

CS2109S: Introduction to AI and Machine Learning

Lecture 2: Solving Problems by Searching

21 January 2024

DO NOT CLOSE YOUR POLLEVERYWHERE APP

There will be activities ahead

New Midterm Timing

- Date/Time: Tuesday, 4 March (Week 7), 6.30pm - 8.00pm
- Venue: MPSH 2A & 2B

Consultation

- **Walk-in:**
 - Office: COM2-02-06
 - If it's open, you can come in
 - If not and the light is on, you can knock
 - Highest availability: Tuesday, 12-3pm
- **Appointment:**
 - Send an email to rizki@nus.edu.sg



Muhammad **Rizki** Maulana

rizki@nus.edu.sg

Deep Reinforcement Learning

Consultation

- **Walk-in:**
 - Office: COM2-04-29
 - Monday, 2-4pm
- **Appointment:**
 - Send an email to cqtfpr@nus.edu.sg



Patrick Rebentrost
cqtfpr@nus.edu.sg
Quantum Machine Learning

For those who are just enrolled

- Please watch the recording or read lecture slides for Lecture 1
- **Important:** Course Policies (also available in Canvas)

Outline

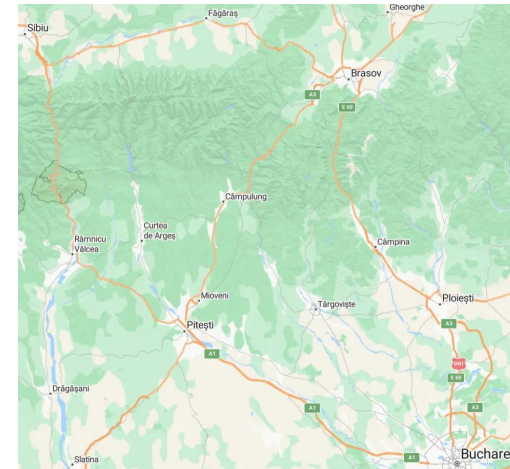
- Designing an Agent
 - Problem solving agents
 - Problem formulation
- Search
 - Uninformed Search
 - Breadth-first, depth-first, and uniform-cost search
 - Depth-limited and iterative-deepening search
 - Informed Search
 - A* search
 - Heuristics

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- **Designing an Agent**
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Preliminary: Search Problems

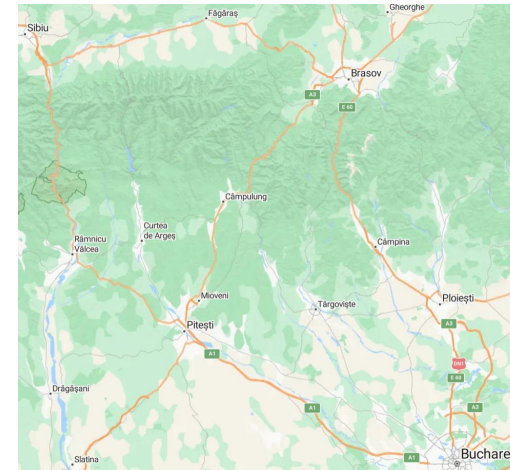
- A **search problem** refers to a type of problem where the goal is to find a state (or a path to a state) from a set of possible states by exploring various possibilities.
- Examples:
 - Path finding
 - Puzzle solving



9	1	3				5		
6		7					2	4
	5			8			7	
	7	9						
		2		9			4	3
					4		9	
	4				1	9		
7		6			9			5
		1			6	4		7

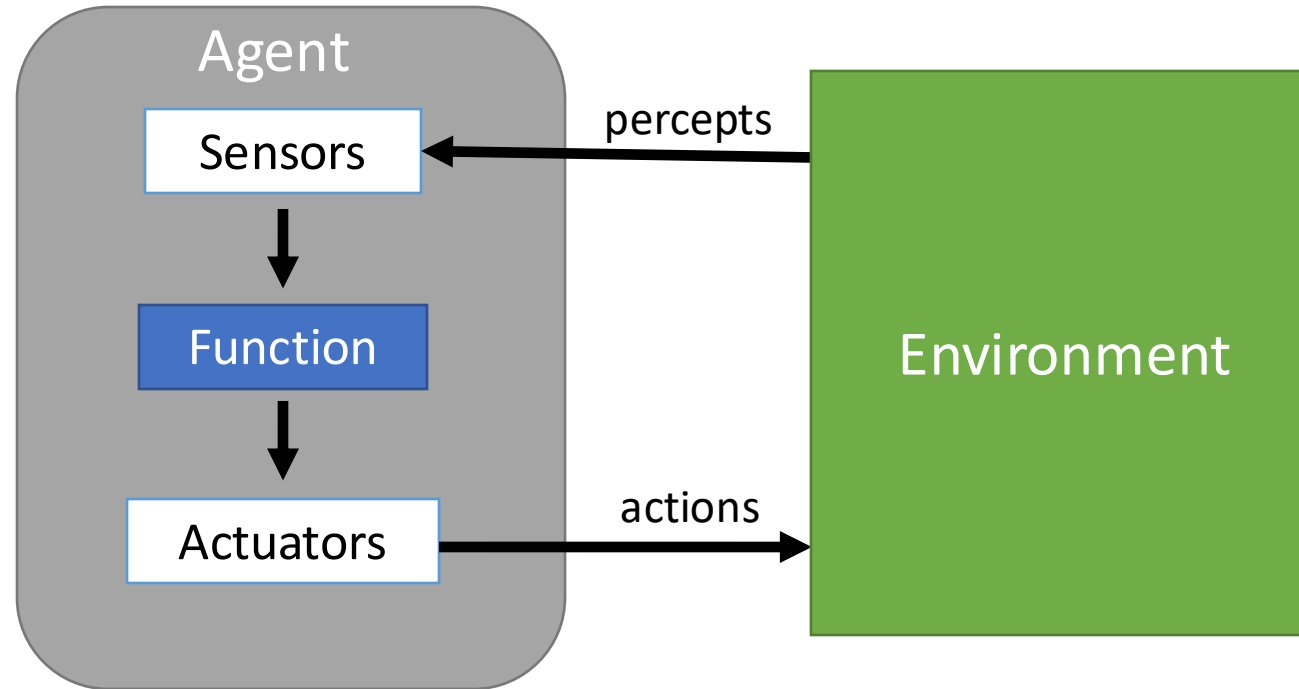
Preliminary: Search Algorithms

- A search algorithm takes in a search problem as input and returns a **solution** / **failure**.
- A **solution** of a search could be a **sequence of actions** or **final state**
 - An **optimal solution** is a solution with least cost, or least number of steps if there is no cost associated with actions
- Search algorithms
 - Linear search (bruteforce)
 - Dijkstra (CS2040S)
 - ...



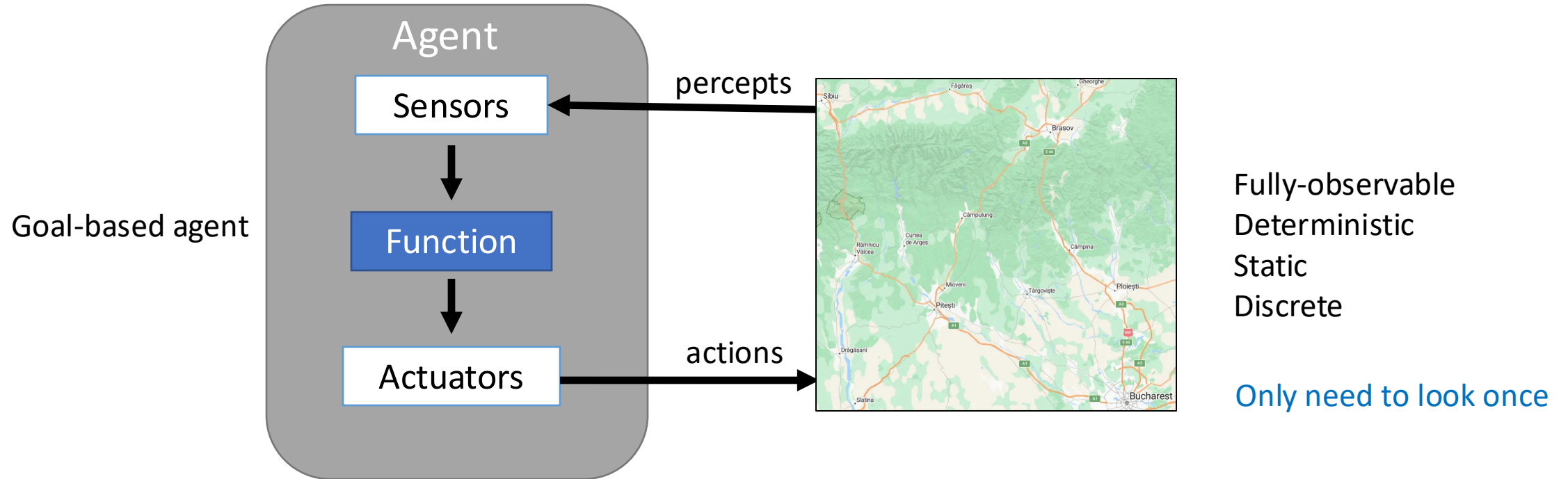
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Designing an Agent



Designing an Agent

for problems that can be solved by **searching**. E.g., path finding



How is search used by the agent?

Designing an Agent

To solve a problem using search, the agent needs to have:

- A goal, or a set of goals
- **A model of the environment**
- **A search algorithm**

Problem Solving Steps

What does the agent want? How does the world work? How to achieve it?



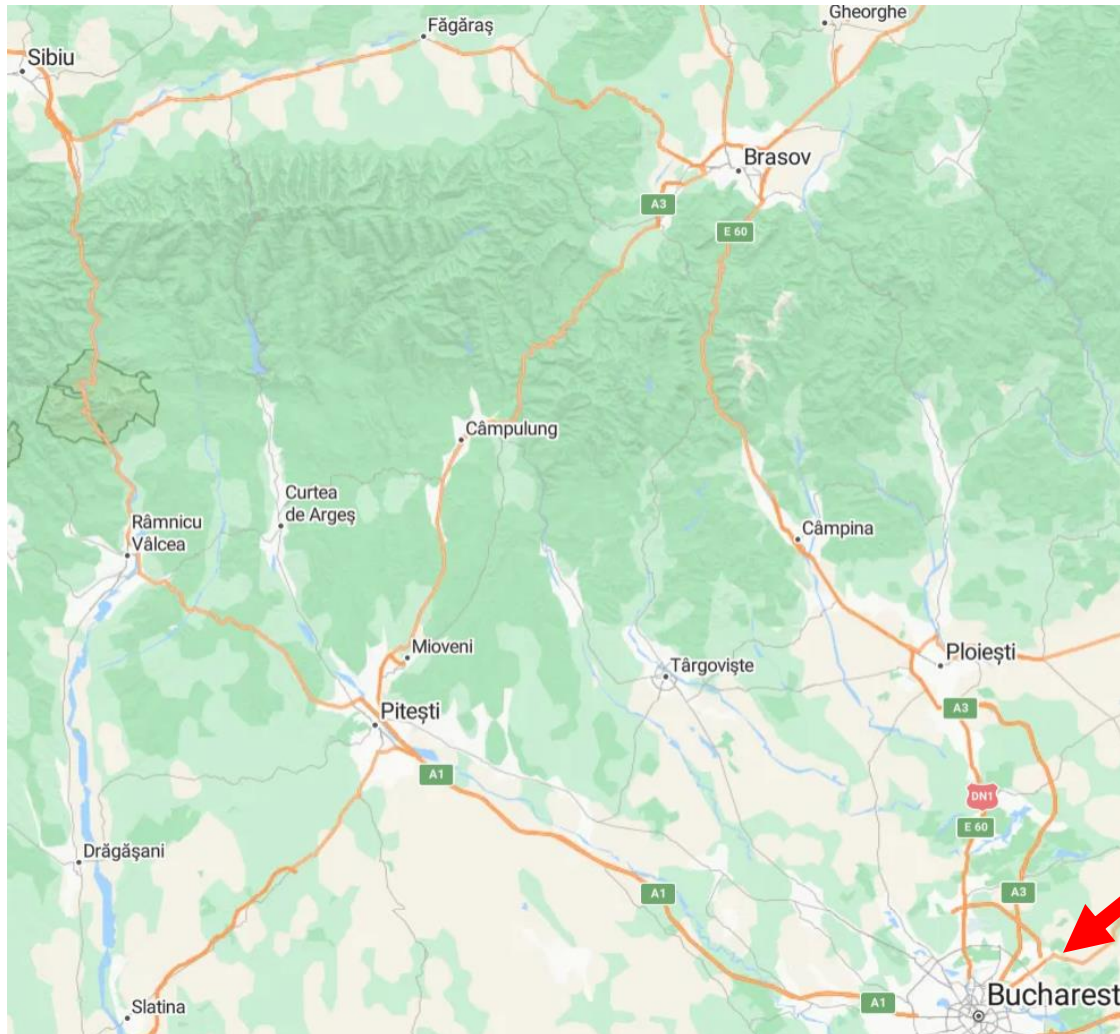
Example: Romania

Goal Formulation

Problem Formulation

Search

Execute



Go to Bucharest

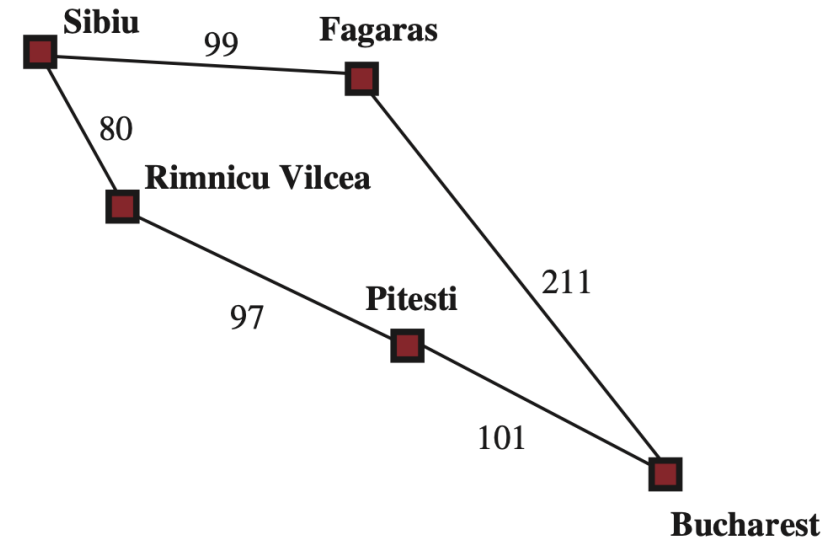
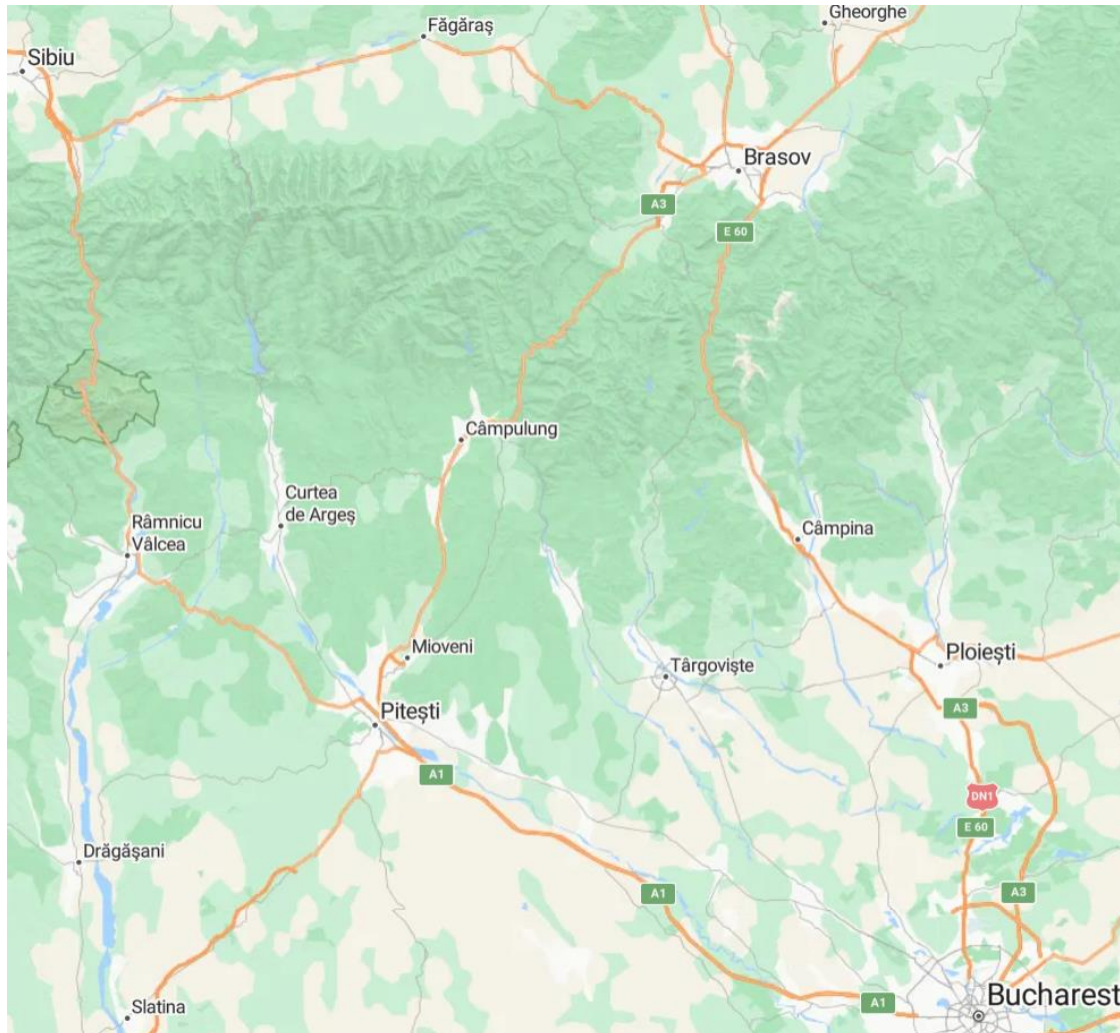
Example: Romania

Goal Formulation

Problem Formulation

Search

Execute



Problem Formulation

- States
- Initial state
- Goal state(s)/test
- Actions
- Transition model
- Action cost function

Cities: {at Sibiu, at Pitesti, ...}

at Sibiu

at Bucharest

Go to a neighboring city

Current state = selected city

See edges

Important facts

Goal Formulation

Problem Formulation

Search

Execute

Representation invariant: ensure that the *abstract states* have corresponding *concrete states*.

