# Network Science: Principles and Applications 

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\text { CS } 695 \text { - Spring } 2019
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(1) Outline of Today's Class
(2) Graphs

- Definition of a Graph
- Types of Graphs
- Asymptotic Notations
(3) Graph Representations
- Adjacency List Representation
- Adjacency Matrix Representation
- Alternative Graph Representations

4 Elementary Graph Algorithms for Path Searching
(5) (Uninformed and Informed) Graph Search Algorithms

- Uninformed Search
- Breadth-first Search (BFS)
- Depth-first Search (DFS)
- Depth-limited Search (DLS)
- Iterative Deepening Search (IDS)
- A* Search


## Components of a Complex System



- components: nodes, vertices ( V )
- interactions: links, arcs, edges (L, E)
- system: network, graph (N, G)


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Networks, or Graphs?

Network = real systems

- WWW
- social network
- metabolic network
- Language: Network, node, link

Graph $=$ mathematical representation of network

- web graph
- social graph (Facebook term)
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We will try to make this distinction whenever appropriate, but in most cases the two terms will be interchangeable.

## What is a Graph?

Graph $G=(V, E)$

- $V$ : set of vertices
- $E$ : set of edges consisting of pairs of vertices from $V$

$$
\begin{aligned}
& V=\left\{v_{0}, v_{1}, v_{2}, v_{3}, v_{4}\right\} \\
& E=\left\{\left(v_{0}, v_{1}\right),\left(v_{0}, v_{3}\right),\left(v_{1}, v_{2}\right),\left(v_{1}, v_{4}\right)\right\}
\end{aligned}
$$



## First Graph Problem

## Seven Bridges of Koenigsberg [1736]:

Find a route that crosses each bridge exactly once. Posed by Leonard Euler [1707-1783].

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What is the minimum number of bridges that need to be added so that there exists a route that crosses each bridge exactly once?

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## Specifically:

What is the minimum number of bridges that need to be added so that there exists a route that crosses each bridge exactly once?
Iff there are exactly two or zero nodes of odd degree

## Applications of Graphs Beyond Network Science

- Compilers
- Databases
- Neural Networks
- Machine Learning
- Artificial Intelligence
- Robotics
- Computational Biology
- ...


