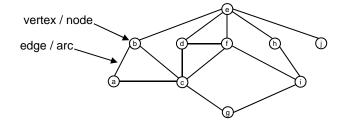
# Graphs

Computer Science E-22 Harvard Extension School

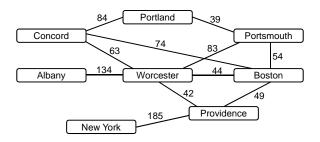
David G. Sullivan, Ph.D.

# What is a Graph?



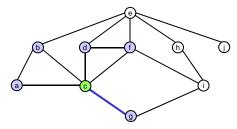
- A graph consists of:
  - a set of vertices (also known as nodes)
  - a set of *edges* (also known as *arcs*), each of which connects a pair of vertices

#### Example: A Highway Graph



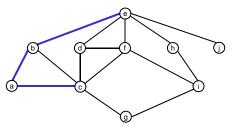
- · Vertices represent cities.
- · Edges represent highways.
- This is a weighted graph, because it has a cost associated with each edge.
  - for this example, the costs denote mileage
- We'll use graph algorithms to answer questions like
   "What is the shortest route from Portland to Providence?"

## Relationships Among Vertices

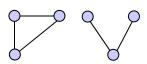


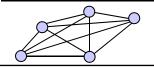
- Two vertices are *adjacent* if they are connected by a single edge.
  - ex: c and g are adjacent, but c and i are not
- The collection of vertices that are adjacent to a vertex v are referred to as v's *neighbors*.
  - ex: c's neighbors are a, b, d, f, and g

# Paths in a Graph



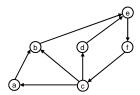
- A path is a sequence of edges that connects two vertices.
  - ex: the path highlighted above connects c and e
- A graph is connected if there is a path between any two vertices.
  - ex: the six vertices at right are part of a graph that is not connected
- A graph is complete if there is an edge between every pair of vertices.
  - ex: the graph at right is complete





## **Directed Graphs**

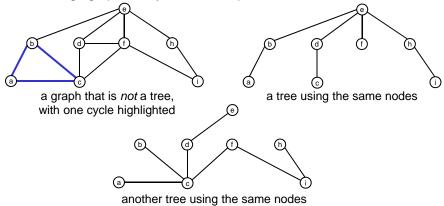
• A *directed* graph has a direction associated with each edge, which is depicted using an arrow:



- Edges in a directed graph are often represented as ordered pairs of the form (start vertex, end vertex).
  - ex: (a, b) is an edge in the graph above, but (b, a) is not.
- A path in a directed graph is a sequence of edges in which the end vertex of edge i must be the same as the start vertex of edge i + 1.
  - ex: { (a, b), (b, e), (e, f) } is a valid path. { (a, b), (c, b), (c, a) } is not.

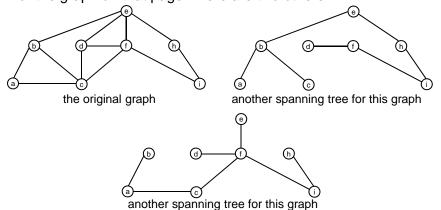
#### Trees vs. Graphs

- A tree is a special type of graph.
  - it is connected and undirected
  - it is *acyclic:* there is no path containing distinct edges that starts and ends at the same vertex
  - we usually single out one of the vertices to be the root of the tree, although graph theory does not require this



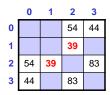
## **Spanning Trees**

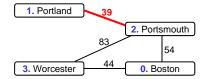
- A spanning tree is a subset of a connected graph that contains:
  - · all of the vertices
  - a subset of the edges that form a tree
- The trees on the previous page were examples of spanning trees for the graph on that page. Here are two others:



#### Representing a Graph Using an Adjacency Matrix

- Adjacency matrix = a two-dimensional array that is used to represent the edges and any associated costs
  - edge[r][c] = the cost of going from vertex r to vertex c
- Example:

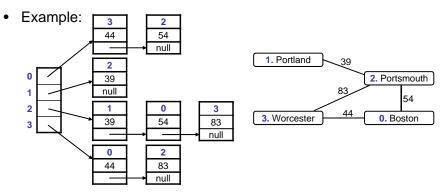




- Use a special value to indicate that you can't go from r to c.
  - either there's no edge between r and c, or it's a directed edge that goes from c to r
  - · this value is shown as a shaded cell in the matrix above
  - we can't use 0, because we may have actual costs of 0
- This representation is good if a graph is dense if it has many edges per vertex – but wastes memory if the graph is sparse – if it has few edges per vertex.