Goal test: Goal defined via a function such as *is_goal(state)*

Actions: a set *actions(state)* with size $|\text{actions}(\text{state})| \leq b$ (branching factor)

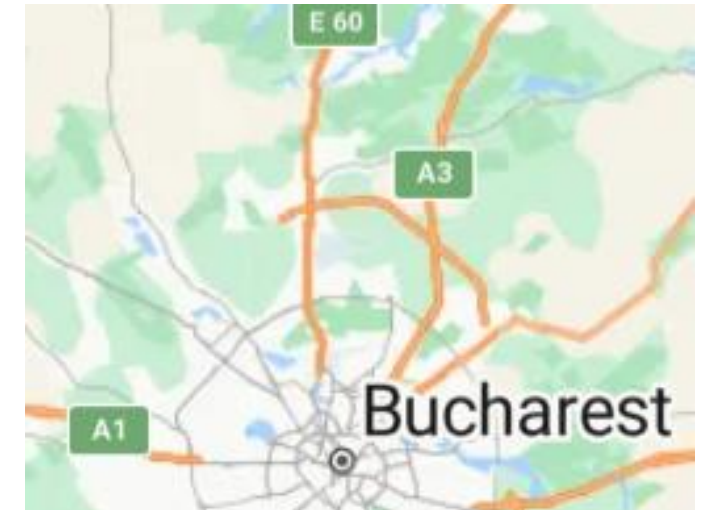
Transition model: *new_state = transition(state, action)*



Bucharest



Credit: Passport & Plates



Example: Sudoku

Goal Formulation

Problem Formulation

Search

Execute

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9x9 Integer Matrix

Problem Formulation

- States
All possible assignments of numbers to a 9x9 matrix
- Initial state
Partially filled matrix
- Goal state(s)/test
Check if all constraints are satisfied
- Actions
Fill matrix
- Transition model
Current state = filled matrix
- Action cost function
1

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- Designing an Agent
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- **Search**
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Review: Data structures

Required operations

- Add element ("add")
- Remove element ("pop")
- Is empty



Credit: freepik.com

Queue

First-in-first-out (FIFO)



Credit: freepik.com

Priority Queue

High-priority-first-out



Credit: iStock

Stack

Last-in-first-out (LIFO)

Search

AIAMA: tree search

```
create frontier
```

```
insert Node(initial_state) to frontier
```

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while frontier is not empty:
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```
    node = frontier.pop()
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    if node.state is goal: return solution
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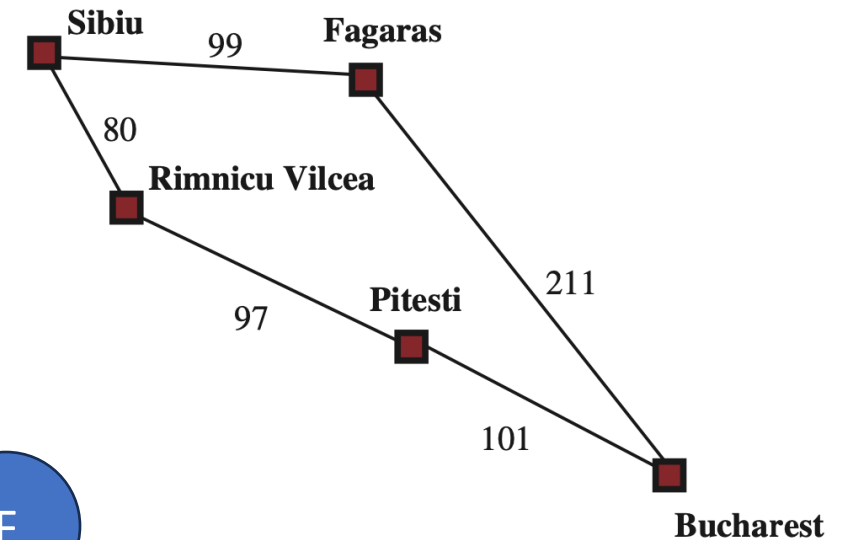
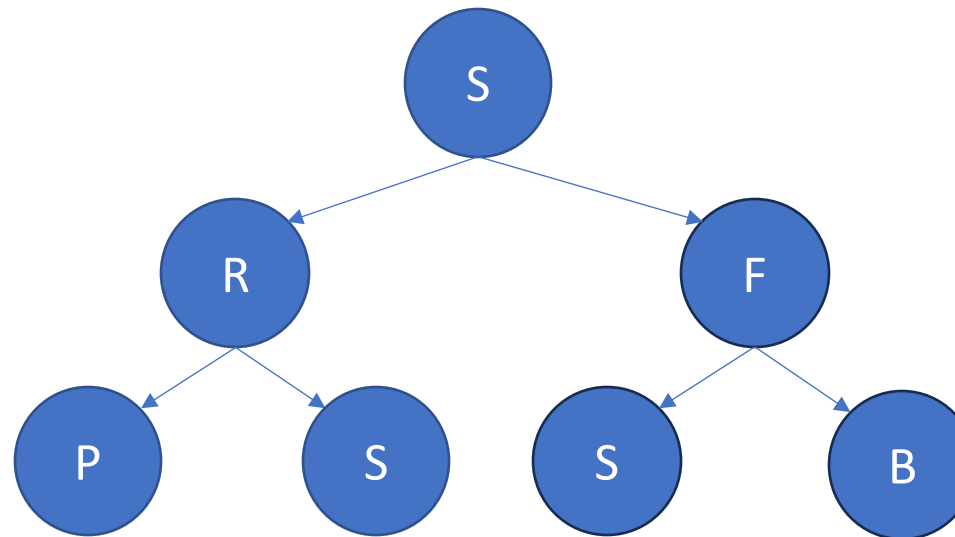
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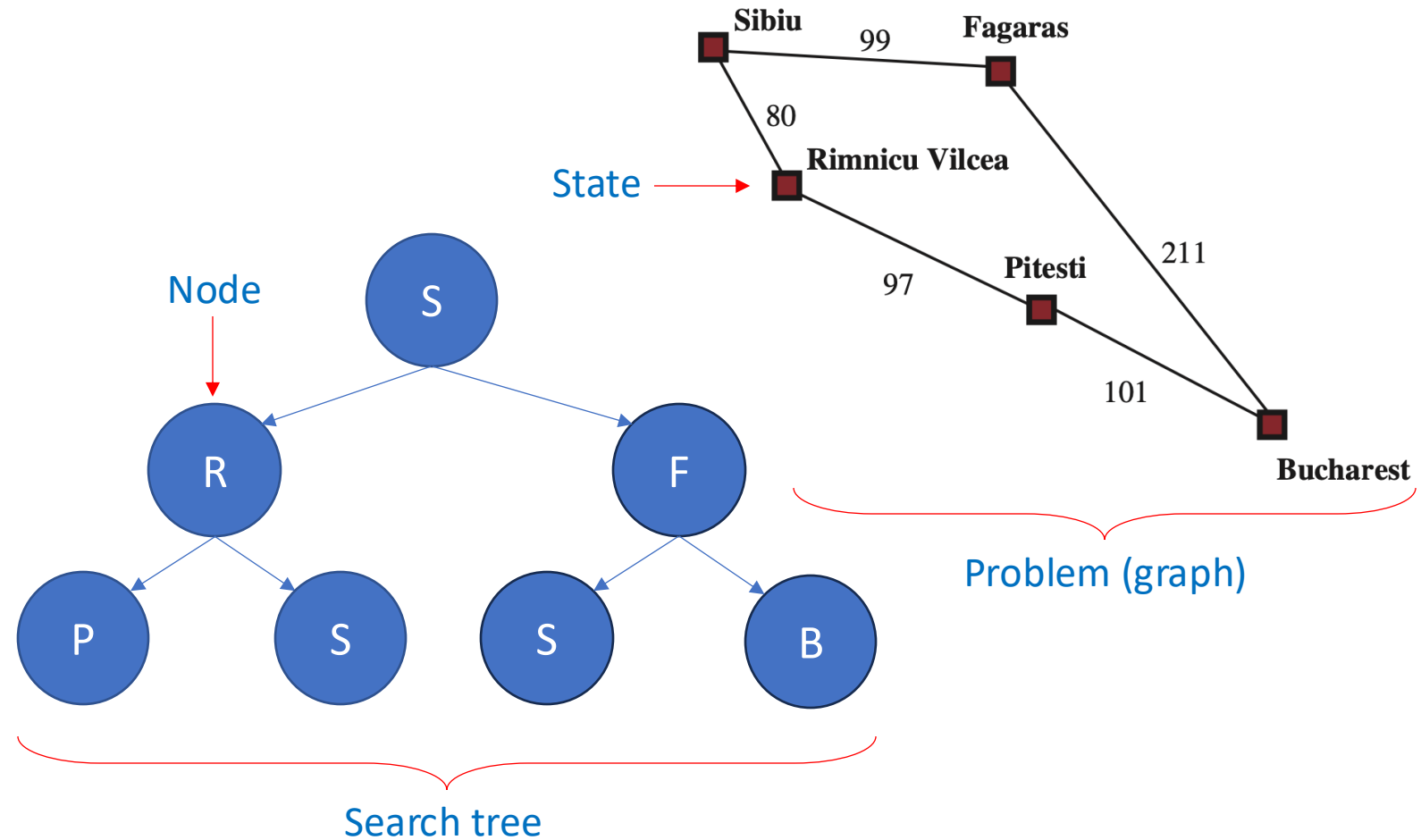
Can be queue, priority queue, stack
Frontier defines the search



Search Terms

Path cost is the cost of a path from any state to any state

Optimal path cost is the cost of the lowest-cost path from any state to any state



Evaluation Criteria

(Worst-case) Complexity:

- **Time complexity**: number of nodes generated or expanded
- **Space complexity**: maximum number of nodes in memory
- Measure: branching factor, optimal depth, maximum depth, ...

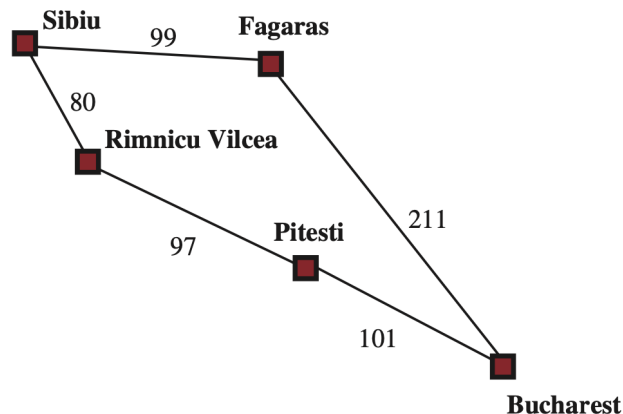
Disclaimer: CS2109S is not an algorithm-oriented course, so we will not discuss this in detail

Others:

- **Completeness**
- **Optimality**

Completeness and Optimality

- **Complete:** An algorithm is complete if, for every problem instance, it will find a solution if one exists. Conversely, an algorithm is incomplete if there exists at least one instance with a solution that the algorithm fails to find.
- **Optimal:** An algorithm is optimal if, for every instance where it produces a solution, that solution is the best possible. In other words, if the algorithm outputs a solution, it is guaranteed to be optimal.
- **Optimal and Incomplete:** An algorithm can be both optimal and incomplete. This means that there exists at least one instance where the algorithm fails to find a solution, even though, when it does find a solution, that solution is guaranteed to be optimal.



```
def search(state):  
    if state == "Fagaras":  
        return "go to Bucharest"  
    return None
```

Break

CAN YOU
SOLVE THE
RIVER CROSSING RIDDLE?

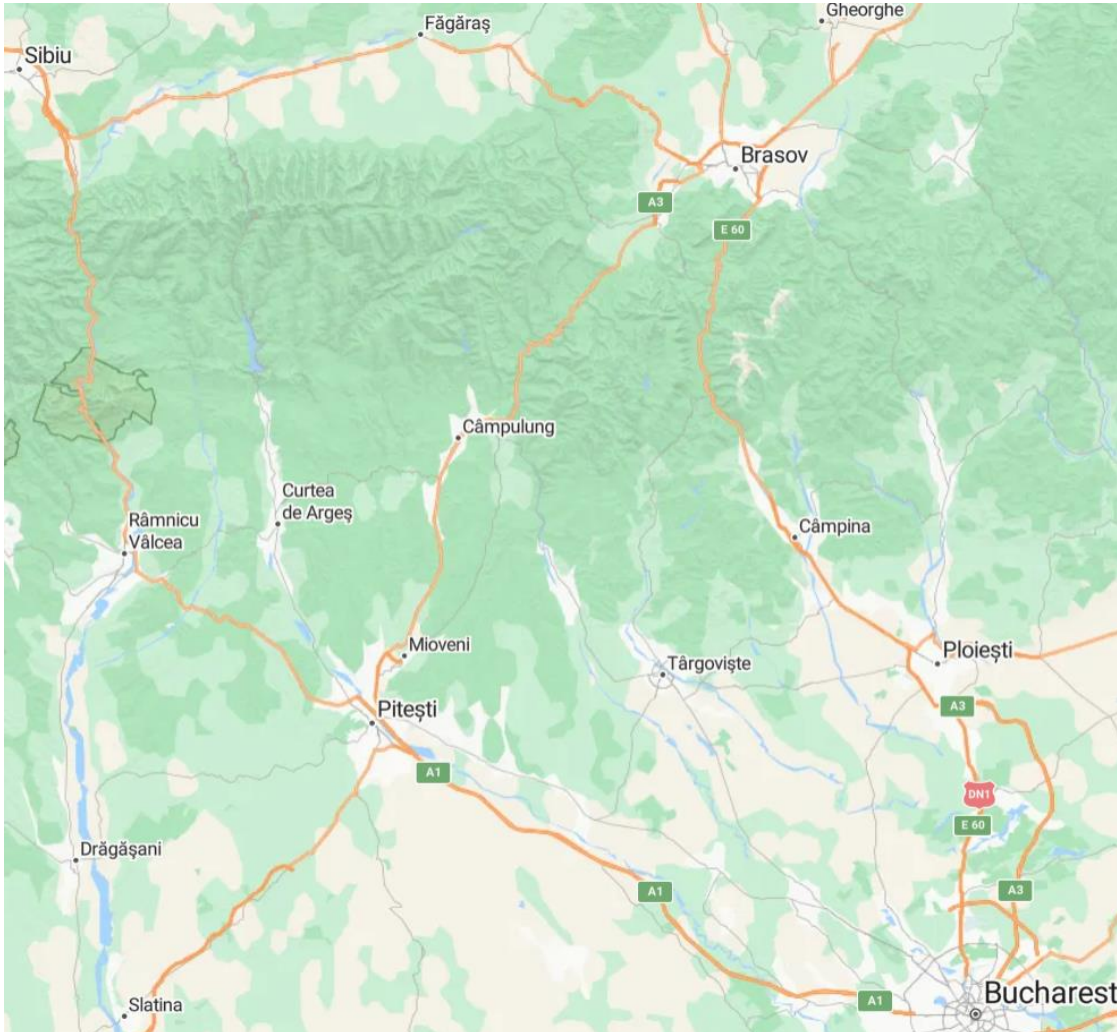


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Uninformed Search Algorithms

No information that could guide the search



Blind search

No clue how good a state is,
e.g., how close it is to the goal

Search

AIAMA: tree search

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create frontier

insert Node(initial_state) to frontier

while frontier is not empty:
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    for action in actions(node.state):
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return failure
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Breadth-first Search (BFS)