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```
Focus of this Lecture:
Primer on Graphs
Terminology, Characteristics, and Algorithms Relevant to Networks
```


## Formal Definition of a Graph

## A graph $G=(V, E)$ is a pair consisting of:

- a set $V$ of vertices (or nodes)
- a set $E \subseteq V \times V$ of edges (or arcs)
- edge $e_{i} \in E$ is a pair $(u, v)$ connecting vertices $u$ and $v$


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A graph $G=(V, E)$ is:

- directed (referred to as a digraph) if $E$ is a set of ordered pairs of vertices. The edges here are often referred to as directed edges or arrows.
- undirected if $E$ is a set of unordered pairs of vertices.
- weighted if there are weights associated with the edges.


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We typically reserve:

- N for number of vertices, $|V|$
- $|E|$ indicates number of edges


## Illustrations of Types of Graphs



Figure: undirected graph


Figure: multigraph


Figure: directed graph


Figure: weighted graph

## More Definitions, Conventions, Nomenclature

- Two vertices are adjacent if they are connected by an edge.
- The neighbors of a vertex are all the vertices adjacent to it.
- The degree of a vertex is the number of its neighbors.
- A path is a sequence of vertices, where each pair of successive vertices is connected by an edge.
- The length of the path is the number of edges in the path.
- A simple path contains unique vertices.
- A cycle is a simple path with the same first and last vertex.


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- A subgraph $H$ of $G=(V, E)$ is $H=\left(V_{1}, E_{1}\right)$ where $V_{1} \subseteq V$ and $E_{1} \subseteq E$, where $\forall e=(k, j) \in E_{1}, k, j \in V_{1}$.


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## Focusing on Simple Graphs

## Simple Graphs

- A simple graph, or a strict graph, is an unweighted, undirected graph containing no loops or multiple edges
- Given that $E \subseteq V \times V,|E| \in O\left(|V|^{2}\right)$.
- If a graph is connected, $|E| \geq|V|-1$
- Combining the two, show that $\lg (|E|) \in \theta(\lg (|V|))$


## Short Detour:

## Asymptotic Notations

## Big-Oh: An Asymptotic Upper Bound

## Definition

A function $g(n) \in O(f(n))$ if
$\exists$ constants $c>0$ and $n_{0}$ s.t $g(n) \leq c \cdot f(n)$ $\forall n \geq n_{0}$.
Note: $O(f(n))$ denotes a set.

## Graphical Illustration



## little-oh: Tight Asymptotic Upper Bound

$g(n) \in o(f(n))$ when the upper bound $<$ holds for all constants $c>0$. Alternative definition: $\lim _{n \rightarrow \infty} \frac{g(n)}{f(n)}=0$

## Big-Omega: An Asymptotic Lower Bound

## Definition

A function $g(n) \in \Omega(f(n))$ if
$\exists$ constants $c>0$ and $n_{0}$ s.t $g(n) \geq c \cdot f(n)$ $\forall n \geq n_{0}$.
Note: $\Omega(f(n))$ denotes a set.

## Graphical Illustration



## little-omega: Tight Asymptotic Lower Bound

 $g(n) \in \omega(f(n))$ when the lower bound $>$ holds for all constants $c>0$. Alternative definition: $\lim _{n \rightarrow \infty} \frac{g(n)}{f(n)}=\infty$
## Theta: Asymptotic Upper and Lower Bounds

## Definition

A function $g(n) \in \Theta(f(n))$ if $g(n) \in O(f(n))$ and $g(n) \in \Omega(f(n))$. Alternatively, $g(n) \in \Theta(f(n))$ if $\exists$ positive constants $c_{1}, c_{2}$ and $n_{0}$ s.t.
$c_{1} \cdot f(n) \leq g(n) \leq c_{2} \cdot f(n) \forall n \geq n_{0}$.

## Graphical Illustration



## Alternative Definition

$g(n) \in \Theta(f(n))$ when $\lim _{n \rightarrow \infty} \frac{g(n)}{f(n)}=O(1)$

## Back to Graphs

## General Definition of a Graph

In a graph $G=(V, E)$ :

- $E$ may be a set of unorderered pairs of vertices not necessarily distinct. More than one edge can connect two vertices.
- An edge in $E$ may connect more than two vertices.
- These graphs are referred to as multigraphs or pseudo-graphs.


