

## Algorithms and Data Structures

Graphs: Introduction and First Algorithms

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## This Course

- Introduction

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- Abstract Data Types 1
- Complexity analysis 1
- Styles of algorithms 1
- Lists, stacks, queues 2
- Sorting (lists)
- Searching (in lists, PQs, SOL)
- Hashing (to manage lists)

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- Trees (to manage lists)
- Graphs (no lists!)
- Sum

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## Content of this Lecture

- Graphs
- Definitions
- Representing Graphs
- Traversing Graphs
- Connected Components
- Shortest Paths


## Graphs

- There are objects and there are relations between objects
- Directed trees can represent hierarchical relations
- Relations that are asymmetric, cycle-free, binary
- Examples: parent_of, subclass_of, smaller_than, ...
- Undirected trees can represent cycle-free, binary relations
- This excludes many (cyclic) real-life relations
- friend_of, similar_to, reachable_by, html_linked_to, ...
- (Classical) Graphs can represent all binary relationships
- N-ary relationships: Hypergraphs
- exam(student, professor, subject), borrow(student, book, library)


## Types of Graphs

- Most graphs you will see are binary
- Most graphs you will see are simple
- Simple graphs: At most one edge between any two nodes
- Contrary: multigraphs
- Some graphs you will see are undirected, some directed
- This lecture: Only binary, simple, finite graphs


## Exemplary Graphs

- Classical theoretical model: Random Graphs
- Create every possible edge with a fixed probability p

$p=0.1$

$p=0.25$

$p=0.5$

- In a random graph, the degree of every node has expected value $\mathrm{p}^{*} \mathrm{n}$, and the degree distribution follows a Poisson distribution


## Web Graph



# Note the strong local clustering 

This is not a random graph

- Graph layout is difficult
[http://img.webme.com/pic/c/chegga-hp/opte_org.jpg]


## Universities Linking to Universities



- Small-World Property
[http://internetlab.cindoc.csic.es/cv/11/world_map/map.html]


## Human Protein-Protein-Interaction Network



- Still terribly incomplete
- Proteins that are close in the graph likely share function
[http://www.estradalab.org/research/index.html]


## Word Co-Occurrence



- Words that are close have similar meaning
- Close: Appear in the same contexts
- Words cluster into topics
[http://www.michaelbommarito.com/blog/]


## Social Networks



- Six degrees of separation
[http://tugll.tugraz.at/94426/files/-1/2461/2007.01.nt.social.network.png]


## Road Network



- Specific property: Planar graphs
[Sanders, P. \&Schultes, D. (2005).Highway Hierarchies Hasten Exact Shortest Path Queries. In 13th European Symposium on Algorithms (ESA), 568-579.]


## More Examples

- Graphs are also a wonderful abstraction


## Coloring Problem

- How many colors do one need to color a map such that never two colors meet at a border?

[http://www.wikipedia.de]
- Chromatic number: Number of colors sufficient to color a graph such that no adjacent nodes have the same color
- Every planar graph has chromatic number of at most 4


## History [wikipedia.de]

- This is not simple to proof
- It is easy to see that one sometimes needs at least four colors
- It is easy to show that one may need arbitrary many colors for general graphs
- First conjecture which until today was proven only by computers

- Falls into many, many subcases - try all of them with a program


## Königsberger Brückenproblem

- Given a city with rivers and bridges: Is there a cycle-free path crossing every bridge exactly once?
- Euler-Path



## Königsberger Brückenproblem

- Given a city with rivers and bridges: Is there a cycle-free path crossing every bridge exactly once?
- A graph has an Euler-Path iff at contains 0 or 2 edges with odd degree

- Hamiltonian path
- ... visits each vertex exactly once
- NP complete


## Recall?



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## Recall from Trees

- Definition

A graph $G=(V, E)$ consists of a set of vertices (nodes) $V$ and a set of edges ( $E \subseteq V x V$ ).