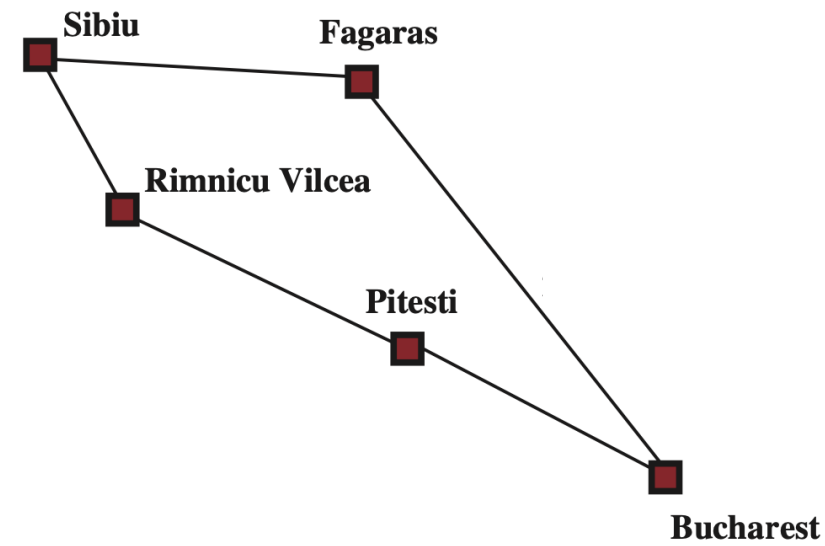
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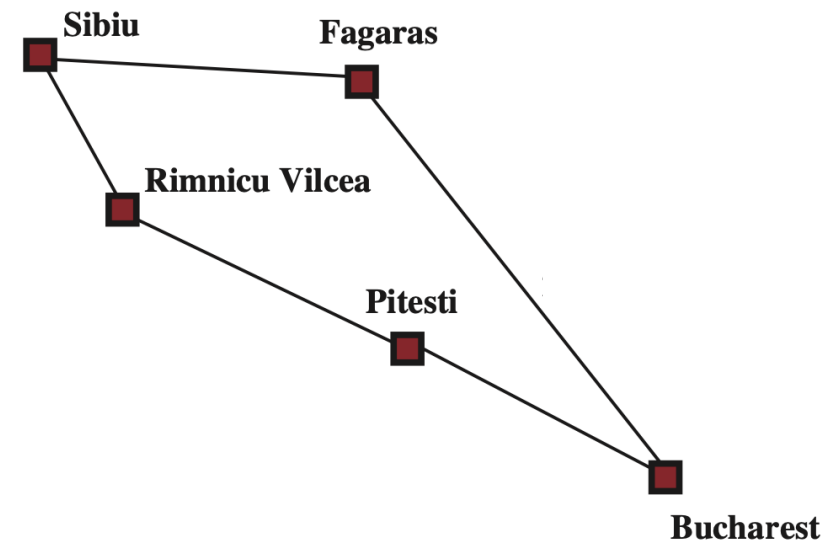
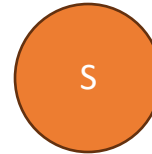
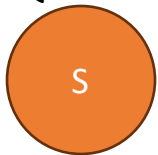
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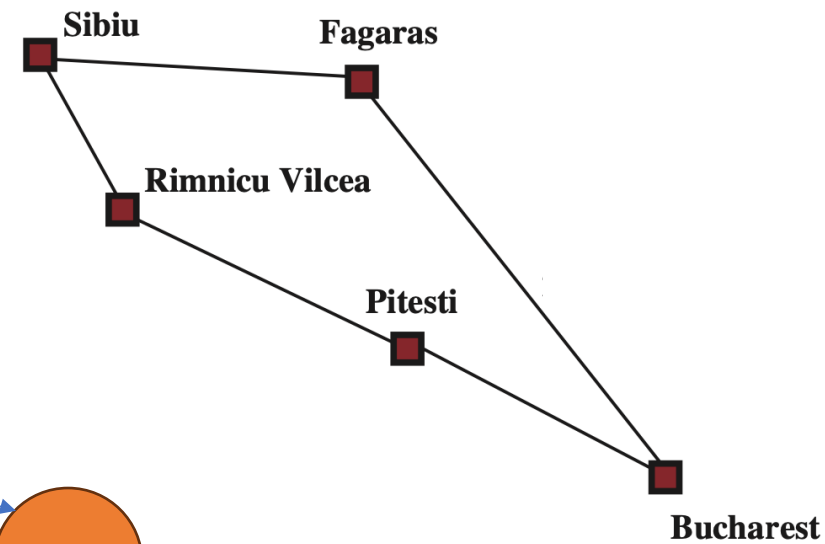
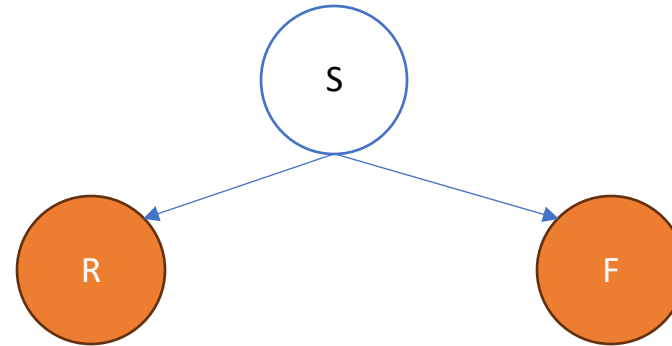
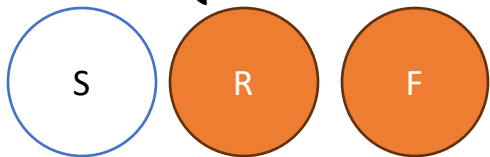
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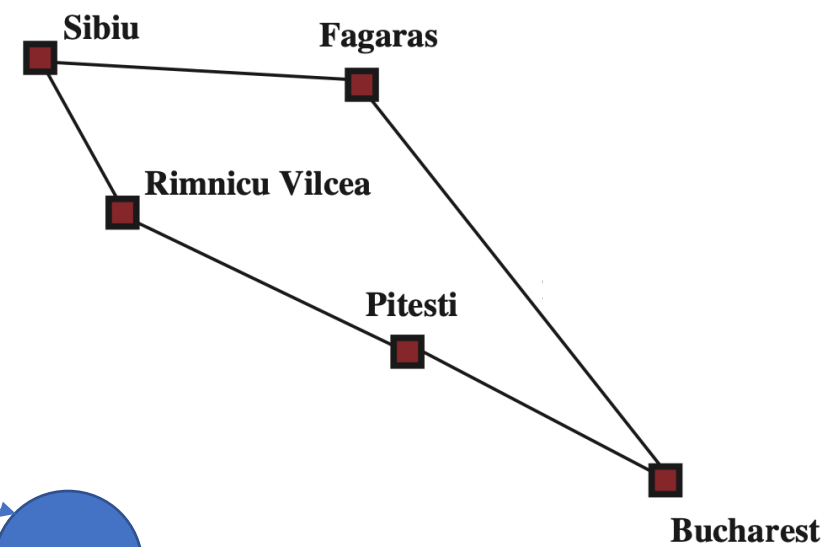
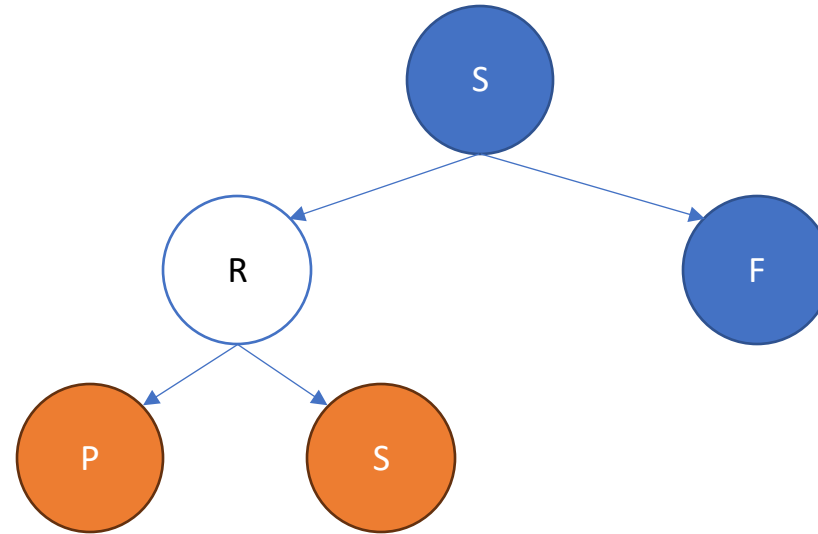
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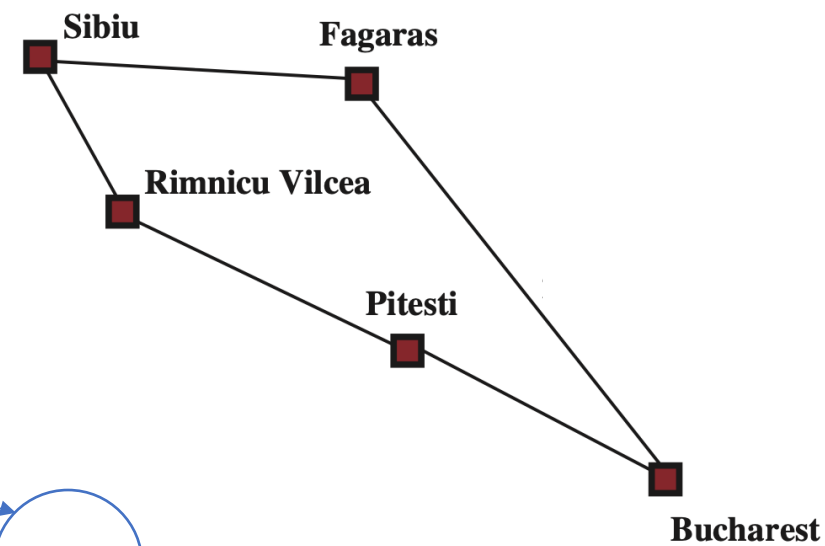
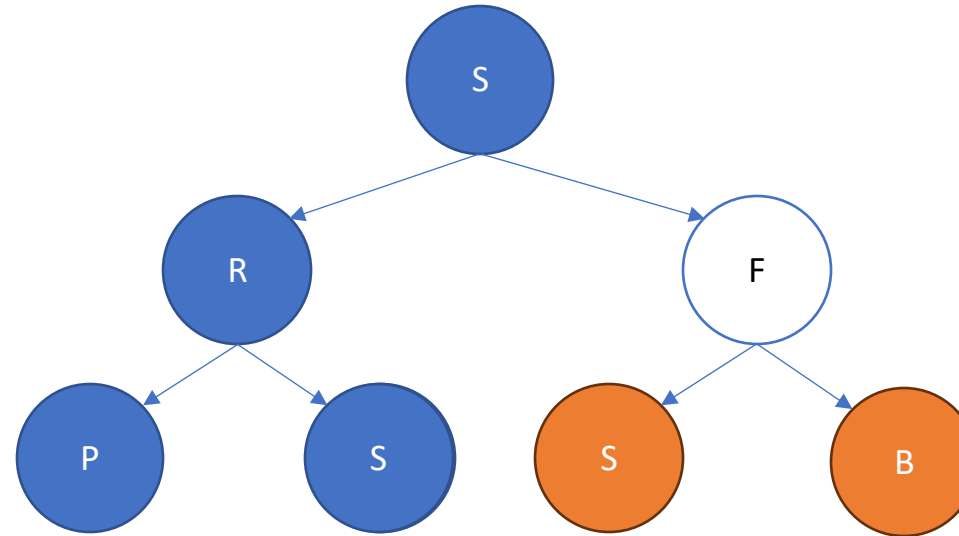
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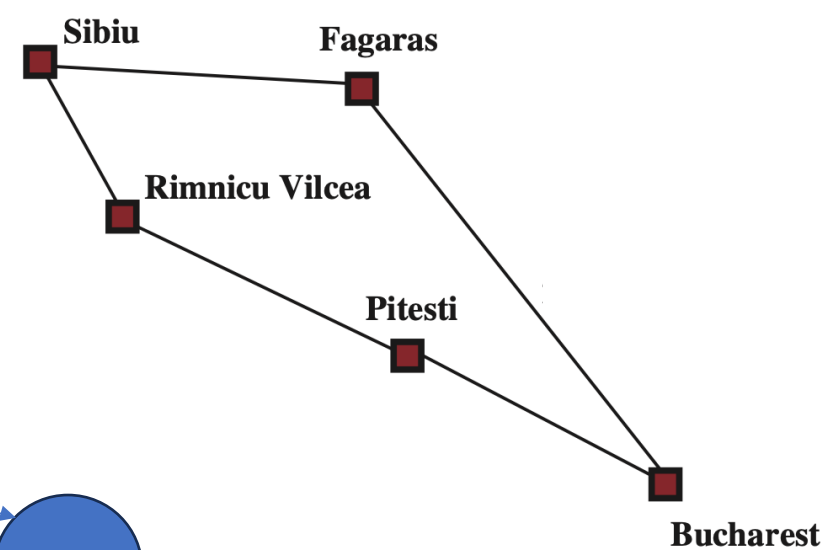
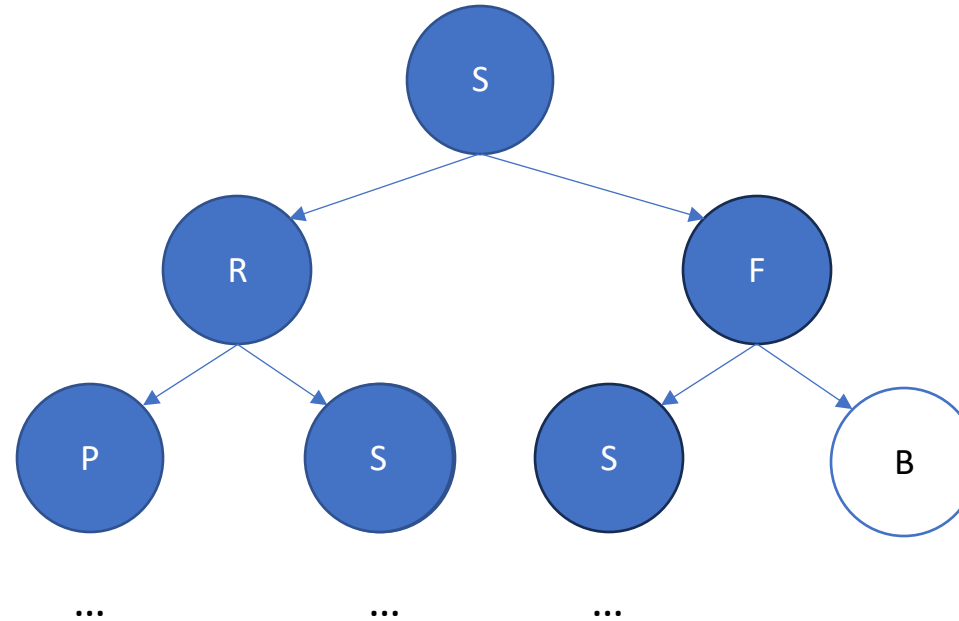
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Queue:

B

...



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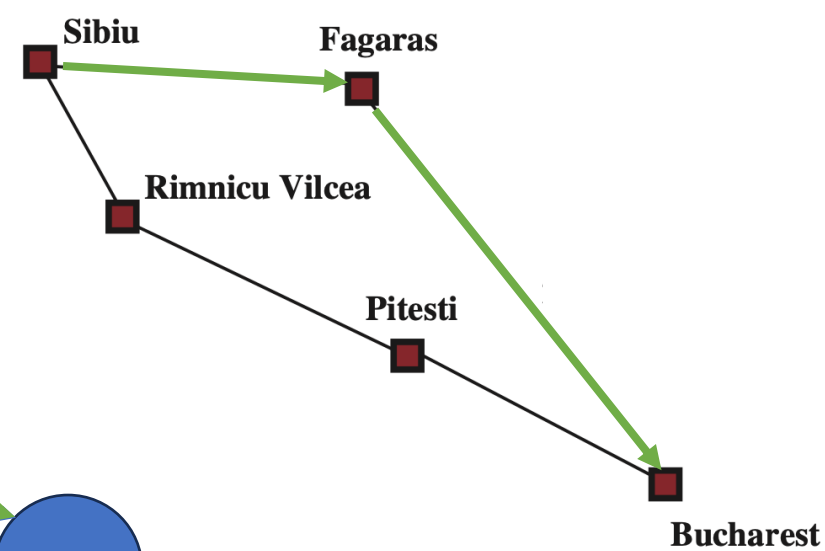
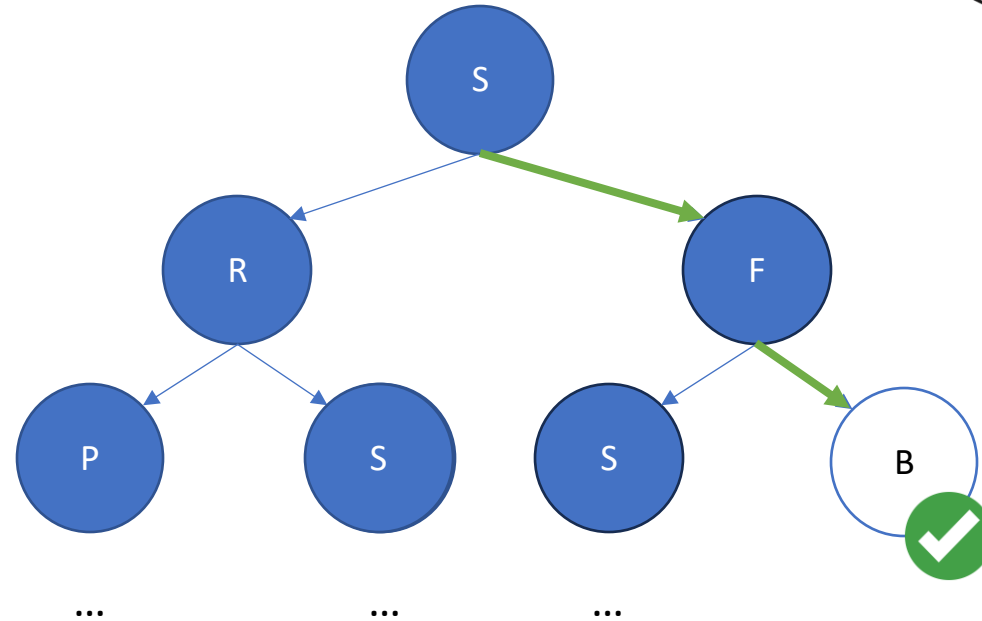
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Queue:

B

...



Breadth-first Search (BFS) - Analysis

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```

Time complexity: (# nodes generated)

Exponential w.r.t. the depth of the optimal solution

Space complexity: (size of frontier)

Exponential w.r.t. the depth of the optimal solution

Complete: Yes, if b is finite

Optimal: Yes, if step cost is the same everywhere

Uniform-cost Search (UCS)