## Representing a Graph Using an Adjacency List

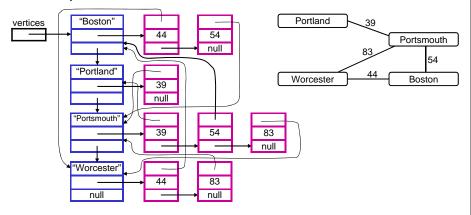
 Adjacency list = a list (either an array or linked list) of linked lists that is used to represent the edges and any associated costs



- No memory is allocated for non-existent edges, but the references in the linked lists use extra memory.
- This representation is good if a graph is sparse, but wastes memory if the graph is dense.

#### Our Graph Representation

- Use a linked list of linked lists for the adjacency list.
- Example:



verti ces is a reference to a linked list of Vertex objects. Each Vertex holds a reference to a linked list of Edge objects. Each Edge holds a reference to the Vertex that is the end vertex.

## **Graph Class**

```
public class Graph {
    pri vate class Vertex {
        private String id;
                                             // adjacency list
        pri vate Edge edges;
        pri vate Vertex next;
        pri vate bool ean encountered;
        pri vate bool ean done;
        pri vate Vertex parent;
        pri vate double cost;
    private class Edge {
        pri vate Vertex start;
        pri vate Vertex end;
        pri vate double cost;
        private Edge next;
                                                  The highlighted fields
                                                are shown in the diagram
    private Vertex vertices;
                                                  on the previous page.
}
```

#### Traversing a Graph

- Traversing a graph involves starting at some vertex and visiting all of the vertices that can be reached from that vertex.
  - visiting a vertex = processing its data in some way
    example: print the data
  - if the graph is connected, all of the vertices will be visited
- We will consider two types of traversals:
  - depth-first: proceed as far as possible along a given path before backing up
  - breadth-first: visit a vertex

visit all of its neighbors

visit all unvisited vertices 2 edges away visit all unvisited vertices 3 edges away, etc.

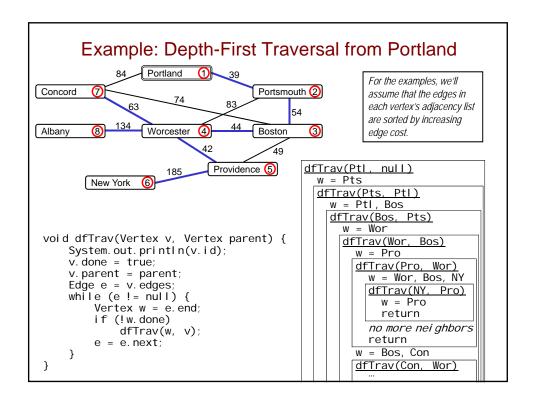
- Applications:
  - determining the vertices that can be reached from some vertex
  - state-space search
  - web crawler (vertices = pages, edges = links)

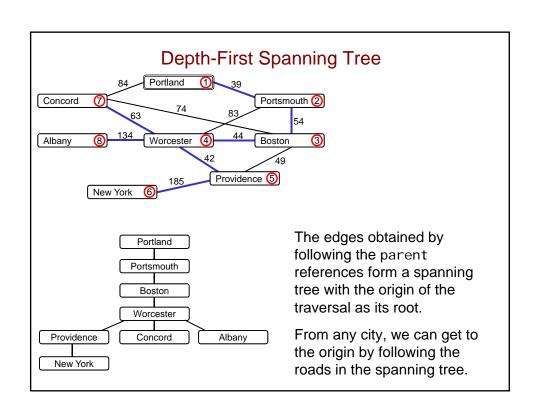
## **Depth-First Traversal**

 Visit a vertex, then make recursive calls on all of its yet-to-be-visited neighbors:

```
dfTrav(v, parent)
visit v and mark it as visited
v.parent = parent
for each vertex w in v's neighbors
if (w has not been visited)
dfTrav(w, v)
```