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- Choice determines ability to use network theory successfully.
- In some cases there is a unique, unambiguous representation; in others, the representation is not unique.
- E.g. the way we assign the links between a group of individuals will determine the nature of the question we can study.
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- E.g. the way we assign the links between a group of individuals will determine the nature of the question we can study.
- Some examples next


## Finding the Right Network Representation



Figure: If you connect individuals that work with each other, you will explore the professional

## Finding the Right Network Representation



## Finding the Right Network Representation



Undirected edges for symmetric relationships

- Co-authorship links
- Actor network
- Protein-protein interactions


Directed edges for asymmetric relationships

- URLs on the www
- phone calls
- metabolic reactions


## Finding the Right Network Representation

Bipartitle graph or bigraph is a graph $G=(V, E)$ whose vertices can be divided into two disjoint sets $V_{1}$ and $V_{2}$ such that every edge connects a vertex in $V_{1}$ to one in $V_{2}$

Specifically: $V=V_{1} \cup V_{2}$ and $V_{1} \cap V_{2}=\{ \}$

## Examples

- Collaboration networks
- Hollywood actor network

- Disease network (diseasome)


## Some More Examples

## GENE NETWORK - DISEASE NETWORK



## Gene network



Disease network

Goh, Cusick, Valle, Childs, Vidal \& Barabási, PNAS (2007)

## Some More Examples

## HUMAN DISEASE NETWORK



## (Internal) Graph Representations

- A graph can be represented as an adjacency list.
- A graph can be represented as an adjacency matrix.


## Adjacency List Representation



## Implementation of Adjacency-list Representation

## The adjacency list of a vertex can be implemented as a linked list

The list of vertices themselves can be implemented using:

- A linked list
- A binary search tree
- A hash table

In a standard implementation, each edge list has two fields, a data field and a pointer:

- The data field contains adjacent vertex name and edge information
- The pointer points to next adjacent vertex


## Basic Graph Operations with Adjacency List Representation

| Function | Worst-case Running Time |
| :--- | :--- |
| find $(v)$ | $O(\|V\|)$ |
| hasVertex $(v)$ | $O(\operatorname{find}(\mathrm{v}))$ |
| hasEdge $\left(v_{i}, v_{j}\right)$ | $O\left(\right.$ find $\left.\left(\mathrm{v}_{\mathrm{i}}\right)+\operatorname{deg}\left(\mathrm{v}_{\mathrm{i}}\right)\right)$ |
| insertVertex $(v)$ | $O(1)$ |
| insertEdge $\left(v_{i}, v_{j}\right)$ | $O\left(\operatorname{find}\left(\mathrm{v}_{\mathrm{i}}\right)\right)$ |
| removeVertex $(v)$ | $O(\|V\|+\|E\|)$ |
| removeEdge $\left(v_{i}, v_{j}\right)$ | $O\left(\operatorname{find}\left(\mathrm{v}_{\mathrm{i}}\right)+\operatorname{deg}\left(\mathrm{v}_{\mathrm{i}}\right)\right)$ |
| outEdges $(v)$ | $O($ find $(\mathrm{v})+\operatorname{deg}(\mathrm{v}))$ |
| inEdges $(v)$ | $O(\|V\|+\|E\|)$ |
| overall memory | $O(\|V\|+\|E\|)$ |

In undirected graphs: $\mid$ elist[v]| $=$ degree( $v$ ).

In digraphs:
$|\operatorname{elist}[\mathrm{v}]|=$ out-degree(v).

## Handshaking Lemma:

$\sum_{v \in V}|\operatorname{elist}(\mathrm{v})|=2|\mathrm{E}|$ for undirected graphs.
$O(|V|+|E|)$ storage $\Rightarrow$ sparse representation.

## Adjacency Matrix Representation


$M[i][j]=1 \quad$ iff $\quad\left(v_{i}, v_{i}\right) \in E$

| M | $V_{0}$ | $V_{1}$ | $V_{2}$ | $V_{3}$ | $V_{4}$ |  | M | $V_{0}$ | $V_{1}$ | $V_{2}$ | $V_{3}$ | $V_{4}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $V_{0}$ | 0 | 1 | 0 | 1 | 0 |  | $V_{0}$ | 0 | 1 | 1 | 0 | 1 |
| $V_{1}$ |  | 0 | 1 | 0 | 1 | bool **M; | $V_{1}$ | 0 | 1 | 0 | 0 | 0 |
| $V_{2}$ |  |  | 1 | 0 | 0 |  | $V_{2}$ | 0 | 1 | 0 | 1 | 0 |
