is. The most common definition is:

A system of machines that can perform tasks that normally require human intelligence.

This is flawed in that intelligence itself also does not have a set definition, and neither does human intelligence.

1.1 What is Intelligence?

1.1.1 Touring Test

Intelligence is often defined by the Touring Test. Hereby it is assumed that an entity is intelligent if it cannot be distinguished from another intelligent entity by observing its behavior.

The Touring Test is set up like this:

1. Human interrogator interacts with two entities, A and B. Hereby one of the two is already assumed to be intelligent (another human).
2. If the interrogator cannot distinguish which entity is the assumed intelligent entity, it is assumed that the other entity is intelligent as well.

This test is also flawed as it does not distinguish between different intelligence levels (knowledge, reasoning, language understanding, learning etc.). It also is very subjective to the interrogator. It is not based on an objective metric and therefore the outcome can differ from person to person.

It also assumes that humans are inherently intelligent, which makes it a circular argument.

1.1.2 Chinese Room Argument

The Chinese Room Argument tries to answer the question whether intelligence is the same as intelligent behavior. It assumes that even if a machine behaves intelligently, that does not mean it is actually intelligent.

The argument goes as follows:

1. A person who doesn't know chinese is put into a room. Outside the room there is a person, who can only interact with this person by slipping them notes written in chinese.
2. The person inside the room has detailed instructions as to how to answer the notes, without any translation or understanding.
3. To the person outside of the room it looks like the person inside is able to understand and answer to these notes, therefore the person outside of the room assumes that the person inside knows chinese.

So the person outside of the room assumes intelligence due to behavior, that does not necessitates the intelligence if the answers are already known.

Is a self-driving car intelligent? Is ChatGPT intelligent?

1.1.3 Does it even matter?

The question of what intelligence is is a long, complex and difficult question. However, as it is a more philosophical question it doesn't actually really affect the scientific field of AI. It's a definition, not a basis.

1.2 Characteristics of AI

AIs are often divided into two categories: general AI and narrow AI.

General & Narrow AI

- General (strong) AI is defined so that it can handle any intellectual task
- Narrow (weak) AI is defined so that it has a specific task or domain it works in.

This mirrors the distinction between intelligence and acting intelligent. Currently, most AIs are considered narrow, general AIs are the goal in most research.

An AI should possess the following characteristics:

Adaptability

The ability to improve performance by learning from experience

Autonomous

The ability to perform tasks without constant guidance from a user / expert

Usually an AI is modelled after one of the two following concepts:

Law of Thoughts

The AI should be able to reason about its own actions, arguments and thought processes.
More akin to human intelligence.

Rational Behavior

The AI should be able to determine what the best action is for a given situation to maximize the achievement.
Based on a mathematical model of rationality that achieves the most desirable outcome given the information available.

Rationality has two advantages

- **More General:** For many situations a provable correct option does not exist. The most likely outcome is a better solution.
- **More amenable:** Rationality can be defined, refined and optimized.

However, rationality rarely displays a good model of reality.

Systems that think and behave like humans are often talked about in the scientific field of **Cognitive Science**.

1.3 Foundations of AI

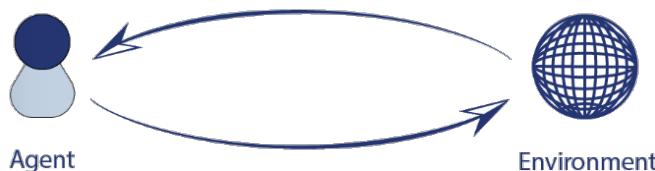
The field of AI is made up by many other fields:

- **Philosophy:** Logic, reasoning, mind as a physical system, foundations of learning, language, rationality
- **Mathematics:** Formal representation and proof algorithms, computation, decidability, tractability, probability
- **Psychology:** Adaptation, phenomena of perception and motor control
- **Economics:** Formal theory of rational decisions, game theory
- **Linguistics:** Knowledge representation, grammar
- **Neuroscience:** Physical substrate for mental processes
- **Control theory:** homeostatic systems, stability, optimal agent design

2 AI Systems

2.1 What is an AI System?

An AI System can be defined as the study of **rational agents** and **their environments**



2.1.1 Environment

- "The surroundings or conditions in which a person, animal, or plant lives or operates" - Oxford Dictionary
- In AI: The surrounding of an (AI) agent, where the agent operates
- Does not have to be real - Can be artificial
- Example:
 - Selfdriving cars: Street, traffic, weather, road signs, ...
 - Chess: Board, pieces,...

Characteristics of Environments

Discrete vs. Continous

Discrete: Environment has countable number of distinct, well defined states

Continous: Not discrete - Uncountable number of states

For Example:

- Discrete: Chess - Every state of the board is mathematically determinable and defined
- Continous: Selfdriving car - Practically infinite positions and conditions

Observable vs. Partially Observable / Unobservable

Observable: State is completely determinable at each point in time

Partially Observable: State is only partially determinable or only determinable at specific points in time

Unobservable: State is never determinable

Static vs. Dynamic

Static: Environment does **not** change while the agent is acting

Dynamic: Environment can change while the agent is acting

For Example:

- Static: Jigsaw puzzle - State does not change without the agents action
- Dynamic: Driving - State still changes even when the agent stops acting

Single Agent vs. Multiple Agents

Single Agent: Environment contains only one agent

Multiple Agents: Environment can contain multiple agents

Accessible vs. Inaccessible

Accessible: Agent can obtain complete and accurate information about the state

Inaccessible: Agent cannot obtain complete or only inaccurate information

Deterministic vs. Stochastic / Probabilistic

Deterministic: Next state is completely determined by the current state and the actions of the agents

Probabilistic: Next state is also influenced by other factors

Episodic vs. Non-episodic / Sequential

Episodic: Each **episode** consists of the agent perceiving and then acting - every action is dependent only on the episode

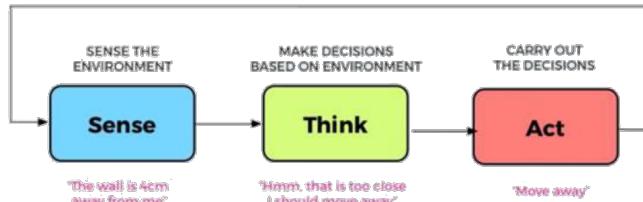
Non-episodic: Actions are also dependent on past memory

These characteristics are important, as the environment specifies the specific needs of the agent:

- Different environments require different agent designs
- Not every algorithm works for a specific environment

2.1.2 Agents

- **Sense:** Perceives its environment
- **Think:** Makes decisions autonomously
- **Act:** Acts upon the environments



Rules of AI Agents

1. Must be able to perceive its environment
2. Observations must be used to make decisions
3. Decisions should be used to act
4. (Action should be rational)

Rational Agents

Maximizes the performance and yield the best positive outcome.

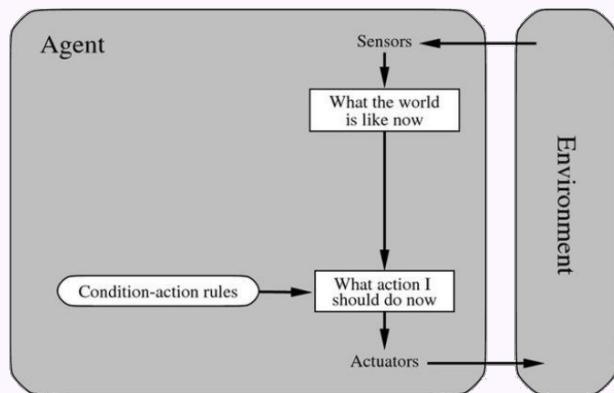
Performance is hereby often measured by a function that evaluates a sequence of actions. This function is task-dependent and cannot be generalized.

2.1.3 Types of Agents

Reflex Agent

Act only on the basis of the current percept, ignores past memory

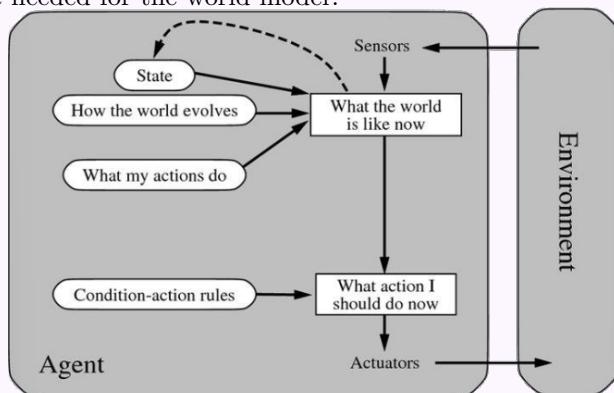
- Implemented through condition-action rules - map state to action
- Problem:
 - Limited decision making
 - No knowledge about anything that cannot be currently perceived
 - Hard to handle in complex environments



Model-Based Agent

Similar decision making to reflex agent, but keep track of the world state

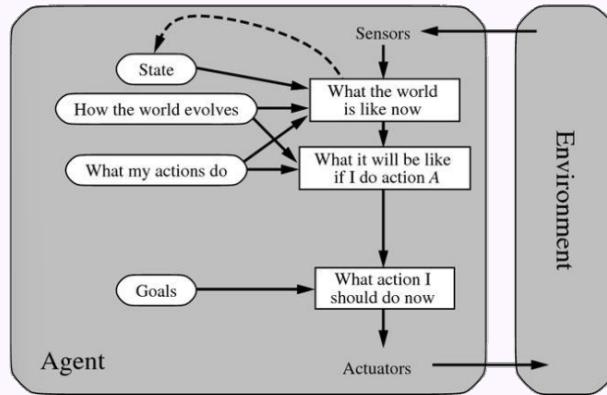
- Input is interpreted and mapped to an internal state representation of the world
- Problem:
 - How do these action affect the internal representation of the world?
 - What details are needed for the world model?



Goal-Based Agent

Essentially a Model-Based Agent with additional functionality that stores desirable states

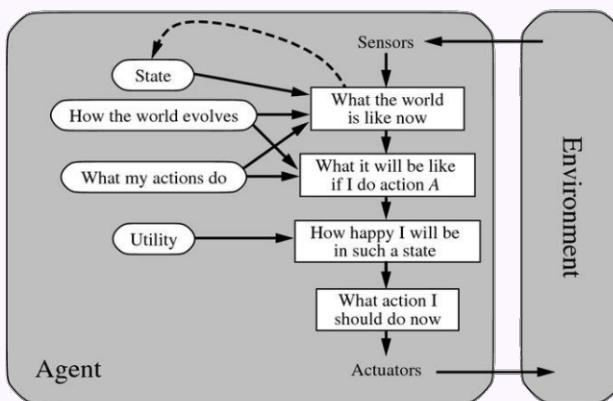
- Knows what states are desirable and acts towards them
- Problem:
 - Difficult to choose actions if a lot of actions are required to achieve a goal



Utility-Based Agent

Similar to Goal-Based Agents, but instead of providing goals it provides a utility function for rating actions and scenarios based on the desirability of the result

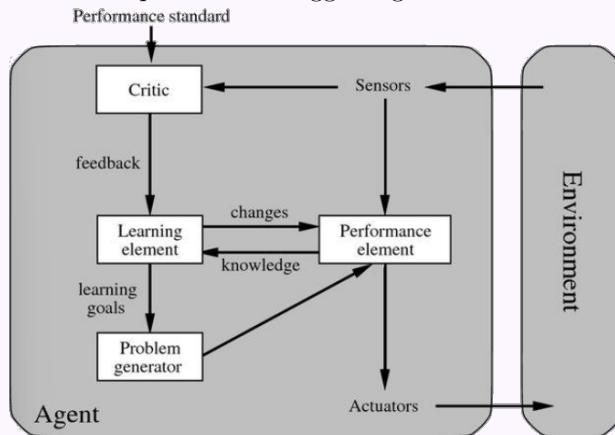
- Goals provide binary distinction, while utility functions provide a continuous measure of desirability
- Can handle selection between two conflicting goals - "Speed or safety"



Learning Agent

Employs additional learning element to gradually improve and become more knowledgeable over time about an environment

- Can learn from past experiences
- Is more robust towards unknown environments
- A learning agent has four conceptual components:
 1. **Learning Element:** Makes improvements by learning from the environment
 2. **Critic:** Gives feedback on the performance of the agent according to a fixed metric
 3. **Performance Element:** Selects the best action according to the critic
 4. **Problem Generator:** Responsible for suggesting actions that will lead to new experiences



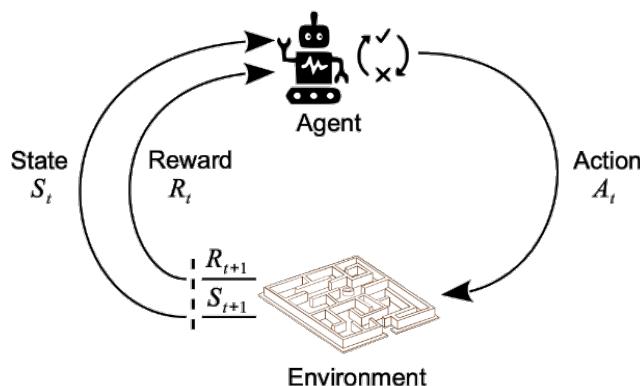
2.2 Creating Intelligent Agents

2.2.1 Search Algorithms

Define "finding a good action" as a search problem and use search algorithm to solve it. Most of these search algorithms are tree based, although Bread-First is used often.

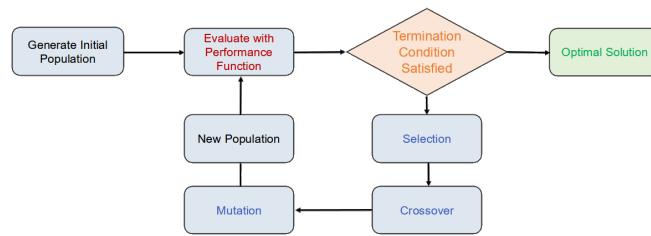
2.2.2 Reinforcement Learning

Developed in psychology, Reinforcement Learning essentially is a process of trial and error - Try something out, have a reaction to it, learn whether it was good or bad. Reactions or actions are based on our observations or experiences.



2.2.3 Genetic Algorithms

Inspired by Darwins "Theory of natural selection", this model build multiple different agents and evaluates every one of them. The agent with the highest performance is selected and new models are built based on it. This is done until the performance is good enough.



3 Uninformed and Informed Search

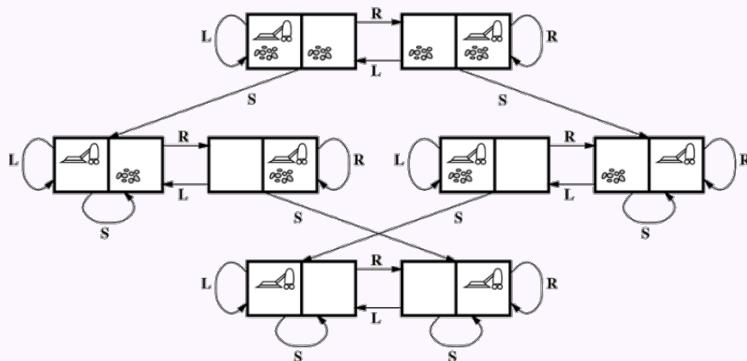
3.1 Problem Solving

3.1.1 Key Terminology

State Space / States

A state is a possible situation in our environment - The State Space is a set of all possible states, reachable from the initial state.

Often visualized as a **state-space graph** that displays all reachable states and its transitions.