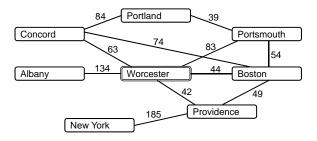
· Java method:



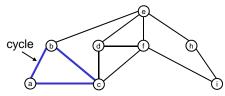


# Another Example: Depth-First Traversal from Worcester

- In what order will the cities be visited?
- Which edges will be in the resulting spanning tree?



## Checking for Cycles in an Undirected Graph



- To discover a cycle in an undirected graph, we can:
  - · perform a depth-first traversal, marking the vertices as visited
  - when considering neighbors of a visited vertex, if we discover one already marked as visited, there must be a cycle
- If no cycles found during the traversal, the graph is acyclic.
- This doesn't work for directed graphs:
  - c is a neighbor of both a and b
  - there is no cycle

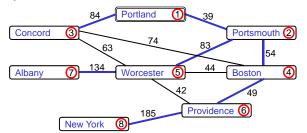


#### **Breadth-First Traversal**

• Use a queue, as we did for BFS and level-order tree traversal:

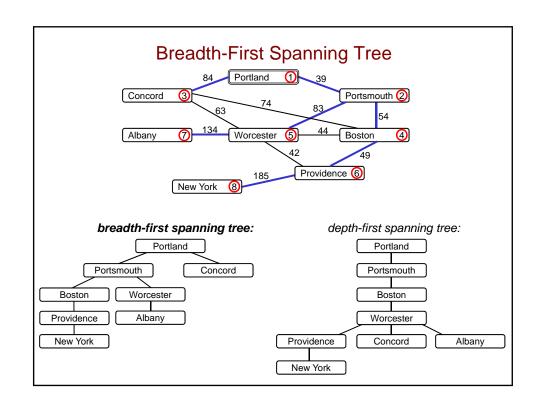
```
private static void bfTrav(Vertex origin) {
     origin.encountered = true;
origin.parent = null;
Queue<Vertex> q = new LLQueue<Vertex>();
     q. i nsert (ori gi n);
     while (!q.isEmpty()) {
          Vertex v = q.remove();
          System. out. println(v.id);
                                                    // Visit v.
          // Add v's unencountered neighbors to the queue.
         Edge e = v. edges;
while (e != null) {
               Vertex w = e. end;
               if (!w.encountered) {
                    w.encountered = true;
                    w.parent = v;
                    q.insert(w);
               e = e. next;
     }
}
```

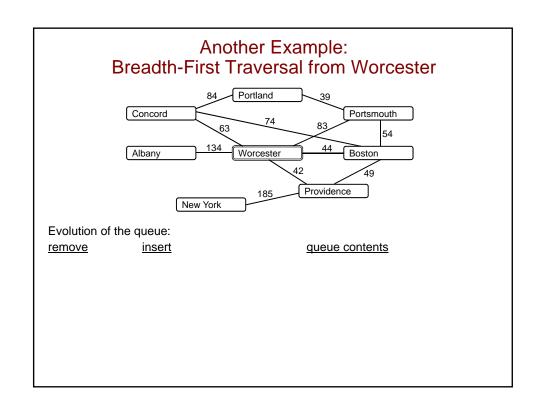




#### Evolution of the queue:

to a seat	
<u>insert</u>	<u>queue contents</u>
Portland	Portland
Portsmouth, Concord	Portsmouth, Concord
Boston, Worcester	Concord, Boston, Worcester
none	Boston, Worcester
Providence	Worcester, Providence
Albany	Providence, Albany
New York	Albany, New York
none	New York
none	empty
	Portsmouth, Concord Boston, Worcester none Providence Albany New York none