Cost from root to a state

```
create frontier : priority queue (path cost)
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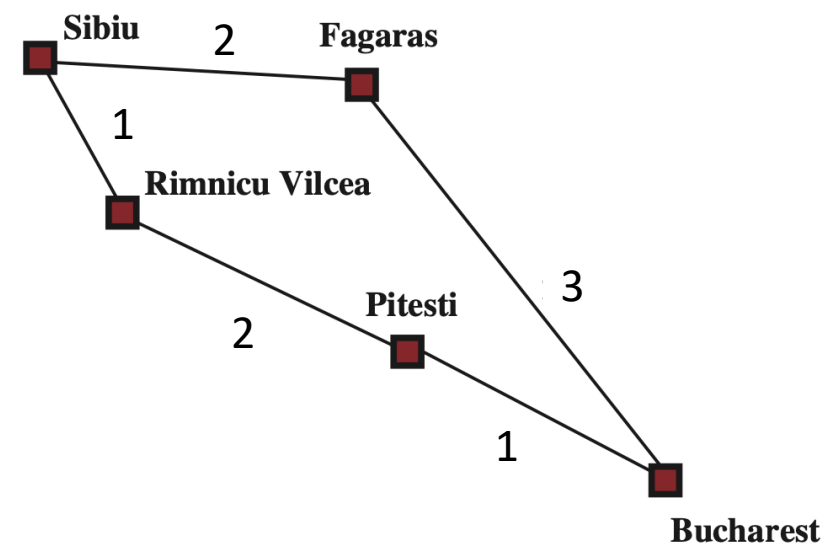
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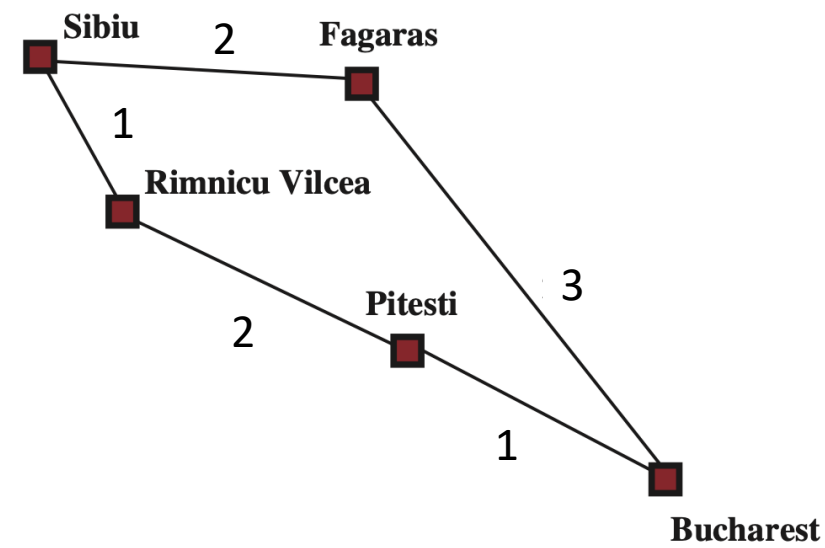
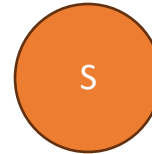
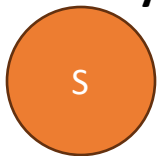
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Priority Queue:



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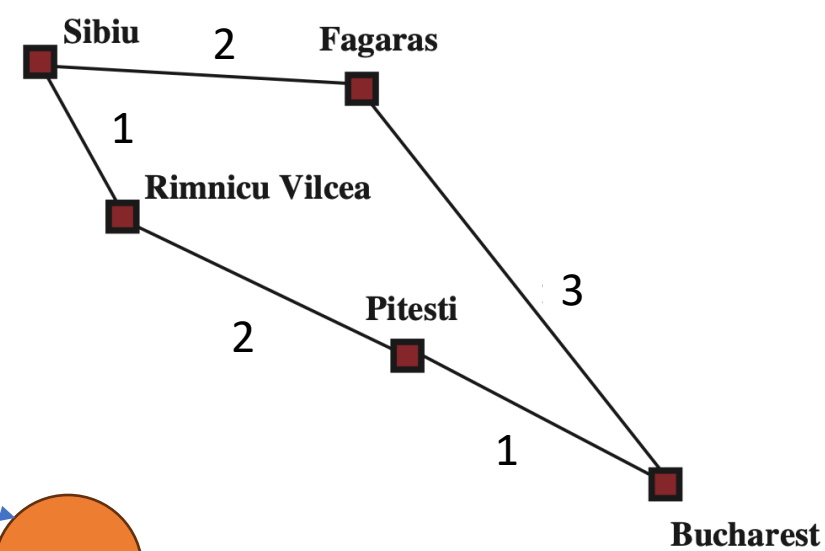
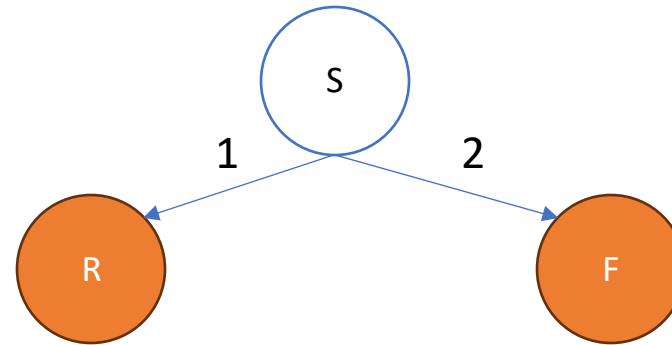
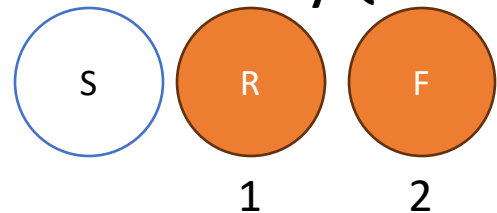
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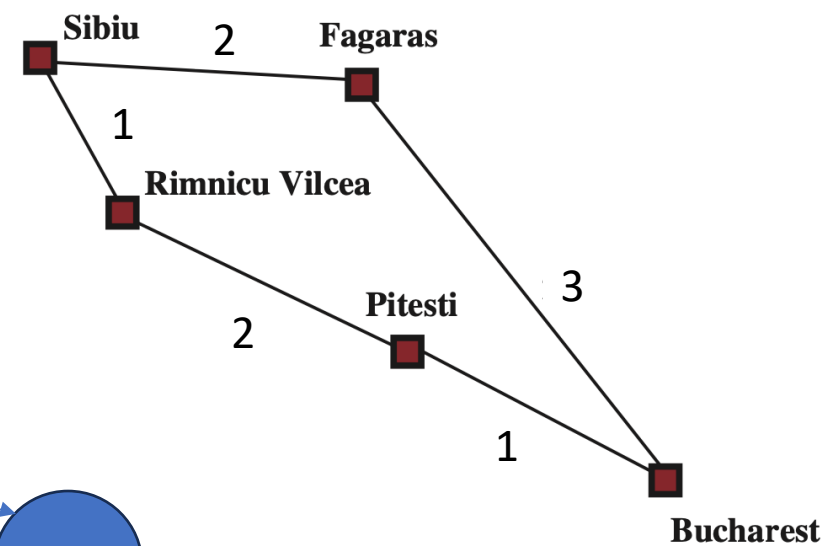
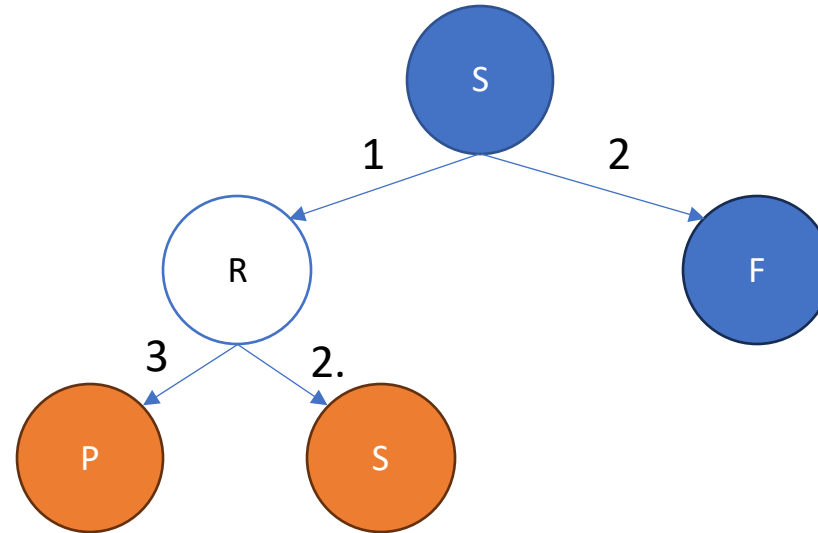
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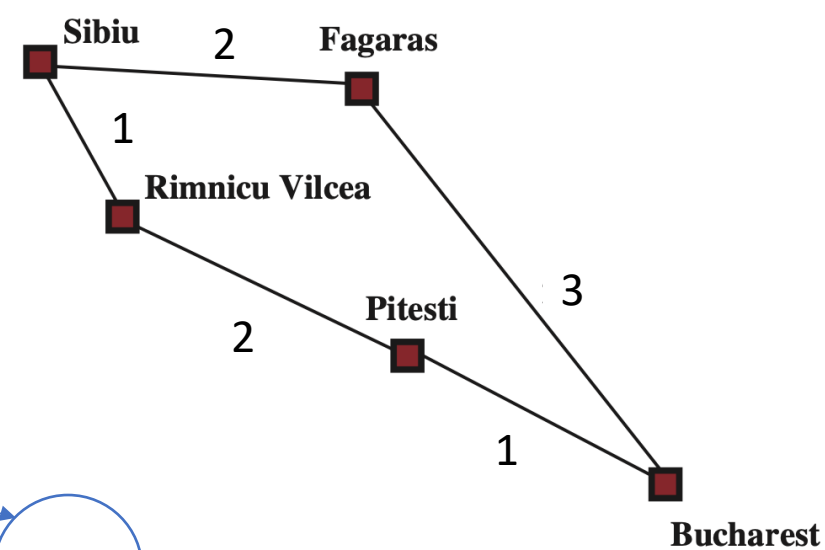
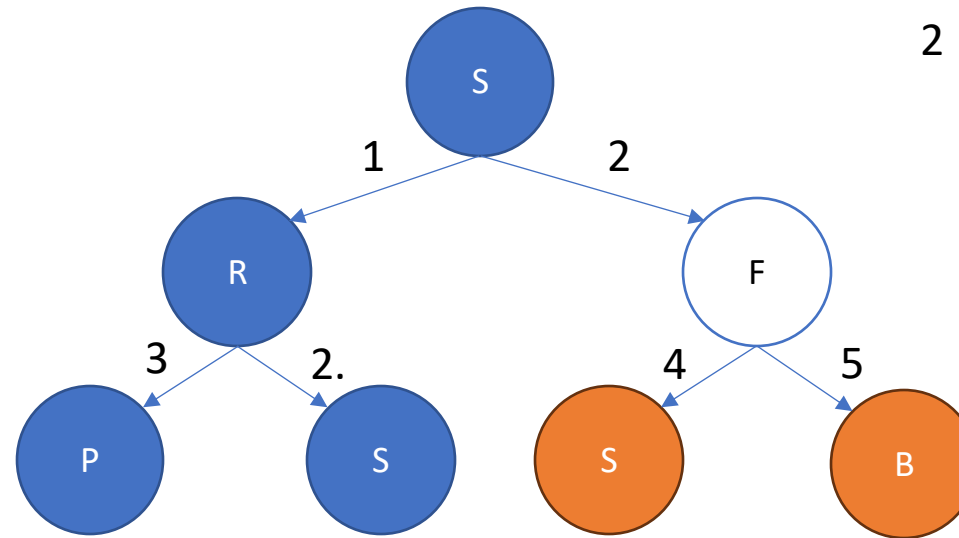
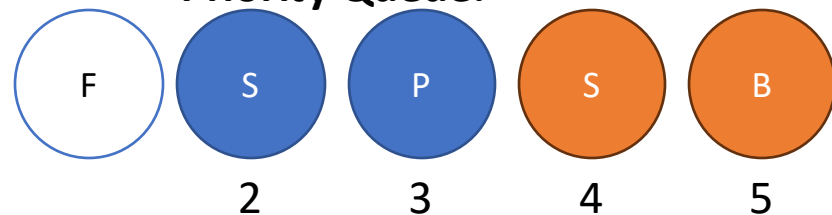
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Priority Queue:



Uniform-cost Search (UCS)

Cost from root to a state

create **frontier** : **priority queue** (path cost)

insert **Node**(initial_state) to **frontier**

while **frontier** is not empty:

node = **frontier**.pop()

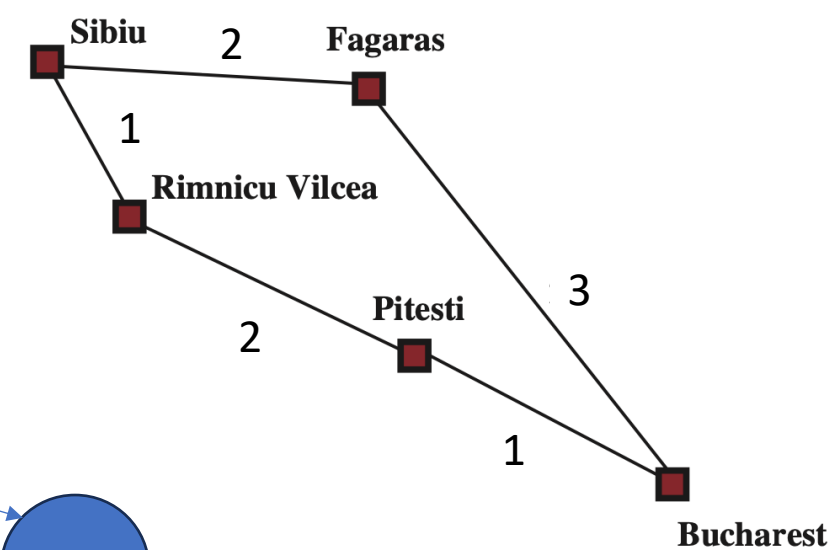
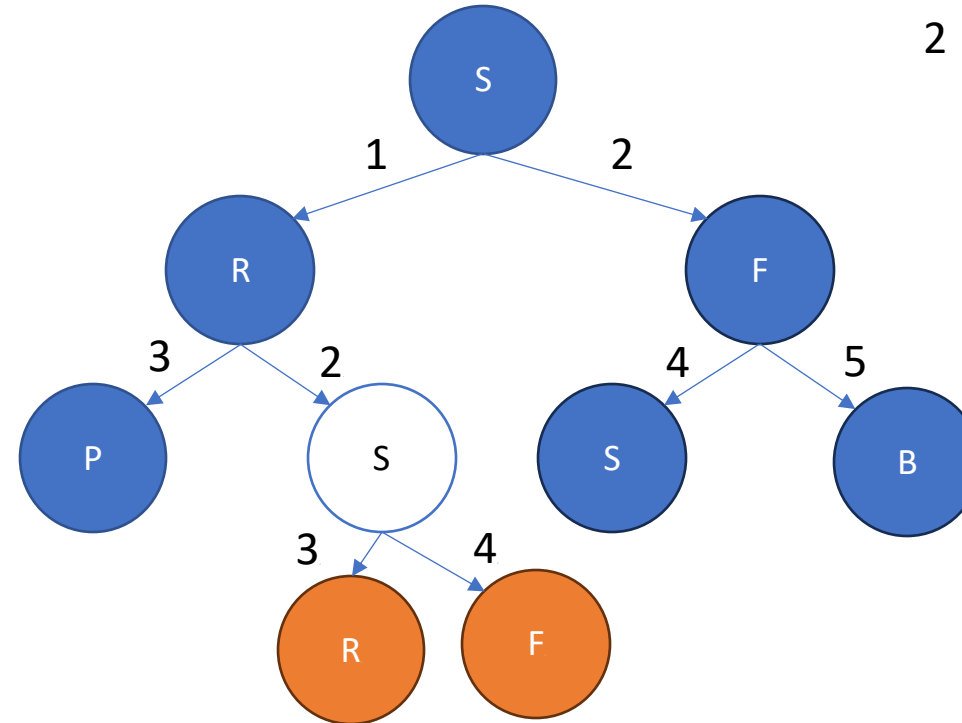
 if **node.state** is goal: return solution

 for **action** in actions(**node.state**):

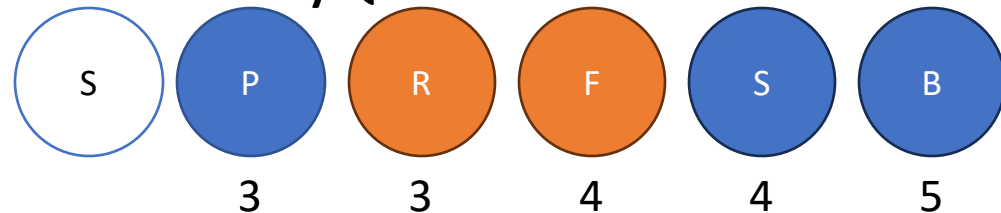
next_state = transition(**node.state**, **action**)

frontier.add(**Node**(**next_state**))

return failure



Priority Queue:



Uniform-cost Search (UCS)

Cost from root to a state

create **frontier** : **priority queue** (path cost)

insert **Node**(initial_state) to **frontier**

while **frontier** is not empty:

node = **frontier**.pop()

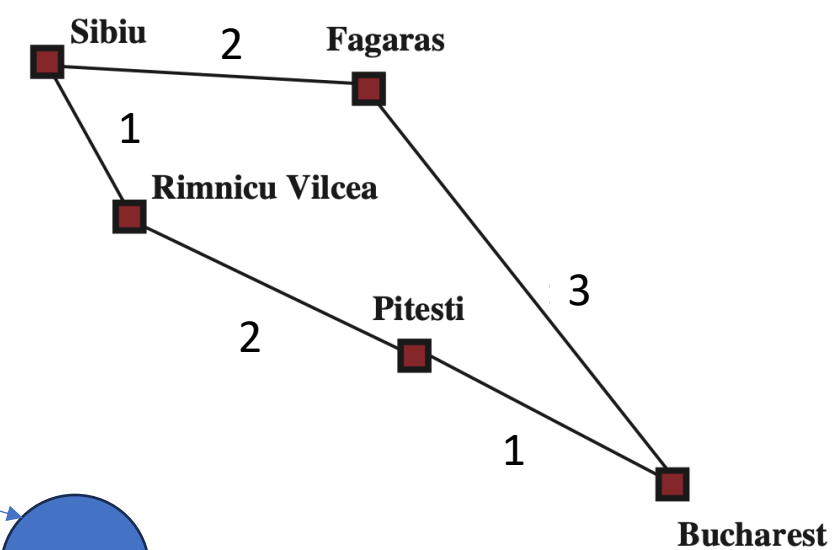
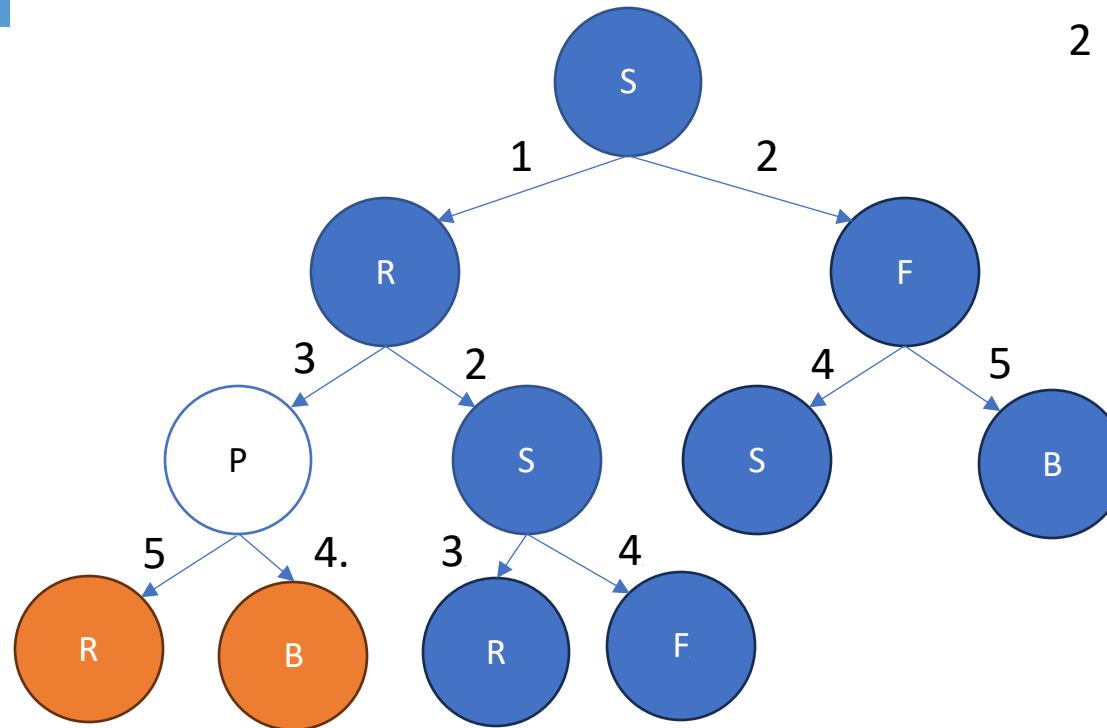
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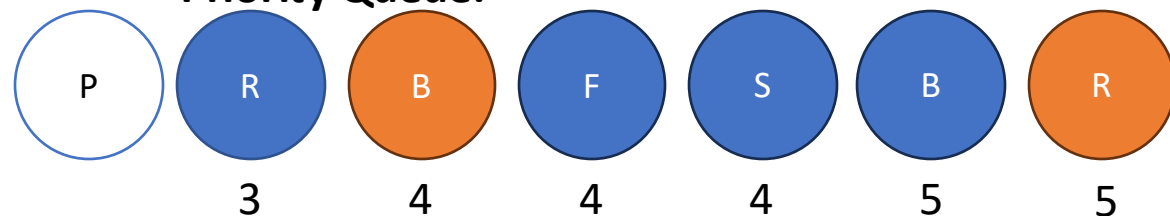
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Priority Queue:



Uniform-cost Search (UCS)

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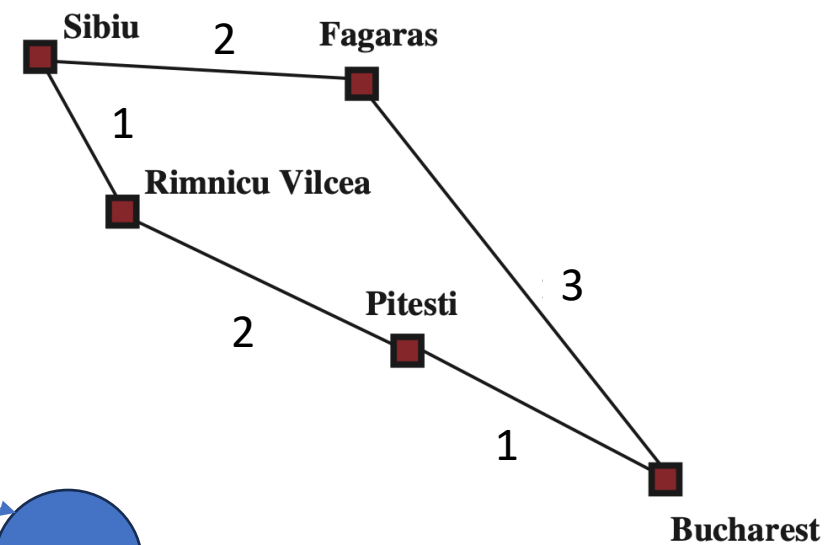
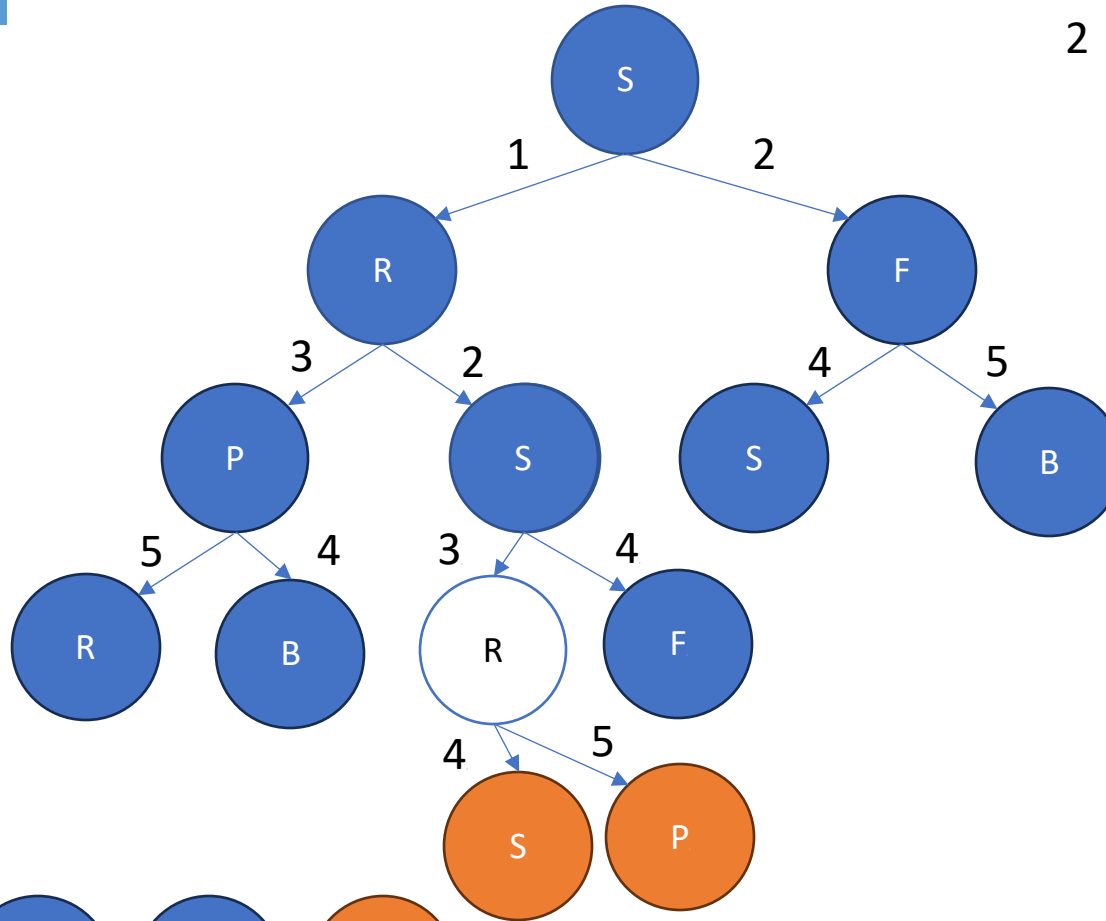
```
if node.state is goal: return solution
```