State-Space Graph of a robot vacuum cleaning

Transition / Action

A Transition describes possible actions to take to get from one state to another. We only count direct transitions between two states (single actions)

Costs

Transitions often differ in different qualities. We add a "cost" to each action, so we can rate an algorithm on how cost effective it is.

Path

A sequence of states connected by a sequence of actions

Solution

A path that leads from the initial state to a goal state

Optimal Solution

The Solution with the minimal path cost

Problem Components:

1. State Space and Initial State:

All possible states and the initial environment as a state

2. Descriptions of Actions:

Function that maps a state to a set of possible actions in this state

3. Goal Test:

Typically a function to test if the current state fulfills the goal

4. Costs:

A cost function that maps actions to costs

An easy way to add costs of all actions taken

Now that we have defined problems, let's go on to solutions. Most problems can be defined as **planning problems**, in which we start from an initial state and transform it into a desired goal considering future actions and outcomes.

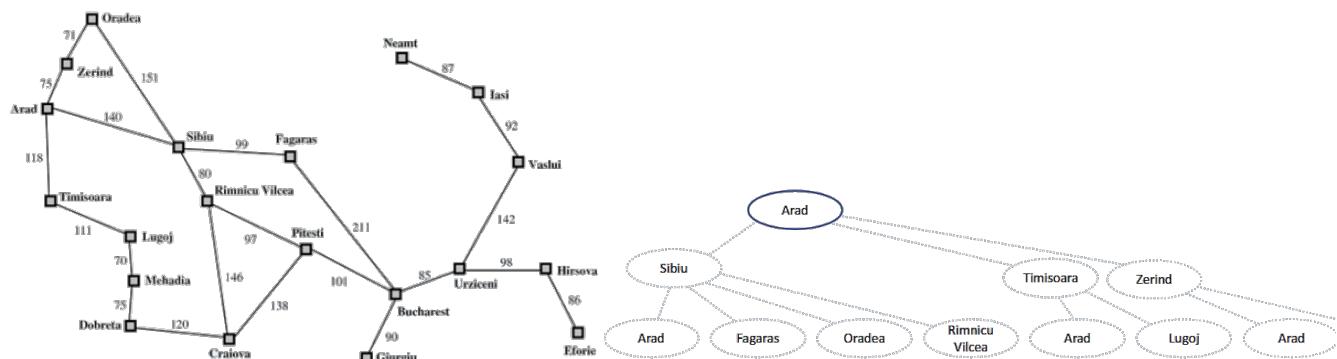
To solve these problems we usually utilize **search** algorithms to find a (optimal) solution in form of a sequence of actions.

3.1.2 Tree Search Algorithms

Hereby we treat the state-space graph as a tree, starting with the initial state. Using this approach we can define iterative or recursive algorithms to search for suitable paths.

Example Tree Search

```
1 Function tree_search(problem, strategy):
2   initialize search tree with initial state of problem;
3   While true do
4     If Node contains goal state then
5       return solution
6     Else If No suitable candidates for expansion then
7       return failure
8     Else
9       Expand node and add resulting nodes to the tree
```



Each Node in the search tree is an entire path in the state-space graph. We construct both on demand - only as much as we need (won't get all solutions)

Node

Describes a part of a tree. Includes **state**, **parent node**, **taken action**, **path cost** and **depth of the tree**

Fringe

Describes the set of nodes at the end of all visited paths

Depth

Number of levels in the search tree

3.2 Uninformed Search

Definition

The uninformed search strategy only has the problem definition, no additional information.

Some algorithms that utilize uninformed search are:

- Uniform-Cost Search (UCS)
- Breadth-First Search (BFS)
- Depth-First Search (DFS)
- Depth-Limited Search (DLS)
- ...

3.2.1 Uniform-Cost Search (UCS)

IN UCS each node is associated with a fixed cost, which accumulate over the path. UCS uses the lowest cumulative cost to find a path.

Only works if each step has a positive cost, as otherwise infinite loops would occur

Complexity: $O(b^{1+\lfloor \text{OptimalCost}/\text{eps} \rfloor})$ with b being the branching factor (average number of children per node) and eps being the minimal cost for a step

3.2.2 Breadth-First Search

BFS is a special case of UCS, when all costs are equal. It starts at the root and goes through each node of a level before progressing to the next level. BFS stops as soon as it finds a solution, while UCS searches for the 'best' solution by lower cost.

Complexity: $O(b^d)$ with b being the branching factor and d being the depth of the search tree

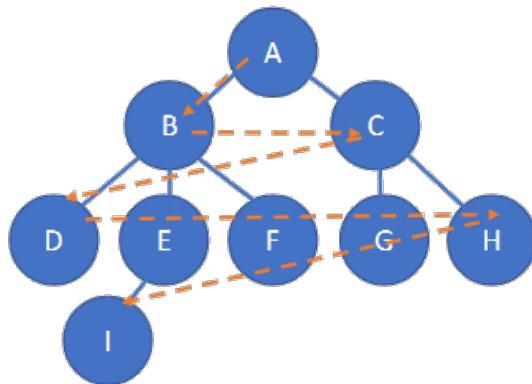
3.2.3 Depth-First Search (DFS)

Depth-First Search starts at the root and continues on one branch until it finds a solution or failure. In case of failure it backtracks to the current parent node and continues on the next branch.

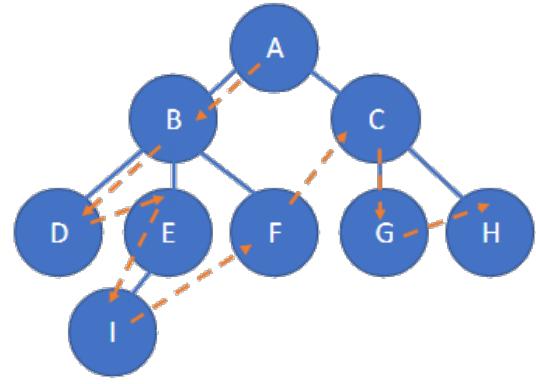
Unlike UCS and BFS DFS is not complete; It fails if the search space is of infinite depth or has loops.

It's also not optimal; More costly solutions may be found before less costly ones.

Complexity: $O(b^m)$ with b being the branching factor and m being the maximum depth of the search tree



BFS: A,B,C,D,E,F,G,H,I



DFS: A,B,D,E,I,F,C,G,H

Criteria	BFS	DFS
Concept	Traversing tree level by level	Traversing tree sub-tree by sub-tree
Data Structure (Queue)	First In First Out (FIFO)	Last In First Out (LIFO)
Time Complexity	$O(\text{Vertices} + \text{Edges})$	$O(\text{Vertices} + \text{Edges})$
Backtracking	No	Yes
Memory	Requires more memory	Less nodes are stored normally (less memory)
Optimality	Yes	Not without modification
Speed	In most cases slower compared to DFS	In most cases faster compared to BFS
When to use	If the target is relatively close to the root node	If the goal state is relatively deep in the tree

Comparison between BFS and DFS algorithms.

3.2.4 Depth-Limited Search (DLS)

DLS is a variant of DFS. Hereby the search is limited to a depth of d . This means that no infinite search can occur, the trade-off being that it might not find all solutions.

Example Depth-Limited Search

```
1 Function depth_limited_search(problem, limit):
2   recursive_dls(make_node(initial_state(problem)), problem, limit)
3 Function recursive_dls(node, problem, limit):
4   cutoff_occurred = false;
5   If goal_test(problem, state(node)) then
6     return node;
7   Else If depth(node) >= limit then
8     return cutoff;
9   Else
10    ForEach successor in expand(node, problem) do
11      result = recursive_dls(successor, problem, limit);
12      If result == cutoff then
13        cutoff_occurred = true;
14      Else If result != failure then
15        return result;
16    If cutoff_occurred then
17      return cutoff;
18    Else
19      return failure
```

This, of course, is neither complete nor optimal.

Complexity: $O(b^l)$ with b being the branching factor and l being the maximum depth of the search tree

3.2.5 Iterative Deepening Search (IDS)

IDS is a variant of DLS. It works like DLS, but instead of a fixed depth, it iteratively increases the depth until a solution is found.

Example Iterative Deepening Search

```
1 Function iterative_deepening_search(problem):
2   For depth = 0 to ∞ do
3     result = depth_limited_search(problem, depth);
4     If result != cutoff then
5       return result
```

This change makes it complete and optimal.

Complexity: $O(b^m)$ with b being the branching factor and d being the depth of the search tree. This makes its time complexity equal to BFS. However, the space complexity of IDS is $O(bd)$, which is much better than BFS' $O(b^d)$.

Criterion	Breadth-First	Uniform-Cost	Depth-First	Depth-Limited	Iterative Deepening
Complete?	Yes*	Yes*	No	Yes, if $l \geq d$	Yes
Time	b^d	$b^{1+\lfloor OptCost/\epsilon \rfloor}$	b^m	b^l	b^d
Space	b^d	$b^{1+\lfloor OptCost/\epsilon \rfloor}$	bm	bl	bd
Optimal?	Yes*	Yes	No	No	Yes*

Comparison of search strategies.

3.3 Heuristics h

Denotes a "rule of thumb", a rule that may be helpful in solving a problem.

In Tree-Search, a heuristic is a function that estimates the remaining cost from the current node to the goal.

Can go wrong!

Admissible Heuristic

A heuristic is admissible if it never overestimates the actual cost to reach the goal.

$$h(n) \leq h^*(n)$$

if $h^*(n)$ is the true cost to reach the goal from node n

Consistent Heuristic

A heuristic is consistent if for every node n and successor n' generated by any action a :

$$h(n) \leq c(n, a, n') + h(n')$$

if $c(n, a, n')$ is the cost of the action a from n to n'

Thus, a heuristic is consistent if, when going from neighboring nodes, the heuristic difference / step cost never overestimates the actual cost.

Lemmas

- If a heuristic is consistent, it is also admissible.
- If $h(n)$ is consistent, then the values of $f(n)$ on any path are non-decreasing.

3.3.1 Relaxed Problems

A relaxed problem is a problem that has fewer constraints on the actions than the original problem.

The cost of the optimal solution to a relaxed problem is an admissible heuristic for the original problem.

Example: Relaxed Problem as Admissible Heuristic

Consider a grid-based pathfinding problem where certain movements are restricted due to obstacles. A relaxed version of this problem might allow movement through obstacles by ignoring some constraints. The cost of the optimal solution to this relaxed problem, which is typically lower or equal to the original problem's optimal cost, serves as an admissible heuristic for the original problem.

This means that looking for relaxed problems is a good way to find admissible heuristics.

3.3.2 Dominance

A heuristic h_2 dominates h_1 if $h_2(n) \geq h_1(n)$ for all nodes n . (Given that h_1 and h_2 are admissible)

This means that a dominant heuristic is always closer to the optimal heuristic h^* , which results in less expansion and thus more efficient search.

3.3.3 Combining Heuristics

If h_1, h_2, \dots, h_m are admissible heuristics, then $h(n) = \max(h_1(n), h_2(n), \dots, h_m(n))$ is also admissible and dominates both h_1 and h_2 .

This is useful if we have multiple admissible non-dominated heuristics and want to combine them to get a better heuristic.

3.4 Informed Search

Definition

The informed search strategy has additional knowledge about "where" to look for solutions, usually in form of a heuristic function.

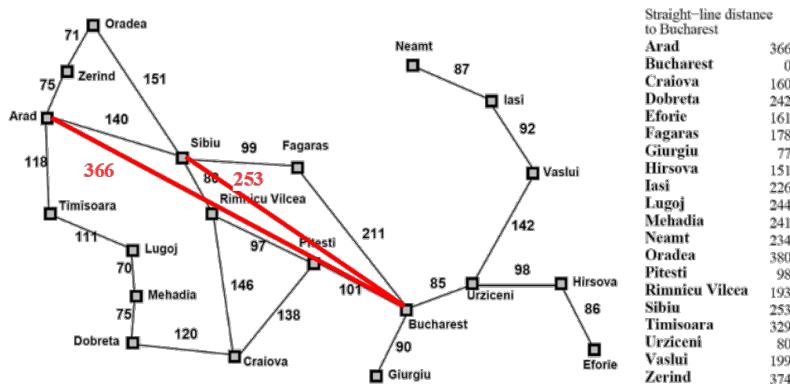
Some algorithms that utilize informed search are:

- Greedy Best-First Search
- A* Search
- Memory-Bounded Heuristic Search

3.4.1 Greedy Best-First Search

Greedy Best-First Search (GBFS) is an informed search algorithm that selects the next node to expand based on a heuristic that estimates the cost from the current node to the goal.

One example of a heuristic is the straight-line distance to the goal.



Example of GBFS with a straight-line distance heuristic.

Complexity: The time complexity of Greedy Best-First Search is $O(b^m)$, and its space complexity is also $O(b^m)$, where b is the branching factor and m is the maximum depth of the search tree. This is the same as DFS, however due to the heuristic it can be significantly faster.

GBFS is not guaranteed to be optimal or complete, especially if the heuristic function is not admissible or consistent. Its efficiency heavily depends on the quality of the heuristic used.

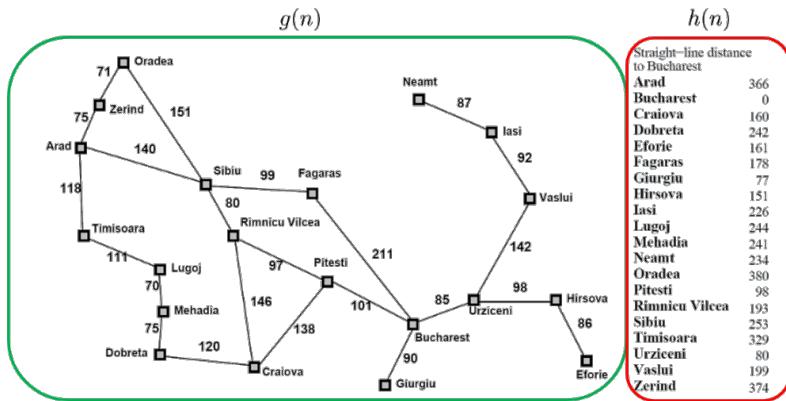
- **Complete?** No, can get stuck in loops.
- **Optimal?** No, does not guarantee an optimal solution as it depends on the heuristic, which may be flawed.

3.4.2 A* Search

Definition

A* Search is an informed search algorithm that combines the strengths of Uniform-Cost Search and Greedy Best-First Search. It searches for the least-cost path to the goal by considering both the cost to reach the current node and an estimated cost to reach the goal.

A* Search tries to avoid paths that are already expensive. It evaluates the complete path cost and the remaining cost to the goal. Its cost function is defined as $f(n) = g(n) + h(n)$, where $g(n)$ is the cost to reach the current node (root to n) and $h(n)$ (the heuristic) is the estimated cost to reach the goal (n to goal).



Example of A* Search with heuristic function.

Complexity: The time complexity of A* Search is $O(b^m)$, and its space complexity is also $O(b^m)$, where b is the branching factor and m is the maximum depth of the search tree.

Completeness and Optimality: A* Search is complete, and can be optimal, if the heuristic is admissible.

3.4.3 Alternatives to A*

1. Iterative-Deepening A* (IDA*)

- Like iterative deepening, it explores nodes level by level, but uses A* to evaluate the nodes.
- Cutoff information is the f-cost ($g + h$) instead of the depth.

2. Recursive Best-First Search (RBFS)

- Recursive algorithm that mimics best-first search with linear space
- Keeps track of f-value of best alternative path
- Path available from any ancestor of the current node and heuristic evaluations are updated with results of successors

3. (Simple) Memory-Bounded A* ((S)MA*)

- Drops the worst leaf node when memory is full
- Its value will be updated to its parent
- May be researched later

3.4.4 Graph Search

When traversing a problem, loops can occur. Failure to detect them can turn linear search into exponential search. To avoid this, we can use **graph search**. Hereby we only expand nodes that have not been visited yet.