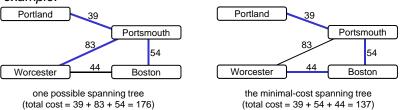


#### Time Complexity of Graph Traversals

- let V = number of vertices in the graph
   E = number of edges
- If we use an adjacency matrix, a traversal requires O(V<sup>2</sup>) steps.
  - why?
- If we use an adjacency list, a traversal requires O(V + E) steps.
  - · visit each vertex once
  - traverse each vertex's adjacency list at most once
    - the total length of the adjacency lists is at most 2E = O(E)
  - O(V + E) << O(V<sup>2</sup>) for a sparse graph
  - for a dense graph, E = O(V<sup>2</sup>), so both representations are O(V<sup>2</sup>)
- In our implementations of the remaining algorithms, we'll assume an adjacency-list implementation.

## Minimum Spanning Tree

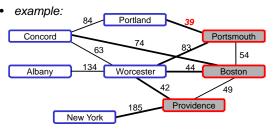
- A minimum spanning tree (MST) has the smallest total cost among all possible spanning trees.
  - example:



- If no two edges have the same cost, there is a unique MST.
   If two or more edges have the same cost, there may be more than one MST.
- Finding an MST could be used to:
  - determine the shortest highway system for a set of cities
  - calculate the smallest length of cable needed to connect a network of computers

## **Building a Minimum Spanning Tree**

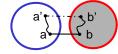
Key insight: if you divide the vertices into two disjoint subsets
 A and B, then the lowest-cost edge joining a vertex in A to a
 vertex in B – call it (a, b) – must be part of the MST.



The 6 bold edges each join an unshaded vertex to a shaded vertex.

The one with the lowest cost (Portland to Portsmouth) must be in the MST.

- · Proof by contradiction:
- assume there is an MST (call it T) that doesn't include (a, b)
- T must include a path from a to b, so it must include one of the other edges (a', b') that spans subsets A and B, such that (a', b') is part of the path from a to b



- adding (a, b) to T introduces a cycle
- removing (a', b') gives a spanning tree with lower cost, which contradicts the original assumption.

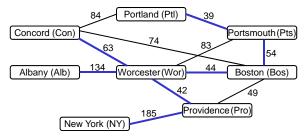
## Prim's MST Algorithm

- Begin with the following subsets:
  - A = any one of the vertices
  - B = all of the other vertices
- Repeatedly select the lowest-cost edge (a, b) connecting a vertex in A to a vertex in B and do the following:
  - add (a, b) to the spanning tree
  - update the two sets: A = A U {b}

 $B = B - \{b\}$ 

· Continue until A contains all of the vertices.

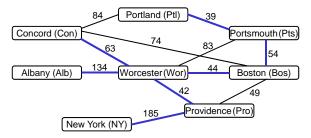




• Tracing the algorithm:

edge added	set A	set B
	{Con}	{Alb, Bos, NY, Ptl, Pts, Pro, Wor}
(Con, Wor)	{Con, Wor}	{Alb, Bos, NY, Ptl, Pts, Pro}
(Wor, Pro)	{Con, Wor, Pro}	{Alb, Bos, NY, Ptl, Pts}
(Wor, Bos)	{Con, Wor, Pro, Bos}	{Alb, NY, Ptl, Pts}
(Bos, Pts)	{Con, Wor, Pro, Bos, Pts}	{Alb, NY, Ptl}
(Pts, Ptl)	{Con, Wor, Pro, Bos, Pts, Ptl}	{Alb, NY}
(Wor, Alb)	{Con, Wor, Pro, Bos, Pts, Ptl, Alb}	{NY}
(Pro, NY)	{Con, Wor, Pro, Bos, Pts, Ptl, Alb, NY}	{}
	'	

## MST May Not Give Shortest Paths



- The MST is the spanning tree with the minimal total edge cost.
- It does <u>not</u> necessarily include the minimal cost path between a pair of vertices.
- Example: shortest path from Boston to Providence is along the single edge connecting them
  - that edge is not in the MST

