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Part I

Graphs
### Examples

- Bristol
- Birmingham
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### Graphs in General

- A
- B
- C
- D
- E
- F
- G
- multiple connections for robustness against failures

- parallel arcs
- loops
- disconnected components

### Definitions

An **(undirected) graph** is a set \( N \) of **nodes** and a set \( A \) of **arcs** such that each \( a \in A \) is associated with an unordered pair of nodes (the **endpoints** of \( a \)).

**Notation**

- \( G \)
- \( \text{nodes}(G) \)
- \( \text{arcs}(G) \)

A graph is **simple** if it has no parallel arcs and no loops.

### Why Parallel Arcs?

- multiple connections for robustness against failures

- Is our network **robust**?

- How many failures can it tolerate before becomes disconnected?
**Degrees**

The degree of a node is the number of arcs incident on it.
- the no of arcs which have that node as an endpoint
  • Count loops twice
Each arc contributes twice to the total of all the degrees
- once for each endpoint

**Sum of Degrees**

There are 8 arcs. Sum of degrees is
\[2 + 2 + 3 + 2 + 1 + 2 + 4 = 2 \times 8.\]

**Theorem**

1) The sum of the degrees of all the nodes of a graph is twice the number of arcs, and therefore even.
2) The number of nodes with odd degree is even.

**Subgraphs**

Here \(G_1\) is a subgraph of \(G_2\):
- nodes\((G_1) \subseteq \text{nodes}(G_2)\)
- arcs\((G_1) \subseteq \text{arcs}(G_2)\)
Of course \(G_1\) and \(G_2\) don’t have to be drawn the same way.
- the connectivity is what counts
**Full and Spanning Subgraphs**

**Full (Induced) Subgraphs**

- Any subset $X \subseteq \text{nodes}(G)$ induces a subgraph $G[X]$ of $G$, where $G[X]$ has nodes $X$ and $G[X]$ contains all arcs of $G$ which join nodes in $X$.
- $G'$ is a full (or induced) subgraph of $G$ if $G' = G[X]$ for some $X \subseteq \text{nodes}(G)$.

**Spanning Subgraphs**
If $G'$ is a subgraph of $G$ and $\text{nodes}(G') = \text{nodes}(G)$, we say that $G'$ spans $G$.

---

**Adjacency Matrices**

Create adjacency matrix. $i,j$ entry: how many arcs connect $i$ to $j$.
- Symmetric because arcs are undirected
- If we order the nodes differently the matrix gets rearranged.

Diagonal entries:
- count each loop twice
- to be consistent with our definition of degree
- so every arc contributes twice to the adjacency matrix

$$
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 2 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
2 & 1 & 0 & 0 & 0 & 1 & 0 \\
\end{pmatrix}
$$

---

**Adjacency Lists**

Create adjacency list: Array of linked lists.
- For each node list nodes which are adjacent.
- If multiple arcs then multiple entries.
- Each arc gets entered twice (apart from loops).
Comparison

The adjacency matrix gives efficient access to any arc in the graph. However certain algorithms rely on looking at all arcs incident on a given node. For these algorithms it can be faster to use adjacency lists. This is particularly the case if the matrix has a lot of zeroes, i.e. the graph is sparse.

Suppose that there are $n$ nodes and $m$ arcs:

- The adjacency matrix has size $n^2$.
- The adjacency list has size $\leq n + 2m$.

Say that a graph is sparse if $m$ is much smaller than $n/2$.

- Storage space will be less with adjacency list.

Big-Oh Notation

Multiplication of $n \times n$ matrices:

$$\begin{pmatrix} 1 & 0 & 2 \\ 3 & 1 & 0 \\ 4 & 2 & 3 \end{pmatrix} \begin{pmatrix} 3 & 6 & 1 \\ 2 & 0 & 5 \\ 1 & 4 & 2 \end{pmatrix} = \begin{pmatrix} 5 & 14 & 5 \\ 11 & 18 & 8 \\ 19 & 36 & 20 \end{pmatrix}$$

Each entry takes $n$ multiplications and $n - 1$ additions.

So total is

- $n^3$ multiplications
- $n^3 - n^2$ additions
- $2n^3 - n^2$ arithmetical operations

Often prefer not to be so precise: $O(n^k)$ means bounded by $n^k$.

- $O(n^3)$ multiplications
- $O(n^3)$ additions
- $O(n^3)$ arithmetical operations

Graph Isomorphism

What does it mean for a graph to be the “same” as another? The graphs look different, but they have the same shape, in the sense that the nodes are connected in the same way.

- Degrees: $1, 2, 3, 4, A, B, C, D$
- parallel arcs: 14, 12 and AB, BC.
- Which nodes correspond?
3 must correspond to D - only nodes with degree 2.
1 must correspond to B, since
1 only node not adjacent to 3 and
B only node not adjacent to D
We now can either have 2 \mapsto A, 4 \mapsto C or
2 \mapsto C, 4 \mapsto A
Suppose we take
1 2 3 4
B A D C
This is a bijection between nodes.
But also must check that connections are the same.
Fairly obvious by mentally transforming the graphs so they look the same.
To check rigorously we need to find the adjacency matrices.

In the standard order (1234 and ABCD) the adjacency matrices are:
\[
\begin{pmatrix}
0 & 2 & 0 & 2 \\
2 & 0 & 1 & 1 \\
0 & 1 & 0 & 1 \\
2 & 1 & 1 & 0 \\
\end{pmatrix}
\quad \begin{pmatrix}
0 & 2 & 1 & 1 \\
2 & 0 & 2 & 0 \\
1 & 2 & 0 & 1 \\
1 & 0 & 1 & 0 \\
\end{pmatrix}
\]
To make them match, reorder RH matrix to correspond to mapping
1 2 3 4
B A D C

Let G, G′ be graphs.

An isomorphism from G to G′ is a bijection f : \text{nodes}(G) \to \text{nodes}(G′)
together with a bijection g : \text{arcs}(G) \to \text{arcs}(G′)
such that if a \in \text{arcs}(G) has endpoints n_1 and n_2 then
the endpoints of g(a) are f(n_1) and f(n_2).

\[
\begin{array}{c}
\text{n}_1 \\
a \\
\text{n}_2 \\
\end{array}
\quad \quad
\begin{array}{c}
f(\text{n}_1) \\
g(a) \\
f(\text{n}_2) \\
\end{array}
\]

G is isomorphic to G′

This amounts to seeing that the adjacency matrices of G and G′ are the same, except that the rows and columns may have been reordered.

When testing whether two graphs are isomorphic, it is simplest to start with the obvious checks:

- # nodes
- # arcs
- # loops
- degrees

If this turns up a difference, then the graphs can’t be isomorphic.
If they are the same on these tests, then attempt to find a bijection on nodes.
Check that it works using adjacency matrices.
**Complexity**

In general, discovering whether two graphs are isomorphic has quite a high complexity.

We need to see whether the adjacency matrices are rearrangements of each other.

There are $n!$ rearrangements if there are $n$ nodes.

This is worse than exponential ($2^n$).

**Remark:**

László Babai (2015): Graph isomorphism can be solved in quasi-polynomial time, i.e. $\exp(\log^k n)$ for some $k$.

Better than exponential though worse than polynomial.

---

**Automorphisms**

An automorphism on a graph $G$ is an isomorphism from $G$ to itself.

Possible automorphism: \[ 1 \ 2 \ 3 \ 4 \\
2 \ 3 \ 4 \ 1 \]

This is a 90 degree clockwise rotation.

Another one is \[ 1 \ 2 \ 3 \ 4 \\
3 \ 2 \ 1 \ 4 \]

This is a flip across the diagonal $2 - 4$.

How many other automorphisms?

**Method**

1 can map to 4 different places.

Fix 1. Then 2 can map to 2 places.

Fix 2. Then 3 can map to 1 place. 4 is also fixed.

Total: $4 \cdot 2 \cdot 1 \cdot 1 = 8$ (including the identity).

---

**Example**

How many automorphisms?

By method:

1 can map to 2 different places.

Fix 1. Then 2 can map to 2 places.

Fix 2. Then 3 and 4 are fixed.

Total: $2 \cdot 2 \cdot 1 \cdot 1 = 4$ (including the identity).

---

**Planar Graphs**

Sometimes it is desirable to avoid arcs crossing.

*e.g. microchips*

**Definition**

A graph is planar if it can be drawn so that no arcs cross.

Planar $K_5$ - the complete graph on 5 nodes.

Not planar
**Cube and $K_5$**

The cube graph is planar:

The best we can do with $K_5$:

There is still one crossing.

**Kuratowski’s Theorem**

It turns out that any non-planar graph contains $K_5$ or $K_{3,3}$ as a subgraph, in a sense.

Two graphs are **homeomorphic** if they can both be obtained from the same graph by a series of operations where an arc $x - y$ is replaced by two arcs $x - z - y$.

**Is a Graph Planar?**

As we have seen, it is not obvious whether a given graph is planar.

But there is a **linear time** algorithm due to Hopcroft & Tarjan (1976).

“Linear time” here means $O(n + m)$ where $n$ is the number of nodes and $m$ is the number of arcs.

So in a sense, testing planarity is “easy”.

- “low complexity”

**Fact**

*If a (simple) graph is planar it can always be redrawn so that all arcs are straight lines which don’t cross.*
Euler's Formula

Any planar graph splits the plane into regions, called faces. The cube graph has 6 faces, including the outside.

Let $G$ have $N$ nodes, $A$ arcs and $F$ faces.

Euler's formula: $F = A - N + 2$ for a connected planar graph

For the cube: $F = 6$, $A = 12$ and $N = 8$.

Map Colouring

A map with six countries:

Problem: Colour the map so that if two countries share a border then they have different colours.

Question: How many different colours do we need?

The Dual Graph

We can turn a map into a planar graph by letting the countries be the nodes, and joining them if they are neighbours on the map.