For example: The graph search version of UCS is **Dijkstra's algorithm**.

4 Local and Adversarial Search

(Un-)Informed Search shows some limitations. Typically these algorithms can only handle search spaces with up to 10^{100} states due to memory constraints. They also only consider "paths" as a solution.

4.1 Optimization Problems

An optimization problem is a problem where every state can be a solution (to different degrees) but the target is to find the state that optimizes (min, max,...) the solution according to an objective function.

This means that there is no explicit goal state and also no path to reach it (no cost).

For example: Darwinian evolution could be seen as an optimization problem.

Objective (Evaluation) Function

An objective function shows how good a state is, also in comparison to other states. Its value is minimized or maximized depending on the problem.

4.1.1 Terminology

Convergence

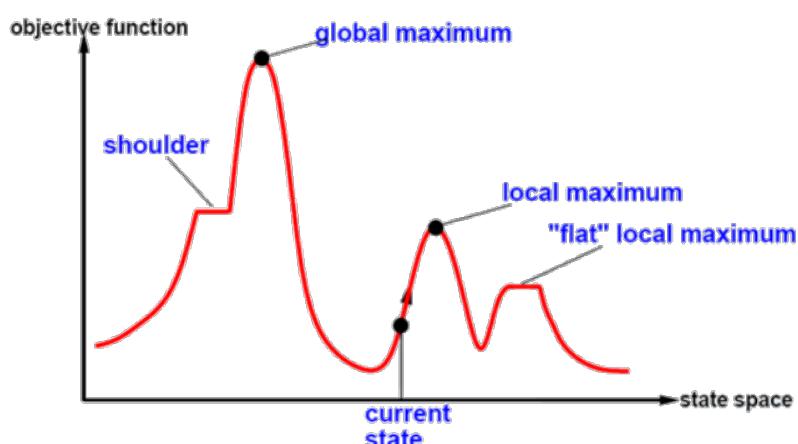
Describes a sequence of (function) values that approach a limit / value more and more.

Global Optimum

The **extremum** of an objective function over the **entire** input search space

Local Optimum

The **extremum** of an objective function over a **subset** of the input search space



4.2 Local Search

Local Search algorithms traverse only a single state rather than saving multiple paths. It modifies its state iteratively, trying to improve a specific criteria.

Optimization problems often times do not care about the path taken, but only to fulfill the goal constraint.

Advantages

- Uses little and constant memory
- Finds reasonable solution in large state spaces

Disadvantages

- No guarantee for completeness or optimality

Basic Idea (Travelling Salesman Problem):

- Start with a complete but likely suboptimal tour
- Modify the tour (e.g. pairwise swap) to improve the objective function
- Repeat until the tour is sufficiently good
- This approach often gets very good results quickly

4.2.1 Hill Climbing

Basic Idea:

- Expand the current state
- Move to the one with the highest value
- Repeat until a maximum is reached

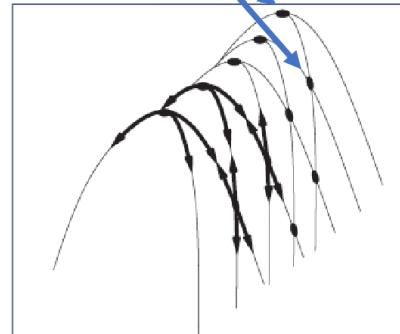
Hill Climbing

```
1 Function hill_climbing(problem):
2     current = make_node(initial_state(problem));
3     neighbor;
4     While true do
5         neighbor = highest_valued_successor(current);
6         If value(neighbor) ≤ value(current) then
7             return state(current);
8         current = neighbor;
```

Ridge Problem:

Most Local Search algorithms are implemented by expanding their neighbors and then selecting the one that increases the objective function the most. Often times the problem space is not as simple as that there's only two neighbors, resulting in a more "3D" or higher search space. This can cause an issue, when all neighbors are worse than the current state, but the search space has an uphill.

States / steps (discrete)

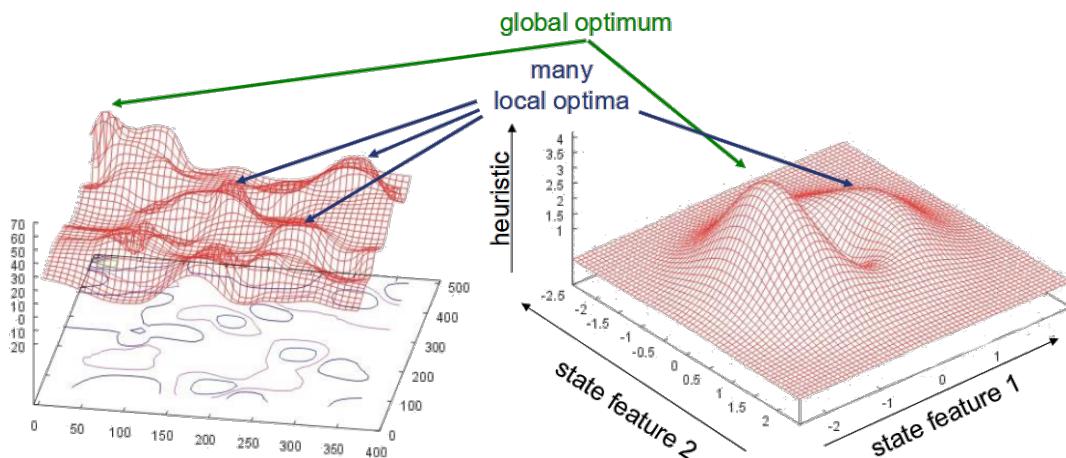


Problem - Local Optima:

- Algorithm will stop at the nearest local optima
- This might be very far from the global optimum (plateaus, ridges, shoulders...)
- Solution: Random Restart
 - Random initial positions result in different local optima
 - → Iterate over multiple local optima and select the best one
- Alternative Solution: Stochastic Hill Climbing
 - Select successor randomly with a higher chance for better successors

4.2.2 Gradient Descent

As mentioned before, search spaces often are not only 2-dimensional, as we might need to consider multiple features. This, of course, makes it much harder to find an optimal solution with higher dimensional search spaces.



Before our objective function only had a single input feature, now we also have to consider more.

Gradient

The **derivative** of a function that has more than one input variable. In mathematics it would be known as the **slope** of a function, which measures the change in all weights with regard to the change in error.

Gradient Descent

The **gradient descent** is an optimization algorithm. It can be considered as Hill-Climbing in continuous state space.

Gradient Descent: Working Principle

Gradient Vector

$$\nabla J(\underline{\theta}) = \left[\frac{\partial J(\underline{\theta})}{\partial \theta_0}, \dots, \frac{\partial J(\underline{\theta})}{\partial \theta_n} \right]$$

Cost Function

$$J(x_1, x_2, \dots, x_n)$$

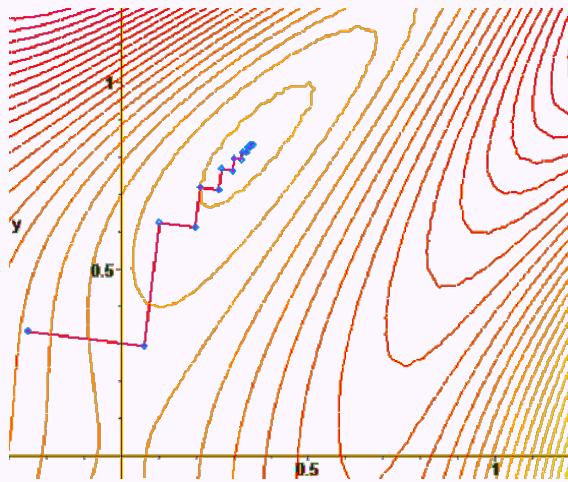
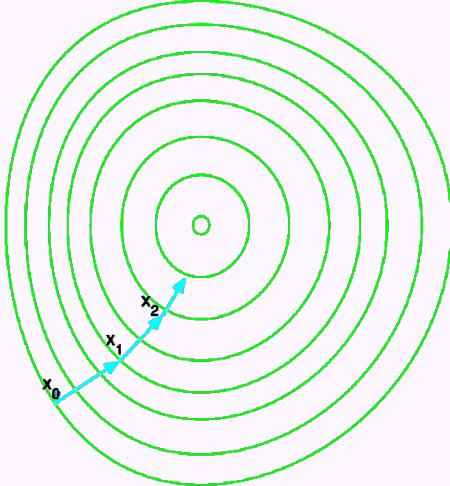
We now want to minimize over the continuous variables x_1, x_2, \dots, x_n .

1. Compute gradient: $\frac{\partial}{\partial x_i} J(x_1, x_2, \dots, x_n) \quad \forall i \in n$

2. Take a step downhill in the direction of the gradient: $x_i' = x_i - \lambda \frac{\partial}{\partial x_i} J(x_1, x_2, \dots, x_n)$

3. If $J(x_1', x_2', \dots, x_n') < J(x_1, x_2, \dots, x_n)$, accept move, else reject.

4. Repeat until desired accuracy is reached



Learning Rate

"The size of the step taken in the gradient descent". The **learning rate** is a hyperparameter, controlling how quickly the model adapts to the problem.

Finding the right learning rate is a very important task. It can be done by trial and error, or by using a learning rate scheduler.

In general:

- **Smaller learning rate:**
 - Smaller changes → requires more training epochs
- **Larger learning rate:**
 - Larger changes → requires fewer training epochs
 - Can converge to local optima or not at all

Determining the gradient can be difficult.

- Derive formula using multivariate calculus
- Ask mathematician or domain expert
- Literature search

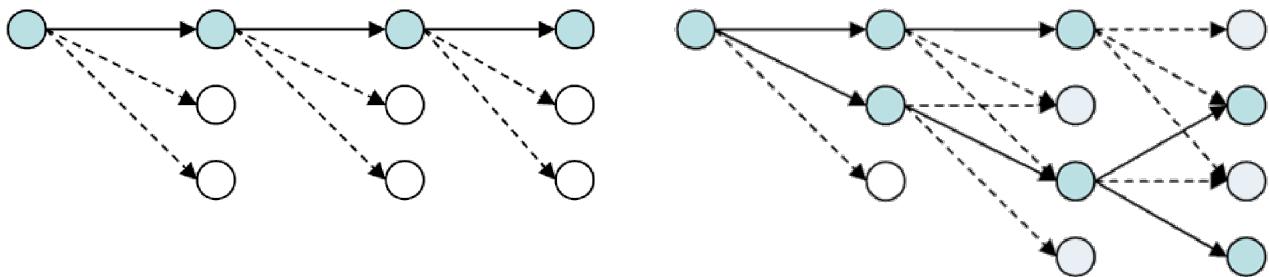
- Automatic differentiation

Gradient Descent in general works well for "smooth" spaces; poorly for "rough" spaces.

4.2.3 Beam Search

Basic Idea:

- Keep track of k states (beam size) rather than just one
1. Start with k randomly generated states
 2. At each iteration, all successors of all k states are generated
 3. Select the k best successors from complete list
 4. Repeat



4.2.4 Simulated Annealing

Basic Idea:

- Use hill-climbing, but occasionally take a step into a direction that does not show improvement
- Reduce the probability of a down-hill step and decrease the size of the step as the number of iterations grows
- Allows some "bad moves" to escape local optima

Simulated Annealing Algorithm

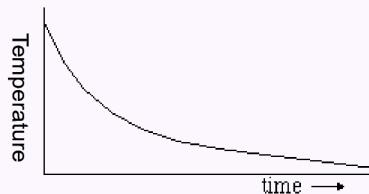
```

1 // schedule maps time t to temperature T
2 Function simulated_annealing(problem, schedule):
3   current = make_node(initial_state(problem));
4   temperature;
5   next;
6   For t = 1 to ∞ do
7     temperature = schedule[t];
8     next = select_random_successor(current);
9     ΔE = value(next) - value(current);
10    If ΔE > 0 then
11      current = next;
12    // Still accepts worse solution with a probability of e^ΔE/temperature
13    Else If random_number(0,1) < e^ΔE/temperature then
14      current = next

```

Temperature

Temperature is a hyperparameter, controlling how frequently we accept worse solutions to escape local optima. Temperature usually decays exponentially.



Simulated Annealing converges to a global optimum if the temperature is lowered slowly enough. This is not a strong claim as even random guessing would eventually yield the global optimum.

As such, simulated annealing can take a very long time.

4.3 Adversarial Search

Adversarial Search assumes an "adversary", who acts against the agent. The goal of adversarial search is to plan ahead, while taking the adversary's actions into account.

Adversarial search is often used to model games as search problems. Each player has to consider other players' actions and their effect on the game state.

Adversarial search is often time constrained, so it is unlikely to find an optimal solution.

4.3.1 Games

Zero-Sum Game

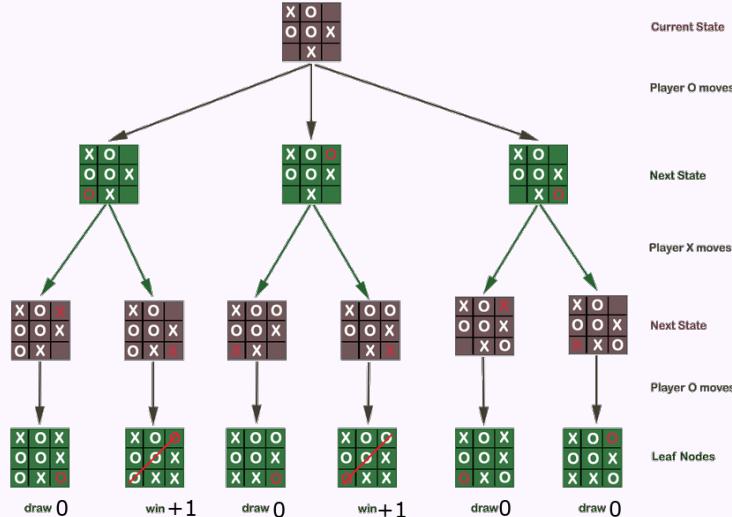
Describes a game whereby, if one party loses, the other must win, therefore the net change in "points" is zero.

A game can be defined as a search problem:

1. **Initial State:** Game set-up
2. **Player(s):** Specifies which players turn it is
3. **Action(s):** Returns all possible moves in state s
4. **Result(s, a):** Specifies the state s' after action a in state s is taken
5. **Terminal(s):** Tests if state s fulfills the goal/terminal constraints
6. **Utility(s, p):** Returns a numeric value for a terminal state s from the perspective of player p

Game Trees

Game Trees are used to represent the possible states of a game. Hereby each level corresponds to a player. The **root node** is always the initial (empty) state with current player. **Leaf Nodes** are always terminal states. Every **terminal node** has a utility value corresponding to the outcome of the game (e.g. +1 for a win, 0 for a draw, -1 for a loss).