- A sequence of edges $e_{1}, e_{2}, . ., e_{n}$ is called a path iff $\forall 1 \leq i<n$ : $e_{i}=\left(v^{\prime}, v\right)$ and $e_{i+1}=\left(v, v^{`}\right)$; the length of this path is $n$
- A path $\left(v_{1}, v_{2}\right),\left(v_{2}, v_{3}\right), \ldots,\left(v_{n-1}, v_{n}\right)$ is acyclic iff all $v_{i}$ are different
- $G$ is acyclic, if no path in $G$ contains a cycle; otherwise it is cyclic
- A graph is connected if every pair of vertices is connected by at least one path
- Definition

A graph (tree) is called undirected, if $\forall\left(v, v^{\prime}\right) \in E \Rightarrow\left(v^{\prime}, v\right) \in E$. Otherwise it is called directed.

## More Definitions

- Definition

Let $G=(V, E)$ be a directed graph. Let $v \in V$

- The outdegree out(v) is the number of edges with v as start point
- The indegree in(v) is the number of edges with $v$ as end point
- $G$ is edge-labeled, if there is a function w: $E \rightarrow L$ that assigns an element of a set of labels $L$ to every edge
- A labeled graph with $L=N$ is called weighted
- Remarks
- Weights can as well be reals; often we only allow positive weights
- Labels / weights max be assigned to edges or nodes (or both)
- Indegree and outdegree are identical for undirected graphs


## Some More Definitions

- Definition. Let $G=(V, E)$ be a directed graph.
- Any $G^{\prime}=\left(V^{\prime}, E^{\prime}\right)$ is called a subgraph of $G$, if $V^{\prime} \subseteq V$ and $E^{\prime} \subseteq E$ and for all $\left(v_{1}, v_{2}\right) \in E^{\prime}: v_{1}, v_{2} \in V^{\prime}$
- For any $V^{\prime} \subseteq V$, the graph $\left(V^{\prime}, E \cap\left(V^{\prime} \times V^{\prime}\right)\right.$ ) is called the induced subgraph of $G$ (induced by $V^{\prime}$ )



## Some More Definitions

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## Some More Definitions

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## Famous Problem

- Subgraph isomorphism problem: Given a graph $\mathrm{G}_{1}=\left(\mathrm{V}_{1}, \mathrm{E}_{1}\right)$ and a graph $\mathrm{G}_{2}=\left(\mathrm{V}_{2}, \mathrm{E}_{2}\right)$ : Is there an isomorphism $\mathrm{f}: \mathrm{V}_{1} \rightarrow \mathrm{~V}_{2}$ such that $f\left(G_{1}\right)$ is a subgraph of $G_{2}$ ?



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## Data Structures

- From an abstract point of view, a graph is a list of nodes and a list of (weighted, directed) edges
- Two fundamental implementations
- Adjacency matrix
- Adjacency lists
- As usual, the representation determines which primitive operations take how long
- Suitability depends on the specific problem under study and the nature of the graphs
- Shortest paths, transitive hull, cliques, spanning trees, ...
- Random, sparse/dense, scale-free, planar, ...


## Example [ow93]

Graph


Adjacency Matrix
Adjacency List


## Adjacency Matrix

- Definition

Let $G=(V, E)$ be a simple graph. The adjacency matrix $M_{G}$ for $G$ is a two-dimensional matrix of size $/ V / * / V /$, where $M[i, j]=1$ iff $\left(v_{j}, v_{j}\right) \in E$

- Remarks
- Allows to test existence of a given edge in $\mathrm{O}(1)$
- Requires $\mathrm{O}(|\mathrm{V}|)$ to obtain all incoming (outgoing) edges of a node
- For large graphs, $M$ is too large to be of practical use
- If G is sparse (much less edges than $|\mathrm{V}|^{2}$ ), M wastes a lot of space
- If $G$ is dense, $M$ is a very compact representation ( 1 bit / edge)
- In weighted graphs, M[i,j] contains the weight
- Since M must be initialized with zero's, without further tricks all algorithms working on adjacency matrices are in $\Omega\left(|\mathrm{V}|^{2}\right)$


## Adjacency List

- Definition

Let $G=(V, E)$. The adjacency list $L_{G}$ for $G$ is a list of all nodes $v_{i}$ of $G$. The entry representing $v_{i} \in V$ is a list of all edges outgoing (or incoming or both) from $v_{i}$.