```
for action in actions(node.state):
```

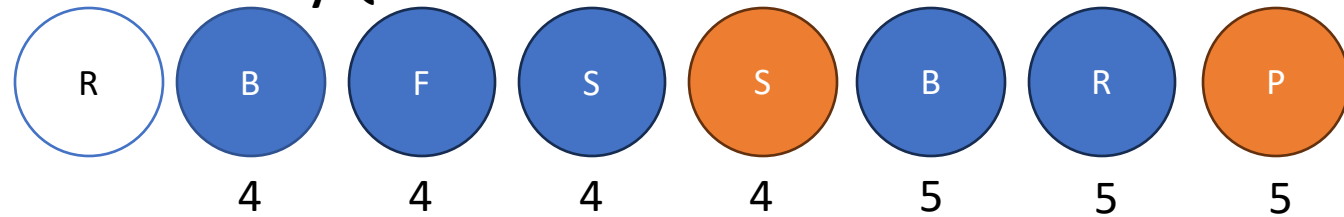
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next_state = transition(node.state, action)
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frontier.add(Node(next_state))
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return failure



Priority Queue:



Uniform-cost Search (UCS)

Cost from root to a state

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create frontier : priority queue (path cost)
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insert Node(initial_state) to frontier
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while frontier is not empty:
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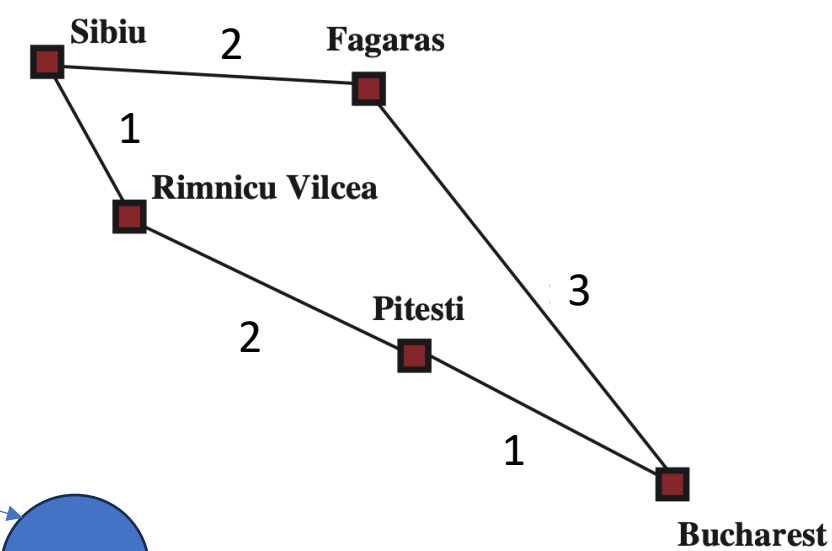
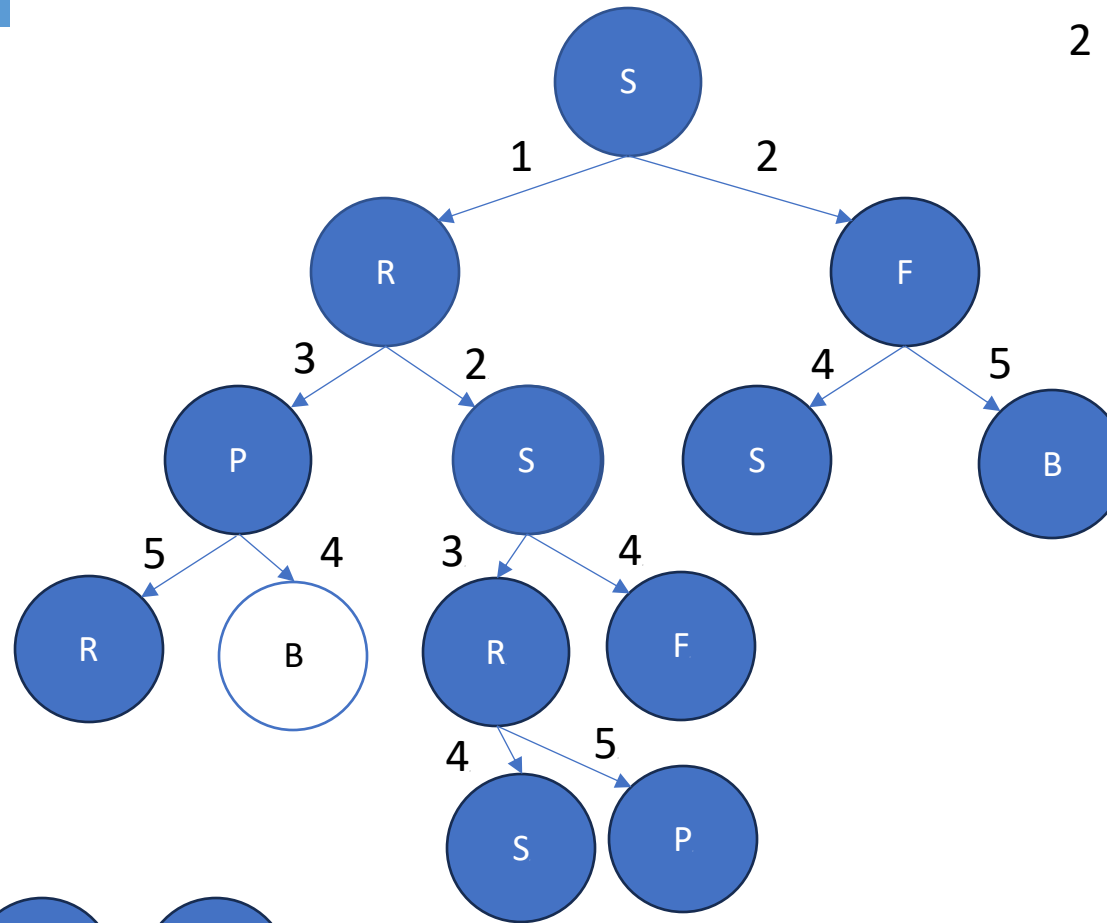
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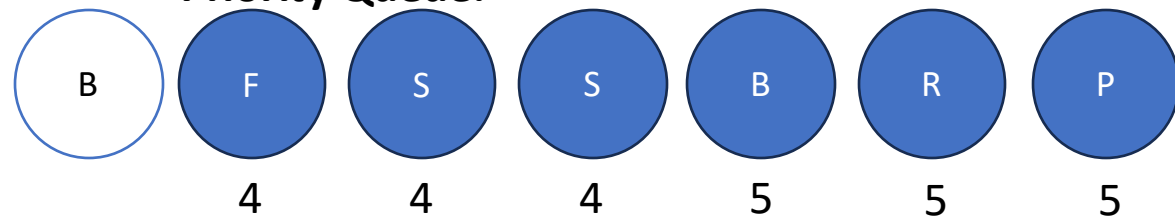
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```

```
        frontier.add(Node(next_state))
```

```
return failure
```



Priority Queue:



Uniform-cost Search (UCS)

Cost from root to a state

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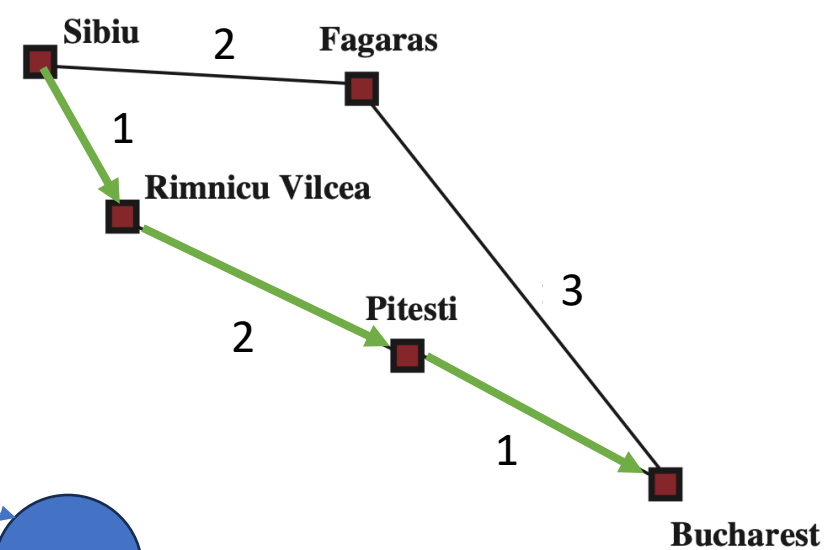
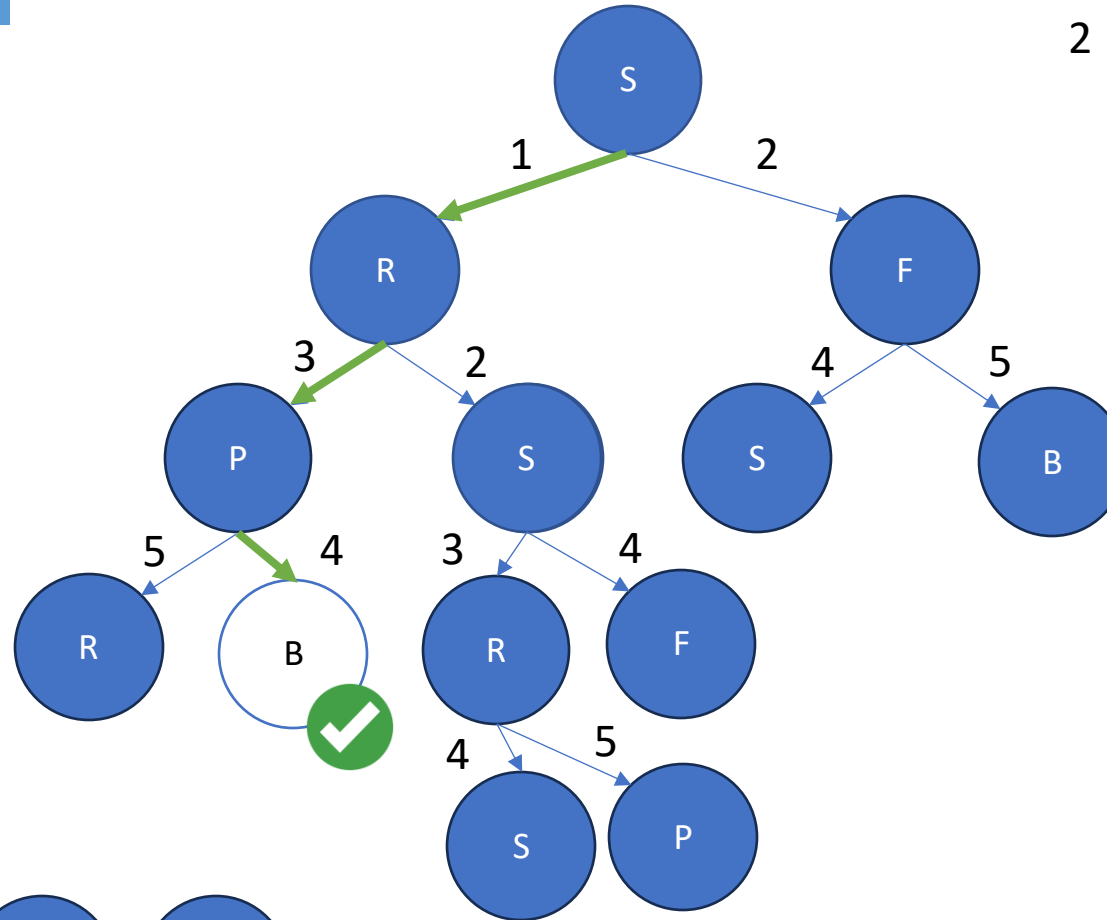
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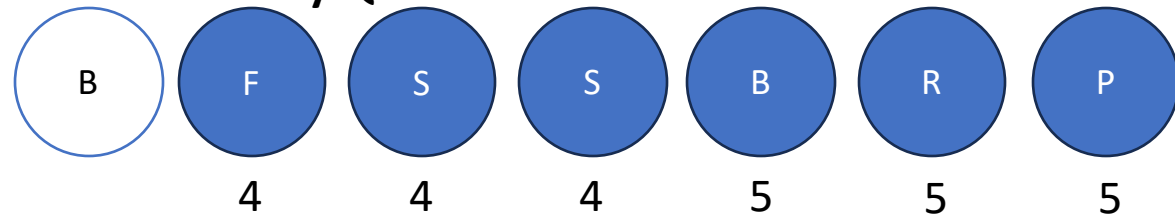
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return failure
```



Priority Queue:



Uniform-cost Search (UCS)

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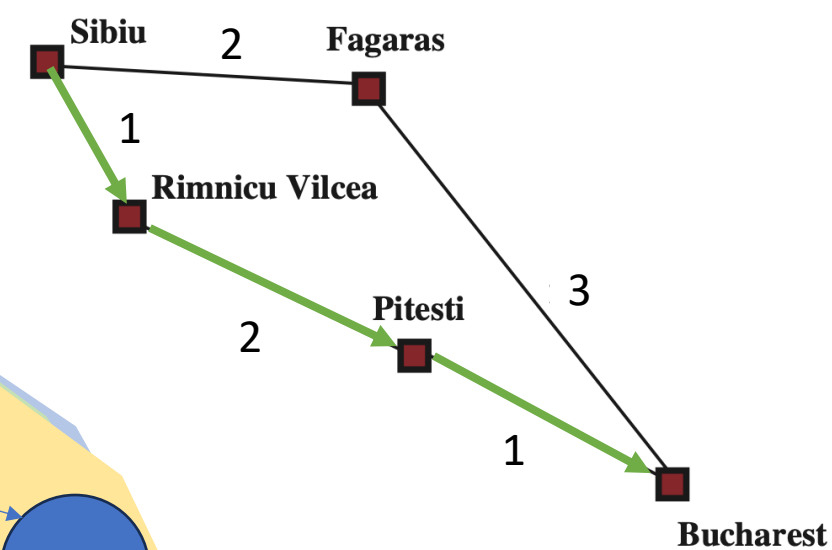
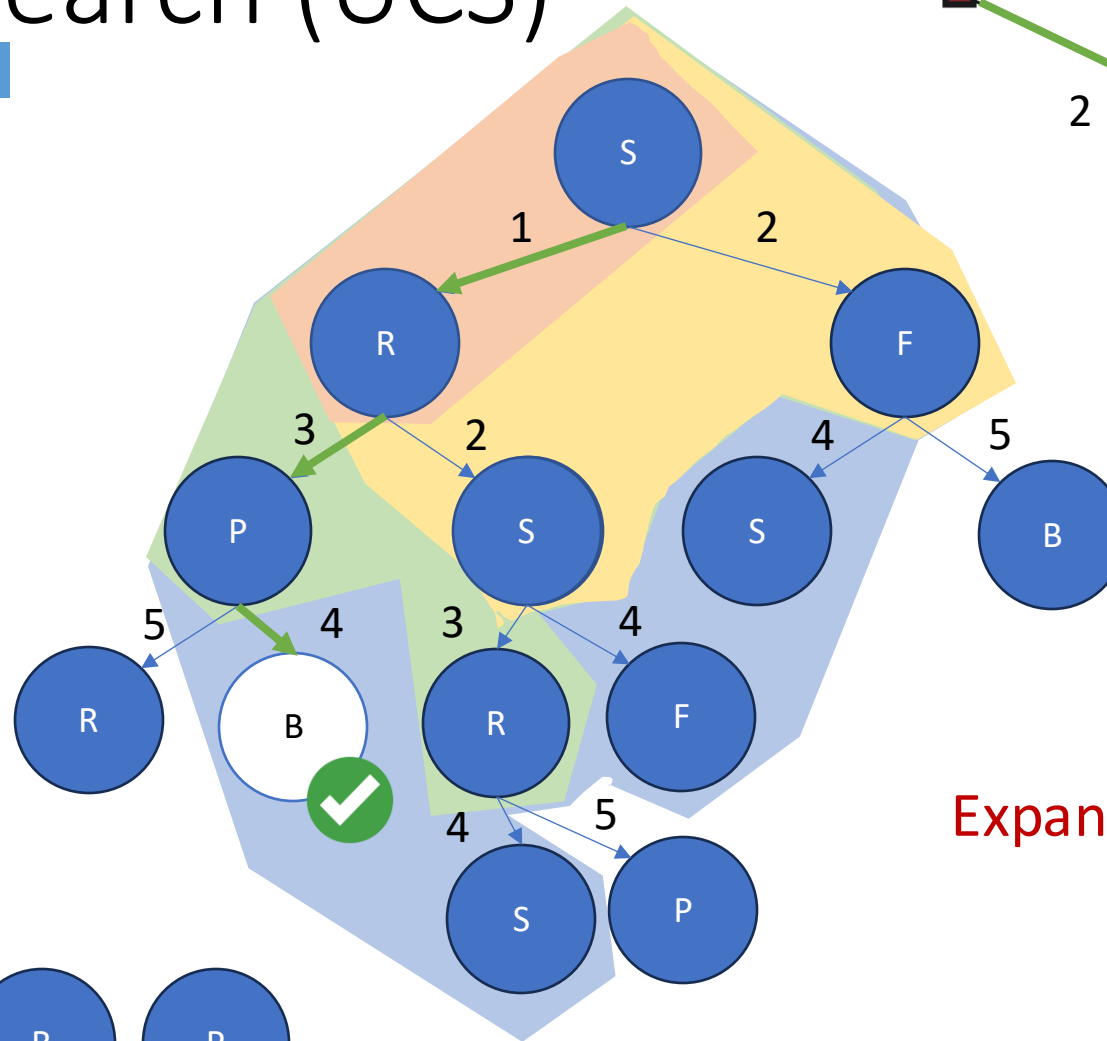
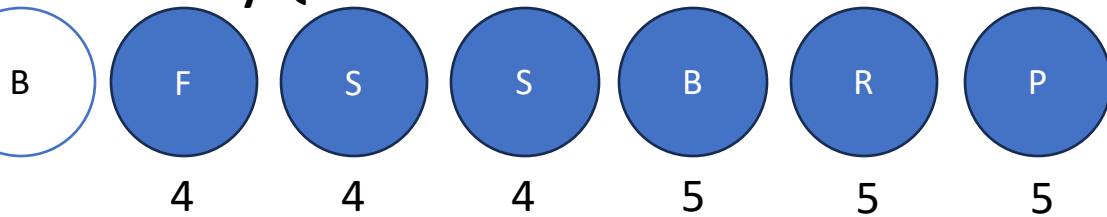
```
    for action in actions(node.state):
```

```
        next_state = transition(node.state, action)
```

```
        frontier.add(Node(next_state))
```

```
return failure
```

Priority Queue:



Expands “tier” by “tier”

Uniform-cost Search (UCS) - Analysis

Cost from root to a state

```
create frontier : priority queue (path cost)

insert Node(initial_state) to frontier

while frontier is not empty:
    node = frontier.pop()
    if node.state is goal: return solution

    for action in actions(node.state):
        next_state = transition(node.state, action)
        frontier.add(Node(next_state))

return failure
```

Time complexity: (# nodes generated)

Exponential w.r.t. the “tier” of the optimal solution

Space complexity: (size of frontier)

Exponential w.r.t. the “tier” of the optimal solution

Complete: *Yes*, if positive step cost everywhere and finite total cost

Optimal: *Yes*, if positive step cost everywhere

Depth-first Search (DFS)

```
create frontier : stack
```

```
insert Node(initial_state) to frontier
```

```
while frontier is not empty:
```

```
    node = frontier.pop()
```

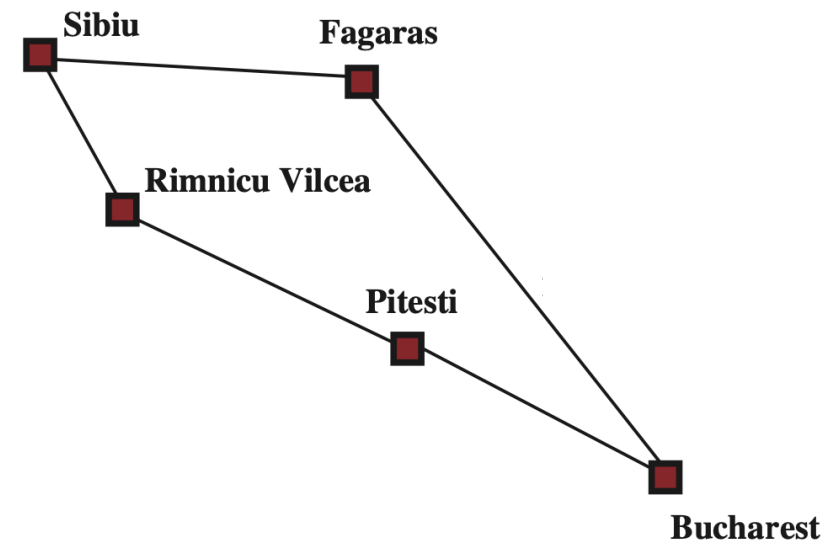
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    if node.state is goal: return solution
```

