

COMPSCI4004/COMPSCI5087 AI (H/M)

Week 3: Solving Problems by Searching

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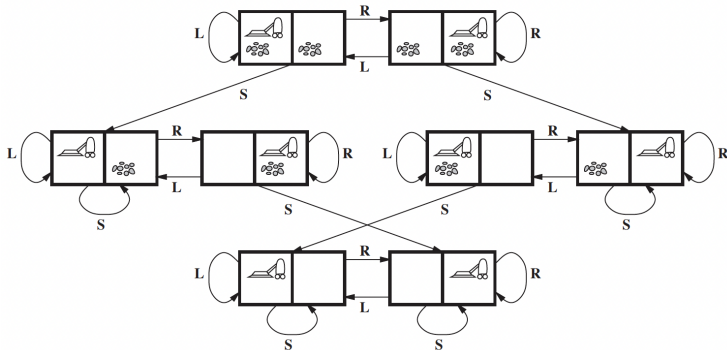
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November 11, 2025

Road Map

- ▶ Last week:
 - ▶ Looked at different agent types.
 - ▶ Recollect: Goal-based agents.
- ▶ This week, we will study:
 - ▶ A generic **state-transition based graph framework** to model a common class of problems.
 - ▶ Discuss **search strategies on these graphs** to solve the problems.
 - ▶ Uninformed Search → Informed Search
 - ▶ Designing Heuristics Functions
 - ▶ Stochastic search for Deterministic problems.
 - ▶ Introduce the coursework (which will be released this week).

State-Space



- ▶ The simple vacuum world.
- ▶ The state-space is **Discrete** and **Deterministic**.

State-Space

- ▶ **State:** A state is a particular snapshot of the environment.
- ▶ **Initial State:** The point from where we start our 'search' for the solution (the goal state).
- ▶ **Actions:** Possible ways to transition across states.
- ▶ **Transition Model:** The entire graph. May need to list some exceptions like 'sucking dirt from a clean room has no effect' (can you spot this in the graph?).
- ▶ **Path cost:** All actions cost equally (unweighted edges). Is this accurate for the vacuum world?

Menti Quiz

Join at menti.com using code "3334 0792".

Some more examples - 8 Puzzle

7	2	4
5		6
8	3	1

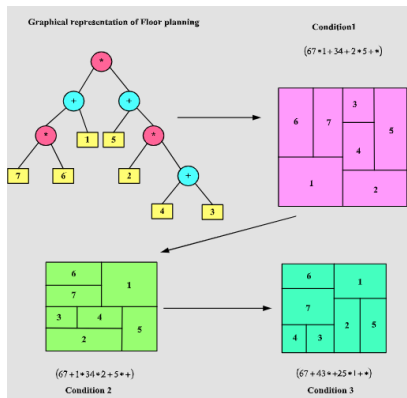
Start State

	1	2
3	4	5
6	7	8

Goal State

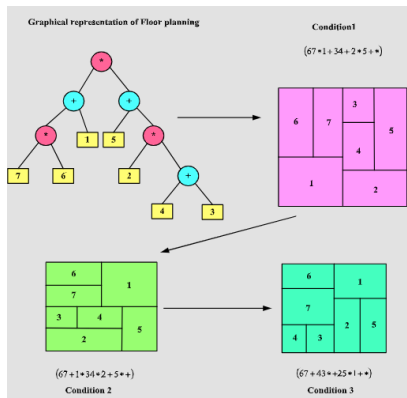
- ▶ **Action:** Left, Right, Up or Down.
'Left' could mean that you swap the tile to the 'right' with the blank tile; this means 'physically moving' the adjacent tile to its 'left'.
- ▶ **Transition Model:** Note that some actions can't be taken from some states, e.g., "right" can't be applied to the 'Goal state' shown.
- ▶ **Path cost:** Uniform? **Is this realistic?**

Some more examples - VLSI Floor Planning



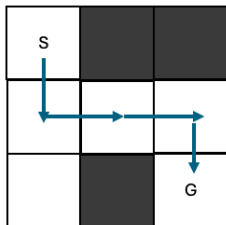
- **State:** A partial floor plan with blocks placed on a grid.
- **Action:** Place a new block, remove a block, transpose a block and so on.
- **Transition Model:** Captures **constraints** like some blocks **need to be adjacent** to others.
- **Path cost:** Uniform?