This graph is called the dual graph.

Problem: Colour the map so that if two countries share a border then they have different colours.

Question: How many different colours do we need?

The problem now is to colour the nodes of a planar graph in such a way that if two nodes are adjacent then they have different colours.
The Dual Graph

A map that needs four colours:

\[
\begin{array}{ccc}
1 & 2 & 3 \\
\end{array}
\]

The dual graph:

\[
\begin{array}{ccc}
3 & 1 & 4 \\
2 \\
\end{array}
\]

This is just $K_4$.

Maps and simple planar graphs

- Dual graphs of maps are always simple and planar.
- Conversely, any simple planar graph is the dual graph of some map.

The Four Colour Theorem

Four Colour Theorem

Every map can be coloured using at most four colours.

- 1976. Original proof by Appel and Haken. Very long. 1482 cases generated and checked by computer. But how to check it?

Graph Colouring

Definition

A graph $G$ is $k$-colourable if the nodes of $G$ can be coloured using no more than $k$ colours.

From the Four Colour Theorem:

- Every simple planar graph is 4-colourable.

Bipartite Graphs

Definition

$G$ is bipartite if nodes($G$) can be partitioned into sets $X$ and $Y$ in such a way that no two nodes of $X$ are joined and no two nodes of $Y$ are joined.

We already saw an example of a bipartite graph - $K_{3,3}$.

Proposition

A graph is bipartite iff it is 2-colourable.
Cube

Not always obvious.
For example, the cube graph is 2-colourable.

Paths and Connectedness

A path in a graph is a sequence of adjacent arcs.
Usually describe paths by nodes passed through.

Paths in example include 1, 2, 3, 4 and 2, 5, 2, 3, 3, 4.

Definition
A path is simple if it has no repeated nodes.

Definition
A graph is connected if there is a path joining any two nodes.

Connected Components

The graph is not connected.
It has two connected components, with nodes A, B, F, G and C, D, E.
**Connected Components**

For any $G$ we can define a relation on $\text{nodes}(G)$ by

$x \sim y$ iff there is a path from $x$ to $y$

We can check that this is an equivalence relation:

- reflexive
- symmetric
- transitive

The equivalence classes of $\sim$ are the nodes of the connected components.

**Cycles**

A cycle (or circuit) is a path which

- finishes where it starts
- has at least one arc
- does not use the same arc twice

Cycles in example include 1, 2, 3, 4, 1 and 3, 3.
However 2, 5, 2 is not a cycle.

**Definition**

A graph with no cycles is called acyclic.

---

**The Königsberg Bridge Problem**

Problem: Start anywhere and cross each bridge exactly once.

Notice the degrees of the nodes.

Problem: Start anywhere and cross each bridge exactly once.
Definitions

• An Euler Path is a path which uses each arc exactly once.
• An Euler Circuit (or Euler Cycle) is a cycle which uses each arc exactly once.

(So an EC is an EP which finishes where it starts)

Euler Paths

An intermediate node must be entered and left the same number of times.

If an intermediate node $n$ has odd degree, then cannot use all the arcs joined to $n$.

• If a graph has an Euler path, then the number of odd nodes must be 0 or 2.
• If a graph has an Euler circuit, then every node must be even.
Euler's Theorem

Theorem (Euler 1736)

- A connected graph has an Euler path iff there are 0 or 2 odd nodes.
- A connected graph has an Euler circuit iff every node has even degree.

Proof. We have shown “⇒”.
For “⇐”, assume that exactly two nodes $n, n'$ have odd degree.
(Case where all nodes have even degree is similar.)

Proof (cont.)

Start at $n$ and carry on until can go no further.
We must have got to $n'$:

- if stop at $n$ then there will be a spare arc ($n$ is odd and have used even no of arcs)
- if stop at $n'' \neq n, n'$ then there will be a spare arc ($n''$ is even and have used odd no of arcs)

Notice that the no of unused arcs at any node is now even.

Proof (cont.)

Now do a side journey:

Keep on adding until all arcs used up.

Example
Identify endpoints of EP (4,7).

Start from 4 (say):
Path so far: 4, 8, 7, 6, 4, 3, 8, 7

Now do side journeys:
- 3, 2, 1, 3
- 4, 5, 4
- 6, 6

Complete path: 4, 5, 4, 8, 7, 6, 4, 3, 2, 1, 3, 8, 7

Hamiltonian Paths
Can we find a path which visits every node exactly once?
Such a path is called a Hamiltonian path.
Similarly Hamiltonian circuit: HP which returns to start node.

Graph has HP but not HC.

We may as well consider simple graphs, since we can never follow a loop, and we can never follow more than one arc between two nodes.

Hamiltonian Circuit Problem (HCP)
Given a graph G determine whether G has a HC.
### Conditions

For HP to exist:

*graph must be connected*

For HC to exist:

*connected and each node must have degree \( \geq 2 \)*

But this is not sufficient:

The graph has no HC, despite every node degree \( \geq 2 \).

### Brute Force Attack

We can solve by “brute force”:

Check every possible circuit

12345(1) - no arc from 5 to 1
21345(2) - no arc from 1 to 3 etc.

How long does this take with \( n \) nodes?
Possible circuit corresponds to a permutation of nodes.
A permutation is a bijection \( \pi : \{1, \ldots, n\} \rightarrow \{1, \ldots, n\} \).
To be an actual circuit we must have \( \pi(i) \) adjacent to \( \pi(i + 1) \) for \( i = 1, \ldots, n \)
(take \( n + 1 \) to be 1 for convenience).

### Improvement

A ‘dynamic programming’ method can solve HCP in \( O(n^2 2^n) \) - still exponential.

Due to Bellman, Held, and Karp (1962)
Will be discussed later in the course.
**Complexity**

The complexity of HCP is much greater than that of the Euler Path Problem (EPP):

*Can solve EPP in polynomial time – $O(n^2)$*

HCP seems to require $O(n \cdot \log n)$

In fact HCP has been shown to be **NP-complete**.
The NP-complete problems are believed not to be solvable in polynomial time.

*i.e. they cannot be solved in $O(n^k)$ for any $k$*

NP-completeness will be discussed later in the course.

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**Trees**

- **A rooted graph** is a graph $G$ together with a distinguished node (the root of $G$).
- **A tree** is an acyclic, connected, rooted graph.
- **A nonrooted tree** is an acyclic, connected graph.

In a tree there is a unique (non-repeating) path between any two nodes:

*two different paths would give a cycle*

The depth of a node $x$ is the distance (along the unique path) from the root to $x$.

If $x$ is not the root, define the **parent** of $x$ to be the unique node adjacent to $x$ on the path from $x$ to the root.

The depth of a tree is the maximum of the depths of all its nodes.

---

**Nodes and Arcs**

**Theorem**

*Let $T$ be a tree with $n$ nodes. Then $T$ has $n - 1$ arcs.*

**Proof.**

Note that there is a 1-1 correspondence between arcs and non-root nodes:

- Any arc $a$ joins a unique non-root node $f(a)$ to its parent.
- Also, if $x$ is a non-root node then there is a unique arc $g(x)$ which joins $x$ to its parent.

Clearly $f$ and $g$ are mutual inverses.

Theorem still holds for nonrooted trees—just make any node into the root.

---

**Spanning Trees**

Find a subgraph which is a tree and which “spans” all the nodes.

The tree has 6 arcs of course.

**Definition**

Let $G$ be a graph.
A nonrooted tree $T$ is said to be a **spanning tree** for $G$ if $T$ spans $G$, i.e.

- $T$ is a subgraph of $G$ and
- $\text{nodes}(T) = \text{nodes}(G)$. 
Existence

**Proposition**
Let $G$ be a connected graph. Then $G$ has a spanning tree.

**Proof.**
Obtain a spanning tree as follows:
If $G$ has a cycle $C$ then remove any arc $x$ to $y$ of $C$.
Still a path from $x$ to $y$ using remainder of $C$.
Hence still connected.
All nodes still present.
Repeat until all cycles removed.
This must terminate—why?
We have a spanning tree.

Uniqueness

Spanning trees are not necessarily unique.

Directed Graphs

So far we have only considered undirected graphs.
For many applications it makes sense for arcs/edges to be directed.

**Definition**
A directed graph is a set $N$ of nodes and a set $A$ of arcs such that each $a \in A$ is associated with an ordered pair of nodes (the endpoints of $a$)

- In diagrams the arcs are shown with arrows from source node to target node.
- In a path $a_1, \ldots, a_n$ in a directed graph the source of $a_{i+1}$ must match the target of $a_i$ (for $i = 1, \ldots, n-1$)
- If for any pair of nodes $x, y$ there is at most one arc from $x$ to $y$ then we can refer to this arc as $(x, y)$.

**Definition**
The indegree of a node $x$ is the number of arcs entering $x$.
The outdegree of a node $x$ is the number of arcs leaving $x$.

For any directed graph:
sum of indegrees of all nodes = sum of outdegrees = number of arcs

**Definition**
A directed graph is strongly connected if for any $x, y \in \text{nodes}(G)$ there is a path from $x$ to $y$.

So we need paths both from $x$ to $y$ and from $y$ to $x$.

**Convention**
In this course (though not necessarily elsewhere) by default a graph is undirected unless we state that it is directed.
Part II

Graph Algorithms

Start at some node.
Visit every node, using some path.
Allowed to backtrack.
Will reach every node if graph connected.
In a network may need to process each node
- check if working properly
- calculate some function (time since last failure)

Traversing a Graph

Two standard traversal procedures are
- Depth-first search
- Breadth-first search

Depth-First search

Start and finish at 1.
**Depth-First search**

Start and finish at 1.
Go to 2 and start DFS from 2.

Start and finish at 1.
Go to 2 and start DFS from 2.
Backtrack from 3 to 2 and then go to 4.