```
    for action in actions(node.state):
```

```
        next_state = transition(node.state, action)
```

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        frontier.add(Node(next_state))
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return failure
```



Depth-first Search (DFS)

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create frontier : stack
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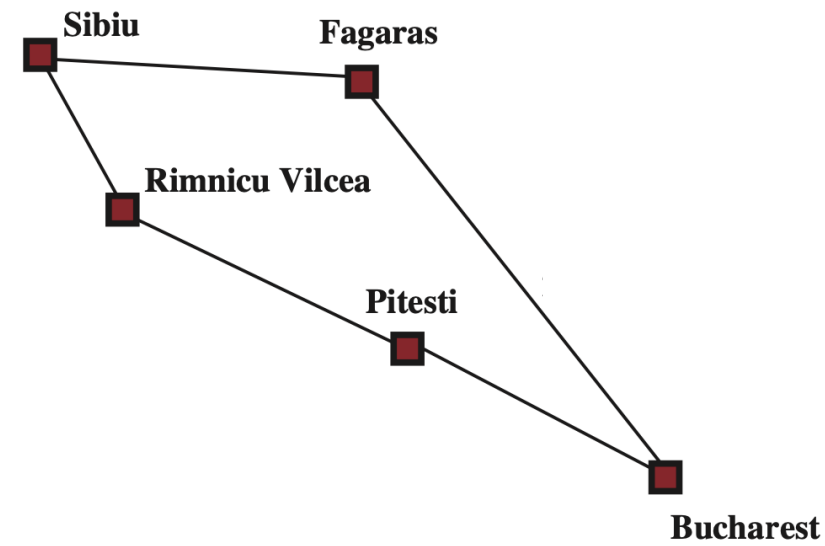
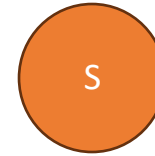
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        next_state = transition(node.state, action)
```

```
        frontier.add(Node(next_state))
```

```
return failure
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Stack:



Depth-first Search (DFS)

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create frontier : stack
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insert Node(initial_state) to frontier
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while frontier is not empty:
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    node = frontier.pop()
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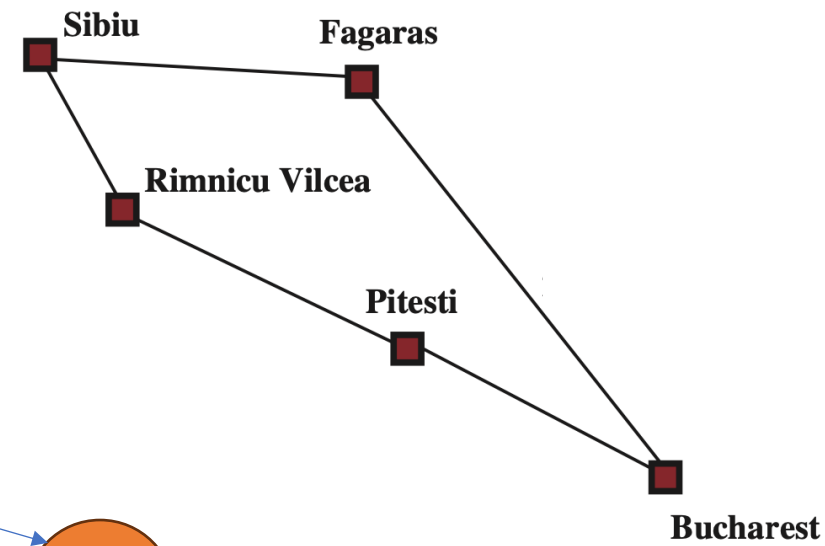
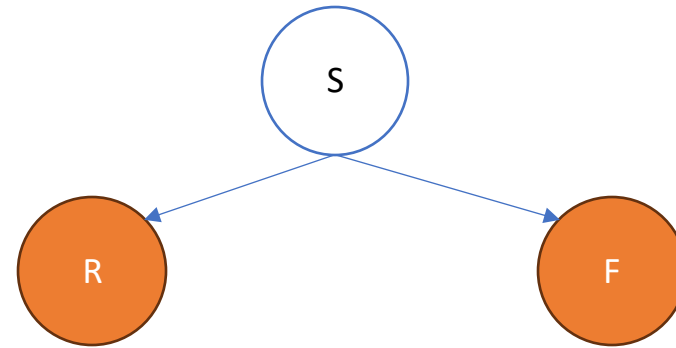
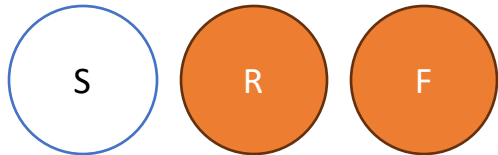
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        frontier.add(Node(next_state))
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Stack:



Depth-first Search (DFS)

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create frontier : stack
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while frontier is not empty:
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    node = frontier.pop()
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```
    if node.state is goal: return solution
```

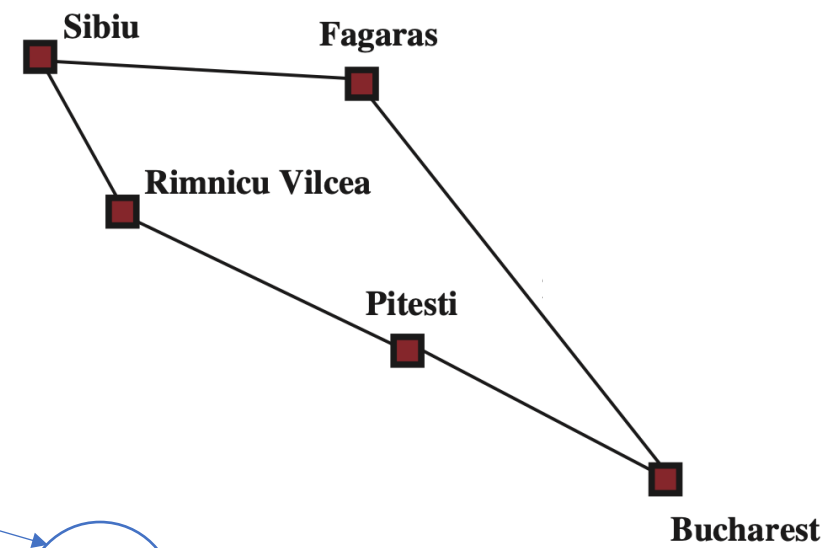
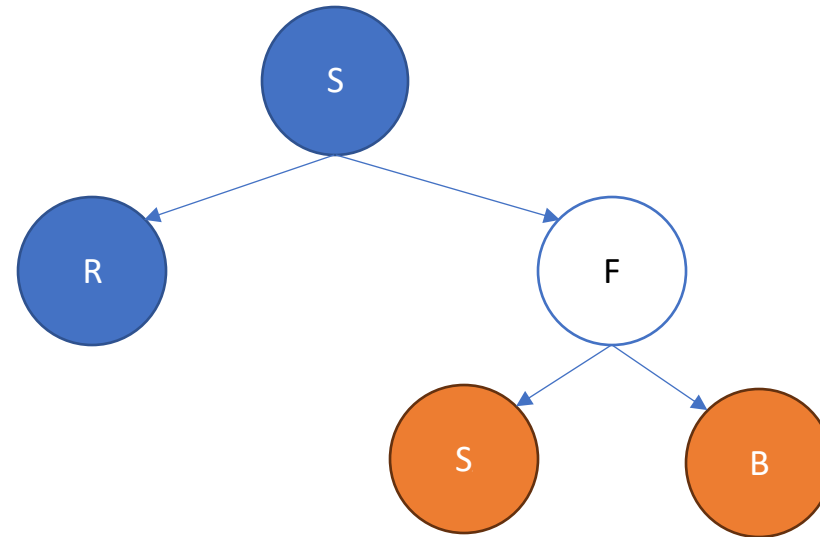
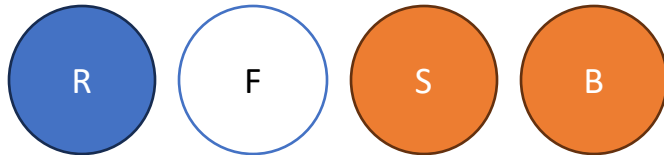
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        next_state = transition(node.state, action)
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        frontier.add(Node(next_state))
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Stack:



Depth-first Search (DFS)

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create frontier : stack
```

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    node = frontier.pop()
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    if node.state is goal: return solution
```

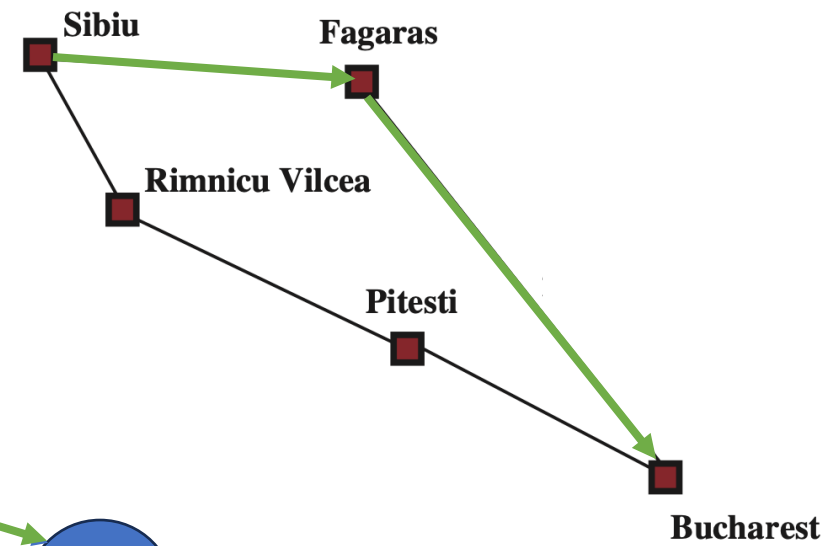
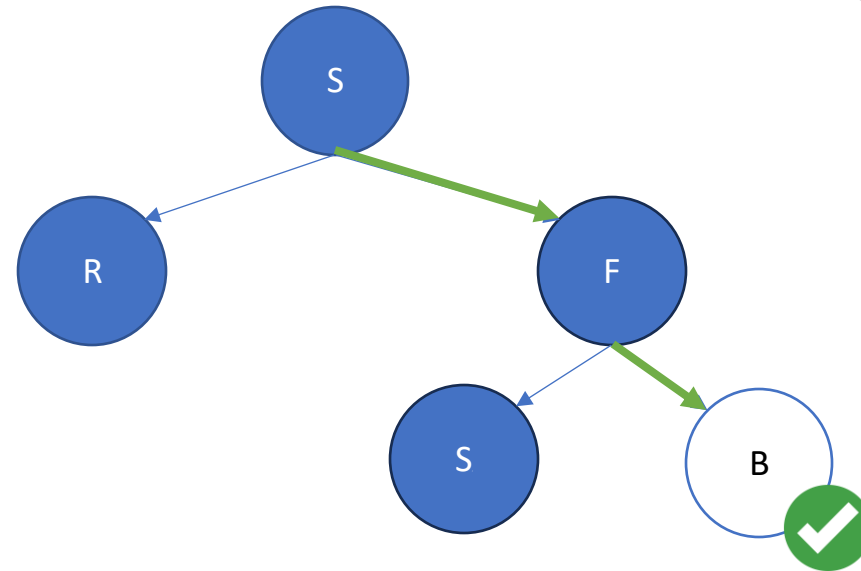
```
    for action in actions(node.state):
```

```
        next_state = transition(node.state, action)
```

```
        frontier.add(Node(next_state))
```

```
return failure
```

Stack:



Depth-first Search (DFS) - Analysis

```
create frontier : stack

insert Node(initial_state) to frontier

while frontier is not empty:
    node = frontier.pop()
    if node.state is goal: return solution

    for action in actions(node.state):
        next_state = transition(node.state, action)
        frontier.add(Node(next_state))

return failure
```

Time complexity: (# nodes generated)

Exponential w.r.t. the maximum depth of the search tree

Space complexity: (size of frontier)

Polynomial w.r.t. the maximum depth of the search tree

Complete: No, when the depth of the search tree is infinite (e.g., when the action is reversible, causing the state to go back and forth)

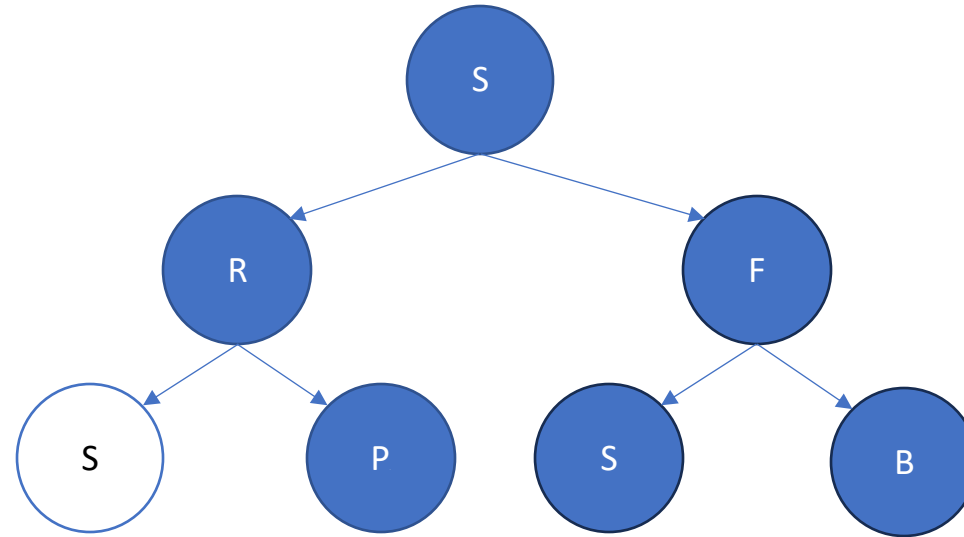
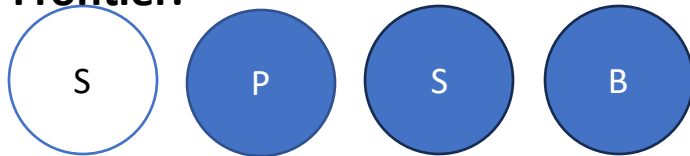
Optimal: No, the optimal solution may be in a shallower depth

Search with visited memory

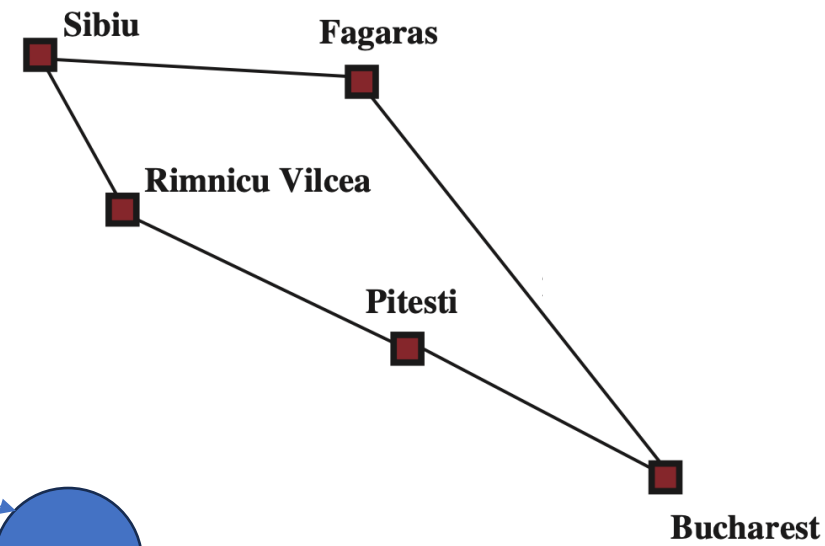
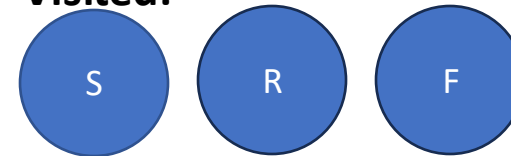
AIAMA: graph search