Some more examples - VLSI Floor Planning



- ▶ **State:** A partial floor plan with blocks placed on a grid.
- ▶ **Action:** Place a new block, remove a block, transpose a block and so on.
- ▶ **Transition Model:** Captures **constraints** like some blocks **need to be adjacent** to others.
- ▶ **Path cost:** Uniform?
- ▶ May be easier to try out transposing a block as compared to inserting or removing a block?

Maze navigation



- ▶ **State:** A partial path navigated through a maze.
- ▶ **Action:** Move *left*, *right*, *up* or *down* from a cell if there are no obstacles in the target cell.
- ▶ **Transition Model:** Captures **constraints** like obstacles.
- ▶ **Path cost:** Uniform? **Real life:** Need more effort to change a robot's direction than to keep on heading along the same direction?

State spaces may not always be finite!

- ▶ Generate a target integer with a sequence of $x!$, \sqrt{x} and $\lfloor x \rfloor$ functions, the only value of x being allowed is 4.
- ▶ Example solution:

$$\lfloor \sqrt{\sqrt{\sqrt{\sqrt{\sqrt{\sqrt{(4!)!}}}}} \rfloor} = \underbrace{5}_{\text{target integer}}$$

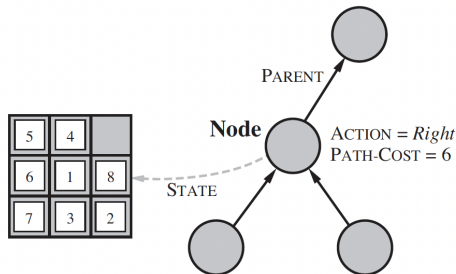
- ▶ What is the state space?
- ▶ What is the action space for this problem?

Finding a solution \equiv Searching a path to Goal



1. Root expanded
2. 1-level successors of root node expanded
3. 2-level successors of root node expanded
4. Note: Realise that we don't need to store the entire graph in memory because we can't do it if the state space is massive.
 - Think about an example state space that is massive.

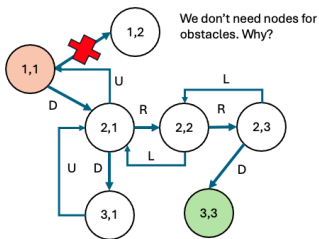
Nodes \equiv States + Book keeping data structures



- ▶ Each state is represented by a unique node.
- ▶ A node however contains additional generic information.
 - ▶ Links to children and parent (helps backtracking)
 - ▶ Edge information, e.g., the cost of the edge and the action type.

Transition Graph for Maze Navigation

(1,1) S	(1,2)	(1,3)
(2,1)	(2,2)	(2,3)
(3,1)	(3,2)	(3,3) G



- Find a path (without loops) from the start to one the goal nodes in this graph.
 - In general, there can be multiple goal nodes.

Uninformed (Blind) Search Strategies

- ▶ Search strategies that don't have any problem-specific information.
- ▶ Capable only of expanding the search tree (traversing the transition graph by generating successors).
- ▶ Can only distinguish a goal state from a non-goal one.
- ▶ We will study three algorithms under this category:
 - ▶ Depth-first Search (DFS) – LIFO
 - ▶ Breadth-first Search (BFS) – FIFO
 - ▶ Iterative Depth First Search (IDFS).

Breadth First Search



- ▶ From a node, generate children (if not already generated before) and add them to a FIFO queue.
- ▶ Remove from queue, and repeat unless goal state is reached.
- ▶ Hypothesis: Exhaust all k -sequence length action consequences before exploring $(k + 1)$ -sequence length ones.
- ▶ Pros:
 - ▶ Guaranteed to find solution if one exists.
 - ▶ Even **works on infinite state spaces** (can you see why?)

Breadth First Search

Space Complexity

- ▶ Let branching factor (average number of actions that can be taken from a state) be b .
 - ▶ For 8-puzzle and maze navigation: $b = 4$ (why?)
 - ▶ What about a VLSI floor planner?
- ▶ Number of children at depth $k = O(b^k)$.

Time Complexity

- ▶ Total #states visited (till depth k) = $b^0 + b^1 + \dots + b^k = O(b^{k+1})$.
 - ▶ Is BFS good for 8-puzzle?
 - ▶ What about a VLSI floor planner?