- Remarks (assume a fixed node v)
- Let k be the maximal outdegree of G . Then, accessing an edge outgoing from v is $\mathrm{O}(\log (\mathrm{k})$ ) (if list is sorted; or use hashing)
- Obtaining a list of all outgoing edges from v is in $\mathrm{O}(\mathrm{k})$
- If only outgoing edges are stored, obtaining a list of all incoming edges is $\mathrm{O}(|\mathrm{V}| * \log (|E|))$ - we need to search all lists
- Therefore, usually outgoing and incoming edges are stored, which doubles space consumption
- If $G$ is sparse, $L$ is a compact representation
- If $G$ is dense, $L$ is wasteful (many pointers, many IDs)


## Comparison

|  | Matrix | Lists |
| :--- | :---: | :---: |
| Test if a given edge exists | $\mathrm{O}(1)$ | $\mathrm{O}(\log (\mathrm{k}))$ |
| Find all outgoing edges of <br> a given v | $\mathrm{O}(\mathrm{n})$ | $\mathrm{O}(\mathrm{k})$ |
| Space of G | $\mathrm{O}\left(\mathrm{n}^{2}\right)$ | $\mathrm{O}(\mathrm{n}+\mathrm{m})$ |

- With $\mathrm{n}=|\mathrm{V}|, \mathrm{m}=|\mathrm{E}|$
- We assume a node-indexed array
- $L$ is an array and nodes are unique numbered
- We find the list for node $v$ in $O(1)$
- Otherwise, L has additional costs for finding v


## Transitive Closure

- Definition

Let $G=(V, E)$ be a digraph and $v_{j} v_{j} \in V$. The transitive closure of $G$ is a graph $G^{\prime}=\left(V, E^{\prime}\right)$ where $\left(v_{i j} v_{j}\right) \in E^{\prime}$ iff $G$ contains a path from $v_{i}$ to $v_{j}$.

- TC usually is dense and represented as adjacency matrix
- Compact encoding of reachability information



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## Graph Traversal

- One thing we often do with graphs is traversal
- "Traversal" means: Visit every node exactly once in a sequence determined by the graph's topology
- Not necessarily on one consecutive path (Hamiltonian path)
- Two popular orders
- Depth-first: Using a stack
- Breadth-first: Using a queue
- The scheme is identical to that in tree traversal
- Difference
- We have to take care of cycles
- No root - where should we start?


## Breaking Cycles

- Any naïve traversal will visit nodes more than once
- If there is at least one node with more than one incoming edge
- Any naïve traversal will run into infinite loops
- If the graphs contains at least one cycle (is cyclic)
- Breaking cycles / avoiding multiple visits
- Assume we started the traversal at a node r
- During traversal, we keep a list S of already visited nodes
- Assume we are in v and aim to proceed to v' using $\mathrm{e}=\left(\mathrm{v}, \mathrm{v}^{\prime}\right) \in \mathrm{E}$
- If $v^{\prime} \in S, v^{\prime}$ was visited before and we are about to run into a cycle or visit v' twice
- In this case, e is ignored


## Example



- Started at $r$ and went $S=\{r, y, z, v\}$
- Testing ( $\mathrm{v}, \mathrm{y}$ ): $\mathrm{y} \in \mathrm{S}$, drop
- Testing ( $\mathrm{v}, \mathrm{r}$ ): $\mathrm{r} \in \mathrm{S}$, drop
- Testing $(\mathrm{v}, \mathrm{x}): \mathrm{x} \notin \mathrm{S}$, proceed