```
create frontier
create visited
insert Node(initial_state) to frontier
while frontier is not empty:
    node = frontier.pop()
    if node.state is goal: return solution
    if node.state in visited: continue
    visited.add(state)
    for action in actions(node.state):
        next_state = transition(node.state, action)
        frontier.add(Node(next_state))
return failure
```

Frontier:



Visited:



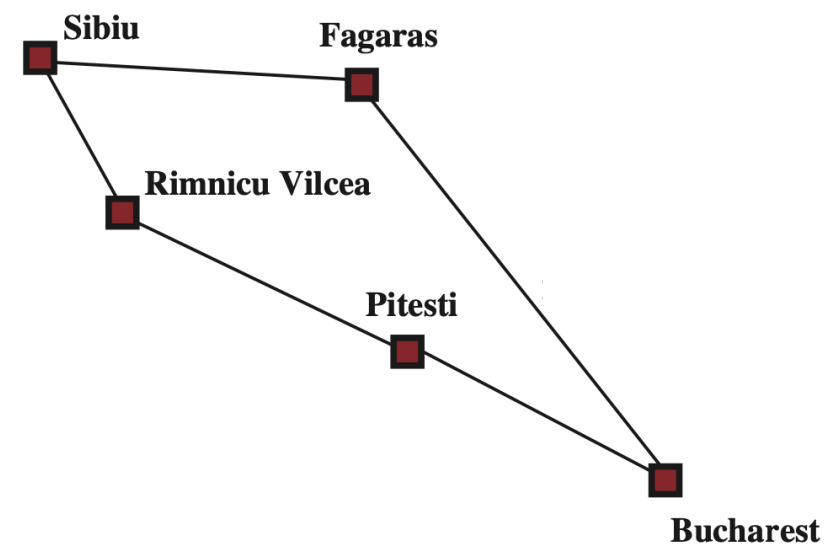
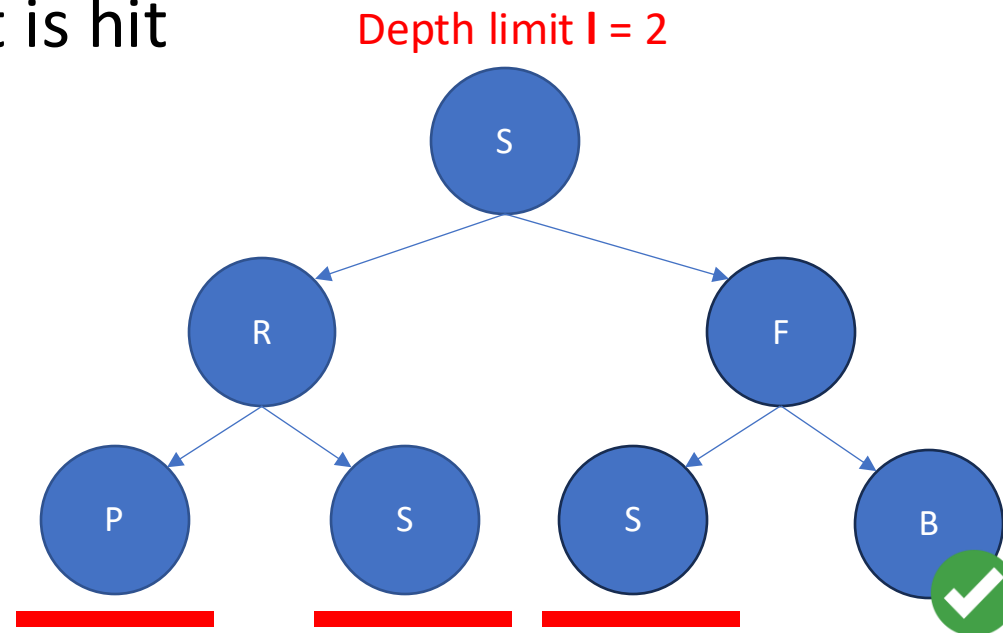
Outline

- Designing an Agent
 - Problem solving agents
 - Problem formulation
- Search
 - **Uninformed Search**
 - Breadth-first, depth-first, and uniform-cost search
 - **Depth-limited and iterative-deepening search**
 - Informed Search
 - A* search
 - Heuristics

Depth-limited Search (DLS)

Limit the search to depth l

Backtrack when limit is hit



Depth-limited Search (DLS)

Limit the search to depth l

Backtrack when limit is hit

Time complexity: (# nodes generated)

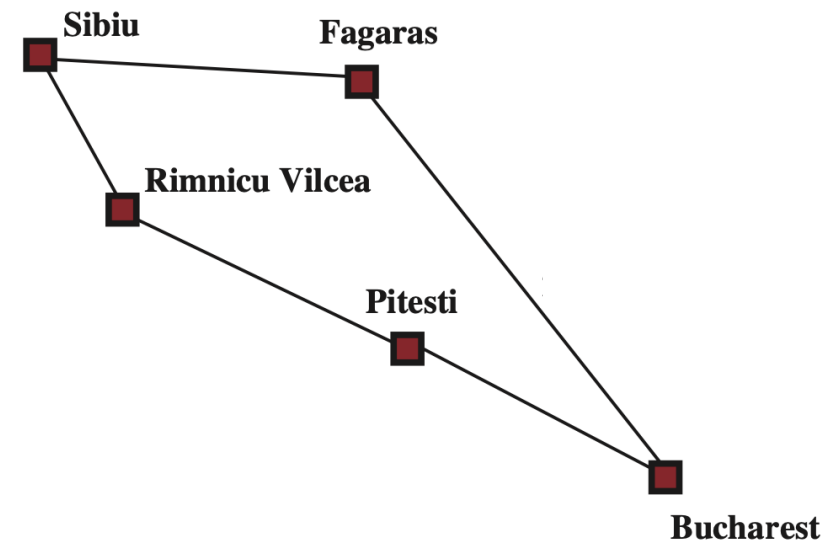
Exponential w.r.t. the depth limit

Space complexity: (size of frontier)

Polynomial w.r.t. the depth limit if used with DFS

Complete: No

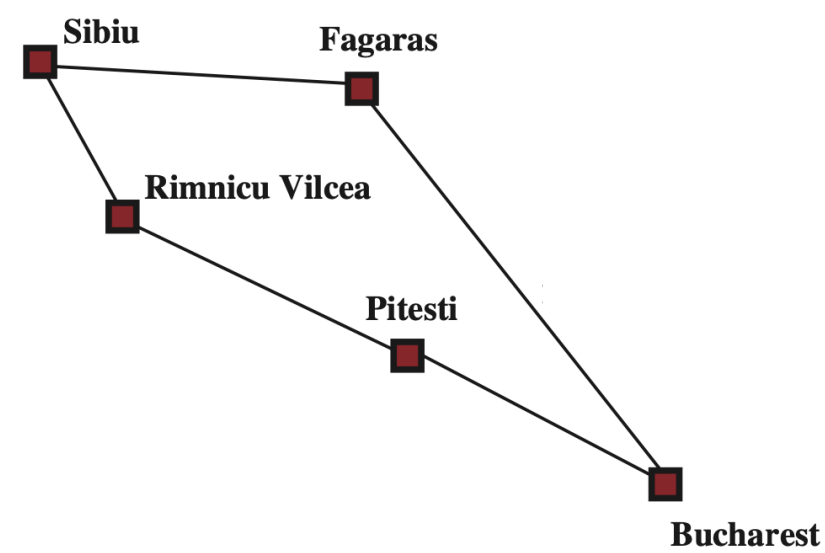
Optimal: No, if used with DFS



Iterative Deepening Search (IDS)

Search with depth limit 0, ..., ∞

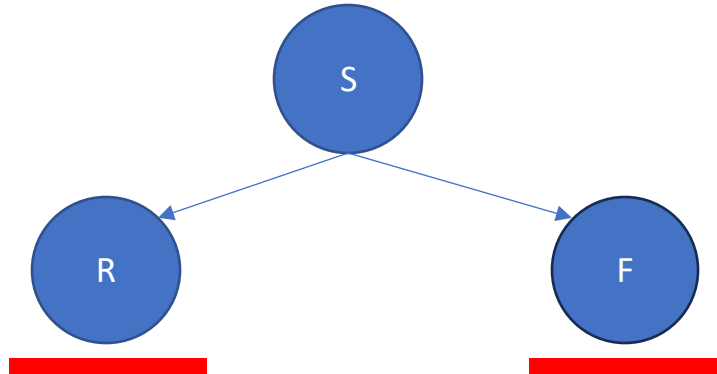
Return solution if found



Depth limit = 0

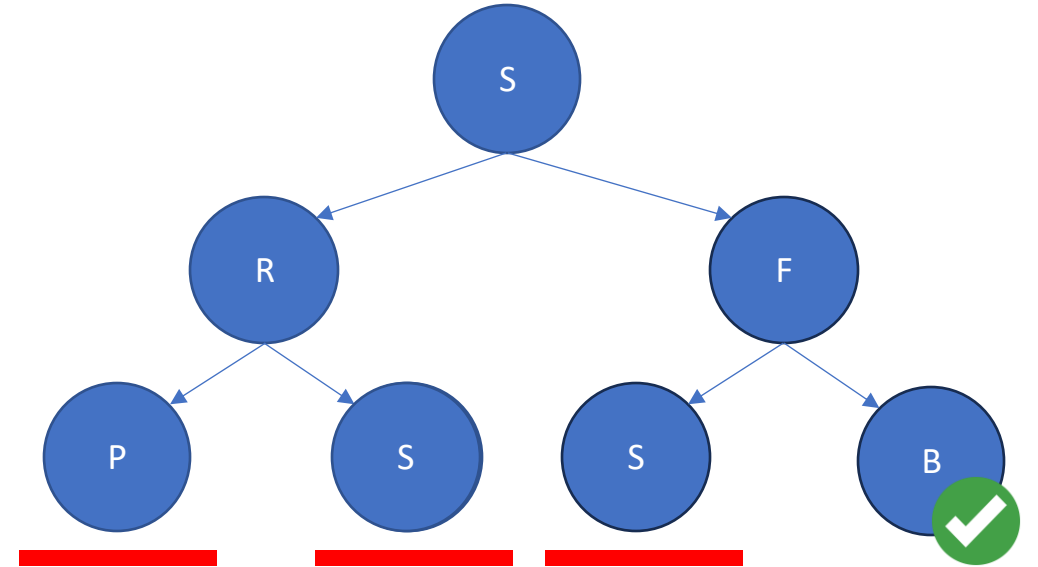


Depth limit = 1



Overhead!

Depth limit = 2



Iterative Deepening Search (IDS)

Search with depth limit $0, \dots, \infty$

Return solution if found

Time complexity: (# nodes generated)

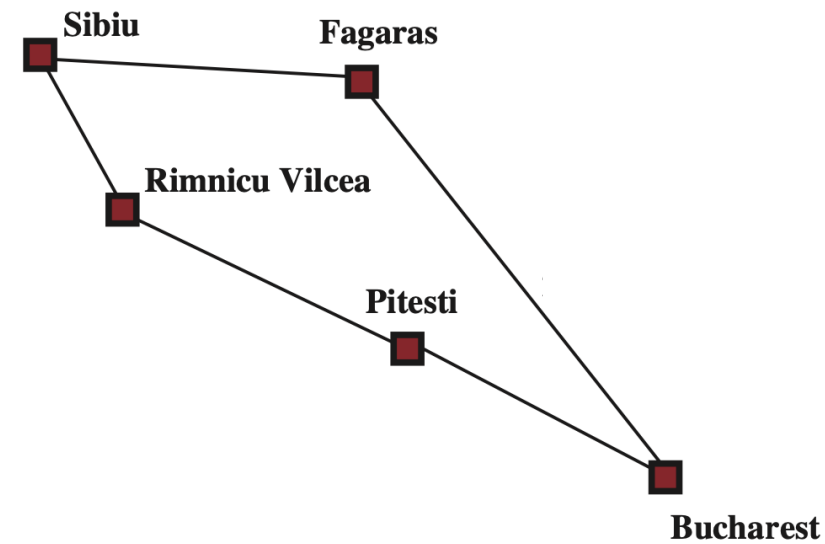
Exponential w.r.t. the depth of optimal solution (with overhead)

Space complexity: (size of frontier)

Polynomial if used with DFS

Complete: Yes

Optimal: Yes, if step cost is the same everywhere



Summary: Uninformed Search Algorithms

- Search algorithms
 - Breadth-first search – **queue**, explore layer by layer
 - Uniform-cost search – **priority queue** (path cost)
 - Depth-first search – **stack**, go deep first then backtrack
- Variants:
 - Depth limited search – **limit max depth** of the search
 - Iterative deepening search – try DLS with depth limit $0, \dots, \infty$

Summary: Uninformed Search Algorithms

Worst-case

Name	Time Complexity*	Space Complexity*	Complete?	Optimal?
Breadth-first Search	Exponential	Exponential	Yes	Yes
Uniform-cost Search	Exponential	Exponential	Yes	Yes
Depth-first Search	Exponential	Polynomial	No	No
Depth-limited Search	Exponential	Polynomial**	No**	No**
Iterative Deepening Search	Exponential	Polynomial**	Yes	Yes

*) In terms of some notion of depth/tier

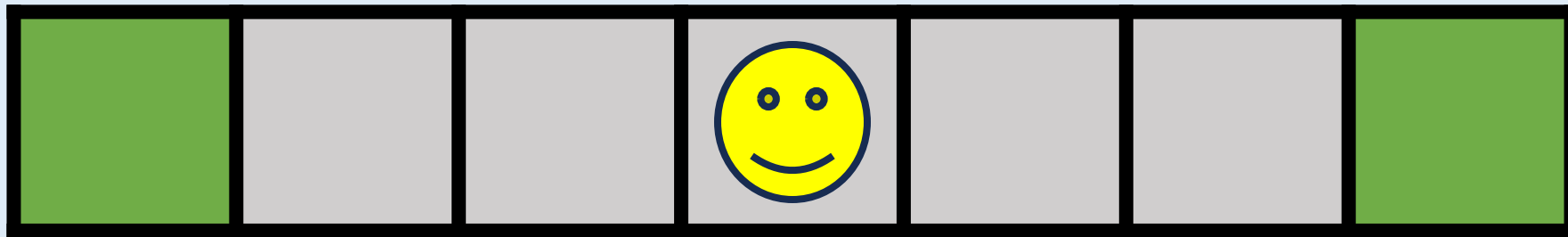
***) If used with DFS

Further Reading (Optional)

- Full analysis of BFS, UCS, DFS, DLS, and IDS (AIAMA 3.4)
- Backward Search (AIAMA 3.4.6)
- Bidirectional Search (AIAMA 3.4.6)

Activity:

Given a maze where the agent is in the middle and there are two goals at the ends, which search algorithm(s) with visited memory is/are **optimal** and the most **space** and **time** efficient (in worst-case)?



Note: we care about overhead in space and time complexities

Name	Time Complexity*	Space Complexity*	Complete?	Optimal?
Breadth-first Search	Exponential	Exponential	Yes	Yes
Uniform-cost Search	Exponential	Exponential	Yes	Yes
Depth-first Search	Exponential	Polynomial	No	No
Depth-limited Search	Exponential	Polynomial**	No**	No**
Iterative Deepening Search	Exponential	Polynomial**	Yes	Yes



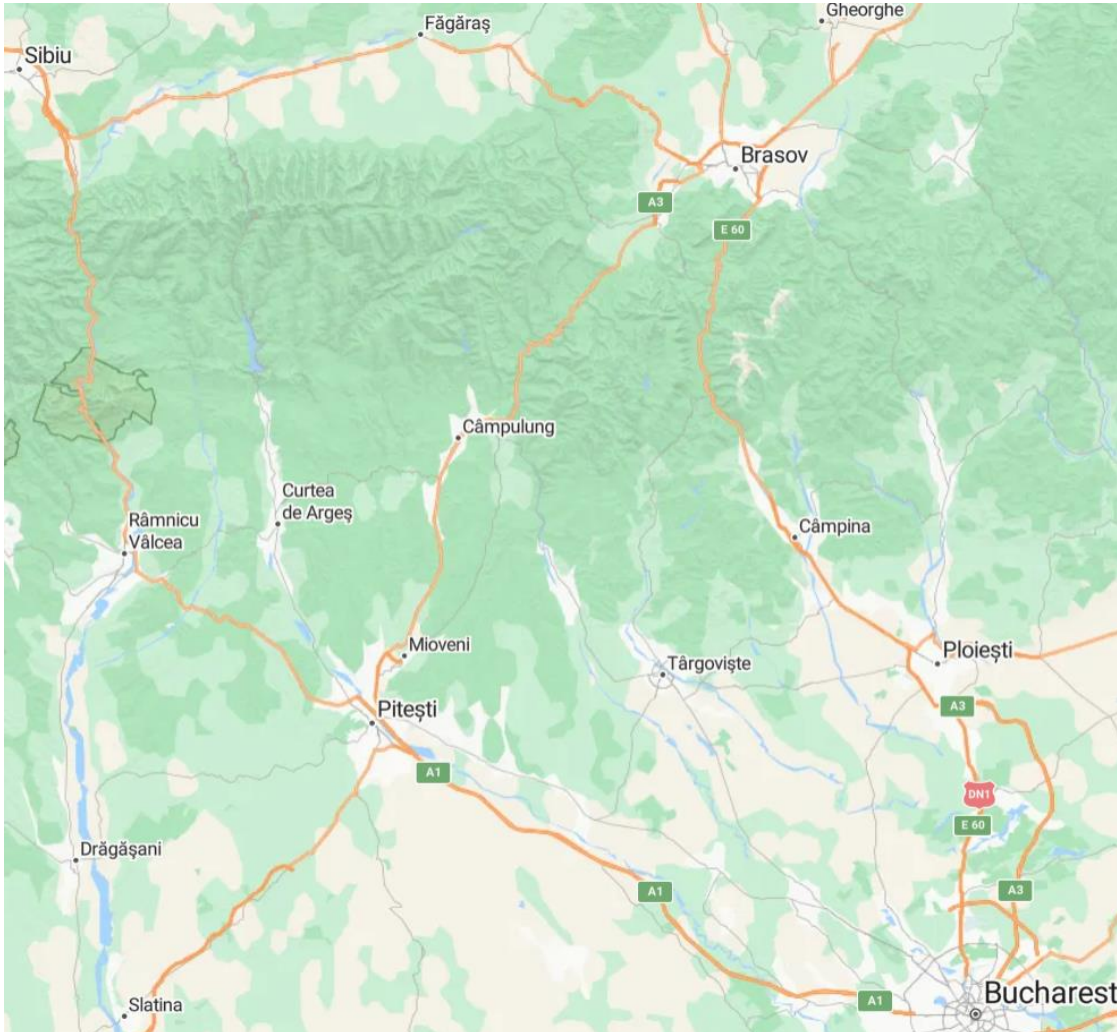
Note: we care about overhead in space and time complexities

Outline

- Designing an Agent
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 - Depth-limited and iterative-deepening search
 - **Informed Search**
 - A* search
 - Heuristics

Uninformed Search Algorithms

No information that could guide the search

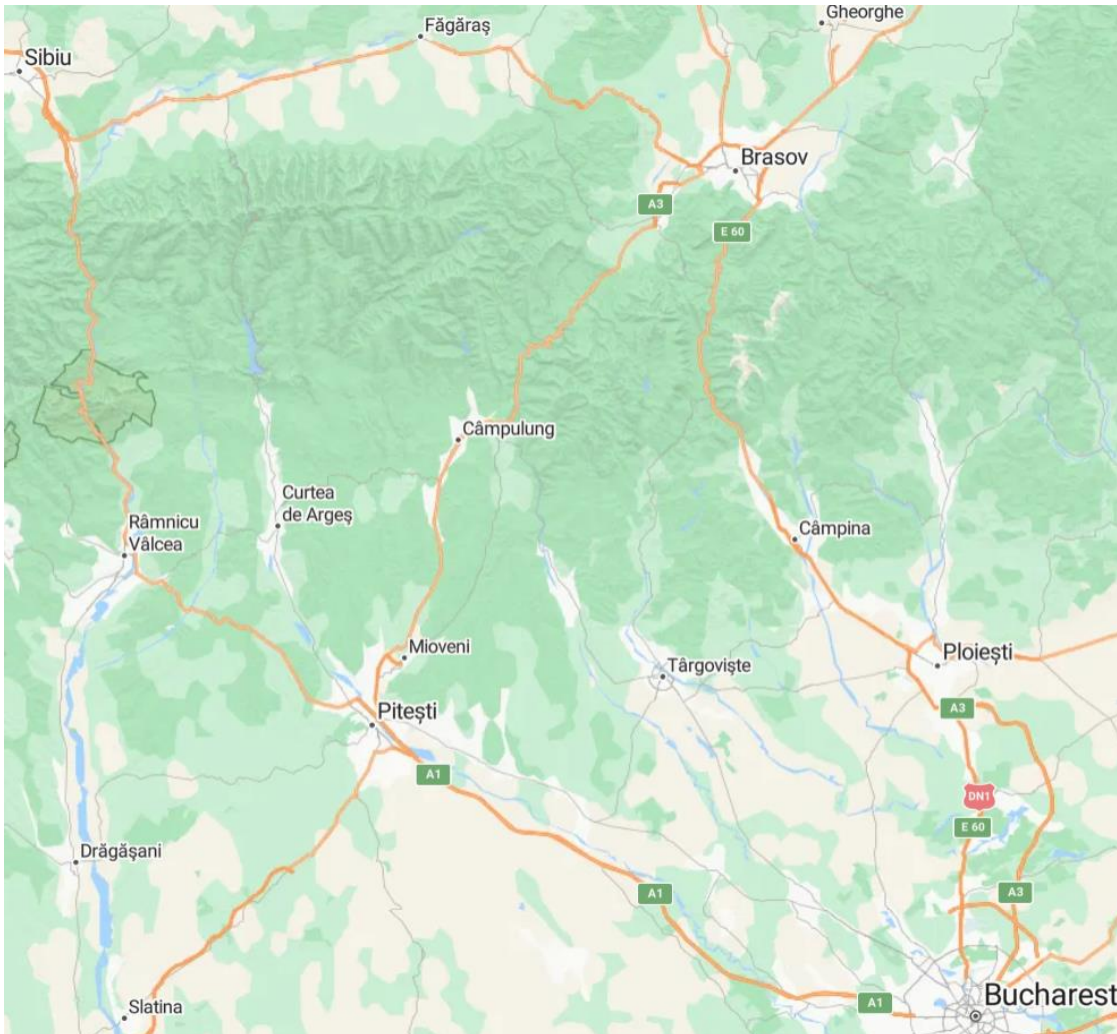


Blind search

No clue how good a state is,
e.g., how close it is to the goal

Informed Search Algorithms

Use information to guide the search

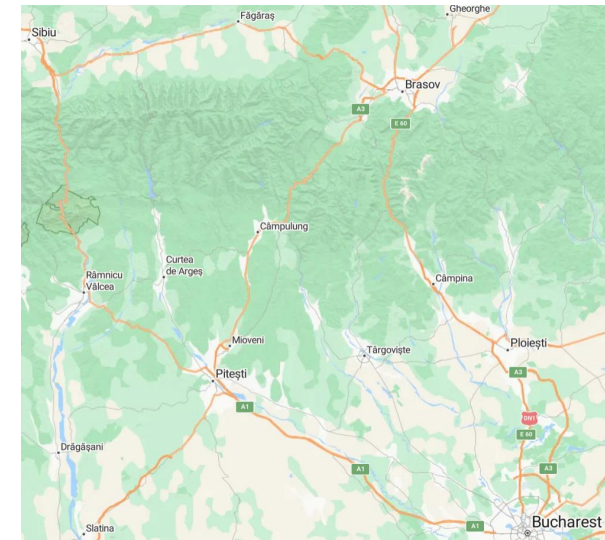


Search with extra info

Has a clue how good a state is,
e.g., how close it is to the goal, estimated
using a **heuristic function**

Heuristic

- Recall that:
 - **Path cost** is the cost of a path from any state to any state
 - **Optimal path cost** is the cost of the lowest-cost path from any state to any state
- A **heuristic** is an estimate of the optimal path cost from any state to the goal state
- Examples (in path finding):
 - Straight-line distance h_{SLD}
 - Manhattan distance h_{MD}



Best-first Search

Evaluation function