Breadth First Search

Space Complexity

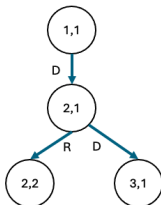
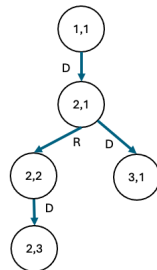
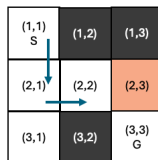
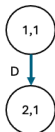
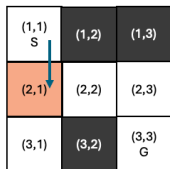
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Time Complexity

- ▶ Total #states visited (till depth k) = $b^0 + b^1 + \dots + b^k = O(b^{k+1})$.
 - ▶ Is BFS good for 8-puzzle?
 - ▶ What about a VLSI floor planner?
- ▶ BFS is excessively slow if the solution occurs somewhere deeper down the search space tree, or in other words you need a relatively **large number of actions to get to the goal state.**

BFS for the Toy Maze Example

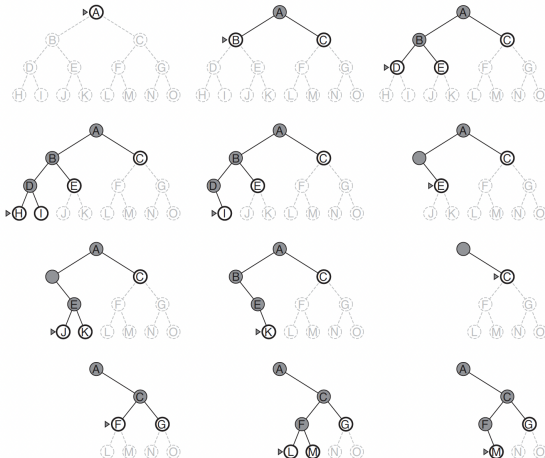
- Actions considered in order:
Right, Down, Left, Up.



Depth First Search

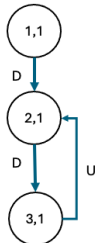
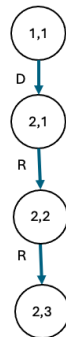
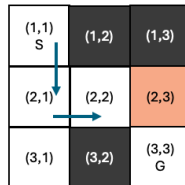
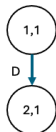
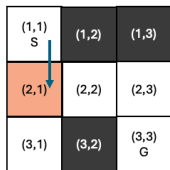
- ▶ From a node, generate children (if not already generated before) and add them to a LIFO queue (stack).
- ▶ Remove from queue, and repeat unless goal state is reached.
- ▶ Hypothesis: Continue expanding along a particular direction.
- ▶ Pros:
 - ▶ Can find a goal state quicker if the path to the goal state is considerably large (**alleviates the limitation of BFS**).
- ▶ Cons:
 - ▶ No guarantee to find a solution for infinite state spaces (**Why?**).

Depth First Search



DFS for the Toy Maze Example

- Actions considered in order:
Right, Down, Left, Up.



DFS/BFS Animation

Can we do better Uninformed Search?

Depth Limited Search

- ▶ Run a DFS to a maximum depth, say l .
- ▶ Intuition: Forces to backtrack and explore along other paths.
- ▶ Doesn't work if the shallowest goal's depth (d) is beyond the depth limit, i.e., $l < d$.
- ▶ What could be a reasonable depth limit for 8-puzzle?

Iterative Depth First Search (IDFS)

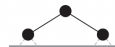
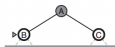
- ▶ Run a DFS to a maximum depth, say l .
- ▶ Repeat with $l \leftarrow l + 1$.
- ▶ Not sensitive to the choice of l .
- ▶ But has to repeat the exploration every time.

IDFS

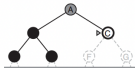
Limit = 0



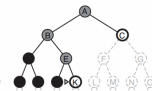
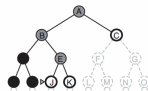
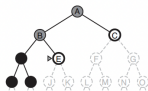
Limit = 1



Limit = 2



Limit = 3



Space Complexity Comparisons

Number of states required to be stored

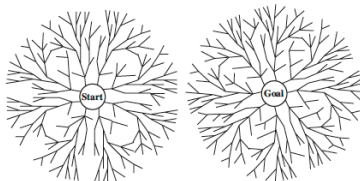
- ▶ BFS: $b^0 + b^1 + \dots + b^d = O(b^{d+1})$
- ▶ DFS: $O(bd)$ (only required to save the parent nodes along a path for backtracking)