#### Implementing Prim's Algorithm in our Graph class

- · Use the done field to keep track of the sets.
  - if v. done == true, v is in set A
  - if v. done == fal se, v is in set B
- Repeatedly scan through the lists of vertices and edges to find the next edge to add.
  - → O(EV)
- We can do better!
  - use a heap-based priority queue to store the vertices in set B
  - priority of a vertex x = -1 \* cost of the lowest-cost edge connecting x to a vertex in set A
    - why multiply by -1?
  - · somewhat tricky: need to update the priorities over time
  - → O(E log V)

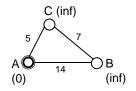
#### The Shortest-Path Problem

- It's often useful to know the shortest path from one vertex to another – i.e., the one with the minimal total cost
  - example application: routing traffic in the Internet
- For an *unweighted* graph, we can simply do the following:
  - start a breadth-first traversal from the origin, v
  - stop the traversal when you reach the other vertex, w
  - the path from v to w in the resulting (possibly partial) spanning tree is a shortest path
- A breadth-first traversal works for an unweighted graph because:
  - the shortest path is simply one with the fewest edges
  - a breadth-first traversal visits cities in order according to the number of edges they are from the origin.
- Why might this approach fail to work for a *weighted* graph?

#### Dijkstra's Algorithm

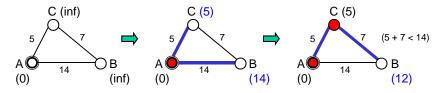
- One algorithm for solving the shortest-path problem for weighted graphs was developed by E.W. Dijkstra.
- It allows us to find the shortest path from a vertex v (the origin) to all other vertices that can be reached from v.
- Basic idea:
  - maintain estimates of the shortest paths from the origin to every vertex (along with their costs)
  - gradually refine these estimates as we traverse the graph
- Initial estimates:

the origin itself: stay put! 0
all other vertices: unknown infinity



# Dijkstra's Algorithm (cont.)

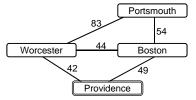
- We say that a vertex w is *finalized* if we have found the shortest path from v to w.
- We repeatedly do the following:
  - find the unfinalized vertex w with the lowest cost estimate
  - mark w as finalized (shown as a filled circle below)
  - examine each unfinalized neighbor x of w to see if there is a shorter path to x that passes through w
    - if there is, update the shortest-path estimate for x
- Example:



#### Another Example: Shortest Paths from Providence

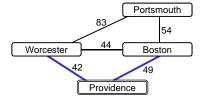
Initial estimates:

**Boston** infinity infinity Worcester Portsmouth infinity Providence



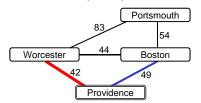
- Providence has the smallest unfinalized estimate, so we finalize it.
- We update our estimates for its neighbors:

**Boston** 49 (< infinity) **42** (< infinity) Worcester Portsmouth infinity Providence 0



#### Shortest Paths from Providence (cont.)

49 **Boston 42** Worcester Portsmouth infinity Providence 0

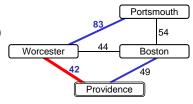


- Worcester has the smallest unfinalized estimate, so we finalize it.
  - any other route from Prov. to Worc. would need to go via Boston, and since (Prov → Worc) < (Prov → Bos), we can't do better.
- We update our estimates for Worcester's unfinalized neighbors:

**Boston** 49 (no change) Worcester 42

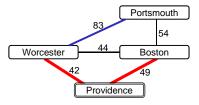
Portsmouth 125 (42 + 83 < infinity)

Providence 0



#### Shortest Paths from Providence (cont.)

Boston 49
Worcester 42
Portsmouth 125
Providence 0

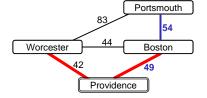


- Boston has the smallest unfinalized estimate, so we finalize it.
  - we'll see later why we can safely do this!
- We update our estimates for Boston's unfinalized neighbors:

Boston 49
Worcester 42
Portsmouth 103

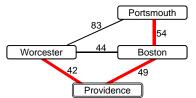
Portsmouth 103 (49 + 54 < 125)

Providence 0



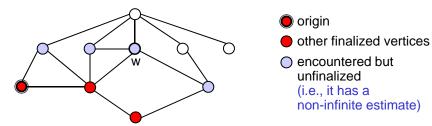
## Shortest Paths from Providence (cont.)