Start and finish at 1.
Go to 2 and start DFS from 2.
Backtrack from 3 to 2 and then go to 4.
At 8 all adjacent nodes are visited: backtrack to start.
Order of visiting: 1, 2, 3, 4, 5, 6, 7, 8
We get a spanning tree. Notice that 8 is distance 5 from start.

**Breadth-First Search**

Start at 1.
Breadth-First Search

Start at 1.
Fan out to visit adjacent nodes at distance 1: 2, 8

Then visit nodes at distance 2: 3, 4, 7
Finally visit 5, 6
Again get a (different) spanning tree.

Depth of any node is its distance from start.

Comparison

Both DFS and BFS traverse all nodes in a connected graph, but the order of visiting is different.
Sometimes either procedure will do; other times one procedure is to be preferred.
Formalising DFS and BFS

Graph to be traversed is given as an adjacency list.

- visited: Boolean array of nodes
- parent: parent node in search tree
- output nodes in order visited
- initialise: no nodes visited

DFS Algorithm

DFS uses recursion.
Each time we visit a new node $y$, we perform DFS completely at $y$ before backtracking to parent node $x$.

**procedure dfs($x$)**

<table>
<thead>
<tr>
<th>visited[$x$] = true</th>
</tr>
</thead>
<tbody>
<tr>
<td>print $x$</td>
</tr>
<tr>
<td>for $y$ in adj[$x$]:</td>
</tr>
<tr>
<td>if not visited[$y$]:</td>
</tr>
<tr>
<td>parent[$y$] = $x$</td>
</tr>
<tr>
<td>dfs($y$)</td>
</tr>
<tr>
<td># backtrack to $x$</td>
</tr>
</tbody>
</table>

Once DFS is completed every node has a parent except for the start node. Of course, the parent information can be omitted.

Analysis

- dfs($x$) is applied to each node at most once (in fact exactly once if the graph is connected).
- Also each application of dfs($x$) runs through the arcs incident on $x$ exactly once.

Therefore the running time of DFS is $O(n + m)$, where $n$ is the number of nodes and $m$ is the number of arcs.

- Note that we are just counting accesses to the graph (stored as adjacency lists).
- Each access counts as 1 unit.
- We are ignoring overheads due to recursion.

Breadth-First Search

BFS is naturally expressed using a queue of nodes.
FIFO (first in, first out)
Queue is initialised with start node $x$.
We then process nodes from the front of the queue.
For each node we visit its immediate neighbours, adding them to the back of the queue.

**Algorithm: Breadth-first Search**

<table>
<thead>
<tr>
<th>visited[$x$] = true</th>
</tr>
</thead>
<tbody>
<tr>
<td>print $x$</td>
</tr>
<tr>
<td>enqueue($x$, $Q$)</td>
</tr>
<tr>
<td>while not isempty($Q$):</td>
</tr>
<tr>
<td>$y$ = front($Q$)</td>
</tr>
<tr>
<td>for $z$ in adj[$y$]:</td>
</tr>
<tr>
<td>if not visited[$z$]:</td>
</tr>
<tr>
<td>visited[$z$] = true</td>
</tr>
<tr>
<td>print $z$</td>
</tr>
<tr>
<td>parent[$z$] = $y$</td>
</tr>
<tr>
<td>enqueue($z$, $Q$)</td>
</tr>
<tr>
<td>dequeue($Q$)</td>
</tr>
</tbody>
</table>
Example

Head of the queue to the left; nodes added to the right. Initially the queue is [1].
Process 1, and add 2, 8 to get [2,8].
Process 2 to get [8,3,4].
   etc.
Nodes are added to the queue in the order 1,2,8,3,4,7,5,6
   Removed in the same order.

Discussion

Queue grows and shrinks during the computation.
Size of the queue represents “breadth” of the front on which BFS working.

Analysis
As with DFS each node is processed once and each adjacency list is processed once.
Again $O(n + m)$.

Is a Graph Connected?

• So far we have assumed that the graph to be traversed is connected.
• But we can traverse non-connected graphs as well.
• Of course we will only visit nodes which are in the same connected component as the start node.
• We can easily adapt either DFS or BFS to return a list of visited nodes.
• Clearly the graph is connected iff this list is the same (up to reordering) as the complete list of nodes.
• This gives us an $O(n + m)$ algorithm to determine whether a graph is connected.

Does a Graph Have a Cycle?

• Suppose a connected graph has $n$ nodes.
• If it has $\geq n$ arcs then it contains a cycle (exercise: in fact true even if graph not connected).
• We can use this to check easily whether a graph has a cycle.
• But this method does not find a cycle.
• As an alternative, use DFS.
Does a Graph Have a Cycle?

Suppose that we are using DFS to traverse a graph.

**Example**

When reach 8 we find that 1 (and 4) already visited.

Backtrack from 8 to get cycle 8, 7, 6, 4, 2, 1, (8).

If we encounter a node which we have already visited (except by backtracking), this tells us that the node can be approached by two different routes from the start node.

*Hence there is a cycle in the graph.*

Conversely, if we never encounter an already visited node, the graph is in fact a tree, with no cycles.

(We omit the proof.)

---

Distance from the Start Node

BFS finds the shortest path from the start node to any reachable node, while DFS may well give a longer distance than necessary.

- Easily adapt BFS to calculate the distance from the start node.
- Record the depth of each visited node in the BFS tree.
- The shortest path from a node \( y \) to the start node can be read off from the parent function as:
  
  \[ y, \text{parent}[y], \text{parent}[	ext{parent}[y]], \ldots, \text{start} \]

---

Does a Graph Have a Cycle?

Therefore we can adapt DFS to test whether a graph has a cycle.

**Fact (exercise)**

Let \( G \) be a connected graph, and let \( T \) be a spanning tree of \( G \) obtained by DFS starting at node \( \text{start} \).

If \( a \) is any arc of \( G \) (not necessarily in \( T \)), with endpoints \( x \) and \( y \), then either \( x \) is an ancestor of \( y \) in \( T \) or \( y \) is an ancestor of \( x \) in \( T \).

Here ‘\( x \) is an ancestor of \( y \) in \( T \)’ means that \( x \) lies on the (unique) path from \( \text{start} \) to \( y \) in \( T \).

---

Does a Graph Have a Cycle?

Return \( x, y \) if from node \( x \) we find that \( y \) (not the parent of \( x \)) has already been visited.

In this case there must be a cycle.

By the Fact, \( y \) must be an ancestor of \( x \).

Cycle is \( x, \text{parent}[x], \ldots, y, x \).
**Topological Sorting**

Suppose that we have a list of tasks to be completed and some tasks have to be completed before others.

Can view as a directed graph:

```
1  2  7
6  4  5
3  4
```

This graph must be **acyclic** or else we cannot find an order in which to complete the tasks.

Given a directed acyclic graph (DAG) $G$ with $n$ nodes, find a total ordering of the nodes $x_1, \ldots, x_n$ such that for any $i, j \leq n$, if $j > i$ then there is no path from $x_j$ to $x_i$ in $G$.

Such a total ordering is called a **topological sort** of $G$.

It could be presented as a list or array of nodes. For the example diagram a TS could be $1, 6, 3, 2, 4, 7, 5$ or $6, 1, 2, 7, 3, 4, 5$, etc.

---

**DAGs and partial orderings**

Given a DAG $G$, let $x \leq y$ iff there is a path from $x$ to $y$.

Then $\leq$ is a (weak) partial ordering:

1. reflexive
2. transitive
3. antisymmetric

Conversely, if $(X, \leq)$ is a partial ordering, let $G$ be the directed graph with nodes $X$ and arcs $\{(x, y) : x \leq y\}$. Then $G$ is acyclic.

So a topological sorting of a DAG amounts to a **linearisation** of a partial ordering, i.e. a linear order which extends the partial ordering.

---

**Topological Sorting using DFS**

Can perform topological sorting using DFS.

The idea is that when we have finished processing a node $x$ we must have finished with all nodes which are reachable from $x$, and which must come after $x$ in the sorting.

So we can add a node to the sorted list (starting from the top end) once we have finished processing it (once we exit the node).

In the example we enter (visit) the nodes in the order $1, 2, 5, 7, 3, 4, 6$ assuming that the adjacency lists are given in numerical order.

We exit the nodes in the order $5, 7, 2, 1, 4, 3, 6$.

We get the sort $6, 3, 4, 1, 2, 7, 5$.
### Topological Sorting using DFS

**Given:** a directed graph $G$ with $n$ nodes.

**Return:** topological sort of $G$ as array $ts$ of nodes if $G$ acyclic (else abort).

**procedure dfsts($x$)**
- $entered[x] = true$
- for $y$ in $adj[x]$
  - if $entered[y]$:  
    - if not $exited[y]$: abort  
    - else:
      - $parent[y] = x$
      - $dfsts(y)$
  - end if
- $exited[x] = true$
- $ts[index] = x$; $index = index - 1$

Note that we add nodes to the array as they are exited.
Correctness follows from

**Proposition**

*When performing DFS on a DAG, when we exit a node $x$ we have already exited all nodes reachable from $x.*

### Weighted Graphs

Many networks have a **cost** associated with each arc.

Transport network: distance, time or fuel

Call these costs **weights**.

**Definition**

A **weighted graph** $(G, W)$ is a simple graph $G$ together with a weight function $W : arcs(G) \to \mathbb{R}^+$ (reals $\geq 0$).

We shall investigate these problems:
- finding a minimum spanning tree
- finding shortest paths
- finding a shortest circuit

### Why Simple Graphs?

We are trying to minimise cost, and so the restriction to simple graphs is sensible:

- if there are two parallel arcs then we will always choose the cheaper
- if there is a loop then we will never wish to use it.

With simple graphs an arc can be specified uniquely by giving its endpoints: $(1, 2)$

Can regard the weight function as acting on pairs of nodes: $W(1, 2)$

($= W(2, 1)$ of course)
Minimum Spanning Trees

Recall that every connected graph has a spanning tree

- connects all nodes with least number of arcs

When dealing with weighted graphs we want to find a minimum spanning tree, that is, a spanning tree where the sum of the weights of its arcs is as small as possible.