Space Complexity Comparisons

Number of states required to be stored

- ▶ BFS: $b^0 + b^1 + \dots + b^d = O(b^{d+1})$
- ▶ DFS: $O(bd)$ (only required to save the parent nodes along a path for backtracking)
- ▶ IDFS: Same as DFS (why?)
 - ▶ What about the number of times a node is generated due to the multiple DFS calls in IDFS?
 - ▶ $(d)b + (d-1)b^2 + \dots + \underbrace{(d-i)b^{i-1}}_{\substack{\text{(\#times a node at i-th depth is generated)} \\ \text{\#nodes at depth i}}} + \dots (1)b^d = O(b^{d+1}).$

Bidirectional Search

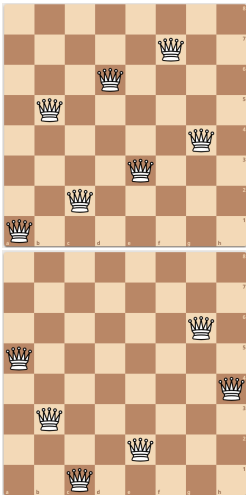


- ▶ Search both from the start and goal (usually BFS or IDFS **why?**), and hope to **meet in the middle**.
- ▶ If the goal is d -depth away, #states expanded = $b^{d/2+1} + b^{d/2+1} \ll b^d$ (for large d).
- ▶ Questions:
 - ▶ Can we use DFS as the forward or backward searches?
 - ▶ What should be done for multiple goal states?

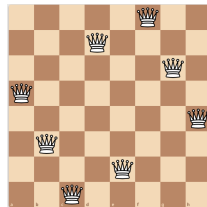
Informed (Heuristics-based) Search Strategies

- ▶ Search strategies that use **problem-specific knowledge** to **find solutions more efficiently**.
- ▶ Relies on two **key cost functions**:
 - ▶ Evaluation function $g(n)$ - How good is the current state or how much effort/cost did it take to reach here?
 - ▶ Evaluation function $h(n)$ - An estimate on how 'close' is this to the goal state?
 - ▶ As these are cost functions, we interpret them as: **lower the better**.

Good $g(n)$ does not imply good $h(n)$!



- ▶ 7 queens placed: better $g(n)$
- ▶ But no way to reach goal state from the position shown.
- ▶ 6 queens state admits a solution.



Two key search strategies

- ▶ **Greedy Best First** - Expands the node with the minimum $h(n)$, i.e., $f(n) = h(n)$.
- ▶ **A* search** - Minimizes the total estimated solution cost. i.e., $f(n) = g(n) + h(n)$.
- ▶ Note:
 - ▶ $g(n)$ is an exact function
 - ▶ $h(n)$ is only an approximation because if we had known the exact path to the goal, then there's nothing left to solve!

Best First Search

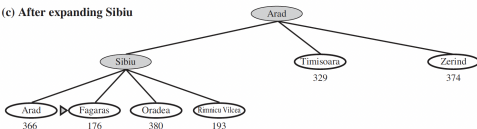
(a) The initial state



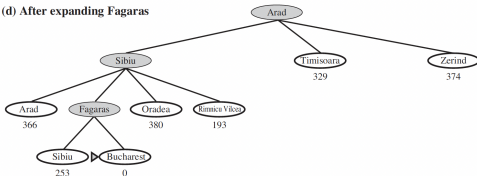
(b) After expanding Arad



(c) After expanding Sibiu



(d) After expanding Fagaras



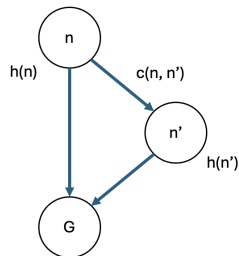
- Combines benefits of both BFS (exploit more, explore less) and DFS (explore more, exploit less).
- Not optimal because it ignores the cost that it took to reach the current node.
 - Example: There may be a shorter route from Timisoara (node not expanded) to Fagaras which is shorter than the distance from Sibiu to Fagaras.

A* Search

- ▶ Instead of using $h(n)$ use $g(n) + h(n)$ as the criteria to select a state for expansion.
- ▶ $g(n)$ is the cost from the root to node n .
- ▶ Balances: current cost (exploitation) + future cost (exploration).

Conditions for Optimality

- ▶ **Admissibility:** *Never overestimates* the cost to the goal (underestimation is good; **don't be pessimistic; better be optimistic!**).
- ▶ **Consistency:**
 $\forall a, h(n) \leq c(n, a, n') + h(n')$.