Boston 49
Worcester 42
Portsmouth 103
Providence 0



Only Portsmouth is left, so we finalize it.

#### Finalizing a Vertex



- Let w be the unfinalized vertex with the smallest cost estimate. Why can we finalize w, before seeing the rest of the graph?
- We know that w's current estimate is for the shortest path to w that passes through only *finalized* vertices.
- Any shorter path to w would have to pass through one of the other encountered-but-unfinalized vertices, but we know that they're all further away from the origin than w is.
  - their cost estimates may decrease in subsequent stages of the algorithm, but they can't drop below w's current estimate!

## Pseudocode for Dijkstra's Algorithm

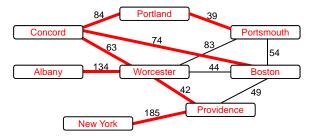
```
dijkstra(origin)
    origin.cost = 0
    for each other vertex v
        v.cost = infinity;

while there are still unfinalized vertices with cost < infinity
        find the unfinalized vertex w with the minimal cost
        mark w as finalized

for each unfinalized vertex x adjacent to w
        cost_via_w = w.cost + edge_cost(w, x)
        if (cost_via_w < x.cost)
            x.cost = cost_via_w
        x.parent = w
```

- At the conclusion of the algorithm, for each vertex v:
  - v.cost is the cost of the shortest path from the origin to v;
     if v.cost is infinity, there is no path from the origin to v
  - starting at v and following the parent references yields the shortest path

## **Example: Shortest Paths from Concord**

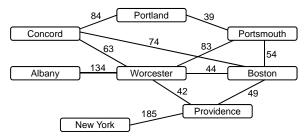


Evolution of the cost estimates (costs in bold have been finalized):

Albany	inf	inf	197	197	197	197	197	
Boston	inf	74	74					
Concord	0							
New York	inf	inf	inf	inf	inf	290	290	290
Portland	inf	84	84	84				
Portsmouth	inf	inf	146	128	123	123		
Providence	inf	inf	105	105	105			
Worcester	inf	63						

Note that the Portsmouth estimate was improved three times!

## Another Example: Shortest Paths from Worcester



Evolution of the cost estimates (costs in bold have been finalized):

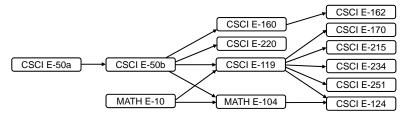
Albany				
Boston				
Concord				
New York				
Portland				
Portsmouth				
Providence				
Worcester				

#### Implementing Dijkstra's Algorithm

- Similar to the implementation of Prim's algorithm.
- Use a heap-based priority queue to store the unfinalized vertices.
  - priority = ?
- Need to update a vertex's priority whenever we update its shortest-path estimate.
- Time complexity = O(ElogV)

## **Topological Sort**

- Used to order the vertices in a <u>directed acyclic graph</u> (a DAG).
- Topological order: an ordering of the vertices such that, if there is directed edge from a to b, a comes before b.
- Example application: ordering courses according to prerequisites



- a directed edge from a to b indicates that a is a prereq of b
- There may be more than one topological ordering.

#### **Topological Sort Algorithm**

- A successor of a vertex v in a directed graph = a vertex w such that (v, w) is an edge in the graph (v→→•w)
- Basic idea: find vertices that have no successors and work backward from them.
  - there must be at least one such vertex. why?
- Pseudocode for one possible approach:

```
topolSort

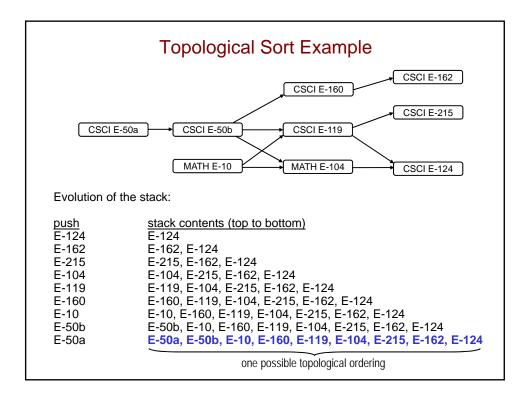
S = a stack to hold the vertices as they are visited while there are still unvisited vertices

find a vertex v with no unvisited successors mark v as visited

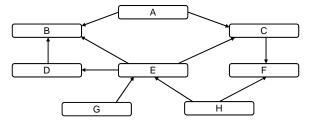
S.push(v)

return S
```

 Popping the vertices off the resulting stack gives one possible topological ordering.