For instance, if we had to build a road network joining some cities, a minimum spanning tree would represent the cheapest network which would connect all the cities.

Example

We have a spanning tree above with weight 12, but we can do better:

These both have weight 9.

They are minimum—easy to check.

Shows MSTs need not be unique.

Definition

Let $G$ be a weighted graph.

- The weight of a spanning tree $T$ for $G$ is the sum of the weights of the arcs of $T$.
- $T$ is a minimum spanning tree (MST) for $G$ if
  - $T$ is a spanning tree for $G$, and
  - no other spanning tree for $G$ has smaller weight.

Prim's Algorithm

Build MST starting from root node 1.

Add the shortest arc which will extend the tree.

So-called greedy approach

- do what gives a short-term advantage, even if it may not be the best overall.
Prim's Algorithm

Build MST starting from root node 1.

(1, 2)

Add the shortest arc which will extend the tree.

So-called greedy approach

• do what gives a short-term advantage, even if it may not be the best overall.

Prim's Algorithm

Build MST starting from root node 1.

(1, 2)

Then (1, 4) or (2, 3).

Add the shortest arc which will extend the tree.

So-called greedy approach

• do what gives a short-term advantage, even if it may not be the best overall.

Fringe Nodes

At an arbitrary stage in Prim's algorithm, there are three kinds of nodes:

• tree nodes
• candidates to join at the next stage: fringe nodes adjacent to a tree node
• the rest—unseen nodes

Initially all nodes are unseen.
**Prim's Algorithm—Scheme**

Choose any node $\text{start}$ as the root
Reclassify $\text{start}$ as tree
Reclassify all nodes adjacent to $\text{start}$ as fringe
while fringe nonempty:
    Select an arc of minimum weight between a tree node $t$ and a fringe node $f$ (*)
    Reclassify $f$ as tree
    Add arc $(t,f)$ to the tree
    Reclassify all unseen nodes adjacent to $f$ as fringe

---

**Analysis**

$n$ nodes, $m$ arcs
Each time the while loop is executed another node is added to the tree.
Hence the while loop is executed $O(n)$ times.

(*) involves finding the shortest arc among all possible arcs between $O(n)$ tree nodes and $O(n)$ fringe nodes.
Therefore $O(n + m)$.
So the whole algorithm $O(n(n + m))$.

---

**Improvement**

Keep track of which arcs might be used—candidate arcs.
Example. Initially just 1 in tree.

```
     1
    /\  \\
   4  \ 2
   \   3
    \ 4
     3
```

Fringe nodes 2,3,4.

Now (1,4) added:
```
     1
    /\  \\
   4  \ 5
   \   4
    \ 2
     3
```

Fringe nodes 2,3,4.
Candidate arc for 3 has changed again.

Fringe node 3.
Candidate arc for 3 has changed again.

```
     1
    /\  \\
   4  \ 2
   \   3
     4
```

Implement using parent function (as for graph traversal).
Defined for tree and fringe nodes.
Let the parent of a fringe node $f$ be the tree node $t$ such that $(t,f)$ has least weight.
Prim's MST Algorithm ('classic' version)

Choose any node \( \text{start} \) as the root

```plaintext
# initialise tree
tree[\text{start}] = true

# initialise fringe
for \( x \) in adj[\text{start}]:
    # add \( x \) to fringe
    fringe[\( x \)] = true
    parent[\( x \)] = \text{start}
    weight[\( x \)] = \( W[\text{start}, x] \)

# end of initialisation
```

while fringe nonempty:
    Select fringe node \( f \) s.t. weight[\( f \)] is minimum
    fringe[\( f \)] = false
    tree[\( f \)] = true

    for \( y \) in adj[\( f \)]:
        if not tree[\( y \)]:
            if fringe[\( y \)]:
                # update candidate arc if lower weight poss.
                if weight[\( y \)] < \( W[f, y] \):
                    weight[\( y \)] = \( W[f, y] \)
                    parent[\( y \)] = \( f \)
            else:
                # \( y \) is unseen—add to fringe
                fringe[\( y \)] = true
                weight[\( y \)] = \( W[f, y] \)
                parent[\( y \)] = \( f \)

Discussion

Weight of the MST: add weights of nodes (apart from \( \text{start} \)).

Analysis

- As before there are \( O(n) \) executions of the while loop.

Executing the while loop:

- Testing whether the fringe is empty is \( O(n) \).
- Finding the fringe node \( f \) such that weight[\( f \)] is minimum is \( O(n) \).
- The updating of the candidate arc for each \( y \) in adj[\( f \)] is \( O(1) \).

Hence the for loop is \( O(n) \).

We conclude that the algorithm is \( O(n^2) \).

Improves our earlier estimate of \( O(n(n + m)) \).

(Recall that \( m \) can be as large as \( n^2 \), so that \( O(n(n + m)) \) is \( O(n^3) \).)
Correctness

**Theorem**

Let $G$ be a connected weighted graph. Then Prim's algorithm constructs an MST for $G$.

Let $G$ have $n$ nodes.
Let the trees constructed at each stage be $T_0, \ldots, T_k, \ldots$.

$T_0$: just the node start
$T_{k+1}$ got from $T_k$ by adding arc $a_{k+1}$.
Then $T_k$ has $k + 1$ nodes.

There are $n - 1$ stages, with $T_{n-1}$ being returned by the algorithm.
We show by induction on $k$ that

**each $T_k$ is a subgraph of an MST $T'$ of $G$.**

**Base case** $k = 0$. $T_0$ has one node and no arcs.
Clearly $T_0 \subseteq T'$ for any MST $T'$ of $G$.

**Induction step**. Assume that $T_k \subseteq T'$, some MST $T'$ of $G$.

If $a_{k+1} \in \text{arcs}(T')$ then $T_{k+1} \subseteq T'$ as required.

So suppose $a_{k+1} \notin \text{arcs}(T')$.
Since $T'$ is a spanning tree, there must be a path in $T'$ from $x$ to $y$.

Form a new spanning tree $T''$ from $T'$ by removing $a$ and adding $a_{k+1}$.
Since the algorithm chose $a_{k+1}$ rather than $a$, we have $W(a_{k+1}) \leq W(a)$.
Hence $W(T'') \leq W(T')$ and so $T''$ is an MST.
(Since all MSTs have the same weight, actually $W(a_{k+1}) = W(a)$.)
Also, $T_{k+1} \subseteq T''$ as required.
This completes the induction step.
Now $T_{n-1}$ has $n - 1$ arcs, and $T_{n-1} \subseteq T'$ some MST $T'$.
Since all spanning trees for $G$ have $n - 1$ arcs, we must have $T_{n-1} = T'$.
Hence $T_{n-1}$ is an MST, as required.
Remarks

1. We can regard the induction hypothesis as an invariant.
   - Established initially
   - Maintained through each execution of the while loop of the code
2. Each $T_k$ constructed by Prim’s algorithm is connected.
3. Also, in fact $T_k$ is an MST for the subgraph of $G$ induced by
   $\text{nodes}(T_k)$:
   the subgraph with nodes $\text{nodes}(T_k)$ and all arcs of $G$ which join
   nodes in $\text{nodes}(T_k)$
   
   We did not require either (2) or (3) for the proof.

Priority Queues

- Each item $x$ of the queue has a priority $\text{key}[x]$—usually a natural number.
- Key represents cost
- Items removed lowest key first.

Operations:
- $Q = \text{PQcreate}()$
- $\text{isEmpty}(Q)$
- $\text{insert}(Q, x)$
- $\text{getMin}(Q)$
- $\text{deleteMin}(Q)$
- $\text{decreaseKey}(Q, x, \text{newkey})$ — updates $\text{key}[x] = \text{newkey}$

Prim’s algorithm with priority queues

$Q = \text{PQcreate}()$
for $x$ in $\text{nodes}(G)$:
   $\text{key}[x] = \infty$; $\text{parent}[x] = \text{nil}$
insert($Q, x$)
decreaseKey($Q, \text{start}, 0$)
while not $\text{isEmpty}(Q)$:
   $f = \text{getMin}(Q)$; deleteMin($Q$)
   $\text{tree}[f] = \text{true}$
   for $y$ in $\text{adj}[f]$:
      if not $\text{tree}[y]$:
         # so $y$ in $Q$
         if $W[f, y] < \text{key}[y]$:
            decreaseKey($Q, y, W[f, y]$)
            $\text{parent}[y] = f$

Example

\begin{center}
\begin{tabular}{cccc}
node & 1 & 2 & 3 & 4 \\
key & $\infty$ & $\infty$ & $\infty$ & $\infty$ \\
& 0 & $\infty$ & $\infty$ & $\infty$ \\
& $-$ & 3 & 5 & 4 \\
& $-$ & $-$ & 4 & 4 \\
& $-$ & $-$ & 2 & $-$ \\
& $-$ & $-$ & $-$ & $-$ \\
\end{tabular}
\end{center}
**Analysis**

With $n$ nodes and $m$ arcs the number of PQ operations is:

- $O(n)$ inserts
- $O(n)$ isEmptys
- $O(n)$ getMins
- $O(n)$ deleteMins
- $O(m)$ decreaseKeys

Good implementation of priority queue via Binary Heap (later in these lectures).

For a PQ of length $N$ all operations $\log N$ apart from isEmpty and getMin which are $O(1)$.

So Prim with PQ overall $O(m \log n)$ assuming that $n < m$ as is usually the case.

Which is better—'classic' Prim with candidate arcs or Prim with PQ?

If graph is sparse, say $m \leq n \log n$:

$O(m \log n) = O(n \log^2 n)$

Better than $O(n^2)$

So Prim with PQ is better.

If graph is dense:

$O(m \log n) = O(n^2 \log n)$

Worse than $O(n^2)$

So classic Prim is better.