| $V_{3}$ |  |  |  | 0 | 0 | using namespace std; | $V_{3}$ | 0 | 0 | 0 | 0 | 1 |
| $V_{4}$ |  |  |  |  | 1 | vector < vector<bool>> M; | $V_{4}$ | 1 | 0 | 1 | 1 | 0 |

## Basic Graph Operations with Adjacency Matrix Representation

| Function | Worst-case Running Time |
| :--- | :--- |
| find $(v)$ | $O(1)$ |
| hasVertex $(v)$ | $O(1)$ |
| hasEdge $\left(v_{i}, v_{j}\right)$ | $O(1)$ |
| insertVertex $(v)$ | $O\left(\|V\|^{2}\right)$ |
| insertEdge $\left(v_{i}, v_{j}\right)$ | $O(1)$ |
| removeVertex $(v)$ | $O\left(\|V\|^{2}\right)$ |
| removeEdge $\left(v_{i}, v_{j}\right)$ | $O(1)$ |
| outEdges $(v)$ | $O(\|V\|)$ |
| inEdges $(v)$ | $O(\|V\|)$ |
| overall memory | $O\left(\|V\|^{2}\right)$ |

$O\left(|V|^{2}\right)$ storage $\Rightarrow$ dense representation.

## Comparing The Two Representations

| Function | Adjacency List | Adjacency Matrix |
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| find $(v)$ | $O(\|V\|)$ | $O(1)$ |
| hasVertex $(v)$ | $O($ find $(\mathrm{v}))$ | $O(1)$ |
| hasEdge $\left(v_{i}, v_{j}\right)$ | $O\left(\operatorname{find}\left(\mathrm{v}_{\mathrm{i}}\right)+\operatorname{deg}\left(\mathrm{v}_{\mathrm{i}}\right)\right)$ | $O(1)$ |
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| removeVertex $(v)$ | $O(\|V\|+\|E\|)$ | $O\left(\|V\|^{2}\right)$ |
| removedgge $\left(v_{i}, v_{j}\right)$ | $O\left(\operatorname{find}\left(\mathrm{v}_{\mathrm{i}}\right)+\operatorname{deg}\left(\mathrm{v}_{\mathrm{i}}\right)\right)$ | $O(1)$ |
| outEdges $(v)$ | $O(\operatorname{indnd}(\mathrm{v})+\operatorname{deg}(\mathrm{v}))$ | $O\|V\|)$ |
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## Time and Space

- What data structure choice to make to support faster, $O(1)$ operations?
- What happens when memory is a concern for the very large networks of millions or more nodes?


## Graph Representation: Hash Map

- Vertex set as a hash map
- key: vertex
- data: outgoing edges
- Outgoing edges of each vertex as a hash set



## Graph Representation: Hashmap

| HashMap |  | $O(1)$ |
| :--- | :--- | ---: |
| Fast to query | [hasVertex, hasEdge] | $O(\|V\|)$ |
| Fast to scan | [outEdges] | $O(1)$ |
| Fast to insert | [insertVertex, insertEdge] | $O(1)$ |
| Fast to remove | [removeEdge] | $O$ |

## Comparing The Three Representations

| Function | Adj. List | Adj. Matrix | Hash Map |
| :--- | :--- | :--- | :--- |
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| hasEdge $\left(v_{i}, v_{j}\right)$ | $O\left(\|V\|+\operatorname{deg}\left(\mathrm{v}_{\mathrm{i}}\right)\right)$ | $O(1)$ | $O(1)$ |
| insertVertex $(v)$ | $O(1)$ | $O\left(\|V\|^{2}\right)$ | $O(1)$ |
| insertEdge $\left(v_{i}, v_{j}\right)$ | $O(\|V\|)$ | $O(1)$ | $O(1)$ |
| removeVertex $(v)$ | $O(\|V\|+\|E\|)$ | $O\left(\|V\|^{2}\right)$ | $O(\|V\|)$ |
| removeEdge $\left(v_{i}, v_{j}\right)$ | $O\left(\|V\|+\operatorname{deg}\left(v_{i}\right)\right)$ | $O(1)$ | $O(1)$ |
| outEdges $(v)$ | $O(\|V\|+\operatorname{deg}(v))$ | $O(\|\|\mid)$ | $O(\operatorname{deg}(v))$ |
| inEdges $(v)$ | $O(\|V\|+\|E\|)$ | $O(\|\|\mid)$ | $O(\|V\|)$ |
| overall memory | $O(\|V\|+\|E\|)$ | $O\left(\|V\|^{2}\right)$ | linear-quadratic |

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## What about space concerns?

- Study/store specific subgraphs
- Consider distributed environment (example: Weaver - weaver.systems)


## Finding Distances

Many measures of interest in a network involve distances, that are often related to the length or weight of the shortest/least-weight path connecting two nodes of interest

How do we find a path connecting two nodes?

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## Refresher: Graph Search Algorithms

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How do we find a path connecting two nodes?
Refresher: Graph Search Algorithms

## General Search Template

## - Important insight:

- Any search algorithm constructs a tree, adding to it vertices of graph $G$ in some order