A* Search Implementation

- ▶ Like DFS and BFS, implemented by adding nodes to a queue (children states as candidates to be expanded later).
- ▶ Unlike DFS and BFS, the queue is no longer a LIFO/FIFO. Rather it is a **priority queue**.
- ▶ Standard data structure is a heap, with `extract_min` operation's time complexity is $O(\log N)$.
- ▶ The priority value is the cost $f(n) = g(n) + h(n)$, i.e., the cost it took to reach that node plus the estimated cost from there to reach the goal.

How to design good heuristics?

- ▶ Realise that the performance gains of A* over uninformed search strategies **depends on well-defined heuristics** functions.
- ▶ **Good heuristic function**: lets **explore promising paths** that **potentially lead to goal states much faster**.
- ▶ There is no single general heuristic function (or a class of such functions) that work for all discrete combinatorial optimization problems.
- ▶ Good heuristics are derived (logic and ingenuity) from the **knowledge about a problem task itself**.
- ▶ Of course, if you design a heuristics function you need to check if it is **admissible** and **consistent**. Just by being so, it doesn't always mean that it would be efficient in finding a goal state.

8-puzzle

7	2	4
5		6
8	3	1

Consider the two heuristics functions:

- ▶ h_1 : #misplaced tiles.
 - ▶ Admissible? Yes
 - ▶ You have to place each incorrect tile in its correct position and that will take at least one step.
- ▶ h_2 : Sum of L1 distance of each tile from its goal position.
 - ▶ Admissible? Yes
 - ▶ Each tile would need to go to its correct position in at least d steps, where d is the L1 distance between its current position and the goal.

Heuristics by Constraints-Relaxed Sub-problems

- ▶ $h_1 \equiv$ Cost to the goal state for the relaxed action space - swap a tile A with tile B.
- ▶ $h_2 \equiv$ Cost to the goal state for the relaxed action space - swap a tile A with tile B if they are adjacent.
- ▶ In general, #state transitions leading to a goal state of a relaxed sub-problem is a **good heuristic** for **any** actual problem task.
 - ▶ No more assumptions specific to a problem task like #misplaced tiles.
 - ▶ Just make the action space less constrained (quite easy to do).

Disjoint Pattern Databases for Heuristics

*	2	4
*		*
*	3	1

Start State

	1	2
3	4	*
*	*	*

Goal State

- ▶ Split a problem into disjoint subproblems, e.g., place the tiles '1, 2, 3, 4' in order without worrying about the other tiles (suppose they are not numbered).
- ▶ #steps to solution from start to goal of this relaxed subproblem is a good heuristic of the 8-puzzle.
 - ▶ **Homework:** Can you see why this is admissible/consistent?
- ▶ How to compute the heuristics?
 - ▶ Do a backward search from the goal state to one of the states of the relaxed subproblem
 - ▶ Save the states and the cost in a dictionary.

Finding a Heuristic may not always be easy!

- ▶ Generate a target integer with a sequence of $x!$, \sqrt{x} and $\lfloor x \rfloor$ functions, the only value of x being allowed is 4.

▶ Example: $\lfloor \sqrt{\sqrt{\sqrt{\sqrt{\sqrt{(4!)!}}}}} \rfloor = 5$

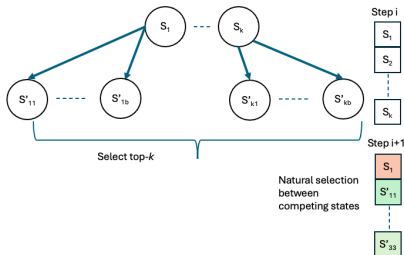
- ▶ Difficult to come up with an admissible heuristic, i.e., an $h(n)$ which never overestimates the cost to goal.

Stochastic Search on Discrete Deterministic Problems

- ▶ Looked at deterministic search algorithms that operate on Discrete Deterministic Problems.
- ▶ Main limitations -
 - ▶ Inefficient if branching factor is too high.
 - ▶ Efficiency mainly relies on the heuristics function that estimates the cost to goal.
- ▶ Using a **stochastic search** helps address these problems.
- ▶ We will cover:
 - ▶ Simulated Annealing
 - ▶ Beam Search
 - ▶ Genetic Algorithm