**Kruskal's MST Algorithm**

Prim’s algorithm is greedy:

*always chooses the shortest candidate arc, pursuing short-term advantage.*

Remarkably, this turned out to give optimal results:

*the algorithm is guaranteed to construct an MST.*

An even "greedier" strategy:

*At each stage choose the shortest arc not yet included, except when this would give a cycle.*

This is **Kruskal's MST algorithm**.

**Example**

At intermediate stages get a forest (acyclic graph) rather than a tree (connected acyclic graph).
Kruskal's MST algorithm

**Scheme**

- **F** = ∅  # forest being constructed
- **R** = arcs(G)  # remaining arcs

while **R** nonempty:
  - remove a of smallest weight from **R**
  - if a does not make a cycle when added to **F**:
    - add a to **F**

return **F**

- Arcs are added in increasing order of weight.
- Possible implementation strategy: work on a list of arcs sorted by weight in increasing order.

Correctness

**Theorem**

Let **G** be a connected weighted graph.

Then Kruskal's algorithm constructs an MST for **G**.

Proof strategy much the same as Prim's algorithm.

We show that stage k we have forest **F** ⊆ **T**′, some MST **T**′ of **G**.

See lecture notes for the details.

Implementation

We have to do two things:

1. Look at each arc in ascending order of weight.
   - We can use a priority queue here
     (or just sort the arcs at the start).
2. Check whether adding the arc to the forest so far creates a cycle.
   - Use dynamic equivalence classes.
   - Put nodes in the same equivalence class if they belong to the same connected component of the forest constructed so far.
   - Map each node to the representative of its equivalence class.
   - An arc (x, y) can be added if x and y belong to different equivalence classes.
   - If (x, y) is added, then **merge** the equivalence classes of x and y.

Example

[Diagram of a graph with labeled nodes and edges]
Union-Find

Dynamic equivalence classes can be handled using the Union-Find data type.
Each set has a leader element which is the representative of that set.
  • find: find the leader of the equivalence class
  • union: merge two classes

Operations:
  • sets — creates a family of singleton sets \{1\}, \{2\}, \ldots, \{n\}
  • x’ = find(sets, x) — finds the leader x’ of x within sets
  • union(sets, x, y) — merge the sets led by x and y
    and use one of x or y as the new leader
    NB x and y must be the leaders of their sets:
    x = find(sets, x)
    y = find(sets, y)

Implementing union-find

A naive implementation:
Maintain an array leader of nodes:
  • leader[x] stores the leader of the set to which node x belongs.
  • Initially leader[x] = x for all nodes.

Find is now O(1).
However union takes O(n).
That means that it takes O(n^2) to perform the O(n) unions required for Kruskal.

Implementation scheme for Kruskal

Let G have n nodes numbered from 1 to n.
Build a priority queue Q of the edges of G with the weights as keys
sets = UFcreate(n)  # initialise Union-Find with singletons
\{1\}, \ldots, \{n\}
F = {}  # forest being constructed
while not isEmpty(Q):
  (x, y) = getMin(Q); deleteMin(Q)
  x’ = find(sets, x); y’ = find(sets, y)
  if x’ != y’:  # no cycle
    add (x, y) to F
    union(sets, x’, y’)  # merge the two components

Non-binary trees

Instead: each set is stored as a (non-binary) tree.
The root node is the representative (leader) of the set.
We merge two sets by appending one tree to the other,
so that the root of one tree is the child of the root of the other tree.
Non-binary trees

To store the tree structure, for each node \( x \) we maintain \( \text{parent}[x] \), where \( \text{parent}[x] = x \) if \( x \) is the root (the leader)

Initially \( \text{parent}[x] = x \) for any node \( x \).

union(sets, \( x \), \( y \)) just involves setting \( \text{parent}[y] = x \) (or vice versa) — constant time \( O(1) \)

However find involves following \( \text{parent}[x] \) up to the root.

Time taken is bounded by the depth of the tree.

With naive merging of trees as above, this can be as much as \( n \), so that find becomes \( O(n) \).

Reducing the depth

We clearly need to keep the depth as low as possible.

Weighted union:
since can append trees in either order, always append the tree of lower size to the one of greater size.

This requires us to store the size of the tree and update this — easy to do.

Bound on depth

Lemma

Using weighted union, the depth of a tree of size \( k \) is \( \leq \lfloor \log k \rfloor \).

Proved by (strong) induction on \( k \).
See the lecture notes.

Complexity

Using the Lemma, with weighted union, each find takes \( O(\log n) \), and each union takes \( O(1) \).

For Kruskal, there will be:

- \( O(m) \) inserts to build the PQ — time taken \( O(m \log m) \)
- \( O(m) \) getMins and \( O(m) \) deleteMins — time taken \( O(m \log m) \)
- \( O(m) \) finds — time taken \( O(m \log n) \)
- \( O(n) \) unions — time taken \( O(n) \)

So overall time taken is \( O(m \log m) \) (assuming \( m \geq n \), as is normally the case).

The number of arcs \( m \) is bounded by \( n^2 \).

So \( O(m \log m) = O(m \log n) \).

Overall complexity for Kruskal: \( O(m \log n) \).

Same as Prim with PQ.
**Complexity**

**Remark**
In fact can build the PQ in time $O(m)$ rather than $O(m \log m)$. Does not bring down the overall complexity here.

Can improve union-find using **path compression**. The complexity for the union-find part of Kruskal then reduces to $O((n + m) \log^* n)$.

Here $\log^* n$ is an extremely slow-growing function. $\log^* n \leq 5$ for any conceivable $n$ that might be used.

**Path compression**

When finding the root (leader) for a node $x$, if this is not parent[$x$] then make parent[$y$] = root for all $y$ on the path from $x$ to the root.

We have extra work in updating parent, but we keep the depth of the nodes lower so that future finds are faster. Combines well with weighted union (on size) since size is unchanged by path compression.

**Comparison**

Kruskal: $O(m \log n)$
Prim with PQ (binary heap): $O(m \log n)$
Classic Prim: $O(n^2)$

Which is better?

As when comparing classic Prim and Prim with PQ:

- On dense graphs where $m$ is large (order $n^2$) then Kruskal gives $O(n^2 \log n)$ and classic Prim is to be preferred.
- On sparse graphs, where $m$ is small (say $O(n \log n)$), then Kruskal (or Prim with PQ) give better results than classic Prim:

$$O(m \log n) = O(n \log^2 n)$$
Fibonacci heaps

Priority queues can also be implemented with Fibonacci heaps rather than binary heaps.
All operations are $O(1)$ apart from deleteMin, which is $O(\log n)$.
Complexity of Prim with PQ (Fibonacci heap):

$$O(m + n \log n)$$

In practice the memory usage and constant factors can be high.

The Shortest Path Problem

Network of cities joined by roads.
Wish to find the shortest route between two cities.
Find shortest path from 1 to 7.
The path 1,2,6,7 has length 10+7+4 = 21.
Can we do better?

Single Pair Shortest Path Problem

Given a weighted graph $G$, and two nodes $\text{start}$ and $\text{finish}$, find the shortest path from $\text{start}$ to $\text{finish}$ in $G$.

All Pairs versus Single Pair

Contrast with

All Pairs Shortest Path Problem

Given a weighted graph $G$, find the shortest paths between all pairs of nodes of $G$.

Algorithm due to Floyd later in these lectures.
Excellent algorithm for finding all shortest paths between any pairs of nodes.
It runs in $O(n^3)$ time.
Suppose instead that we only want to find the shortest distance from a single start node to a single finish node.
Seems to be no way to speed up Floyd.
But there is an $O(n^2)$ algorithm due to Dijkstra.
It is very closely related to Prim's MST algorithm.

Idea

As in Prim's algorithm, we build up a spanning tree starting from the start node.
We classify nodes into

- **tree** nodes: already included
- **fringe** nodes: not in the tree yet, but adjacent to a tree node
- **unseen** nodes: the rest

The new idea:

- We have already computed the shortest path from start to all the tree nodes:
it is the path given by the tree.
- As far as the fringe nodes are concerned, we know the shortest path using the tree constructed so far.
  This path might be improved as the tree grows.
Add 3. Update candidate arcs.

Now we add 2 rather than 5 since $\text{distance}[5] = 13$.


Here we computed shortest paths from start for all nodes, but in general we stop as soon as finish joins the tree.

We got a spanning tree, but it is not an MST.
**Implementation**

We store two values for each tree or fringe node:
- its parent node in the tree
- the distance of the shortest path known.

At each stage the next node to be added to the tree is the fringe node with the smallest distance.

We then update the fringe, possibly improving the current shortest path.

We can obtain the shortest path to a node \(x\) in reverse order from the parent function:

\[x, \text{parent}[x], \text{parent}[	ext{parent}[x]], \ldots, \text{start}\]

**Dijkstra’s Shortest Path Algorithm**

Input: Weighted graph \((G, W)\) together with a pair of nodes \(\text{start}, \text{finish}\)

Output: Length of shortest path from \(\text{start}\) to \(\text{finish}\)

\[\text{tree}[\text{start}] = \text{true}\]

for \(x\) in \(\text{adj}[\text{start}]\):

  # add \(x\) to fringe
  fringe\([x]\) = \text{true}
  parent\([x]\) = \text{start}
  distance\([x]\) = \(W[\text{start}, x]\)

# end of initialisation

[continued]

while not \(\text{tree}[\text{finish}]\) and fringe nonempty:

  Select a fringe node \(f\) s.t. \(\text{distance}[f]\) is minimum
  fringe\([f]\) = \text{false}
  tree\([f]\) = \text{true}

[continued]

for \(y\) in \(\text{adj}[f]\):

  if not \(\text{tree}[y]\):

    if fringe\([y]\):

      # update distance and candidate arc
      if distance\([f]\) + \(W[f, y]\) < distance\([y]\):

        distance\([y]\) = distance\([f]\) + \(W[f, y]\)
        parent\([y]\) = \(f\)

      else:

        # \(y\) is unseen
        fringe\([y]\) = \text{true}
        distance\([y]\) = distance\([f]\) + \(W[f, y]\)
        parent\([y]\) = \(f\)

    return distance\([\text{finish}]\)
Discussion

When terminates, read off the path using parent.