- $G=(V, E)$ - look at it as split in two: set $S$ on one side and $V-S$ on the other
- search proceeds as vertices are taken from $V-S$ and added to $S$
- search ends when $V-S$ is empty or goal found
- First vertex to be taken from $V-S$ and added to $S$ ?
- Next vertex? (... expansion ...)
- Where to keep track of these vertices? (... fringe/frontier ...)
- Important ideas:
- Fringe (frontier into $V-S /$ border between $S$ and $V-S$ )
- Expansion (neighbor generation so can add to fringe)
- Exploration strategy (what order to grow S?)
- Main question:
- which fringe/frontier nodes to explore/expand next?
- strategy distinguishes search algorithms from one another


## Search Strategies

A strategy is defined by picking the order of node expansion

Strategies are evaluated along the following dimensions:

- completeness-does it always find a solution if one exists?
- time complexity—number of nodes generated/expanded
- space complexity-maximum number of nodes in memory
- optimality-does it always find a least-cost solution?

Time and space complexity are measured in terms of:

- b-maximum branching factor of the search tree
- d-depth of the least-cost solution
- m—maximum depth of the state space (may be $\infty$ )


## Uninformed Graph Search

## Characteristics of Uninformed Graph Search/Traversal:

- There is no additional information about states/vertices beyond what is provided in the problem definition.
- All that the search does is generate successors/neighbors and distinguish a goal state from a non-goal state.


The systematic search "lays out" all paths from initial vertex; it traverses the search tree of the graph.


## Uninformed Graph Search

## F: search data structure (fringe)

 parent array: stores "edge comes from" to record visited states1: F.insert(v)
parent[v] $\leftarrow$ true
3: while not F.isEmpty do
4: $\quad \mathrm{u} \leftarrow$ F.extract()
5: if isGoal(u) then
6: return true
7: for each $v$ in outEdges( $u$ ) do
8: if no parent[v] then
9: $\quad$ F.insert(v)
10: $\quad$ parent $[\mathrm{v}] \leftarrow \mathrm{u}$


Figure: Graph


## Uninformed Search Algorithms

- Breadth-first Search (BFS)
- Depth-first Search (DFS)
- Depth-limited search (DLS)
- Iterative Deepening Search (IDS)


## Breadth-first Search (BFS)



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## Strategy: Expand shallowest unexpanded node

Implementation:
fringe $=$ first-in first-out (FIFO), i.e., unvisited successors go at end $F$ is a queue


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## BFS vs. DFS



- When will BFS outperform DFS?
- When will DFS outperform BFS?


## Another Advantage of DFS

RecursiveDFS( $v$ )
1: if $v$ is unmarked then
2: mark $v$
3: for each edge $v, u$ do
4: RecursiveDFS( $u$ )

## Undiscovered

Unfinished Active Finished

Color arrays can be kept to indicate that a vertex is undiscovered, the first time it is discovered, when its neighbors are in the process of being considered, and when all its neighbors have been considered.

DFS can be used to timestamp vertices with when they are discovered and when they are finished. These start and finish times are useful in various applications of DFS regarding constraint satisfaction.

## Depth-limited Search (DLS)

- Problem with DFS is presence of infinite paths
- DLS limits the depth of a path in search tree of DFS
- Modifies DFS by using a predetermined depth limit $d_{1}$
- DLS is incomplete if the shallowest goal is beyond the depth limit $d_{l}$
- DLS is not optimal if $d<d_{l}$
- Time complexity is $O\left(b^{d_{l}}\right)$ and space complexity is $O\left(b \cdot d_{l}\right)$


## Depth-limited Search (DLS)

$=$ DFS with depth limit $d_{l}$ [i.e., nodes at depth $d_{l}$ are not expanded]

## Recursive implementation:

function DEPTH-LIMITED-SEARCH( problem, limit) returns soln/fail/cutoff