#### Another Topological Sort Example

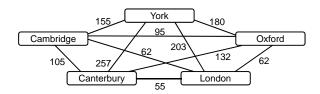


Evolution of the stack:

push

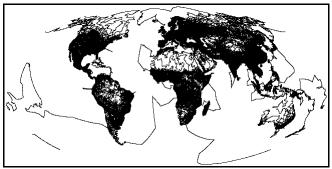
stack contents (top to bottom)

## Traveling Salesperson Problem (TSP)



- A salesperson needs to travel to a number of cities to visit clients, and wants to do so as efficiently as possible.
- · As in our earlier problems, we use a weighted graph.
- A *tour* is a path that begins at some starting vertex, passes through every other vertex *once* and *only once*, and returns to the starting vertex. (The actual starting vertex doesn't matter.)
- TSP: find the tour with the lowest total cost
- TSP algorithms assume the graph is complete, but we can assign infinite costs if there isn't a direct route between two cities.

#### TSP for Santa Claus



source: http://www.tsp.gatech.edu/world/pictures.html

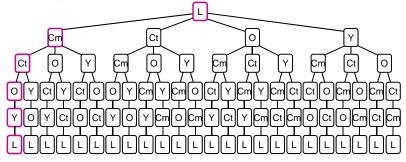
A "world TSP" with 1,904,711 cities.

The figure at right shows a tour with a total cost of 7,516,353,779 meters – which is at most 0.068% longer than the optimal tour.

- Other applications:
  - · coin collection from phone booths
  - · routes for school buses or garbage trucks
  - minimizing the movements of machines in automated manufacturing processes
  - · many others

## Solving a TSP: Brute-Force Approach

- Perform an exhaustive search of all possible tours.
- One way: use DFS to traverse the entire state-space search tree.



- The leaf nodes correspond to possible solutions.
  - for n cities, there are (n-1)! leaf nodes in the tree.
  - half are redundant (e.g., L-Cm-Ct-O-Y-L = L-Y-O-Ct-Cm-L)
- Problem: exhaustive search is intractable for all but small n.
  - example: when n = 14, ((n 1)!) / 2 = over 3 billion

## Solving a TSP: Informed State-Space Search

- Use A\* with an appropriate heuristic function for estimating the cost of the remaining edges in the tour.
- This is much better than brute force, but it still uses exponential space and time.

## Algorithm Analysis Revisited

Recall that we can group algorithms into classes (n = problem size):

<u>name</u>	example expressions	big-O notation
constant time	1, 7, 10	0(1)
logarithmic time	3l og <sub>10</sub> n, l og <sub>2</sub> n + 5	O(I og n)
linear time	5n, 10n – 2l og <sub>2</sub> n	O(n)
n log n time	$4n \log_2 n$ , $n \log_2 n + n$	O(n I og n)
quadratic time	$2n^2 + 3n$ , $n^2 - 1$	$O(n^2)$
$n^{c}$ (c > 2)	$n^3 - 5n$ , $2n^5 + 5n^2$	O(n <sup>c</sup> )
exponential time	2 <sup>n</sup> , 5e <sup>n</sup> + 2n <sup>2</sup>	0(c <sup>n</sup> )
factorial time	(n – 1)! /2, 3n!	O(n!)