Running time \(O(n^2)\), just as Prim's algorithm.

Correctness

The algorithm terminates, since we clearly increase the tree each time we execute the while loop.

To see why the algorithm is correct we need to formulate an invariant.

Correctness

Invariant

1. If \(x\) is a tree or fringe node (other than start) then parent\([x]\) is a tree node.
2. If \(x\) is a tree node (other than start) then distance\([x]\) is the length of shortest path, and parent\([x]\) is its predecessor along that path.
3. If \(f\) is a fringe node then distance\([f]\) is the length of the shortest path where all nodes except \(f\) are tree nodes. Furthermore, parent\([f]\) is its predecessor along that path.

When the program terminates, finish is a tree node, and by (2) we then have the required shortest path.

So it remains to show that the invariant is

- established before the while loop
- maintained during the while loop

We just show that (2) is maintained, and omit the rest of the proof.
Suppose $f$ is added to the tree.
We need to check that we have found the shortest path.
The path given by the algorithm: $\text{start}, \ldots, \text{parent}[f], f$
Suppose we have a different and shorter path $P$ (not necessarily in the tree).

Let $y$ be the first node on $P$ not to belong to the tree.
By (3) $\text{distance}[y] \leq \text{distance from start to } y$ using $P$.
Hence length of $P \geq \text{distance}[y]$.
But $\text{distance}[y] \geq \text{distance}[f]$ by our choice of $f$.
Hence $P$ is at least as long as $\text{path}(f)$.

**Analysis**

Very much the same as for Prim's algorithm.
Dijkstra with PQ (binary heap) overall $O(m \log n)$ assuming that $n < m$ as is usually the case.
Dijkstra with PQ (Fibonacci heap) overall $O(m + n \log n)$.

**Dijkstra's algorithm with priority queues**

$Q = \text{PQcreate}()$

for $x$ in $\text{nodes}(G)$:
  key[$x$] = $\infty$; parent[$x$] = nil
  insert($Q, x$)

decreaseKey($Q, \text{start}, 0$)

while not $\text{tree}[\text{finish}]$ and not isEmpty($Q$):
  $f = \text{getMin}(Q); \text{deleteMin}(Q)$
  $\text{tree}[f] = \text{true}$
  for $y$ in $\text{adj}[f]$:
    if not $\text{tree}[y]$: # so $y$ in $Q$
      if $\text{key}[f] + W[f, y] < \text{key}[y]$:
        decreaseKey($Q, y, \text{key}[f] + W[f, y]$)
        parent[$y$] = $f$

**A* algorithm**

We now consider a different algorithm for the single pair shortest path problem.

We assume that we have a heuristic function $h(x)$ which underestimates the distance from any node $x$ to the finish node.
If we are dealing with cities on a map, $h$ could be the Euclidean distance (as the crow flies).
Example

Each node \( x \) has heuristic value \( h(x) \) shown in red.

Using Dijkstra's algorithm we have to compute the entire shortest path tree before reaching node \( D \).

We had to find the shortest paths to all the nodes which are closer to \( \text{start} \) than \( D \).

Of course we did not use the heuristic information.

Example (continued)

With A*:

Example (continued)

With A*:
Example (continued)

With A*:

0 finish
start
4
3
A
B
D
EF
HI
J
K
3 3
4 5
2 3
3
2
2
4
10
12
22
3
11
3
4
2 8
10 7
C
G
8
5
9
12
10
12
14
13
11
12
13
17
3

/one.osf/six.osf/zero.osf

Example (continued)

With A*:

0 finish
start
4
3
A
B
D
EF
HI
J
K
3 3
4 5
2 3
3
2
2
4
10
12
22
3
11
3
4
2 8
10 7
C
G
8
5
9
12
10
12
14
13
11
12
13
17
3

/one.osf/six.osf/two.osf

Example (continued)

With A*:

0 finish
start
4
3
A
B
D
EF
HI
J
K
3 3
4 5
2 3
3
2
2
4
10
12
22
3
11
3
4
2 8
10 7
C
G
8
5
9
12
10
12
14
13
11
12
13
17
3

/one.osf/five.osf/nine.osf

Example (continued)

With A*:

0 finish
start
4
3
A
B
D
EF
HI
J
K
3 3
4 5
2 3
3
2
2
4
10
12
22
3
11
3
4
2 8
10 7
C
G
8
5
9
12
10
12
14
13
11
12
13
17
3

/one.osf/six.osf/one.osf
**Consistent heuristic**

A heuristic function is consistent if

1. for any adjacent nodes \(x, y\) we have \(h(x) \leq W(x, y) + h(y)\)
2. \(h(\text{finish}) = 0\)

This is clearly satisfied by the Euclidean distance heuristic function if \(W(x, y)\) represents distances on a map.

**Proposition**

Let \(h\) be a consistent heuristic function, and let \(P\) be a path from node \(x\) to node \(y\). Then \(h(x) \leq \text{len}(P) + h(y)\).

A heuristic function is admissible if for any node \(x\) we have \(h(x) \leq \) the weight of the shortest path from \(x\) to the goal \(\text{finish}\).

It is easy to check that if \(h\) is consistent then \(h\) is admissible (exercise).

**A* algorithm**

Input: Weighted graph \((G, W)\) together with a pair of nodes \text{start}, \text{finish} and consistent heuristic function \(h\)

Output: Length of shortest path from \text{start} to \text{finish}

1. \text{tree}[\text{start}] = true
2. \(g[\text{start}] = 0\)
3. \(f[\text{start}] = g[\text{start}] + h[\text{start}]\)
4. for \(x\) in \text{adj}[\text{start}]:
   - # add \(x\) to fringe
   - fringe[\(x\)] = true
   - parent[\(x\)] = \text{start}
   - \(g[\text{x}] = W[\text{start}, \text{x}]\)
   - \(f[\text{x}] = g[\text{x}] + h[\text{x}]\)
5. for \(y\) in \text{adj}[\(x\)]:
   - if not \text{tree}[\(y\)]:
     - if fringe[\(y\)]:
       - # update \(g(y), f(y)\) and candidate arc
       - if \(g[\text{x}] + W[\text{x}, \text{y}] < g[\text{y}]\):
         - \(g[\text{y}] = g[\text{x}] + W[\text{x}, \text{y}]\)
         - \(f[\text{y}] = g[\text{y}] + h[\text{y}]\)
         - parent[\(y\)] = \(x\)
       - else:
         - # \(y\) is unseen
         - fringe[\(y\)] = true
         - \(g[\text{y}] = g[\text{x}] + W[\text{x}, \text{y}]\)
         - \(f[\text{y}] = g[\text{y}] + h[\text{y}]\)
         - parent[\(y\)] = \(x\)
   - else:
     - # \(y\) is unseen
     - fringe[\(y\)] = true
     - \(g[\text{y}] = g[\text{x}] + W[\text{x}, \text{y}]\)
     - \(f[\text{y}] = g[\text{y}] + h[\text{y}]\)
     - parent[\(y\)] = \(x\)
6. return \(g[\text{finish}]\)
Remarks

1. The set of tree nodes is often called the closed set and the set of fringe nodes is the open set.
2. If we set \( h(x) = 0 \) for all nodes \( x \) then \( h \) is consistent, and the A* algorithm is just Dijkstra's algorithm.
3. We deduce that the running time for A* is the same as for Dijkstra in the worst case, though we hope to do better on average, depending on \( h \).
4. We have presented A* for consistent heuristics, for simplicity and for its closeness to Dijkstra’s algorithm.
5. There is a more general version of A* which is guaranteed to give the correct solution for admissible heuristics. The difference is that we may have to re-examine nodes that are already in the closed set (the tree).

Correctness

We now show that A* correctly computes the shortest path. The algorithm terminates, since we clearly increase the tree each time we execute the while loop.

To see why the algorithm is correct we need to formulate an invariant, which is essentially the same as for Dijkstra’s algorithm.

**Invariant**

1. If \( x \) is a tree or fringe node (other than start) then parent[\( x \)] is a tree node.
2. If \( x \) is a tree node (other than start) then \( g[\( x \)] \) is the length of shortest path, and parent[\( x \)] is its predecessor along that path.
3. If \( x \) is a fringe node then \( g[\( x \)] \) is the length of the shortest path where all nodes except \( x \) are tree nodes. Furthermore, parent[\( x \)] is its predecessor along that path.

When the program terminates, finish is a tree node, and by (2) we then have the required shortest path.

So it remains to show that the invariant is

- established before the while loop
- maintained during the while loop

We just show that (2) is maintained, and omit the rest of the proof.
Suppose \( x \) is added to the tree.

We need to check that we have found the shortest path.

The path given by the algorithm: \( \text{start}, \ldots, \text{parent}[x], x \) has length \( g[x] \).

Suppose we have a different and shorter path \( P \) (not necessarily in the tree).

Then \( \text{len}(P) < g[x] \).
Let \( y \) be the first node on \( P \) not to belong to the tree.
Let \( P_1 \) be \( P \) from \( \text{start} \) to \( y \), and \( P_2 \) be \( P \) from \( y \) to \( x \).

\[ f[y] = g[y] + h[y] \]
\[ \leq g[y] + \text{len}(P_2) + h[x] \]
(consistency of \( h \))
\[ \leq \text{len}(P_1) + \text{len}(P_2) + h[x] \]
(by (3) for \( y \))
\[ = \text{len}(P) + h[x] \]
\[ < g[x] + h[x] \] (assumption)
\[ = f[x] \]
But \( f[x] \leq f[y] \) by our choice of \( x \).
Contradiction.