4.3.2 Games vs. Search Problems

- "Unpredictable" opponent
 - Specify a move for every possible reply
 - Different goals for every agent
- Time limits
 - Likely not enough time to find a goal state
 - Needs approximation
- Most games are
 - Deterministic, turn-based, two-player, zero-sum
- Real problems are
 - Stochastic, parallel, multi-agent, utility based

4.3.3 Minimax Algorithm

Basic Idea:

- Build a game tree where nodes represent the states of the game and edges represent the possible moves.
- The players:
 - **MIN:** Decreases the chances of **MAX** winning (Opponent)
 - **MAX:** Increases his own chances of winning (Agent)
- Players take alternating turns following their respective strategies.
- Choose move to position with the highest **minimax value**
- Assume opponent to play the best response to their own action

Minimax Algorithm

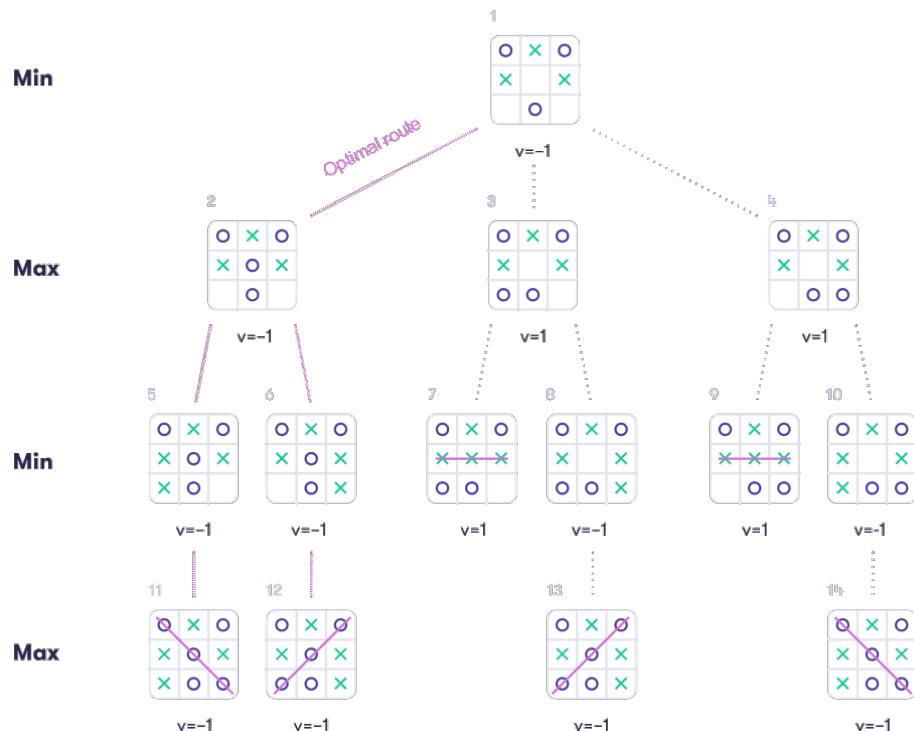
```

1 Function minimax_decision(state):
2   v = maximizer(state);
3   // Returns the action that leads to state with utility value v
4   return get_action(v, get_successors(state));
5 Function maximizer(state):
6   If is_terminal(state) then
7     return utility(state);
8   v = -∞;
9   For s in get_successors(state) do
10    v = max(v, minimizer(s));
11   return v;
12 Function minimizer(state):
13   If is_terminal(state) then
14     return utility(state);
15   v = ∞;
16   For s in get_successors(state) do
17     v = min(v, maximizer(s));
18   return v;

```

Characteristics

- **Optimality:** Yes, assuming an optimal opponent
- **Completeness:** Yes, if the tree is finite (e.g. no infinite game loops)
- **Time Complexity:** $O(b^m)$
- **Space Complexity:** $O(b \cdot m)$
- (b is the branching factor, m is the maximum depth)



Problem:

Many games have too many possible moves and go on for too long which causes the time complexity to grow exponentially. Go for example has a branching factor of about 250 and can go on for 150+ turns, which would result in approximately $5 \times 10^{359} +$ iterations in the worst case.

4.3.4 Alpha-Beta Pruning

A modified, optimized version of **Minimax Algorithm**. It uses **pruning** to reduce the amount of exploration without compromising the correctness of minimax.

Alpha-Beta Pruning is based on two parameters

- **Alpha:** The best (highest-valued) choice found so far at any point along the path of the Maximizer to the root. Initial Value: $-\infty$
- **Beta:** The best (lowest-valued) choice found so far at any point along the path of the Minimizer to the root. Initial Value: $+\infty$

Basic Idea:

Remove all nodes which are not affecting the final decision, but slow down the algorithm.

Alpha-Beta Pruning Algorithm

```
1 Function alpha_beta(state):
2     alpha = -∞;
3     beta = +∞;
4     v = maximizer(state, alpha, beta);
5     return v;
6 Function maximizer(state, alpha, beta):
7     If is_terminal(state) then
8         return utility(state);
9     v = -∞;
10    For s in get_successors(state) do
11        eval = minimizer(s, alpha, beta);
12        v = max(v, eval);
13        alpha = max(alpha, v);
14        If beta ≤ alpha then
15            break;
16    return v;
17 Function minimizer(state, alpha, beta):
18     If is_terminal(state) then
19         return utility(state);
20     v = +∞;
21     For s in get_successors(state) do
22         eval = maximizer(s, alpha, beta);
23         v = min(v, eval);
24         beta = min(beta, v);
25         If beta ≤ alpha then
26             break;
27     return v;
```

Differences to Minimax:

- Max Player will only update alpha
- Min Player will only update beta
- While backtracking, the node values will be passed to upper nodes instead of alpha and beta
- Alpha and beta will only be passed to child nodes

Problems:

- Needs a fast evaluation function
- Games with large branching factors (e.g. Go) exploration with alpha-beta pruning is very slow

5 Constraint Satisfaction Problems

Constraint Satisfaction Problem

Constraint Satisfaction is a technique where a problem is solved when its solution satisfies certain constraints or rules of the problem.

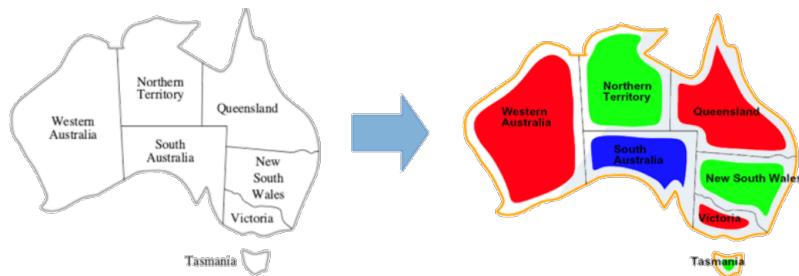
Components:

- A state, defined by **variables** X_i with **d** values from **domain** D_i
- A goal test, defined as a set of **constraints** C specifying allowable combinations of values for subsets of variables.

Solving Constraint Satisfaction Problems:

- A state space
- Notion of the solution

Example of a Constraint Satisfaction Problem



Problem: Assign each territory a colour such that no two adjacent territories have the same colour.

Variables: $X = \{WA, NT, Q, NSW, V, SA, T\}$

Domain of Variables: $D = \{\text{red, green, blue}\}$

Constraints: $C = \{SA \neq WA, SA \neq NT, SA \neq Q, \dots\}$

5.1 Assignment of Values to Variables

A state in state-space is not a "blackbox" as in standard search, but defined by assigning values to some or all variables.

$$X_1 = v_1, X_2 = v_2, \dots, X_d = v_d$$

The assignment of these values can be done in different ways:

1. **Consistent/Legal Assignment:** An assignment is consistent if it satisfies all constraints or rules.
2. **Complete Assignment:** An assignment is complete if every variable is assigned a value, and the solution to the CSP remains consistent.
3. **Partial Assignment:** An assignment is partial if some variables are not assigned values.

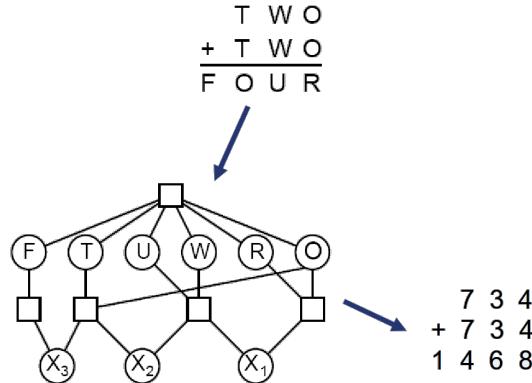
5.2 Constraint Graphs

Constraint Graphs are often constructed because abstraction of the problem makes it easier to solve and understand.

A constraint graph is usually denoted with

- Every variable is represented by a node
- Every edge indicates a constraint between two variables

Example of a Constraint Graph



Problem: Assign unique values to the variables of each letter, so that resulting equation is true.

Variables: $X = \{T, W, O, F, U, R\}$

Domain of Variables: $D = \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$

Constraints: $C = \{T \neq W \neq O \neq F \neq U \neq R\}$

$$\cup \quad \text{int}(T'' + W'' + O'') + \text{int}(T'' + W'' + O'') = \text{int}(F'' + O'' + U'' + R'')$$

Here the connected nodes are involved in (in-)equations:

$2 \cdot O = 10 \cdot X_1 + R$
$2 \cdot W + X_1 = 10 \cdot X_2 + U$
$2 \cdot T + X_2 = 10 \cdot X_3 + O$
$F = X_3$
$T \neq W \neq O \neq F \neq U \neq R$

5.3 Types of Constraints

- **Unary constraints:** Involve a single variable (e.g. South Australia \neq green)
- **Binary constraints:** Involve two variables (e.g. South Australia \neq Wester Australia)
- **Higher-order constraints:** Involve more than two variables (e.g. $2 \cdot W + X_1 = 10 \cdot X_2 + U$)

Preferences / Soft constraints:

- Not binding, but should be considered during search
→ Constrained optimization problems
- e.g. Red is better than green

5.4 Solving CSPs: Search

Basic Idea:

1. Successively assign values to variable
2. Check constraints
3. If constraint is violated → backtrack
4. Repeat until all variables have assigned values that satisfy constraints

To do this we map CSPs into search problems:

- Nodes = assignments of values to a subset of the variables
- Neighbors of a node = nodes in which values are assigned to one additional variable
- Start node = empty assignment
- Goal node = a node which assigns a value to each variable and satisfies all constraints

5.4.1 Naive Search

Naive Search is practically a **brute-force** method. It systematically explores all possible assignments of v values to n variables. This, of course, is incredibly inefficient and results in exponential time complexity. The number of leaves in the search tree grows with $n!v^n$.

5.4.2 Backtracking Search

Basic Idea: As assignments are commutative ($[WA = \text{red} \text{ then } NT = \text{green}] = [NT = \text{green} \text{ then } WA = \text{red}]$) we can reduce the number of leaves in the search tree by only considering nodes that have not been visited before.

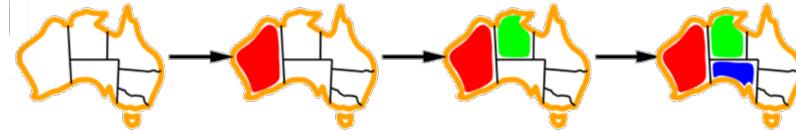
Backtracking Algorithm

```
1 Function backtrack_search(csp):
2   return recursive_backtrack(csp, {});
3 Function recursive_backtrack(csp, assignment):
4   If is_complete(assignment) then
5     return assignment;
6   var = get_unassigned_variable(get_variables(csp), assignment, csp);
7   ForEach value in order_domain_values(var, assignment, csp) do
8     If value is consistent with assignment given constraints(csp) then
9       assignment.add({var = value});
10      result = recursive_backtrack(csp, assignment);
11      If result != failure then
12        return result;
13      assignment.remove({var = value});
14  return failure;
```

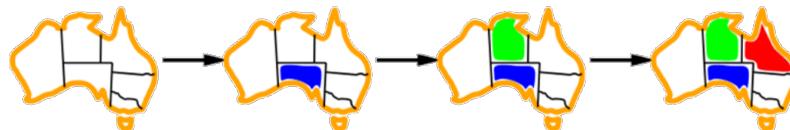
This is still not ideal as in the worst case the complexity is still exponential. This can be improved by including heuristics.

5.5 Heuristics for CSPs

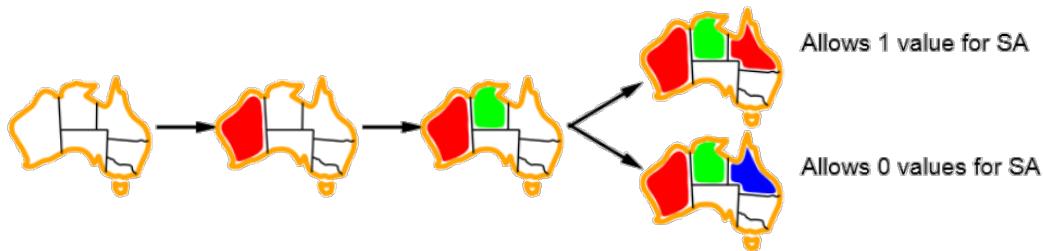
- **Domain-Specific Heuristics:** Depend on the particular characteristics of the problem.
- **General-Purpose Heuristics:** Can work on any CSP.
 - **Minimum Remaining Value:** Choose variable with fewest consistent values



- **Degree Heuristic:** Choose variable with the most constraints on remaining variables



- **Least Constraining Value Heuristic:** Given a variable, choose the value that rules out the fewest values in the remaining variables



If utilized in this order, these heuristics will greatly improve search speed.

5.6 Constraint Propagation

Node Consistency

A variable (node) is consistent if the possible values of this variable are conform to all unary constraints.

Local Consistency

Local consistency is defined by a graph where each of its nodes is consistent with its neighbors. This is done by iteratively enforcing the constraint corresponding to the edges.

Arc

A constraint involving two variables is called an **arc** or binary constraint.

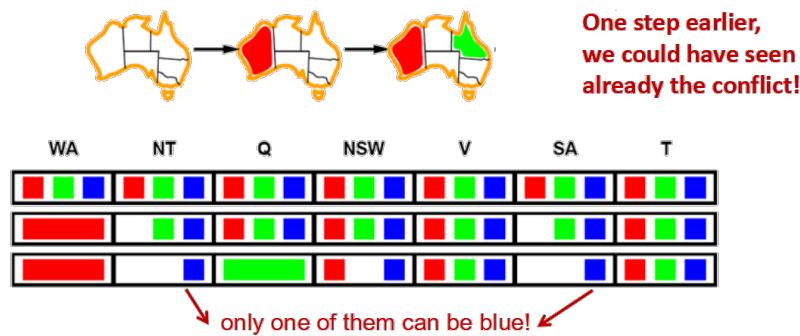
Arc Consistency

An arc is consistent if for each value of X in the domain of X there exists a value Y in the domain of Y such that the constraint $\text{arc}(X, Y)$ is satisfied.

$$\forall X \in \text{dom}(X), \exists Y \in \text{dom}(Y) : \text{arc}(X, Y) \text{ is satisfied}$$

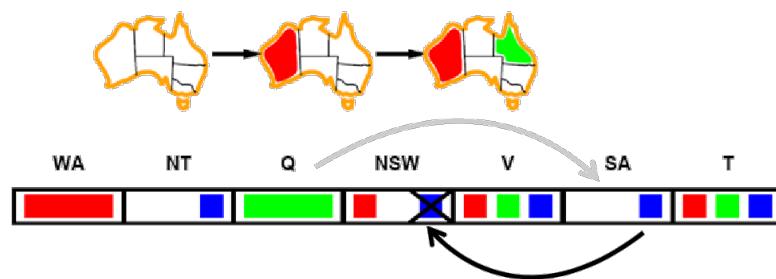
5.6.1 Forward Checking

Basic Idea: Keep track of remaining legal values for unassigned variables and terminate search, when any variable has no legal values left.