- Algorithms that fall into one of the classes above the dotted line are referred to as *polynomial-time* algorithms.
- The term *exponential-time algorithm* is sometimes used to include *all* algorithms that fall below the dotted line.
  - algorithms whose running time grows as fast or faster than c<sup>n</sup>

#### Classifying Problems

- Problems that can be solved using a polynomial-time algorithm are considered "easy" problems.
  - we can solve large problem instances in a reasonable amount of time
- Problems that don't have a polynomial-time solution algorithm are considered "hard" or "intractable" problems.
  - they can only be solved exactly for small values of n
- Increasing the CPU speed doesn't help much for intractable problems:

·		CPU 2
	<u>CPU 1</u>	(1000x faster)
max problem size for O(n) alg:	Ν	1000N
O(n²) alg:	Ν	31.6 N
O(2 <sup>n</sup> ) alg:	Ν	N + 9.97

#### Classifying Problems (cont.)

- The class of problems that can be solved using a polynomial-time algorithm is known as the class P.
- Many problems that don't have a polynomial-time solution algorithm belong to a class known as NP
  - for non-deterministic polymonial
- If a problem is in NP, it's possible to guess a solution and verify if the guess is correct in polynomial time.
  - example: a variant of the TSP in which we attempt to determine if there is a tour with total cost <= some bound b</li>
  - given a tour, it takes polynomial time to add up the costs of the edges and compare the result to b

#### Classifying Problems (cont.)

- If a problem is NP-complete, then finding a polynomial-time solution for it would allow you to solve a large number of other hard problems.
  - thus, it's extremely unlikely such a solution exists!
- The TSP variant described on the previous slide is NP-complete.
- Finding the optimal tour is at least as hard.
- For more info. about problem classes, there is a good video of a lecture by Prof. Michael Sipser of MIT available here:

http://claymath.msri.org/sipser2006.mov

## **Dealing With Intractable Problems**

- When faced with an intractable problem, we resort to techniques that quickly find solutions that are "good enough".
- Such techniques are often referred to as heuristic techniques.
  - heuristic = rule of thumb
  - there's no guarantee these techniques will produce the optimal solution, but they typically work well

#### **Iterative Improvement Algorithms**

- One type of heuristic technique is what is known as an *iterative improvement algorithm*.
  - start with a randomly chosen solution
  - gradually make small changes to the solution in an attempt to improve it
    - · e.g., change the position of one label
  - stop after some number of iterations
- There are several variations of this type of algorithm.

## Hill Climbing

- Hill climbing is one type of iterative improvement algorithm.
  - start with a randomly chosen solution
  - repeatedly consider possible small changes to the solution
  - · if a change would improve the solution, make it
  - if a change would make the solution worse, don't make it
  - stop after some number of iterations
- It's called hill climbing because it repeatedly takes small steps that improve the quality of the solution.
  - "climbs" towards the optimal solution

#### Simulated Annealing

- Simulated annealing is another iterative improvement algorithm.
  - start with a randomly chosen solution
  - repeatedly consider possible small changes to the solution
  - if a change would improve the solution, make it
  - if a change would make the solution worse,
     make it some of the time (according to some probability)
  - the probability of doing so reduces over time

#### **Take-Home Lessons**

- Object-oriented programming allows us to capture the abstractions in the programs that we write.
  - creates reusable building blocks
  - key concepts: encapsulation, inheritance, polymorphism
- Abstract data types allow us to organize and manipulate collections of data.
  - a given ADT can be implemented in different ways
  - fundamental building blocks: arrays, linked nodes
- Efficiency matters when dealing with large collections of data.
  - some solutions can be *much* faster or more space efficient than others!
  - what's the best data structure/algorithm for the specific instances of the problem that you expect to see?
    - example: sorting an almost sorted collection

#### Take-Home Lessons (cont.)

- Use the tools in your toolbox!
  - · generic data structures
  - lists/stacks/queues
  - trees
  - heaps
  - hash tables
  - recursion
  - · recursive backtracking
  - divide-and-conquer
  - state-space search
  - ...

## From the Introductory Lecture...

- · We will study fundamental data structures.
  - · ways of imposing order on a collection of information
  - · sequences: lists, stacks, and queues
  - trees
  - hash tables
  - graphs
- We will also:
  - study algorithms related to these data structures
  - learn how to compare data structures & algorithms
- Goals:
  - learn to think more intelligently about programming problems
  - acquire a set of useful tools and techniques