**A* algorithm with priority queues**

\[ Q = PQcreate() \]
for \( x \) in nodes(\( G \)):
\[ g[x] = \infty; \text{key}[x] = \infty; \text{parent}[x] = \text{nil} \]
insert(\( Q, x \))
\[ g[\text{start}] = 0; \text{decreaseKey}(Q, \text{start}, g[\text{start}] + h[\text{start}]) \]
while not tree[\text{finish}] and not isEmpty(\( Q \)):
\[ x = \text{getMin}(Q); \text{deleteMin}(Q) \]
\[ \text{tree}[x] = \text{true} \]
for \( y \) in adj[\( x \)]:
if not tree[\( y \)]:
so \( y \) in \( Q \)
if \( g[x] + W[x, y] < g[y] \):
\[ g[y] = g[x] + W[x, y]; \text{decreaseKey}(Q, y, g[y] + h[y]) \]
\[ \text{parent}[y] = x \]

**Transitive closure**

Let \( R \subseteq X^2 \) be a binary relation.

Recall from Discrete Structures that the transitive closure of \( R \) is

\[ R^+ = \bigcup_{k=1}^{\infty} R^k \]

If \( X \) is finite and \( |X| = n \) then

\[ R^+ = \bigcup_{k=1}^{n} R^k \]

We can interpret \( R \) as a directed graph \( G \). The nodes of \( G \) are just the members of \( X \). Arc from \( x \) to \( y \) iff \( R(x, y) \).

NB No parallel arcs. We could have loops where \( R(x, x) \).

It is easy to see that \( R^k(x, y) \) iff there is a path of length \( k \) from \( x \) to \( y \).
So \( R^+(x, y) \) iff there is a path of length \( \geq 1 \) from \( x \) to \( y \).
Suppose \( X = \{1, \ldots, n\} \). Clearly if we set
\[
A[i, j] = \begin{cases} 
1 & \text{if } R(i, j) \\
0 & \text{otherwise}
\end{cases}
\]
then \( A \) is the adjacency matrix of \( G \).
We can compute \( R^k \) using matrix multiplication:
\[
R^k(i, j) \iff A^k[i, j] > 0
\]
Let
\[
B = \sum_{k=1}^{n} A^k
\]
Then
\[
R^+(i, j) \iff B[i, j] > 0
\]
So far we have been building up the transitive closure by looking for paths of length \( k \) for \( k = 1, \ldots, n \).
We now look at a quite different and more efficient method.

### Warshall’s algorithm

Now we just need to calculate \( B_k \) from \( B_{k-1} \) (for \( k = 1, \ldots, n \)).
Suppose we have a path \( p \) from \( i \) to \( j \) using intermediate nodes \( \leq k \).
There are two cases:
1. \( k \) is not an intermediate node of \( p \). Then \( B_{k-1}[i, j] \) already.
2. \( k \) is an intermediate node of \( p \).
   We can assume that \( k \) occurs only once, since if it occurs multiple times we can shorten the path by removing the cycle(s) from \( k \) to \( k \).
   But then we have paths \( i \) to \( k \) and \( k \) to \( j \) which just use intermediate nodes \( \leq k-1 \). So \( B_{k-1}[i, k] \) and \( B_{k-1}[k, j] \).
This is the idea behind Warshall’s algorithm.

### Warshall’s algorithm

Suppose that the nodes are \( \{1, \ldots, n\} \).
Consider a path \( p = x_1, x_2, \ldots, x_k \) from \( x_1 \) to \( x_k \).
We say that nodes \( x_2, \ldots, x_{k-1} \) are intermediate nodes of \( p \).
We look for paths which use nodes \( \leq i \) as intermediate nodes.
Let \( B_k[i, j] = 1 \) iff there is a path from \( i \) to \( j \) which uses intermediate nodes \( \leq k \) (set \( B_0[i, j] = 0 \) otherwise).
Clearly \( B_0[i, j] = A[i, j] \) since we only have paths of length one, as there can be no intermediate nodes \( \leq 0 \).
Also \( R^+(i, j) \iff B_n[i, j] = 1 \), since \( B_n \) allows all possible intermediate nodes, and so all possible paths.

input \( A \)
copy \( A \) into \( B \) (array of Booleans) \# \( B = B_0 \)
for \( k = 1 \) to \( n \):
  \# \( B = B_{k-1} \)
  for \( i = 1 \) to \( n \):
    for \( j = 1 \) to \( n \):
      \( b_{ij} = b_{ij} \) or (\( b_{ik} \) and \( b_{kj} \))
      \# \( B = B_k \)
  \# \( B = B_n \)
return \( B \)
Complexity is clearly \( O(n^3) \).
**Floyd's algorithm**

We return to:

**All Pairs Shortest Path Problem**

Given a weighted directed graph $G$, find the shortest paths between all pairs of nodes of $G$.

This can be solved efficiently using a simple modification of Warshall's algorithm.

Let $G$ be a weighted directed graph with nodes $\{1, \ldots, n\}$ and adjacency matrix $A$.

Let $B_k[i,j]$ be the length of the shortest path from $i$ to $j$ which uses intermediate nodes $\leq k$.

If there is no such path set $B_k[i,j] = \infty$.

Clearly $B_0[i,j] = \begin{cases} A[i,j] & \text{if } A[i,j] \\ \infty & \text{otherwise} \end{cases}$

Also $B_n[i,j]$, will be the length of the shortest path from $i$ to $j$.

---

**Dynamic Programming**

Warshall’s algorithm and Floyd’s algorithm are both examples of dynamic programming.

In dynamic programming:

- break the main problem down into sub-problems
- the sub-problems are ordered (e.g. increasing size) and culminate in the main problem

To solve the main problem:

- move through the sub-problems in order
  - solve each sub-problem using the stored solutions of the previous sub-problems and storing the new solution for later use
  - solve the main problem as the final sub-problem
The Travelling Salesman Problem

Given some cities and roads between them, a travelling salesman wants to find a tour of all the cities with the shortest distance.

Given a complete weighted graph \((G, W)\), find a way to tour the graph visiting each node exactly once and travelling the shortest possible distance.

The Travelling Salesman Problem (TSP)

The restriction to complete graphs is not that strong: if arcs were missing from the graph we could make it complete by adding fictitious arcs with weights made high enough to ensure that they would never be chosen.

Complexity

TSP is clearly related to
- Hamiltonian Circuit Problem (HCP)
- Shortest Path Problem

We have to find a Hamiltonian circuit (HC) which is of minimum weight.

The difficulty is not in finding an HC, since we have assumed that the graph is complete.

But to find the shortest HC involves potentially checking \(n!\) different tours if \(G\) has \(n\) nodes.

Just like HCP, TSP is NP-complete and so unlikely to have a polynomial solution.

A better algorithm than just checking every possible tour yields a running time of \(O(n^2 2^n)\) (Bellman, Held & Karp).
- still worse than exponential

Bellman-Held-Karp algorithm

Another example of dynamic programming.

Let \((G, W)\) have \(\text{Nodes} = \{1, \ldots, n\}\).

Idea: Fix a start node, say 1.

For each \(x \neq 1\) and each \(S \subseteq \text{Nodes} \setminus \{1, x\}\):
find and store the minimum cost \(C(S, x)\) of a path from node 1 to node \(x\) using set of intermediate nodes precisely \(S\).

A TS tour can start at 1 wlog.
Let the last node before returning to 1 be \(x\).

The least cost of such a tour is \(C(\text{Nodes} \setminus \{1, x\}, x) + W(x, 1)\).

So solution to TSP is
\[
\min_{x \neq 1} C(\text{Nodes} \setminus \{1, x\}, x) + W(x, 1)
\]
Calculating $C(S, x)$

We calculate $C(S, x)$ in increasing order of size: do all $S$ of size 0, then 1, up to $n - 2$.

Clearly $C(\emptyset, x) = W(1, x)$ as no intermediate nodes are allowed.

Assume we know $C(S, x)$ for all $S$ of size $k$.

Suppose $|S| = k + 1$.

Consider the last intermediate node $y$ in a least cost path from 1 to $x$ using intermediate nodes $S$ (including $y$).

Cost must be $C(S \setminus y, y) + W(y, x)$.

So

$$C(S, x) = \min_{y \in S} C(S \setminus y, y) + W(y, x)$$

Bellman-Held-Karp algorithm in pseudocode

Input $(G, W)$

Choose $\text{start} \in \text{nodes}(G)$

for $x \in \text{Nodes} \setminus \{\text{start}\}$:

$C[\emptyset, x] = W[\text{start}, x]$

# Process sets $S$ in increasing order of size.

for $S \subseteq \text{Nodes} \setminus \{\text{start}\}$ with $S \neq \emptyset$:

for $x \in \text{Nodes} \setminus (S \cup \{\text{start}\})$:

    # Find $C[S, x]$

    $C[S, x] = \infty$

    for $y \in S$:

        $C[S, x] = \min(C[S \setminus \{y\}, y] + W[y, x], C[S, x])$

# Now have calculated and stored all values of $C[S, x]$

[continued]

Complexity

For each subset of $\text{Nodes}$ (roughly speaking) we do $O(n^2)$ work with the two for loops.

Overall $O(n^2 2^n)$

Hamiltonian circuit problem

The Bellman-Held-Karp algorithm can be adapted to solve the HCP.

Complexity is still $O(n^2 2^n)$.
Approximate Methods for TSP

Despite exact solutions taking too long, we still want to solve TSP—there are applications in circuit design, etc.

Approximate methods.

For instance, we could try a “greedy” algorithm which always chooses the shortest available arc, the so-called nearest neighbour heuristic (NNH).

Starting from node 1 we get the tour 1, 4, 5, 2, 3, 1 with a total weight of $1 + 2 + 4 + 7 + 5 = 19$ which is quite good.

However such a short-sighted method can also fail dramatically.