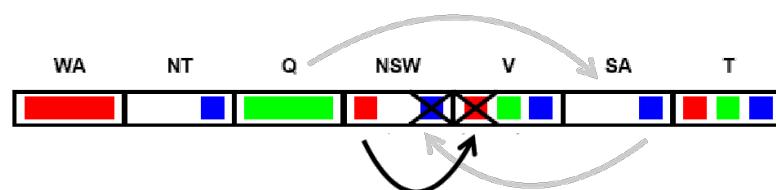


5.6.2 Maintaining Arc Consistency (MAC)

After each assignment of a value to a variable, possible values of the neighbors have to be updated.



If one variable (NSW) loses a value (blue), we need to recheck its neighbors as well because they might have lost a possible value.



AC-3 Algorithm

```
1 Function AC-3(csp):
2   queue = get_all_arcs(csp);
3   While queue is not empty do
4     ( $X_i, X_j$ ) = remove_first(queue);
5     If remove_inconsistent_values( $X_i, X_j$ ) then
6       ForEach  $X_k$  in get_neighbors( $X_i$ ) do
7         queue.add( $X_k$ );
8 Function remove_inconsistent_values( $X_i, X_j$ ):
9   removed = false;
10  ForEach  $x$  in get_domain( $X_i$ ) do
11    If no value  $y$  in get_domain( $X_j$ ) satisfies arc( $X_i, X_j$ ) then
12      get_domain( $X_i$ ).remove( $x$ );
13      removed = true;
14  return removed;
```

5.6.3 Path Consistency

Arc consistency is often sufficient to:

- Solve the problem (all variable domains reduced to one value)
- Show that the problem cannot be solved (some domains empty)

but sometimes may not be enough, for example if there's always a consistent value in the neighboring region.

Path consistency tightens the binary constraint by considering triples of values.

A pair of variables (X_i, X_j) is path-consistent with X_m if

- for every assignment that satisfies the constraint on the arc (X_i, X_j)
- there is an assignment that satisfies the constraints on the arcs (X_i, X_m) and (X_j, X_m)

5.6.4 k-Consistency

k-Consistency is a generalization of path consistency. A set of k values need to be consistent. It may lead to a faster solution but checking for k-consistency is computationally expensive with exponential time in the worst case.

In practice, arc consistency is most frequently used.

5.6.5 Constrain Propagation & Backtracking Search

Basic Idea: Each time a variable is assigned, a constraint propagation algorithm is run in order to reduce the number of choice points in the search. This can improve the speed of backtracking search further. This algorithm can be implemented using Forward Checking or AC-3.

5.7 Local Search for CSPs

Necessary Modifications for CSPs:

- work with complete states
- allow states with unsatisfied constraints
- operators reassign variable values

Min-Conflicts Heuristic:

- Randomly select a conflicted variable
- Choose the value that violates fewest constraints
- Hill climbing with $h(n) = \#$ of violated constraints

Performance:

- Can solve randomly generated CSPs with a high probability
- Except in a narrow range $R = \frac{\# \text{ of constraints}}{\# \text{ of variables}}$

5.8 Problem Decomposition

Assume search space for a constraint satisfaction with **n variables**, each of which can have **d values** $= O(d^n)$

Basic Idea: Decompose the problem into subproblems with **c variables** each

- Each problem has complexity $O(d^c)$
- There are n/c problems \rightarrow total complexity $O(n/c \cdot d^c)$
- Unconditional independence is rare

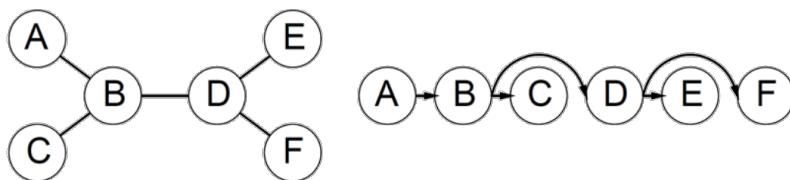
This can reduce the total complexity from exponential to linear, assuming c is constant.

5.9 Tree-Structured CSPs

A CSP is tree-structured if in the constraint graph any two variables are connected by a single path. Any tree structured CSP can be solved in linear time in the number of variables $= O(n \cdot d^2)$

5.9.1 Linear Algorithm

1. Choose variable as root, order nodes so that parent always comes before its children (only one parent per node)
2. For $j = n$ downto 2
 - Make the arc (X_i, X_j) arc-consistent, calling `remove_inconsistent_value(X_i, X_j)`
3. For $i = 1$ to n
 - Assign to X_i any value that is consistent with its parent



5.9.2 Nearly Tree-Structured Problems

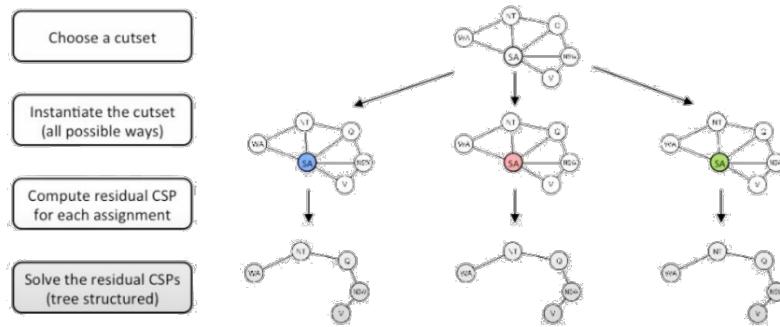
Tree structured problems are rare.

Approaches for making them tree-structured:

1. **Cutset Conditioning:**
 - Removing nodes so that the remaining nodes form a tree
2. **Collapsing nodes together:**
 - Decompose the graph into a set of independent tree-shaped subproblems

Cutset Conditioning

1. Choose a subset S of the variables such that the constraint graph becomes a tree after removal of S (cycle cutset)
2. Choose a consistent assignment of variables for S
3. Remove from the remaining variables all values that are inconsistent with the variables of S
4. Solve the CSP problem with the remaining variables
5. If no solution: Choose different S in **2**



6 Logic & AI: Propositional Logic

Search Algorithms only evaluate states, but do not have an "understanding" of the environment. This does mean, that a goal might not even be able to exist logically, but the search algorithms will still search for it.

Propositional Logic aims to improve on that aspect.

6.1 Logic

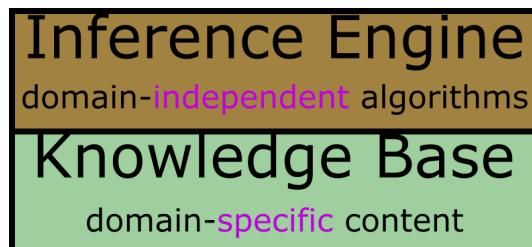
Logic is the key behind any formal knowledge. It allows to filter necessary information from a set of information and to draw conclusions. In AI, any representation of knowledge is based on logic.

Knowledge Base (KB)

A knowledge base represents actual facts which exist in the real world. It is a central component of any knowledge-based agent. It is a collection of "sentences" in a formal language which describe the information related to the world.

Inference Engine

The inference engine is responsible for inferring new knowledge from the knowledge base. It is a central component of any knowledge-based agent.



Knowledge-Based Agents

A knowledge-based agent is a type of **intelligent agent** that uses a knowledge base and an inference engine to make decisions.

```
1 kb; // The knowledge base           t; // counter, indicating time
2 Function knowledge_based_agent(percept):
3   tell(kb, make_percept_sentence(percept,t));
4   action = ask(kb, make_action_query(t));
5   tell(kb, make_percept_sentence(action,t)) t++;
6   return action
```

- Represent states, actions...
- Incorporate new percepts and update knowledge base
- Deduce properties of the world and make decisions / actions

6.2 Syntax

A sentence in propositional logic follows the **Backus-Naur Form (BNF)**:

Symbol:	P, Q, R,...	Descriptor of a sentence
Sentence:	True False Symbol \neg (Sentence) (Sentence \wedge Sentence) (Sentence \vee Sentence) (Sentence \Rightarrow Sentence)	Logical implication of a sentence

6.3 Semantics

Interpretation specifies which symbols are true and which are false. Given a interpretation it should be possible to evaluate a sentence.

A truth table defines semantics of operators:

a	b	$\neg a$	$a \wedge b$	$a \vee b$	$a \Rightarrow b$
false	false	true	false	false	true
false	true	true	false	true	true
true	false	false	false	true	false
true	true	false	true	true	true

6.4 Tautology

A tautology is a sentence that is true for all possible interpretations.

P	Q	$P \vee Q$	$\neg P \wedge \neg Q$	$(P \vee Q) \vee (\neg P \wedge \neg Q)$
false	false	false	true	true
false	true	true	false	true
true	false	true	false	true
true	true	true	false	true

6.5 Logical Equivalence

Two sentences are **logically equivalent** if they have the same truth value for every setting of their propositional variables.

P	Q	$P \vee Q$	$\neg(\neg P \wedge \neg Q)$
false	false	false	false
false	true	true	true
true	false	true	true
true	true	true	true

Logical Law	Equivalence
Commutativity	$(a \vee b) \equiv (b \vee a)$ $(a \wedge b) \equiv (b \wedge a)$
Associativity	$((a \wedge b) \wedge c) \equiv (a \wedge (b \wedge c))$ $((a \vee b) \vee c) \equiv (a \vee (b \vee c))$
Double Negation Elimination	$\neg(\neg a) \equiv a$
Contraposition	$(a \Rightarrow b) \equiv (\neg b \Rightarrow \neg a)$
Implication Elimination	$(a \Rightarrow b) \equiv (\neg a \vee b)$
De Morgan's Laws	$\neg(a \wedge b) \equiv (\neg a \vee \neg b)$ $\neg(a \vee b) \equiv (\neg a \wedge \neg b)$
Distributivity	$(a \wedge (b \vee c)) \equiv ((a \wedge b) \vee (a \wedge c))$ $(a \vee (b \wedge c)) \equiv ((a \vee b) \wedge (a \vee c))$

6.6 Inference / Entailment

A sentence is **entailed** by the knowledge base if, for every setting of the propositional variables, for which knowledge base is true, the sentence is also true.

Assume 2 sentences, A and $A \Rightarrow B$:

A	B	Knowledge base
false	false	false
false	true	false
true	false	false
true	true	true

To find out whether a sentence A is entailed by knowledge base as simple algorithm can be used:

Basic Idea:

1. Go through all possible setting of the propositional variables
2. If knowledge base is true and A is false \Rightarrow return false
3. Else \Rightarrow return true

Problem: Not very efficient: The number of setting increases with $2^{\#}$ propositional variables

6.6.1 Principle of Non-Contradiction

"A cannot be $\neg A$ "

Two contradictionary statements cannot be true at the same time, as that would mean that anything could be true.

Example:

$\text{PetIsABird} \Rightarrow \text{PetCanFly}$

$\text{PetIsAPenguin} \Rightarrow \text{PetIsABird}$

$\text{PetIsAPenguin} \Rightarrow \neg(\text{PetCanFly})$

PetIsAPenguin

This would imply that a penguin can both fly and not fly. If you would work with this contradictionary predicate it could imply anything like:

$\text{PetCanFly} \vee \text{MoonMadeOfCheese} \equiv \text{True}$

6.7 Conjunctive Normal Form (CNF)

The CNF is a way to write any knowledge base as a single formula:

CNF Formula

$$(\dots \vee \dots \vee \dots) \wedge (\dots \vee \dots \vee \dots) \wedge \dots$$

- Can be a symbol x or $\neg(x)$ (**Literals**)
- Multiple facts in knowledge base are "AND"ed together

Example: $\text{RoommateWet} \Rightarrow (\text{RoommateWetOfRain} \vee \text{RoommateWetOfSprinklers})$

becomes

$(\neg(\text{RoommateWet}) \vee \text{RoommateWetOfRain} \vee \text{RoommateWetOfSprinklers})$

6.8 Modus Ponens

Modus Ponens allows to form new sentences from existing ones:

Assume two sentences, A and $A \Rightarrow B$: From this we can conclude the new sentence B .

6.8.1 Unit Resolution

Assume the sentences $l_1 \vee l_2 \vee \dots \vee l_k$ and $\neg(l_i)$.

From this we can conclude the new sentence: $l_1 \vee l_2 \vee \dots \vee l_{i-1} \vee l_{i+1} \vee \dots \vee l_k$

6.8.2 General Resolution

Assume two sentences $l_1 \vee l_2 \vee \dots \vee l_k$ and $m_1 \vee m_2 \vee \dots \vee m_n$ where for some i, j $l_i = \neg(m_j)$.

From this we can conclude the new sentence: $l_1 \vee l_2 \vee \dots \vee l_{i-1} \vee l_{i+1} \vee \dots \vee l_k \vee m_1 \vee m_2 \vee \dots \vee m_{j-1} \vee m_{j+1} \vee \dots \vee m_n$

The same literal may appear multiple times; these need to be removed.

6.9 Resolution

Satisfiable

There exists a model that makes the modified knowledge base true, i.e., the modified knowledge base is consistent.

To see if a knowledge base is satisfiable, one can use a resolution algorithm.

6.9.1 Resolution Algorithm

Basic Idea: CNF formula for modified knowledge base is satisfiable if and only if sentence A is **not entailed**. So to see if a sentence A is entailed we can simply add $\neg A$ to the knowledge base and see if it becomes inconsistent.

1. **Find** two clauses with complementary literals
2. **Apply** resolution
3. **Add** resulting clause (if not already there)
4. **Test**, if it results in the empty clause \rightarrow formula is not satisfiable

Special Case: Horn Clauses

Horn Clauses

Horn clauses are implications with only positive (no negations) literals:

$$\begin{aligned} X_1 \wedge X_2 \wedge X_4 &\Rightarrow X_3 \wedge X_6 \\ \text{True} &\Rightarrow X_1 \end{aligned}$$

To find out whether a literal X_j is entailed:

1. Start from known implications as far as possible
2. If X_j is reachable it is entailed

To increase efficiency of this approach we can maintain a count of how many implications are already known to reduce the necessary computations.

6.10 Limitations of Propositional Logic

- No notion of objects or relations:
 - Identifiers are merely suggestive, it does not necessarily mean that the implied objects and relations actually exist or are real.
 - To this end, every identifier might as well be a single letter $A, B \dots$

7 Logic & AI: First-Order Logic

As established before, Propositional Logic does not have any notion of relations or objects. This does of course limit the possible applications of Propositional Logic.

First-Order Logic (FOL) extends on propositional logic to allow for relations and objects.

Some commonly used terms in FOL and scientific papers:

Axioms

Basic facts about the domain, the "initial" knowledge base.

Theorems

Statements that are logically derived from axioms.

7.1 Elements in FOL

- **Objects:**

- Represent entities in the real world - Can be named accordingly: Person1, John, Earth...

- **Relations:**

- Represent relations between objects - Can be named accordingly: Has(·, ·), Is[Something](·)...

- Relations with only one object are called **Unary Relations or Properties:** Has[Something](·), Is[Something](·)...

- **Functions:**

- Functions refer to objects without a name

- E.g. Roommate(·) → Roommate(Person1) = Person2

- Can be used to encode integers and data structures:

- * $\text{succ}(0) = 1, \text{succ}(1) = 2, \text{succ}(2) = 3\dots$

- * $\text{tree}(\text{value1}, \text{tree}(\text{value2}, \dots), \text{tree}(\text{value3}, \dots))$

- Not specific to specific object: Roommate(Umbrella) is valid, but might be nonsensical

7.2 Quantifiers

Quantifiers can be used to refer to multiple objects at once.