Recursive-DLS(Make-Node(Initial-State[problem]), problem, limit)
function RECURSIVE-DLS(node, problem, limit) returns soln/fail/cutoff cutoff-occurred? $\leftarrow$ false
if Goal-TEST(problem, State[node]) then return node else if DEPTH[node] $=$ limit then return cutoff else for each successor in EXPAND(node, problem) do result $\leftarrow$ RECURSIVE-DLS(successor, problem, limit)
if result $=$ cutoff then cutoff-occurred? $\leftarrow$ true else if result $\neq$ failure then return result
if cutoff-occurred? then return cutoff else return failure

## Iterative Deepening Search (IDS)

- Finds the best depth limit by incrementing $d_{l}$ until goal is found at $d_{l}=d$
- Can be viewed as running DLS with consecutive values of $d_{l}$
- IDS combines the benefits of both DFS and BFS
- Like DFS, its space complexity is $O(b \cdot d)$
- Like BFS, it is complete when the branching factor is finite, and it is optimal if the path cost is a non-decreasing function of the depth of the goal node
- Its time complexity is $O\left(b^{d}\right)$
- IDS is the preferred uninformed search when the state space is large, and the depth of the solution is not known


## Iterative Deepening Search (IDS)

function Iterative-Deepening-Search ( problem) returns a solution inputs: problem, a problem
for depth $\leftarrow 0$ to $\infty$ do
result $\leftarrow$ Depth-Limited-Search (problem, depth)
if result $\neq$ cutoff then return result
end

## Iterative Deepening Search (IDS) @ $d_{l}=0$

Limit $=0$ (4)

## Iterative Deepening Search (IDS) @ $d_{l}=1$



## Iterative Deepening Search (IDS) @ $d_{l}=2$



## Iterative Deepening Search (IDS) @ $d_{l}=3$



## Summary of Uninformed Search Algorithms

| Criterion | Breadth- <br> First | Depth- <br> First | Depth- <br> Limited | Iterative <br> Deepening |
| :--- | :---: | :---: | :---: | :---: |
| Complete? | Yes $^{*}$ | No | Yes, if $d_{l} \geq d$ | Yes |
| Time | $b^{d+1}$ | $b^{m}$ | $b^{d_{l}}$ | $b^{d}$ |
| Space | $b^{d+1}$ | $b m$ | $b d_{l}$ | $b d$ |
| Optimal? | Yes $^{*}$ | No | No | Yes $^{*}$ |

## Uninformed Search Summary

- Problem formulation usually requires abstracting away real-world details to define a state space that can feasibly be explored
- Variety of uninformed search strategies
- IDS uses only linear space and not much more time than other uninformed algorithms
- Graph search can be exponentially more efficient than tree search
- What about least-cost paths with non-uniform state-state costs?
- That is next


## Most popular: Dijkstra and A*

## Differences from uninformed search algorithms:

- work with weighted graphs
- process nodes in order of attachment cost
- employ priority queue (min-heap) for this purpose instead of stack or queue
- Dijkstra: overkill, finds least-cost path from a given start node to all nodes in graph
- A*: works only with given start and goal pair
- Dijkstra: attachment cost of a node is current least cost from given start to that node
- A*: adds to this the estimated distance to goal node, where esimation uses an optimistic heuristic


## Essence of All Informed Search Algorithms

All you need to remember about informed search algorithms

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- Until $F$ is empty, one vertex extracted from $F$ at a time


## Essence of All Informed Search Algorithms

All you need to remember about informed search algorithms

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- What should $d[v]$ be? There are options...
- backward cost (cost of $s \rightsquigarrow v$ )
- forward cost (estimate of cost of $v \rightsquigarrow g$ )
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## Dijkstra's Algorithm in Pseudocode

- Fringe: F is a priority queue/min-heap
- arrays: $d$ stores attachment (backward) costs, $\pi[v]$ stores parents
- $S$ not really needed, only for clarity below