## Where do we Start?



## Where do we Start?

- Definition

Let $G=(V, E)$. Let $V V^{\prime} \subseteq V$ and $G^{\prime}$ be the subgraph of $G$ induced by $V^{\prime}$

- $G^{\prime}$ is called connected if it contains a path between any pair $v, v^{\prime} \in V^{\prime}$
- G' is called maximally connected, if no subgraph induced by a superset of $V^{\prime}$ is connected
- If G is undirected, any maximal connected subgraph of G is called a connected component of $G$
- If G is directed, any maximal connected subgraph of G is called a strongly connected component of $G$


## Example



## Where do we Start?

- If a undirected graph falls into several connected components, we cannot reach all nodes by a single traversal, no matter which node we use as start point
- If a digraph falls into several strongly connected components, we might not reach all nodes by a single traversal
- Remedy: If the traversal gets stuck, we restart at unseen nodes until all nodes have been traversed


## Depth-First Traversal on Directed Graphs

```
func void DFS ((V,E) graph) {
    U := V; # Unseen nodes
    S := \emptyset; # Seen nodes
    while U\not=\varnothing do
        v := any_node_from( U);
        traverse( v, S, U);
    end while;
}
Called once for every connected component
```

```
func void traverse (v node,
```

func void traverse (v node,
S,U list)
S,U list)
{
{
t := new Stack();
t := new Stack();
t.put( v);
t.put( v);
while not t.isEmpty() do
while not t.isEmpty() do
n := t.getNext();
n := t.getNext();
print n; \# Do something
print n; \# Do something
U := U \ {n};
U := U \ {n};
S := S \cup {n};
S := S \cup {n};
c := n.outgoingNodes();
c := n.outgoingNodes();
foreach x in c do
foreach x in c do
if x\inU then
if x\inU then
t.put( x);
t.put( x);
end if;
end if;
end for;
end for;
end while;
end while;
}

```
}
```


## Analysis

- We put every node exactly once on the stack
- Once visited, never visited again
- We look at every edge exactly once
- Outgoing edges of a visited node are never considered again
- $S$ and $U$ can be implemented as bit-array of size |V|, allowing O(1) operations
- Setting, removing, testing nodes

```
func void traverse (v node,
            S,U list) {
    t := new Stack();
    t.put( v);
    while not t.isEmpty() do
        n := t.getNext();
        print n;
        U := U \ {n};
        S := S \cup {n};
        c := n.outgoingNodes();
        foreach x in c do
        if x\inU then
            t.put( x);
        end if;
        end for;
    end while;
}
```

- Altogether: $\mathrm{O}(\mathrm{n}+\mathrm{m})$


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## In Undirected Graphs

- In an undirected graph, whenever there is a path from $r$ to $v$ and from $v$ to $v^{\prime}$, then there is also a path from $v$ ' to $r$
- Simply go the path $r \rightarrow v \rightarrow v^{\prime}$ backwards
- Thus, DFS (and BFS) traversal can be used to find all connected components of a undirected graph G
- Whenever you call traverse(v), create a new component
- All nodes visited during traverse(v) are added to this component
- Obviously in $\mathrm{O}(\mathrm{n}+\mathrm{m})$


## In Digraphs

- The problem is considerably more complicated for digraphs
- Previous conjecture does not hold
- Still: Tarjan's or Kosaraju's algorithm find all strongly connected components in $\mathrm{O}(\mathrm{n}+\mathrm{m})$
- See next lecture


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- Single-Source-Shortest-Paths: Dijkstra's Algorithm
- Shortest Path between two given nodes
- Other


## Distance in Graphs

- Definition

Let $G=(V, E)$ be a graph. The distance $d(u, v)$ between any two nodes $u, v \in V$ for $u \neq V$ is defined as

- G un-weighted: The length of the shortest path from u to v, or $\infty$ if no path from u to v exists
- G weighted: The minimal aggregated edge weight of all non-cyclic paths from $u$ to $v$, or $\infty$ if no path from $u$ to $v$ exists
- If $u=v, d(u, v)=0$
- Remark
- Distance in un-weighted graphs is the same as distance in weighted graphs with unit costs
- Beware of negative cycles in directed graphs