Universal: For All \forall

Asserts that a statement is true for all objects.
 $\forall x : \text{Lion}(x) \Rightarrow \text{Cat}(x)$: All lions are cats

Existential: Exists \exists

Asserts that a statement is true for at least one object.
 $\exists x : \text{Cat}(x) \Rightarrow \neg(\text{Lion}(x))$: At least one cat is not a lion

$\forall x : A$ is equivalent to $\neg(\exists x : \neg(A))$.

7.3 Substitution

Substitution: SUBST(·)

The SUBST method replaces one or more variables with something else in a sentence.

Example:

$$\begin{aligned} \text{SUBST}(\{x / \text{John}\}, \text{IsHealthy}(x) \Rightarrow \neg(\text{HasACold}(x))) \\ \text{becomes} \\ \text{IsHealthy}(\text{John}) \Rightarrow \neg(\text{HasACold}(\text{John})) \end{aligned}$$

7.3.1 Instantiating Quantifiers with SUBST

Universal \forall

Assuming a statement $\forall x : A$ we can obtain a new clause for **any** concrete **ground term g**:
 $\text{SUBST}(\{x / g\}, A)$

Example:

$$\begin{aligned} \forall x : x > 0 \Rightarrow x^2 > 0 \\ \text{Substituting any concrete ground term } g, \text{ in this} \\ \text{case } g = 3, \text{ yields:} \\ \text{SUBST}(\{x / 3\}, x > 0 \Rightarrow x^2 > 0) = \\ 3 > 0 \Rightarrow 3^2 > 0 \end{aligned}$$

Existential \exists

Assuming a statement $\exists x : A$ we can obtain a new clause for **only one Skolem constant k**:
 $\text{SUBST}(\{x / k\}, A)$

Example:

$$\begin{aligned} \exists x : x^2 = 9 \\ \text{In this case we do not assign a concrete value, but} \\ \text{assign a "placeholder", the } \text{Skolem constant } k, \\ \text{that can later be instantiated:} \\ \text{SUBST}(\{x / k\}, x^2 = 9) = k^2 = 9 \end{aligned}$$

Skolem Constant

Important:

- k is a constant, that does not appear elsewhere in the knowledge base
- The result of $\text{SUBST}(\{x / k\}, A)$ is a clause that **replaces** the original clause, as they are **equivalent**
-

One must act carefully when Instantiating existentials **after** universals:

Assume the statement $\forall y \exists x : \text{Parent}(x, y)$: "Every person y has a parent x".

Correct Instantiation:

1. Choose a specific person y - Let's say $y = \text{John}$
2. The statement then becomes $\exists x : \text{Parent}(x, \text{John})$: "John has a parent x".
3. We can now substitute x with a skolem constant k_{John} to get a more specific sentence: $\text{Parent}(k_{\text{John}}, \text{John})$: "John has a parent k_{John} ".
4. Assigning a concrete value to k_{John} later on does not disturb this logic.

Incorrect Instantiation:

1. Assign x a skolem constant k
2. The statement then becomes $\forall y : \text{Parent}(k, y)$: "Every person y has a parent k". This would mean that every person y has **the same parent** k, which might not be correct.

7.4 Generalized Modus Ponens

7.4.1 Unification

Assume two sentences: $\forall x : \text{Loves}(\text{John}, x)$ "John loves everything" and $\forall y : (\text{Loves}_y, \text{Jane} \Rightarrow \text{FeelsAppreciatedBy}(\text{Jane}, y))$ "Jane feels appreciated by everything that loves her".

We can now use substitution:

1. $\{x / \text{Jane}\} \rightarrow \text{Loves}(\text{John}, \text{Jane})$
2. $\{y / \text{John}\} \rightarrow \text{Loves}(\text{John}, \text{Jane}) \Rightarrow \text{FeelsAppreciatedBy}(\text{Jane}, \text{John})$
3. As 1 fulfills the condition of 2, we can infer that $\text{FeelsAppreciatedBy}(\text{Jane}, \text{Jane})$

7.5 First-Order Conjunctive Normal Form

1. Convert to **Negation Normal Form**: Negation symbols only occur immediately before predicate symbols
2. If variable names are used twice within scopes of different quantifiers, rename one of them such that the name is not used elsewhere
3. **Skolemize statements**:
 - (a) Move quantifiers out, so that we got $\forall x_1, x_2 \dots \exists y_1, y_2 \dots : A$. Quantifiers only occur in the prefix, not inside conjuncts.
 - (b) Replace existentially quantified variables with skolem constants.
 - (c) Discard universal quantifiers
4. **Convert** into clause set

Example:

Assume the sentence: $\forall x, y : \text{eats}(x, y) \wedge \neg(\text{killed}(x)) \Rightarrow \text{food}(y)$ "Anything anyone eats and is not killed is food"

1. Eliminate Implications: $\forall x, y : \neg(\text{eats}(x, y) \wedge \neg(\text{killed}(x))) \vee \text{food}(y)$
2. Move negations inwards (De Morgan): $\forall x, y : \neg(\text{eats}(x, y)) \vee \neg(\neg(\text{killed}(x))) \vee \text{food}(y)$
3. Drop universal quantifiers: $\neg(\text{eats}(x, y)) \vee \neg(\neg(\text{killed}(x))) \vee \text{food}(y)$

Inference in FOL is **not decidable** but **semidecidable**. This means that we can not always conclude that a sentence is not entailed.

7.6 Prolog

Prolog (Programming in Logic) is a FOL based logic programming language.

It is based on three basic components:

- **Facts**: Statements that are unconditionally true. E.g.:
 - `cat(john)` "John is a cat".
 - `parent(john, tom)` "John is the parent of Tom"
- **Rules**: Conditional statements that define relationships. E.g.:
 - `animal(X) :- cat(X)` "X is an animal if X is a cat"
- **Queries**: Questions asked to the program to derive answers. If multiple answers are possible, Prolog will return one per iteration in order. E.g.:
 - `?- cat(tom)` "Is Tom a cat?"

7.6.1 Atoms and Variables

Atom	Variable
<p>A constant term that represents fixed values. It is denoted by lowercase letters.</p> <p>Not every constant is an atom: Numbers, empty lists, some constructs (e.g. <code>parent(john, tom)</code>) are not atoms but constant.</p>	<p>A term that represents unknown or general values. It is denoted by uppercase letters or <code>_</code>.</p>

7.6.2 Prolog as a Database

Prolog can be regarded as a standard relational database, that stores facts and rules, which can be accessed and manipulated using Prolog queries. One caveat is that prologs backtracking strategy to retrieve all queries can be inefficient.

7.7 Gödels Incompleteness Theorem

Gödel's Incompleteness Theorem states that in any formal arithmetic system, there exists a sentence that cannot be proven. This is due to the fact, that there is no formal system that is sufficiently powerful so that it is both **complete** (able to prove all statements within the system) and **consistent** (no contradiction exists).

8 Uncertainty

Up until now we assumed that every statement is either true or false (or unknown) and that every action taken behaves exactly as expected.

In the real world, this is not always the case. Agents almost never have access to the entire state (incomplete information).

This means that in many cases, **agents must deal with uncertainty**.

8.1 Probabilities

One way to deal with uncertainty is to use **probabilities**.

We can assign a probability to every event, to summarize effects of uncertainty, due to:

- **Laziness:**
 - Agent is too lazy to consider all possible outcomes and possible events
- **Theoretical Ignorance:**
 - Some things are impossible to know (e.g. Weather cannot be definitely predicted)
- **Practical Ignorance:**
 - Some things might just not be known about an event or situation (e.g. traffic conditions)

Probabilities often are not based on objective truths but rather **subjective beliefs**: A probability p means that I believe that the statement will be true in $p \cdot 100\%$ of cases.

- **Degree of Belief:** There is a traffic jam in 10% of the cases
- **Degree of Truth:** The street is 10% jammed (blocked off a bit)

Probability theory is about **degree of belief** not **degree of truth**.

8.1.1 Basics

The state or **sample space** Ω can be seen as a set of all **samples** ω :

$$\begin{array}{c} \Omega \\ \omega \in \Omega \end{array}$$

The **probability space** or probability model is a sample space with an assignment of probabilities to all samples:

$$\forall \omega \in \Omega : \exists P(\omega) : \sum_{\omega \in \Omega} P(\omega) = 1$$

An event A is any subset of the sample space:

$$\forall A \subseteq \Omega : \exists P(A) : \sum_{\omega \in A} P(\omega) = P(A)$$

8.1.2 Kolmogorov's Axioms of Probability

1. All probabilities are between 0 and 1

$$0 \leq P(A) \leq 1$$

2. Necessarily true proposition have probability 1, false propositions have probability 0

$$P(\text{true}) = 1, P(\text{false}) = 0$$

3. The probability of a disjunction is:

$$P(A \vee B) = P(A) + P(B) - P(A \wedge B)$$

4. Axioms restrict the set of beliefs that an agent can hold:

e.g. A and $\neg A$ cannot both be true.

Just as in logic, the violation of the axioms leads to inconsistent beliefs that may result in nonsensical or wrong conclusions and actions.

8.1.3 Random Variables

Specific events are often a bit complicated to work with. We can use **random variables** in combination with **atomic events** to map outcomes to atomic events:

Example: Roulette

- **Atomic Events:** Numbers 0-36
- **Random Variables:**
 - Red | Black
 - Odd | Even
 - High | Low (1-18 | 19-36)
 - Street | Square | Split
 - Dozens
 - ...

Then for every atomic event we can apply a random variable to check whether it is true (e.g. `red(36) = true`).

The probability of an event X taking a specific value x_i $P(X = x_i)$ is obtained by summing the probabilities of all atomic event ω that result in $X(\omega) = x_i$:

$$P(X = x_i) = \sum_{\omega: X(\omega) = x_i} P(\omega)$$

8.1.4 Propositions

A proposition is a disjunction of atomic events in which it is true:

$$\begin{aligned}(a \vee b) &\equiv (\neg a \wedge b) \vee (a \wedge \neg b) \vee (a \wedge b) \\ \rightarrow P(a \vee b) &= P(\neg a \wedge b) + P(a \wedge \neg b) + P(a \wedge b)\end{aligned}$$

Syntax of Propositions

- **Propositional or Boolean** random can be true or false
 - `hasUmbrella = true` is a proposition and can be written as `hasUmbrella`
- **Discrete** random variables (finite or infinite)
 - e.g. Weather is one of {sunny, cloudy, rainy, snow}
 - `Weather = rainy` is a proposition
 - Values must be mutually exclusive and exhaustive (All possible cases are covered by values)
- **Continuous** random variables (bounded or unbounded)
 - e.g. Temperature
 - `Temp = 25.5`, `Temp > 23` are propositions

8.2 Joint Distribution

A joint distribution is the probability of combined events e.g. The probability that $X = x$ and $Y = y$ is true:

$$P(x, y) \equiv P(X = x \wedge Y = y)$$

Applying this to a whole set we can obtain a **joint probability distribution truth table**:

Smoking	No	Benign	Malignant
No	0.768	0.024	0.008
Few	0.132	0.012	0.006
Many	0.035	0.010	0.005

Joint Probability Distribution of Smoking and Cancer

8.2.1 Marginalization

Often we don't want to talk about the joint distribution of two events, but get the marginal distribution of one event:

For any set of variables X and Y we can compute the probability

$$P(Y) = \sum_{i=1}^n P(x_i, Y)$$

Smoking	No	Benign	Malignant
No	0.768	0.024	0.008
Few	0.132	0.012	0.006
Many	0.035	0.010	0.005

Joint Probability Distribution of Smoking and Cancer

So for example:

$$P(Y = \text{few}) = P(\text{no}, \text{few}) + P(\text{benign}, \text{few}) + P(\text{malignant}, \text{few}) = 0.132 + 0.012 + 0.006 = 0.15$$

8.2.2 Conditional Probabilities

The probability of $X = x$ under the assumption that $Y = y$ is true:

$$P(x|y) = \frac{P(x \wedge y)}{P(y)} = \frac{P(x,y)}{P(y)}$$

The product rule yields an alternative representation for the joint probability:

$$P(x,y) = P(x|y) \cdot P(y) = P(y|x) \cdot P(x)$$

Expanding this onto the **Chain rule**:

$$\begin{aligned} P(X_1, \dots, X_n) &= P(X_1, \dots, X_{n-1})P(X_n|X_1, \dots, X_{n-1}) \\ &= P(X_1, \dots, X_{n-2})P(X_{n-1}|X_1, \dots, X_{n-2})P(X_n|X_1, \dots, X_{n-1}) \\ &= \prod_{i=1}^n P(X_i|X_1, \dots, X_{i-1}) \end{aligned}$$

8.2.3 Independence

X and Y are independent from another if one of the following is true:

- 1 : $P(X|Y) = P(X)$
- 2 : $P(Y|X) = P(Y)$
- 3 : $P(X|Y) = P(X)P(Y)$

Independent variables are not affected by the other variable. This reduces the amount of possible variables.

However, absolute independent variables are rare.

8.2.4 Bayes Theorem

$$\underbrace{P(x|y)}_{\text{Posterior}} = \frac{\overbrace{P(y|x)}^{\text{Likelihood}} \overbrace{P(x)}^{\text{Prior}}}{\underbrace{P(y)}_{\text{Marginalization}}}$$

- **Posterior:** Probability of hypothesis X after evidence Y
- **Likelihood:** Probability of evidence Y given hypothesis X is true
- **Prior:** Probability of the hypothesis X before considering evidence Y
- **Marginalization:** Probability of evidence Y

8.3 Uncertainty in AI

Joint distribution is done by enumerating everything:

- **Worst-Case Run Time:** $O(2^n)$
 - n = number of random variables
- **Space Complexity:** $O(2^n)$ = size of the table

Due to this we mainly use **independencies** to compress the representation.

9 Bayesian Networks

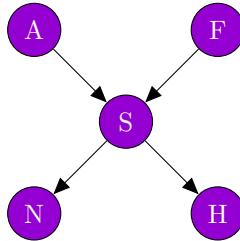
Bayesian Networks are a simple graphical notation for **conditional independence** assertions, hence for **compact specifications of full joint distributions**.

A Bayesian Network is **directed, acyclic graph** with

- **Nodes:** One node per variable
- **Edges:** A directed edge from node N_i to node N_j indicates that the corresponding variable X_i has a direct influence on X_j

Set of random variables $\{X_1, \dots, X_n\}$

Directed Acyclic Graph (DAG)



Conditional Probability Distribution (CPD)

- Each random variable X_i in the network is associated with a CPD given its parents ($Pa(X_i)$)
$$P(X_i|Pa(X_i))$$
- Each variable is probabilistically dependent on its parents

Joint Distribution:

$$P(X_1, \dots, X_n) = \prod_{i=1}^n P(X_i|Pa(X_i))$$

Local Markov Assumption:

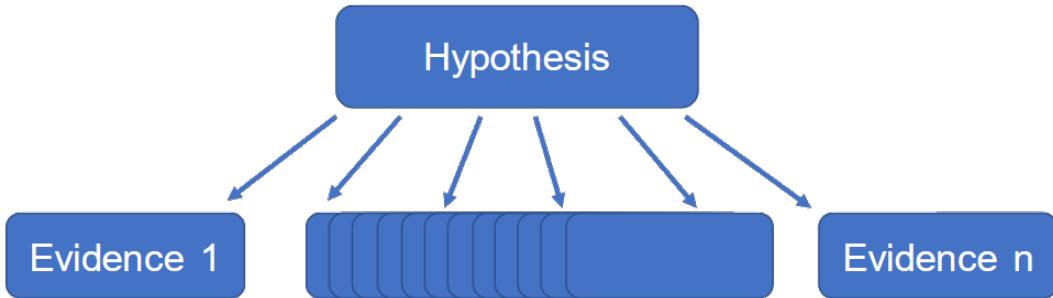
Each random variable X_i is conditionally independent of its non-descendants, given its parents.

$$X_i \perp \text{nonDescendants} | Pa(X_i)$$

9.1 Naïve Bayes

A **naïve Bayes** model assumes that all effects are independent given the cause:

$$P(\text{hypothesis}, \text{evidence}_1, \dots, \text{evidence}_n) = P(\text{hypothesis}) \cdot \prod_{i=1}^n P(\text{evidence}_i | \text{hypothesis})$$



9.2 Inference in Bayesian Networks

Query $P(X|e)$

Definition of conditional probability: $P(X|e) = \frac{P(X, e)}{P(e)}$

Up to normalization: $P(X|e) \propto P(X, e)$

Can be rewritten as:

$$P(Y) = \underbrace{\sum_{X_i \notin Y}}_{\text{Marginalization}} \underbrace{\prod_{i=1}^n P(X_i | Pa(X_i))}_{\text{BN Semantics}}$$

9.2.1 Variable Elimination

Given a Bayesian Network and a query $P(X|e)/P(X, e)$.