```
Dijkstra(G, s, w)
    F}\leftarrows,S\leftarrow{
    d[v]}\leftarrow\infty\mathrm{ for all v}\in
    d[s]\leftarrow0
    4: while F\not={} do
    5:
    6:}\quadS\leftarrowS\cup{u
    for each v}\in\operatorname{Adj(u) do
            F\leftarrowv
        Relax(u,v,w)
```

```
\(\operatorname{Relax}(u, v, w)\)
    1: if \(d[v]>d[u]+w(u, v)\) then
    2: \(\quad d[v] \leftarrow d[u]+w(u, v)\)
    3: \(\quad \pi[\mathrm{v}] \leftarrow \mathrm{u}\)
```

- The process of relaxing tests whether one can improve the shortest-path estimate $d[v]$ by going through the vertex $u$ in the shortest path from $s$ to $v$
- If $d[u]+w(u, v)<d[v]$, then $u$ replaces the predecessor of $v$
- Where would you put an earlier termination to stop when $s \rightsquigarrow g$ found?


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    while F\not={} do
    u\leftarrow Extract-Min(F)
    S\leftarrowS\cup{u}
    for each v}\in\operatorname{Adj(u) do
        F\leftarrowv
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```

in another implementation, F is
initialized with all $V$, and line 8 is
removed.

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## Dijsktra's Algorithm in Action



Figure: Graph $G=(V, E)$


Figure: Shortest paths from $B$

|  | Initial |  | Pass1 |  | Pass2 |  | Pass3 |  | Pass4 |  | Pass5 |  | Pass6 |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Vertex | d | $\pi$ | d | $\pi$ | d | $\pi$ | d | $\pi$ | d | $\pi$ | d | $\pi$ | d | $\pi$ |
| A | $\infty$ |  | 3 | $B$ | 3 | B | 3 | $B$ | 3 | $B$ | 3 | B | 3 | $B$ |
| B | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - |
| C | $\infty$ |  | 5 | $B$ | 4 | A | 4 | $A$ | 4 | A | 4 | A | 4 | A |
| D | $\infty$ |  | $\infty$ |  | $\infty$ |  | 6 | C | 6 | C | 6 | C | 6 | C |
| E | $\infty$ |  | $\infty$ |  | $\infty$ |  | 8 | C | 8 | C | 8 | C | 8 | C |
| F | $\infty$ |  | $\infty$ |  | $\infty$ |  | $\infty$ |  | 11 | D | 9 | E | 9 | E |

## Dijsktra's Algorithm in Action



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| Vertex | d | $\pi$ | d | $\pi$ | d | $\pi$ | d | $\pi$ | d | $\pi$ | d | $\pi$ | d | $\pi$ |
| A | $\infty$ |  | 3 | $B$ | 3 | $B$ | 3 | B | 3 | $B$ | 3 | $B$ | 3 | $B$ |
| B | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - | 0 | - |
| C | $\infty$ |  | 5 | $B$ | 4 | A | 4 | A | 4 | A | 4 | A | 4 | A |
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| E | $\infty$ |  | $\infty$ |  | $\infty$ |  | 8 | C | 8 | C | 8 | C | 8 | C |
| F | $\infty$ |  | $\infty$ |  | $\infty$ |  | $\infty$ |  | 11 | D | 9 | $E$ | 9 | $E$ |

If not earlier goal termination criterion, Dijkstra's search tree is spanning tree of shortest paths from s to any vertex in the graph.

## Take-home Exercise



|  | Initial |  | Pass1 |  | Pass2 |  | Pass3 |  | Pass4 |  | Pass5 |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Vertex | $d$ | $\pi$ | $d$ | $\pi$ | $d$ | $\pi$ | $d$ | $\pi$ | $d$ | $\pi$ | $d$ | $\pi$ |
| a | 0 | - |  |  |  |  |  |  |  |  |  |  |
| b | $\infty$ |  |  |  |  |  |  |  |  |  |  |  |
| c | $\infty$ |  |  |  |  |  |  |  |  |  |  |  |
| d | $\infty$ |  |  |  |  |  |  |  |  |  |  |  |
| e | $\infty$ |  |  |  |  |  |  |  |  |  |  |  |

## Analysis of Dijkstra's Algorithm

- Dijkstra's is optimal: proof relies on corollary that when a vertex $v$ is extracted from fringe $F$ (thus "added" to $S$ ), shortest path from $s$ to $v$ has been found (not true with negative weights).
- Updating the heap takes at most $O(\lg (|V|))$ time
- The number of updates equals the total number of edges
- So, the total running time is $O(|E| \cdot \lg (|V|))$
- Running time can be improved depending on the actual implementation of the priority queue

| Time $=\theta(V) \cdot T($ Extract - Min $)+\theta(\mathrm{E}) \cdot \mathrm{T}($ Decrease - Key $)$ |  |  |  |
| :--- | :--- | :--- | :--- |
| $F$ | $T($ Extr.-Min $)$ | $T($ Decr.-Key $)$ | Total |
| Array | $O(\|V\|)$ | $O(1)$ | $O\left(\|V\|^{2}\right)$ |