## Single-Source Shortest Paths in a Graph



- Task: Find the distance between X and all other nodes
- Only positive edge weights allowed
- Bellman-Ford algorithm solves the general case


## Algorithmic Idea

- Enumerate paths by iteratively extending already found shortest paths by all possible extensions
- All edges outgoing from the end node of a short path
- These extensions
- ... either lead to a node which we didn't reach before - then we found a path, but cannot yet be sure it is the shortest
- ... or lead to a node which we already reached but we are not yet sure of we found the shortest path to it - update current best distance
- ... or lead to a node which we already reached and for which we also surely found a shortest path already - these can be ignored
- Eventually, we enumerate nodes by their distance


## Algorithm

```
1. G = (V, E);
2. x : start_node; # x\inV
3. A : array_of_distances_from_x;
4. \foralli: A[i]:= m;
5. L := V; # organized as PQ
6. A[x] := 0;
7. while L\not=\emptyset
8. k := L.get_closest_node();
9. L := L \ k;
10. forall (k,f,w)\inE do
11. if f\inL then
12. new_dist := A[k]+w;
13. if new_dist < A[f] then
14. A[f] := new_dist;
15. update( L);
16. end if;
17. end if;
18. end for;
19.end while;
```

- We enumerate nodes by length of their shortest paths
- In the first loop, we pick x and update distances (A) to all adjacent nodes
- When we pick a node $k$, we already have computed its distance to x in A
- We adapt the current best distances to all neighbors of $k$ we haven't picked yet
- Once we picked all nodes, we are done


## Dijkstra's Algorithm - Single Operations

1. $\mathbf{G}=(\mathrm{V}, \mathrm{E})$;
2. $x$ : start_node; \# x
3. A : array_of_distances_from_x;
4. $\forall i: A[i]:=\infty$;
5. $\mathrm{L}:=\mathrm{V}$; \# organized as PQ
6. $A[x]:=0$;
7. while $L \neq \emptyset$
8. $k$ := L.get_closest_node();
9. L := L
10. forall $(k, f, w) \in E$ do
11. if $f \in L$ then
12. new_dist := A[k]+w;
13. if new_dist < A[f] then
14. A[f] := new_dist;
15. update( L);
16. end if;
17. end if;
18. end for;
19. end while;

- Assume a heap-based PQ L
- L holds at most all nodes ( n )
- L4: O(n)
- L5: O(n) (build PQ)
- L8: O(1) (getMin)
- L9: O(log(n)) (deleteMin)
- L10: O(m) (with adjacency list)
- L11: O(1)
- Requires additional array LA of size |V| storing membership of nodes in L
- L15: O(log(n)) (updatePQ)
- Store in LA pointers to nodes in L; then remove/insert node


## Dijkstra's Algorithm - Loops

1. $G=(V, E)$;
2. $x$ : start_node; \# x
3. A : array_of_distances;
4. $\forall i: A[i]:=\infty$;
5. L := V; \# organized as PQ
6. $A[x]:=0$;
7. while $L \neq \emptyset$
8. $k$ := L.get_closest_node();
9. L : = L
10. forall $(k, f, w) \in E$ do
11. if $f \in L$ then
12. $n e w \_d i s t:=A[k]+w$;
13. if new_dist < $A[f]$ then
14. $A[f]:=$ new_dist;
15. update( L);
16. end if;
17. end if;
18. end for;
19. end while;

- Central costs
- L9: O(log(n)) (deleteMin)
- L15: O(log(n)) (del+ins)
- Loops
- Lines 7-18: O(n)
- Line 10-17: All edges exactly once
- Together: O(m+n)
- Altogether: O((n+m)*log(n))
- With Fibonacci heaps: Amortized costs are $O(n * \log (n)+m)$ )
- Also possible in $O\left(n^{2}\right)$; this is better in dense graphs ( $\mathrm{m} \sim \mathrm{n}^{2}$ )


## Single-Source, Single-Target



- Task: Find the distance between $X$ and only $Y$
- There is no way to be WC-faster than Dijkstra in general graphs
- We can stop as soon as Y appears at the min position of the PQ
- We can visit edges in order of increasing weight (might help)
- Worst-case complexity unchanged
- Things are different in planar graphs (navigators!)