```
create frontier : priority queue (  $f(n)$  )
```

```
insert Node(initial_state) to frontier
```

```
while frontier is not empty:
```

```
    node = frontier.pop()
```

```
    if node.state is goal: return solution
```

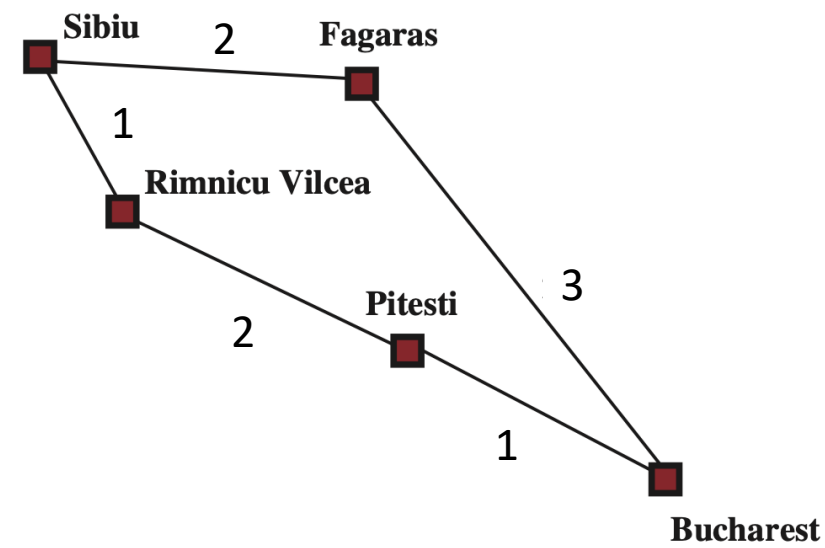
```
    for action in actions(node.state):
```

```
        next_state = transition(node.state, action)
```

```
        frontier.add(Node(next_state))
```

```
return failure
```

$f(n)$ estimates how good a state is



A* Search

Evaluation function

create **frontier**: **priority queue** ($f(n)$)

insert **Node**(initial_state) to **frontier**

while **frontier** is not empty:

node = **frontier**.pop()

if **node.state** is goal: return solution

for **action** in actions(**node.state**):

next_state = transition(**node.state**, **action**)

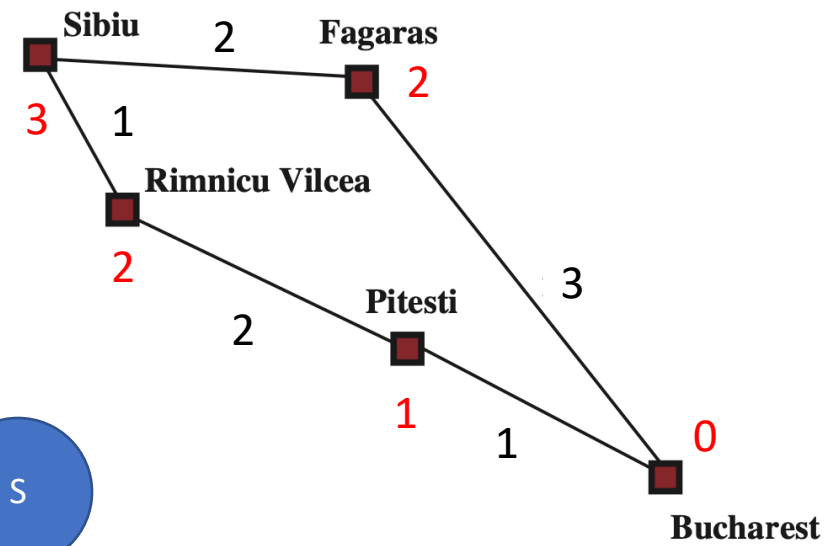
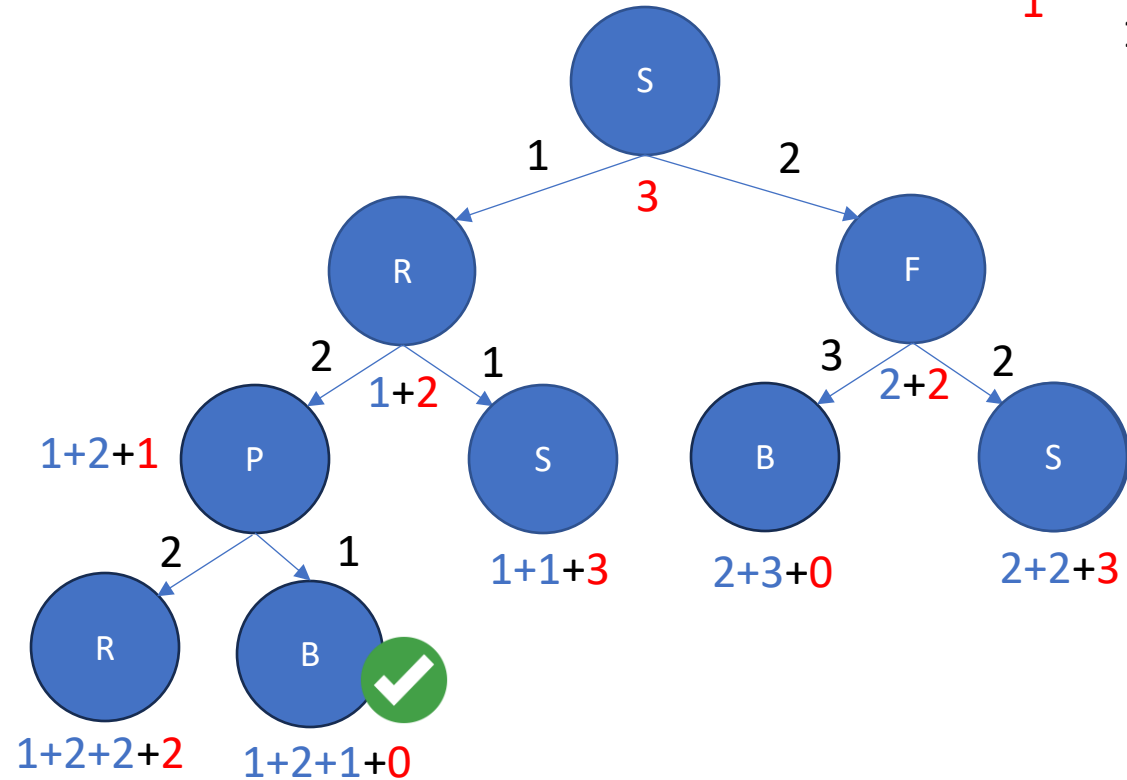
frontier.add(**Node**(**next_state**))

return failure

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

Cost to reach n

Heuristic: estimated cost from n to goal



A* Search - Analysis

Evaluation function

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

Cost to reach n

Heuristic: estimated cost from n to goal

```
create frontier : priority queue ( f(n) )
```

```
insert Node(initial_state) to frontier
```

```
while frontier is not empty:
```

```
    node = frontier.pop()
```

```
    if node.state is goal: return solution
```

```
    for action in actions(node.state):
```

```
        next_state = transition(node.state, action)
```

```
        frontier.add(Node(next_state))
```

```
return failure
```

Time complexity: (# nodes generated)

Exponential, good heuristic can improve

Space complexity: (size of frontier)

Exponential

Complete:

Yes, if edge costs are positive and branching factor is finite
(Hart, Nilsson and Raphael, 1968)

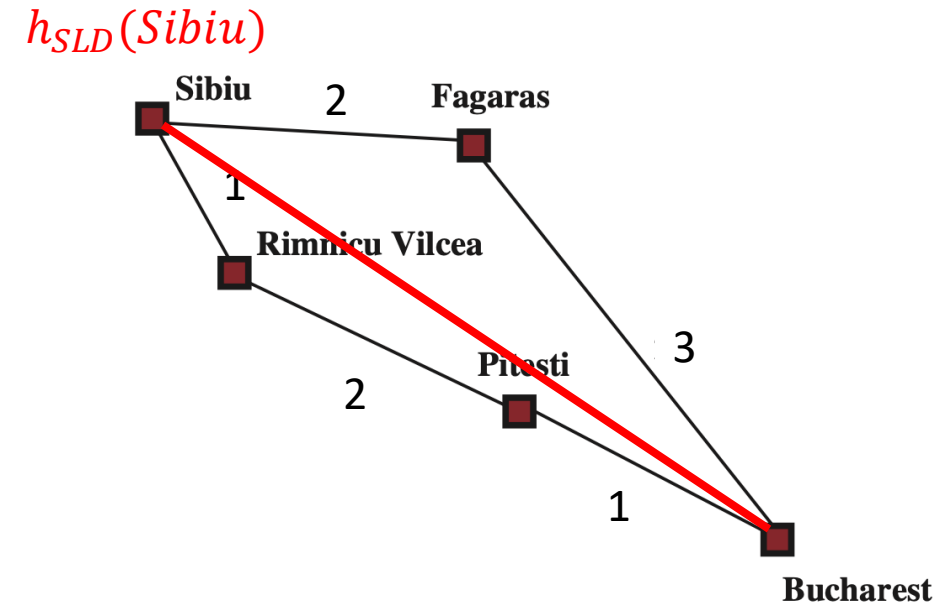
Optimal: Depends on the heuristic

Admissible Heuristics

A **heuristic $h(n)$** is **admissible** if for every node n , $h(n) \leq h^*(n)$, where $h^*(n)$ is the **optimal path cost** to reach the goal state from n .

An admissible heuristic **never over-estimates** the cost to reach the goal, i.e., it is an **optimistic estimate**.

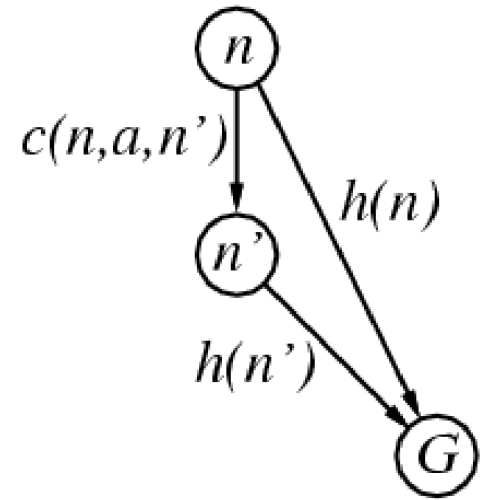
Theorem (Hart, Nilsson and Raphael, 1968):
if $h(n)$ is admissible, A* **search (without visited memory)** is optimal



Example: $h_{SLD}(n)$ never overestimates the actual road distance

Consistent Heuristics

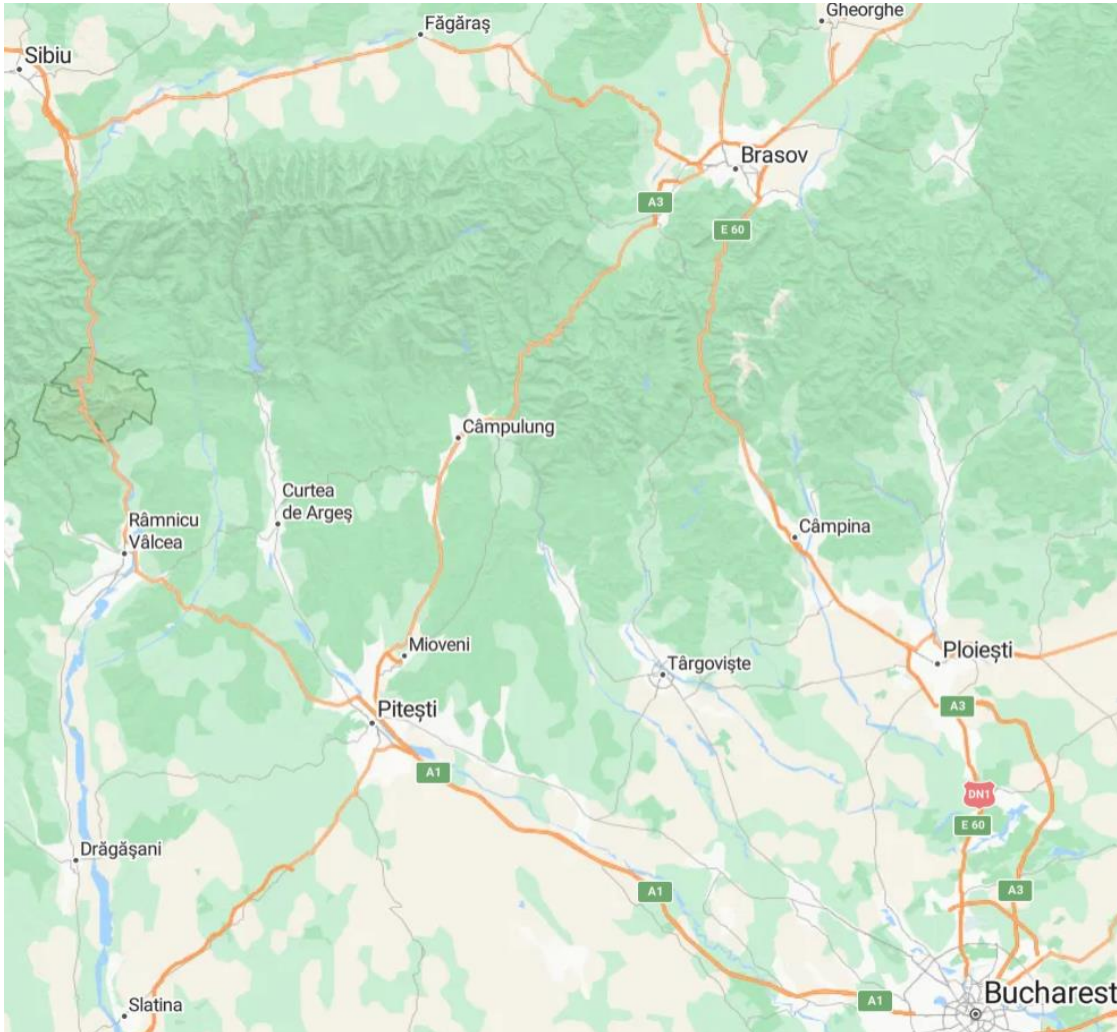
A **heuristic $h(n)$** is **consistent** if for every node n , every successor n' of n generated by any action a , $h(n) \leq c(n,a,n') + h(n')$, and $h(G) = 0$.



Theorem (Hart, Nilsson and Raphael, 1968):

If $h(n)$ is consistent, A* **search with visited memory** is optimal

“Inventing” Admissible Heuristics



A problem with **fewer restrictions** on the actions is called a relaxed problem. The cost of an **optimal solution** to a relaxed problem is an **admissible heuristic** for the original problem.

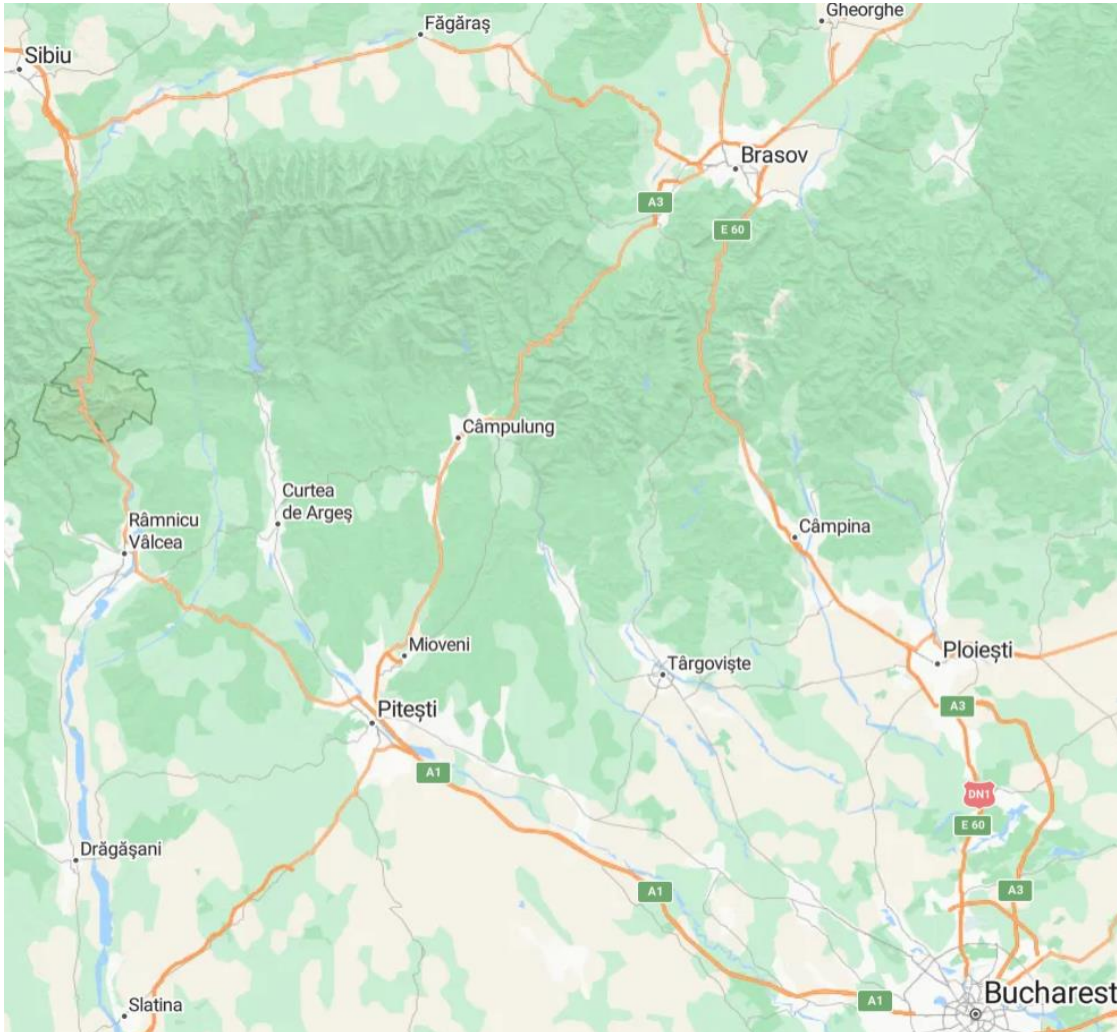
Original:

An agent can only move along the road

Relaxations:

- An agent can move off-road (fly)
 - h_1 straight line distance
- An agent can teleport
 - $h_2 = 1$

Dominance



If $h_1(n) \geq h_2(n)$ for all n , then h_1 dominates h_2 .

- h_1 is better for search if admissible.

Heuristics

- h_1 straight-line distance
- $h_2 = 1$

h_1 dominates h_2

Summary: Informed Search Algorithms

- Informed search: guide search with extra information
- Best-first search
 - A* search
 - $f(n) = g(n) + h(n)$, cost so far + heuristic
- Heuristics
 - Admissible: $h(n) \leq h^*(n)$
 - Consistent: $h(n) \leq c(n,a,n') + h(n')$
 - Dominant: if $h_1(n) \leq h_2(n)$, h_2 dominant
- Creating admissible heuristic: **optimal path cost of the relaxed problem**

Further Reading (Optional)

(Hart, Nilsson and Raphael, 1968)

- Proof: admissible heuristic → optimal search without visited memory
- Proof: consistent heuristic → optimal search with visited memory (AIAMA 3.5.2)
- Greedy best-first search (AIAMA 3.5.1)
- Variants of A* search (AIAMA 3.5.3)
 - Iterative Deepening A* (IDA*)
 - Simplified Memory-bounded A* (SMA*)

Summary

- Problem solving agents:
 - Goal formulation -> problem formulation -> search -> execute
- Uninformed search
 - Breadth-first search (BFS)
 - Uniform-cost Search (UCS)
 - Depth-first Search (DFS)
 - Depth-limited & Iterative deepening search (DLS & IDS)
- Informed search
 - A* Search
 - Heuristics: admissible, consistent, dominant, relaxed problem

Coming Up Next Week

- Local search
 - Hill climbing
 - ...
- Adversarial search
 - Games
 - Minimax
 - Alpha-beta pruning
 - ...

To Do

- **Lecture Training 2**
 - +250 EXP
 - +100 Early bird bonus
- **Problem Set 1**

Will be released later today!