| Binary heap | $O(1)$ | $O(\|g\| V \mid)$ | $O(\|E\| \cdot\|g\| V \mid)$ |
| Fib. heap | $O(\|g\| V \mid)$ | $O(1)$ | $O(\|E\|+\|V\| \cdot\|g\| V \mid)$ |

How does this compare with BFS? How does BFS get away from a $\lg (|V|)$ factor?

## A* Search

Idea: avoid expanding paths that are already expensive
Evaluation function $f(v)=g(v)+h(v)$ :
Combines Dijkstra's/uniform cost with greedy best-first search
$g(v)=$ (actual) cost to reach $v$ from $s$
$h(v)=$ estimated lowest cost from $v$ to goal
$f(v)=$ estimated lowest cost from $s$ through $v$ to goal
Same implementation as before, but prioritize vertices in min-heap by $f[v]$
A* is both complete and optimal provided $h$ satisfies certain conditions: for searching in a tree: admissible/optimistic for searching in a graph: consistent (which implies admissibility)

## Admissible Heuristic

What do we want from $f[v]$ ? not to overestimate cost of path from source to goal that goes through $v$

Since $g[v]$ is actual cost from $s$ to $v$, this "do not overestimate" criterion is for the forward cost heuristic, $h[v]$

A* search uses an admissible/optimistic heuristic i.e., $h(v) \leq h^{*}(v)$ where $h^{*}(v)$ is the true cost from $v$ (Also require $h(v) \geq 0$, so $h(G)=0$ for any goal $G$ )

Example of an admissible heuristic: crow-fly distance never overestimates the actual road distance

A stronger, consistent heuristic: estimated cost of reaching goal from a vertex $n$ is not greater than cost to go from $n$ to its successors and then the cost from them to the goal

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A stronger, consistent heuristic: estimated cost of reaching goal from a vertex $n$ is not greater than cost to go from $n$ to its successors and then the cost from them to the goal

Let's see A* with this heuristic in action

## A* Search in Action

## A* Search in Action



## A* Search in Action



## A* Search in Action



## A* Search in Action



## A* Search in Action



## Optimality of A*

Skipping some details, but essentially if heuristic is consistent: $A^{*}$ expands nodes in order of increasing $f$ value*
Gradually adds "f-contours" of nodes (cf. breadth-first adds layers)
Contour $i$ has all nodes with $f=f_{i}$, where $f_{i}<f_{i+1}$


So, why does this guarantee optimality?
First time we see goal will be the time it has lowest $f=g$ ( $h$ is 0 )
Other occurrences have no lower f (f non-decreasing)

## Summary of A* Search

## Complete??

## Summary of A* Search

## Complete?? Yes, unless there are infinitely many nodes with $f \leq f(G)$

## Summary of A* Search

Complete?? Yes, unless there are infinitely many nodes with $f \leq f(G)$ Time??

## Summary of A* Search

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## Time?? Exponential in [path length $\times \frac{\delta(s, g)-h(s)}{\delta(s, g)}$ ]

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$$
\underline{\underline{\text { Time? }} ? \text { ? Exponential in [path length } \times \frac{\delta(s, g)-h(s)}{\delta(s, g)} \text { ] }}
$$

## Space??

## Summary of A* Search

Complete?? Yes, unless there are infinitely many nodes with $f \leq f(G)$
Time?? Exponential in [path length $\times \frac{\delta(s, g)-h(s)}{\delta(s, g)}$ ]

## Space?? Keeps all generated nodes in memory (worse drawback than time)

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A* expands no nodes with $f(v)>\delta(s, g)$

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## End of Graph Search Algorithms

CS583 additionally considers scenarios where greedy substructure does not lead to optimality

For instance, how can one modify Dijkstra and the other algorithms to deal with negative weights?

How does one efficiently find all pairwise shortest/least-cost paths?
Dynamic Programming is the right alternative in these scenarios

More graph exploration and search algorithms considered in CS583

# Next Lecture: Measures of Interest in Networks 