## Faster SS-ST Algorithms

- Trick 1: Pre-compute all distances
- Transitive closure with distances
- Requires $\mathrm{O}\left(|\mathrm{V}|^{2}\right)$ space: Prohibitive for large graphs
- How? See next lecture


| $\rightarrow$ | $\mathbf{A}$ | $\mathbf{B}$ | $\mathbf{C}$ | $\mathbf{D}$ | $\mathbf{E}$ | $\mathbf{F}$ | $\mathbf{G}$ | $\mathbf{X}$ | $\mathbf{Y}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathbf{A}$ | 0 | - | - | - | - | - | - | - | - |
| $\mathbf{B}$ | 3 | 0 | 2 | - | - | - | - | - | - |
| $\mathbf{C}$ | - | - | 0 | - | - | - | - | - | - |
| $\mathbf{D}$ | 4 | 1 | 3 | 0 | 3 | 4 | 6 | 7 | 3 |
| $\mathbf{E}$ | 6 | 6 | 7 | 5 | 0 | 1 | 11 | 4 | 8 |
| $\mathbf{F}$ | - | - | 6 | - | - | 0 | - | - | - |
| $\mathbf{G}$ | - | - | - | - | - | - | 0 | - | - |
| $\mathbf{X}$ | 2 | 2 | 4 | 1 | 4 | 5 | 7 | 0 | 4 |
| $\mathbf{Y}$ | - | - | 2 | - | - | - | 3 | - | 0 |

## Faster SS-ST Algorithms

- Trick 2: Two-hop cover with distances
- Find a (hopefully small) set $S$ of nodes such that
- For every pair of nodes $\mathrm{v}_{1}, \mathrm{v}_{2}$, at least one shortest path from $\mathrm{v}_{1}$ to $\mathrm{v}_{2}$ goes through a node $s \in S$
- Thus, the distance between $\mathrm{v}_{1}, \mathrm{v}_{2}$ is $\min \left\{\mathrm{d}\left(\mathrm{v}_{1}, \mathrm{~s}\right)+\mathrm{d}\left(\mathrm{s}, \mathrm{v}_{2}\right) \mid \mathrm{s} \in \mathrm{S}\right)$
- S is called a 2-hop cover
- Problem: Finding a minimal $S$ is NP-complete
- And S need not be small



## More Distances

- Graphs with negative edge weights
- Shortest paths (in terms of weights) may be very long (edges)
- Bellman-Ford algorithm is in $\mathrm{O}\left(\mathrm{n}^{2 *} \mathrm{~m}\right)$
- All-pairs shortest paths
- Only positive edge weights: Use Dijkstra $n$ times
- With negative edge weights: Floyd-Warshall in $O\left(n^{3}\right)$
- See next lecture
- Reachability
- Simple in undirected graphs: Compute all connected components
- In digraphs: Use graph traversal or a special graph indexing method


## Possible Examination Questions

- Let G be an undirected graph and S,T be two connected components of G . Proof that S and T must be disjoined, i.e., cannot share a node.
- Let G be an undirected graph with n vertices and $m$ edges, $m<=n^{2}$. What is the minimal and what is the maximal number of connected components G can have?
- Let G be a positively edge-weighted digraph G . Design an algorithm which finds the longest acyclic path in G. Analyze the complexity of your algorithm.
- An Euler path through an undirected graph G is a cyclefree path from any start to any end node that hits every node of G (exactly once). Give an algorithm which tests for an input graph $G$ whether it contains an Euler path.