Instantiate evidence e .

Choose an elimination order over the variables X_1, \dots, X_n .

Initial factors of probability distribution comprised of: f_1, \dots, f_n .

For $i = 1$ to n , if $X_i \notin \{X, E\}$:

Collect factors f_1, \dots, f_k that contain X_i .

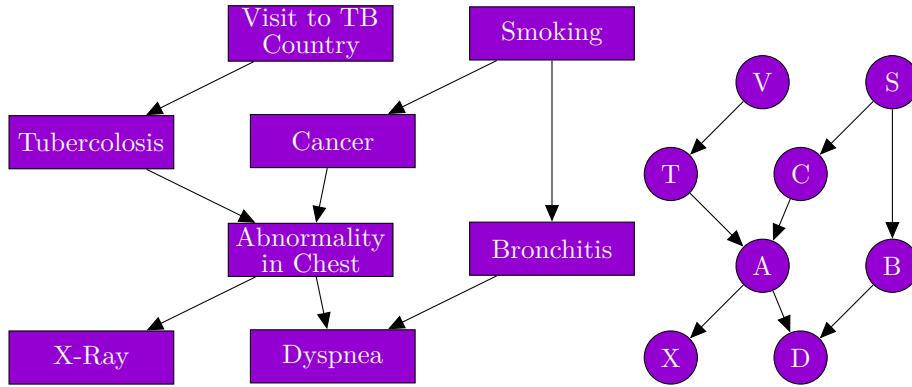
Generate a new factor by eliminating X_i from f_1, \dots, f_k :

$$g = \sum_{X_i} \prod_{j=1}^k f_j$$

Remove all factors f_1, \dots, f_k and add new factor g to the network.

Normalize $P(X, e)$ to obtain $P(X|e)$.

Example



Assume we want to compute $P(d)$, so we need to **eliminate** v, s, t, c, a, b, x .

The **probability distribution** is given as the product of multiple factors:

$$P(v, s, t, c, a, b, x, d) = P(v)P(s)P(t|v)P(c|s)P(b|s)P(a|c, l)P(x|a)P(d|a, b)$$

Lets choose the elimination order: v, s, x, t, c, a, b

From that we get:

$v \Rightarrow$	$P(v, s, x, t, c, a, b, d)$	$= P(v)P(s)P(t v)P(c s)P(b s)P(a c, l)P(x a)P(d a, b)$
$s \Rightarrow$	$P(s, x, t, c, a, b, d)$	$= f_v(t)P(s)P(c s)P(b s)P(a c, l)P(x a)P(d a, b)$
$x \Rightarrow$	$P(x, t, c, a, b, d)$	$= f_v(t)f_s(b, c)P(a t, c)P(x a)P(d a, b)$
$t \Rightarrow$	$P(t, c, a, b, d)$	$= f_v(t)f_s(b, c)f_x(a)P(a t, c)P(d a, b)$
$c \Rightarrow$	$P(a, b, d)$	$= f_s(b, c)f_x(a)f_t(a, c)P(d a, b)$
$a \Rightarrow$	$P(b, d)$	$= f_a(b, d)$
$b \Rightarrow$	$P(d)$	$= f_b(d)$

This unfortunately is not efficient.

Theorem

Inference (even approximate in Bayesien networks is NP-Hard)

9.2.2 Approximate Inference by Stochastic Sampling

Basic Idea:

1. Draw N samples from a sampling distribution S
2. Compute an approximate posterior probability \hat{P}
3. Show this converges to the true probability P

Draw samples

Given:

- Random Variable $X|D(X) = \{0, 1\}$
- $P(X) = \{0.3, 0.7\}$ ($P(X=0) = 0.3$, $P(X=1) = 0.7$)

Sample $X = P(X)$

- Get a random number $r \in [0, 1]$
- If $r < 0.3$ then $X = 0$
- Else $X = 1$

Can be generalized to any domain size.

Sampling from "Empty Network"

Ergo, generating samples from a network that has no evidence associated with it.

Basic Idea:

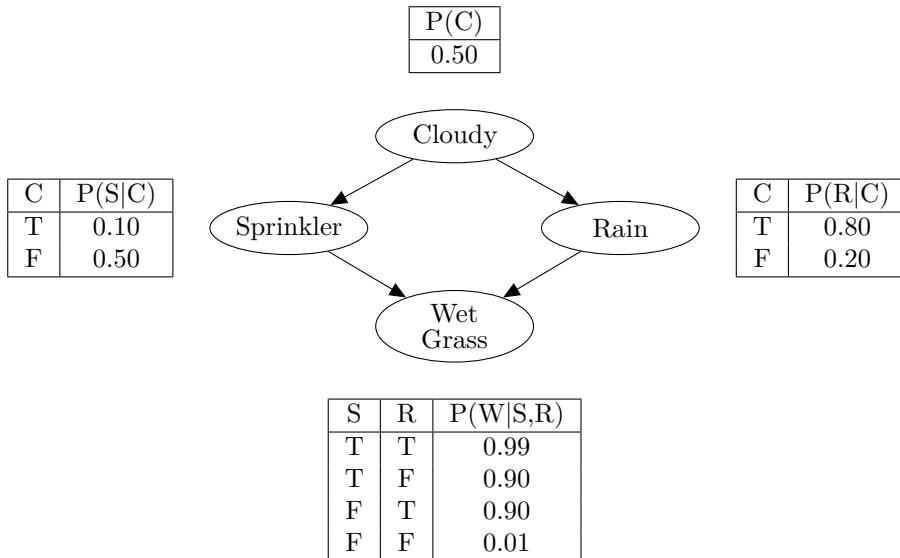
- Sample a value for each variable in topological (in respect to dependencies) order
- Using the specified conditional probabilities

```

1 // belief network specifies joint distribution  $P(X_1, \dots, X_n)$ 
2 Function prior_sample(belief_network) → event sampled from belief network:
3   x = event with n elements;
4   For  $i = 1$  to  $n$  do
5     |  $x_i$  = random sample from  $P(X_i | Pa(X_i))$  given the values of  $Pa(X_i)$  in x;
6   return x

```

Example:



Bayesian Network for Weather and Wet Grass

Probability Estimation using Sampling

Calculating a probability estimation:

- Sample many points using the algorithm above
- Count how often each possible combination x_1, \dots, x_n occurs

- Estimate the probability by the observed percentages

$$\hat{P}(x_1, \dots, x_n) = N_{PS}(x_1, \dots, x_n) / \text{number of samples}$$

This converges towards the joint probability function.

Markov Chain Monte Carlo (MCMC) Sampling

```

1 Function mcmc_ask(X,e,belief_network, num_samples) → estimate of P(X|e):
2   count_X = [] // number of times each X occurs, initially 0 for all
3   Z = [non-evidence variables] // list of non-evidence variables
4   x = e // current state of the network, initially e
5   initialize non-evidence values in x with random values;
6   // Gibbs sampling
7   For j=1 to num_samples do
8     ForEach Z_i ∈ Z do
9       x[Z_i] = sample from P(Z_i|markov_blanket(Z_i))
10    count_X[x] += 1 // x is the value of X in x
11  return normalize(count_X)

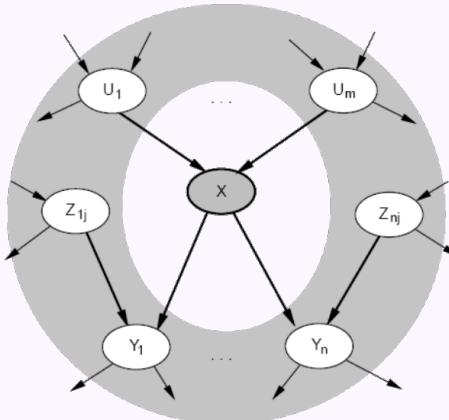
```

More samples result in better approximates.

Markov Blanket

A Markov Blanket is a set of variables that are conditionally independent of a variable given all other variables in the network. It consists of **parents (direct causes)**, **children (direct effects)** and **childrens parents (co-causes)**. Alternatively: A markov blanket includes all variables that **directly influence** or **are influenced** by a variable X . Everything outside of the markov blanket is irrelevant to X . This makes it easier to compute probabilities.

$$P(X|U_1, \dots, U_m, Y_1, \dots, Y_n, Z_{1j}, \dots, Z_{nj}) = P(X|\text{all variables})$$



Gibbs Sampling

Basic Idea:

1. **Initialize** all variables with random values
2. **Iterate through each variable**, updating it based on Markov Blanket
3. **Repeat** until samples converge to the true distribution

Gibbs Sampling utilized Markov Blankets by reducing the number of variables that need to be considered at each step.

Example:

Estimate $P(\text{Rain}|\text{Sprinkler} = \text{true}, \text{WetGrass} = \text{True})$

1. Sample Cloudy or Rain given its Markov Blanket, repeat n times
2. Count number of times Rain is true and false in the samples

E.g. sample 100 states and count 31 times Rain and 69 times not Rain.

$$P(\text{Rain}|\text{Sprinkler} = \text{true}, \text{WetGrass} = \text{True}) = \text{Normalize} < 31, 69 > = < 0.31, 0.69 >$$

Theorem

Chain approaches stationary distribution:

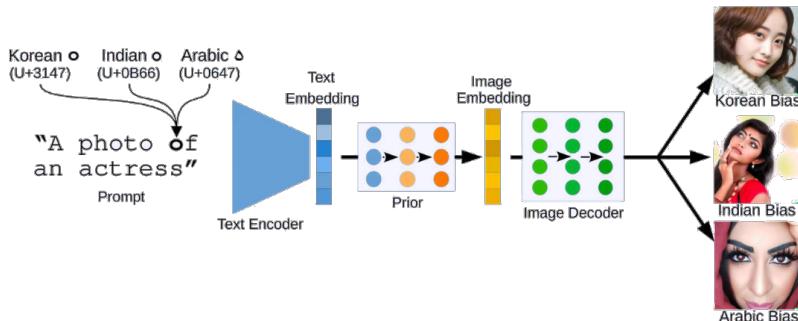
Long-run fraction of time spent in each state is exactly proportional to posterior probability.

10 Machine Ethics

10.1 Concerns

10.1.1 Biases

AI systems are inherently biased, because the data they're trained on is too. One small detail can yield entirely different results.



Bias in Text-to-Image

10.1.2 Data Privacy

Due to the large amounts of data an AI is usually trained on, it is almost inevitable that this data, and by extension the AI model, contains information that it shouldn't have. This may include leaked personal information and the likes, but also things like simply being able to recognize people it isn't trained for.

If we wanted to train a model to be able to recognize one specific person we also have to feed it data that doesn't contain that person. This causes the program to also be able to detect other persons.

10.1.3 Causal Reasoning without Causality

LLMs work on a mostly probabilistic basis. This means that they calculate the string of words that is most likely to correspond to the input. By doing this they mimic the causal reasoning of the data they're trained on, but do not actually employ causal connections.

This leads to a false sense of security when asking LLMs about factual information.

10.2 Mitigation of Concerns

10.2.1 Make AI systems aware of unwanted behaviour

We can try to mitigate the problem of biases by trying to train AI on data that is as unbiased as possible. This, of course, is incredibly hard to do, as AI models need a large amount of data, which is hard to moderate.

Another option is to implement filters. For example, we can implement a filter that makes it impossible to produce pornographic pictures of specific persons, or try to "rework" the result into something better.

Another thing we can do is **train models to be able to detect biases and concerns** (revision engine). Once again, this is hard to do, as first you need to find out what biases and concerns exist, and then train models to detect them and answer responsibly. This results in a long process, that is often still ongoing when an AI is deployed and continues until it is discontinued.

Often **reasoning** models are used for this. If we are able to make an AI be able to explain the reasoning behind its answer, it is more likely to detect when it is doing something it shouldn't.

11 Machine Learning & Neural Networks

11.1 Learning

Learning is an essential process for dealing with unknown environments. An agent is almost **never omniscient**.

Learning also makes an agent "aware" of their environment. Rather than trying to change the environment so that they can take their actions, they might **try to use and adapt to the environment** to fulfill their tasks.

Lastly, Learning improves the agents decision mechanisms the longer it is active. No longer will an agent repeat actions hoping for different results (e.g. local extrema).

11.1.1 Methods of Learning

Memorization (Declarative Knowledge):

Accumulates individual facts and their outcomes. This is limited by the time to observe facts and memory to store facts.

Better: Generalization (Imperative Knowledge):

Deduce new facts from old facts. Limited by accuracy of deduction process, assumes relations between past and future.

11.1.2 Inductive Learning

Inductive learning is the simplest form of learning. It deduces a trend from examples.

Basic Idea:

- f is the (unknown) target function. $f(x)$ is then called the target
- Examples are defined in the form $(x, f(x))$ e.g. Weather data: (1, Rain)
- Use examples to find a hypothesis h such that $h \approx f$

Hypothesis h is **consistent** if $\forall x : h(x) = f(x)$.

Ockhams Razor

The **best explanation** is the **simplest explanation** that fits the data

Overfitting Avoidance

Maximize the combination of consistency and simplicity.

11.2 Machine Learning

Programming an algorithm to automatically learn a program from data or experience.

Machine Learning is **not synonymous** with AI. Many AI algorithms are based on Machine Learning, but not all.

11.2.1 Machine Learning & Human Learning

Human learning is often

- very data- and knowledge efficient
- a complete multitasking, multi-modal system
- time-inefficient

Machine learning is often inspired by human learning, the goal however, is not to recreate human learning.

- May borrow ideas from human learning (e.g. neural networks)

- May perform better or worse

11.2.2 Designing a Learning System

Machine Learning is not the solution to every problem!

1. Do I need a learning approach for my problem?

- Is there a pattern to detect?
- Can I solve the problem analytically?
- Do I have data to train on?

2. What type of problem do we have?

- How to represent it?
- Which algorithm to use?

3. Gather and organize data

- Preprocessing is important

4. Fitting / Training your model

5. Optimization

6. Evaluate and iterate back to step 2

11.2.3 Types of Learning

Supervised Learning

Learning based on labeled datasets. Learns to map inputs to outputs based on pairs in the dataset.

Unsupervised Learning

Learning based on unlabeled datasets. Searches for patterns and similarities in the data.

Reinforcement Learning

Agent acts and receives positive or negative reward. The agent learns to act in a way that maximizes the reward.