-

Beam Search

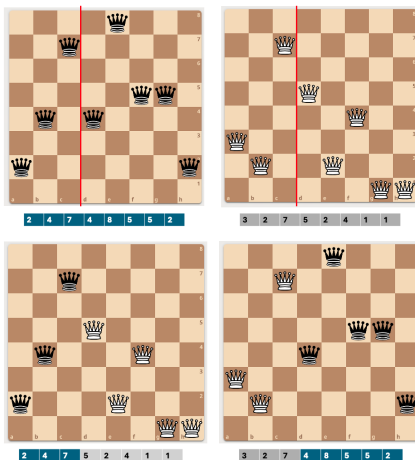


- ▶ SA keeps track of **only one state**. We can do better.
- ▶ Beam Search (BS) keeps track of k states (k - max-size of the queue).
- ▶ For each current state in the buffer S_i ($i = 1, \dots, k$)
- ▶ Generate all successor states $S'_{i,j}$ ($j = 1, \dots, b$) - b_i : branching factor from node S_i .
- ▶ Select the k best states from this candidate pool and repeat.
- ▶ Avg branching factor: kb .

Stochastic Beam Search

- ▶ **Stochastic Beam Search (SBS):** Uses the temperature (similar to SA) to define a probability of selecting a state with a lower 'goodness'.
 - ▶ Prob of selecting a worse state in the candidate pool:
 $\exp(\Delta E \times T)$
- ▶ Introduces more diversity in the state space exploration (otherwise local beam search can get focused on one region of the state space).
- ▶ Favours more exploration during the initial phase.

Genetic Algorithm



- ▶ SBS: Natural selection (asexual reproduction) with mutations.
- ▶ Variant of SBS, where successor states are generated by **combining two parent states** rather than by modifying a single state.

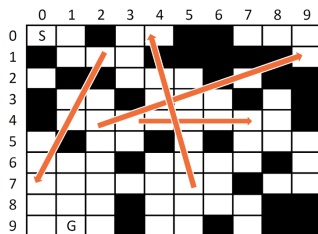
Genetic Algorithm (GA)

- ▶ Biological analogy:
 - ▶ SBS → asexual reproduction.
 - ▶ GA → sexual reproduction.
- ▶ Representation:
 - ▶ A population of **individuals** (states)
 - ▶ Individual represented by a string, each element a **gene**.
- ▶ Fitness (negative cost function):
 - ▶ Evaluate fitness function of the individual.
 - ▶ i.e. how likely are you (or your offspring) to survive?
 - ▶ **Fitness function for the 8-queen's problem?**

GA (Contd.)

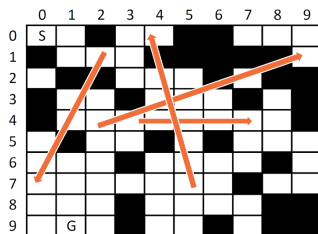
- ▶ Selection:
 - ▶ Select individuals to survive and also to perish. Different strategies but (usually) some form of stochastic selection depending on the fitness level.
- ▶ Crossover:
 - ▶ Have survivors mate and **mix genes**.
 - ▶ Combines parts of the goodness of the solutions.
 - ▶ Recall the relaxed subproblems in A* (Do you see an analogy?)
- ▶ Mutation:
 - ▶ Enforce some mutation of the genes (random changes in the encoded string), usually by a stochastic process.

A modified maze



- ▶ Modified transition graph.
- ▶ $\text{Right}(1, 1) \mapsto (7,0)$ - instead of $(1, 2)$
- ▶ Some wormholes are rewarding, e.g., $(1, 2)$ is rewarding. **Why?**
- ▶ Some are penalizing - e.g., wormhole at $(7,5)$.
- ▶ Which ones do you think work well?
 - ▶ DFS
 - ▶ BFS
 - ▶ IDFS

A modified maze



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- ▶ $\text{Right}(1, 1) \mapsto (7,0)$ - instead of $(1, 2)$
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- ▶ Some are penalizing - e.g., wormhole at $(7,5)$.
- ▶ Which ones do you think work well?
 - ▶ BFS
 - ▶ DFS
 - ▶ A*

Course-work Description

- ▶ Will be released this week.
 - ▶ Tip: Start working on it in an incremental manner.
- ▶ Will ask you to generate a random **maze with wormholes** on a **frozen lake** (code provided).
- ▶ What would be a performance measure in this environment?
- ▶ **Tasks:**
 - ▶ Implement your favorite maze navigation algorithm.
 - ▶ Explain your decision choices.
 - ▶ Conduct experiments and report observations to analyze the effects of you agent's performance measure on the following:
 - ▶ Density of wormholes.
 - ▶ Density of holes in the lake.
 - ▶ Uncertainty of actions, i.e., the slipperiness of the surface?