11.2.4 Supervised Learning

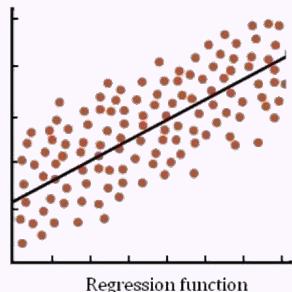
Given: Dataset $(x_1, y_1), \dots, (x_n, y_n)$

Goal: Find a function h such that $h(x_i) \approx y_i$

Regression Task

- y is a continuous value
- Example: Temperature tomorrow

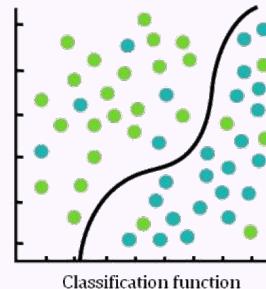
● instances



Classification Task

- y is a discrete class label
- Algorithm tries to predict a continuous value describing the label probability
- Example: Will it be above 0°C tomorrow?

● instances class 1
● instances class 2



11.2.5 Representation

Machine learning algorithms need to handle a lot of different data (e.g. images, audio, etc.).

To make this as easy as possible we represent our input as an **input vector** (in \mathbb{R}^n). Vectors are a great representation as we can transform the data using linear algebra.

Representation

Mapping input to another space, that is **easier** to manipulate.

Feature

Features are the **independent variables** in machine learning models.

Model

The representation of what our algorithm has learned from the data it used in training. The model is the **output representation** of the learned "rule set".

11.2.6 Feature Engineering

Feature engineering is the process of selecting, manipulating and transforming raw data into features that can be used for machine learning.

For this it is important to know your data:

- Data distribution
- Outliers
- Data reflective of reality
- Biased data

- ...

On the basis of these factors we can choose approaches that best fit our needs.

Regression:

- Linear Regression
- Multiple Linear Regression
- Regression Trees
- Non-linear Regression
- Polynomial Regression
- ...

Classification:

- Random Forest
- Decision Trees
- Logistic Regression
- Naïve Bayes
- Support Vector Machines
- ...

11.3 Evaluating a Model

To evaluate a model we need to know the goal we are trying to achieve.

Based on the goal we can use different evaluation metrics. These are the most common ones:

- Accuracy
- Precision
- Recall
- Mean Squared Error
- ...

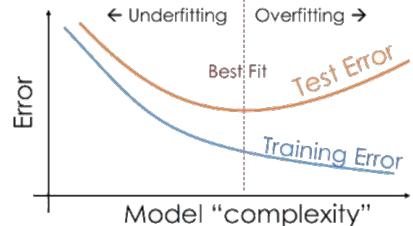
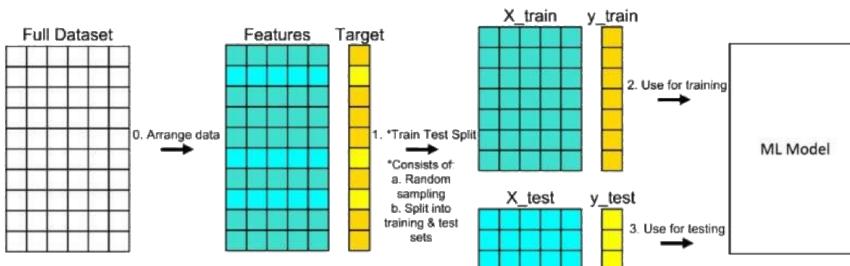
Which metric is best depends on the problem we are trying to solve.

11.3.1 Overfitting

Overfitting describes the problem, that a model is trained "too well" so that it's closer to memorization than generalization. This means that the model is not able to generalize to new data and therefore performs worse on new data.

To deal with overfitting we can:

- Splitting data
 - Split data into training and test data



- Regularization
- Use more data, augment data (adding noise)
- Select different features
- Cross validation
- Ensemble methods

11.4 Neural Networks

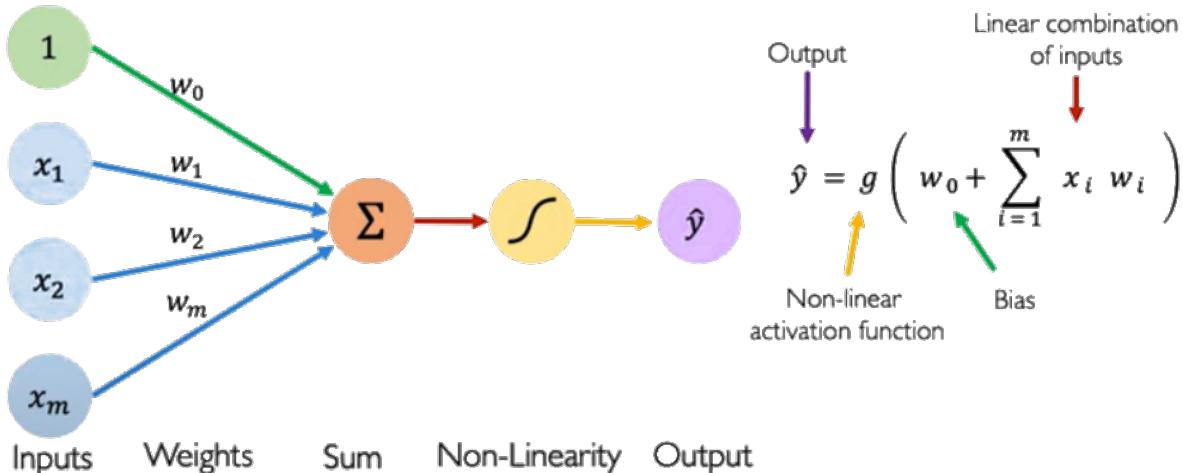
11.4.1 Deep Learning

Up until now we always had to supervise learning in some way, like feature extraction.

But with deep learning we can **learn the underlying features** directly from data without specifying them.

11.4.2 Perceptron

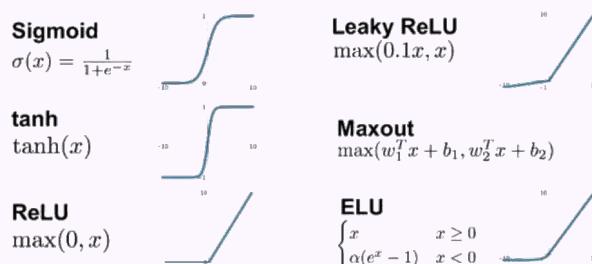
The perceptron can be seen as an **artificial neuron**. It takes multiple inputs, that are weighed individually and summed up to give a single output.



- Neurons correspond to nodes or units
- A link from unit j to unit i propagates activation y from j to i
- The weight $w_{i,j}$ of the link determines the strength and sign of the connection
- All weights together are called W or θ and describe the model
- The **total input activation** is the sum of the input activations
- The **output activation** is determined by the activation function g

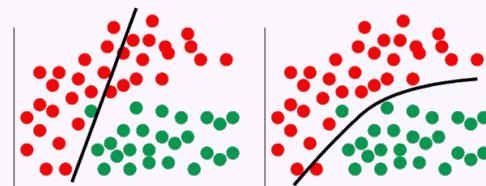
Activation Function

A activation function decides if a neuron should be active. Nowadays they're mostly non-linear.



Why do we need an activation function?

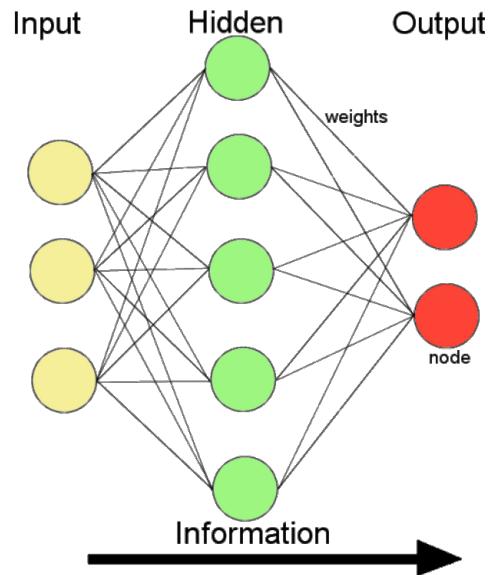
- It adds non-linearity to a neural network
- Without it we would have a linear regression model
- Allows for backpropagation



11.4.3 Perceptron to Neural Network

- Perceptrons may have multiple output nodes which can be combined to other perceptrons
- We can build networks of these nodes: **Multilayer Perceptron (MLP)**
- In a MLP information flow is **unidirectional**
- Information is distributed and processed in parallel
- For each node:

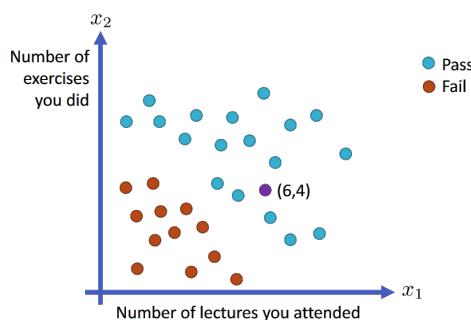
$$z_{k,i} = \sigma(w_{0,i}^k + \sum_{j=1}^{n_{k-1}} z_{k-1,j} \cdot w_{j,i}^k)$$



11.5 Forward Propagation

11.5.1 Applying a NN

Assume a distribution of an exam:

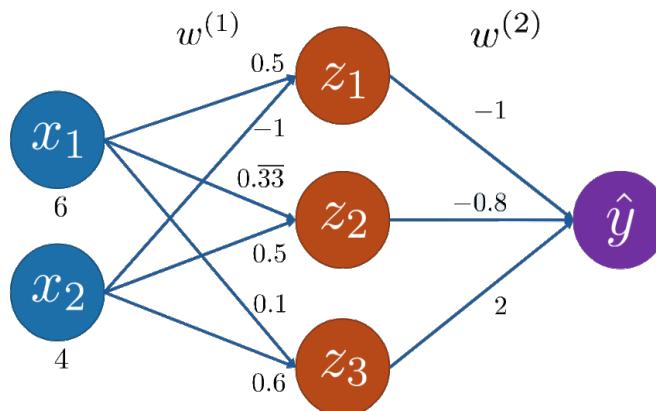


Assume the purple point is $x_1 = 6, x_2 = 4$ and the weights of our NN are:

$w_{1,1}^1 = 0.5$	$w_{2,1}^1 = -1$	$w_{1,1}^2 = -1$
$w_{1,2}^1 = 0.33$	$w_{2,2}^1 = 0.5$	$w_{2,1}^2 = -0.8$
$w_{1,3}^1 = 0.1$	$w_{2,3}^1 = 0.6$	$w_{3,1}^2 = 2$

Further assume a bias $w_{0,i}^k = 0$.

This yields a NN model:



From this we can calculate z :

$$\begin{aligned}
z_1 &= g\left(w_{0,1}^1 + \sum_{j=1}^2 x_j \cdot w_{j,1}^1\right) = g(x_1 w_{1,1}^1 + x_2 w_{2,1}^1) = g(3 + (-4)) = g(-1) \\
z_2 &= g(2 + 2) = g(4) \\
z_3 &= g(0.6 + 2.4) = g(3)
\end{aligned}$$

For the activation function g we use the sigmoid function:
$$g(x) = \frac{1}{1+e^{-x}}$$

This yields $z_1 = 0.26$, $z_2 = 0.98$, $z_3 = 0.95$.

To get the prediction \hat{y} we need to calculate the output activation:

$$\begin{aligned}
\hat{y} &= \sigma\left(w_{0,1}^2 + \sum_{j=1}^3 z_j \cdot w_{j,1}^2\right) \\
&= \sigma(w_{0,1}^2 + z_1 w_{1,1}^2 + z_2 w_{2,1}^2 + z_3 w_{3,1}^2) \\
&= \sigma((-1) \cdot 0.26 + (-0.8) \cdot 0.98 + 2 \cdot 0.95) \\
&= \sigma(0.856) = 0.7
\end{aligned}$$

With this we can conclude, that according to our model, the student has a 70% chance of passing the exam.

11.6 Backpropagation

Assume different weight than in the example above so that $\hat{y} = 0.14$.

Quantifying Loss

$$\mathcal{L}(f(x^i; \theta), y^i)$$

Describes the cost of incorrect predictions.

Empirical Loss

$$J(\theta) = \frac{1}{n} \sum_{i=1}^n \mathcal{L}(f(x^i; \theta), y^i)$$

Measures the total loss over the dataset. Also known as **objective function**, **cost function** or **empirical risk**.

Our goal is to **minimize the empirical loss**:

$$\theta^* = \arg \min_{\theta} J(\theta)$$

θ^* is the weight setting where the empirical loss is minimized.

This can be done using **Gradient descent**, as the **Weight space** is a N-dimensional space where N ist the total number of weights.

Algorithm:

1. Initialize weights randomly
2. Loop until convergence
 - Compute gradient $\frac{\partial J(\theta)}{\partial \theta}$
 - Update weights $\theta \leftarrow \theta - \alpha \frac{\partial J(\theta)}{\partial \theta}$ (with α learning rate)
3. Return weights

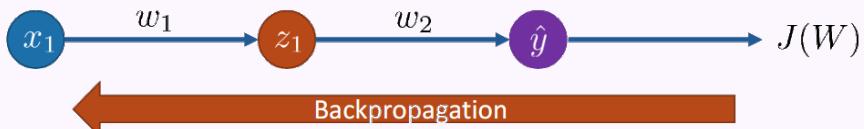
How to compute $\frac{\partial J(\theta)}{\partial \theta}$

Main Question: How much do the weights affect the outcome i.e. the final loss?
Using the chain rule we can describe the problem as:

$$\frac{\partial J(\theta)}{\partial w_2} = \frac{\partial J(\hat{y})}{\partial w_2} \cdot \frac{\partial \hat{y}}{\partial w_2}$$

$$\frac{\partial J(\theta)}{\partial w_1} = \frac{\partial J(\theta)}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z_1} \cdot \frac{\partial z_1}{\partial w_1}$$

We can repeat this for every weight in the network using the gradient from later layers: Propogate the error back to all nodes, through the network.



Example



Given $g = \text{ReLU}(x) = \max(0, x)$, $x_1 = 4$, $y = 1$, $\hat{y} = 2$, $\mathcal{L} = (\hat{y} - y)^2$, $J(\theta) = \mathcal{L}$

ReLU: Rectified Linear Unit

If x is greater than 0 return x else return 0.

Goal: $\frac{\partial J(\theta)}{\partial w_1} = \frac{\partial J(\theta)}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w_1}$

1. $\frac{\partial J(\theta)}{\partial \hat{y}} = 2(\hat{y} - y) = 2(2 - 1) = 2$ (Power rule)
2. $\frac{\partial \hat{y}}{\partial w_1} = \text{ReLU}'(w_0 + \sum_{i=1}^n w_i x_i) \cdot x_1 = 1 \cdot 4 = 4$
3. $\frac{\partial J(\theta)}{\partial w_1} = \frac{\partial J(\theta)}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial w_1} = 2 \cdot 4 = 8$

Now we also need to update the weights $\theta = \theta - \alpha \frac{\partial J(\theta)}{\partial \theta}$ (assume learning rate $\alpha = 0.05$):

$$\begin{aligned}\theta_{\text{new}} &= \theta_{\text{current}} - \alpha \frac{\partial J(\theta)}{\partial \theta} \\ \theta_{\text{new}} &= 0.5 - 0.05 \cdot 8 = 0.1\end{aligned}$$

Loss function in general are hard to optimize as its difficult to find a global minimum.

Basic Idea:

Change weight into the direction of the steepest descent of the error function given a step size - This step size is called the **learning rate α** , but finding a good value is hard.