Suppose that we change the weight of (1, 3) from 5 to 500. Then clearly this arc should be avoided, but NNH is forced to choose it on the last step.

Part III

Algorithm Analysis

Problem $P$

- sort a list
- shortest path in a graph
- multiply two matrices

$S$ the set of all possible solutions for $P$

- MergeSort
- QuickSort, etc.

Which of the available algorithms is best?

We shall rank algorithms according to how fast they run: their time complexity.
Lower Bounds

A harder question:

*Can we improve our existing algorithms, or have we already found the best possible algorithm for P?*

- Can improve $\Rightarrow$ go on looking
- Found best $\Rightarrow$ no need to waste time looking

We must reason about all possible members of $S$, not just the ones we know already.

- a minimum amount of work which every member of $S$ must do (e.g. inspect every element in a list)
- provides a lower bound on the time complexity of any algorithm for $P$.

Which Problems?

We examine *searching* and *sorting*:

1. Frequently used
   - efficiency is particularly important
2. Analysis is well worked out
   - **Optimal** (best possible) algorithms are known

Searching a list

$L$ a list of elements of type $D$

$L[0], \ldots, L[n-1]$ \hspace{1cm} ($n \geq 1$)

Random access $L[k]$

**Problem: Searching an unordered list $L$**

For $x : D$

- if $x$ in $L$ return $k$ such that $L[k] = x$
- if $x$ not in $L$ return “not found”

A particular algorithm:

**Linear Search**

Inspect $L[0], L[1], \ldots, L[n-1]$ in turn.

Stop and return index if $x$ found.

Otherwise return “not found”.

Analysis

How long does LS take?

Count the number of comparisons

$x = L[k]$

This is general:

will work for all algorithms for the problem

Number of comparisons varies.

With $n = 4$, $D = \mathbb{N}$, $x = 5$:

- $[5, 4, 3, 6]$ \hspace{1cm} 1 comparison
- $[3, 4, 6, 2]$ \hspace{1cm} 4 comparisons

With input size $n$ ranges between

1 best case

$n$ worst case

comparisons.
Worst and Average Case

**Worst case analysis**
\[ W(n) = \text{largest number of comparisons for input size } n \]

[Here \( W(n) = n \)]

**Average case analysis**
\[ A(n) = \text{average number of comparisons for input size } n \]

NB We need to know (or make a reasonable assumption about) the probability distribution:
- how likely is \( x \) to be in \( L \)?
- how likely is \( x = L[k] \)?

Which is better?

Average case might seem superior.
But worst case has two advantages:
1. Can guarantee on input size \( n \) that never takes longer than \( W(n) \)
2. \( W(n) \) is easier to compute than \( A(n) \) and often gives similar results
   (same order of complexity)

Best-case analysis is not a good idea:
   *can “tune up” a slow algorithm to look fast on particular inputs.*

Ordered Lists

**Problem**
Search an ordered list.

LS will solve this, but can do better.

**Modified LS**
Inspect \( L[0], L[1], \ldots \) as before.
Stop if find \( x \), or if \( L[k] > x \) (meaning that \( x \) not in \( L \)).

\[ W(n) = n \] still.
Expect that \( A(n) \) has improved.

LS is optimal

LS can be varied, but it cannot be improved.

- **LS is optimal** (in worst case)

Justification:
Take any \( A \) which solves the search problem.

**Claim:** If \( A \) returns “not found” then must have inspected every entry of \( L \).

**Proof:** Suppose for a contradiction that \( A \) did not inspect \( L[k] \).

\[ L : L[0] \ L[1] \ldots \ L[k] \ldots L[n-1] \]
\[ L' : L[0] \ L[1] \ldots x \ldots L[n-1] \]

On input \( L' \), \( A \) will return “not found”, which is wrong. **Contradiction**
Hence in worst case \( n \) comparisons are needed
   — **lower bound**
**Binary Search**

Decision tree for \( n = 8 \)

![Decision tree for n = 8](image)

Big improvement on MLS.
BS is **optimal**.
- Keeps the tree depth low for the same number of nodes.

**Modified Linear Search Tree**

MLS decision tree for \( n = 4 \)

![MLS decision tree for n = 4](image)

The decision tree represents the algorithm.

**Floor and Ceiling**

**Definition**
The floor of \( x \in \mathbb{R} \) is the greatest \( n \in \mathbb{Z} \) such that \( n \leq x \).

Notation \( \lfloor x \rfloor \)

For instance, \( \lfloor 23.18 \rfloor = 23, \lfloor \pi \rfloor = 3 \)

**Definition**
The ceiling of \( x \in \mathbb{R} \) is the least \( n \in \mathbb{Z} \) such that \( n \geq x \).

Notation \( \lceil x \rceil \)

For instance, \( \lceil 0.001 \rceil = 1 \).

**Worst-case analysis for Binary Search**

\[
W(1) = 1 \\
W(n) = 1 + W(\lfloor n/2 \rfloor)
\]

Each half has length \( \leq \lfloor n/2 \rfloor \).

Solve by repeated expansion:

\[
W(n) = 1 + W(\lfloor n/2 \rfloor) \\
= 1 + [1 + W(\lfloor n/4 \rfloor)] \\
= 1 + 1 + 1 + W(\lfloor n/8 \rfloor) \\
= 3 + W(\lfloor n/2^3 \rfloor) \\
= \cdots \\
= 1 + \cdots + 1 + W(1)
\]
**How many ones?**

Examples

\[ W(8) = 1 + 1 + 1 + W(1) \]

\[ W(9) = 1 + W(4) = 1 + 1 + W(2) = 1 + 1 + 1 + W(1) \]

Number of 1s is number of times divisible by 2.

\[ k \text{ where } 2^k \leq n < 2^{k+1} \]

\[ k = \lfloor \log n \rfloor - \log \text{ base } 2 \]

\[ W(n) = 1 + \lfloor \log n \rfloor \]

Can check this against depth of trees.

**Binary Search is Optimal**

We now show that Binary Search is optimal.

Represent any possible search algorithm A by a decision tree.

The tree must have \( n \) nodes at least.

The tree will be binary.

e.g.

```
          x>L[3]
          3
         / \   \
        2   5   \
   6   1   0
```

So it must have at least a certain depth.

**Depth vs. Nodes**

**Proposition**

*If a binary tree has depth \( d \), then it has \( \leq 2^{d+1} - 1 \) nodes.*

Proof by induction:

**Base case.** \( d = 0 \). \( 2^{0+1} - 1 = 1 \). Checked.

**Induction Step.** Assume true for \( d \).

Suppose tree has depth \( d + 1 \). Children have depth \( \leq d \), and \( \leq 2^{d+1} - 1 \) nodes (by inductive hypothesis).

Total number of nodes \( \leq 1 + (2^{d+1} - 1) + (2^{d+1} - 1) = 2^{(d+1)+1} - 1 \)
Minimality of Binary Search

The tree for algorithm A has $\geq n$ nodes.
If the depth is $d$ then

$$n \leq 2^{d+1} - 1 \quad (*)$$

The worst-case performance of A is $d + 1$.
From (*):

$$d + 1 \geq \log(n + 1)$$

In fact

$$d + 1 \geq \lceil \log(n + 1) \rceil$$

For Binary Search,

$$W(n) = 1 + \lceil \log n \rceil$$

We can show

$$\lceil \log(n + 1) \rceil = 1 + \lceil \log n \rceil$$
(see notes)

Orders

Suppose for some algorithm

$$W(n) = 8n^2 + 300n + 70$$

As $n$ gets large, $8n^2$ is the most important term.
If we ignore the constant, $W(n)$ is order $n^2$.
For a different algorithm

$$W'(n) = 2n^3 + n^2 + 4$$

This is order $n^3$.
So the first algorithm is of lower order:

- should be preferred for large $n$, even though possibly $W'(n) < W(n)$ for small $n$.

Constant Factors can be Ignored

When calculating worst-case complexity, it is often desirable to ignore constant factors.
Example: Matrix Multiplication

$$A \cdot B = C$$

$n \times n$ matrices

$$c_{ij} = \sum_{k=1}^{n} a_{ik}b_{kj}$$

This requires $n$ multiplications and $n - 1$ additions
($= 2n - 1$ operations)

$$W(n) = n^2(2n - 1)$$

But if just count multiplications

$$W(n) = n^3$$

However the orders are the same: $n^3$
A Hierarchy of Orders

Polynomial

\[ 1 \quad n \quad n^2 \quad n^3 \quad \ldots \]

Exponential

\[ 2^n \quad 3^n \quad 4^n \quad \ldots \]

We are also interested in logarithms.

E.g. for Binary Search

\[ W(n) \text{ is order } \log n \]

Definitions

\[ \mathbb{R}^+ = \{ x \in \mathbb{R} : x \geq 0 \} \]

Let \( f, g : \mathbb{N} \to \mathbb{R}^+ \)

1. \( f \) is \( O(g) \) iff \( \exists m \in \mathbb{N} \exists c \in \mathbb{R}^+ \) such that \( \forall n \geq m f(n) \leq c \cdot g(n) \)

2. \( f \) is \( \Theta(g) \) iff \( f \) is \( O(g) \) and \( g \) is \( O(f) \).

Example

We know that \( 8n^2 + 300n + 70 \) is \( \Theta(n^2) \).

We prove this just to illustrate the definition.

Clearly \( n^2 \) is \( O(8n^2 + 300n + 70) \).

We need to find \( m \in \mathbb{N}, c \in \mathbb{R}^+ \) such that

\[ 8n^2 + 300n + 70 \leq cn^2 \]

(all \( n \geq m \))

Guess \( c = 9 \):

\[ 9n^2 - (8n^2 + 300n + 70) = n^2 - 300n - 70 \]

This is \( \geq 0 \) for \( n \) sufficiently large

\[ m = 1000 \]

So \( 8n^2 + 300n + 70 \) is \( O(n^2) \).

Order as an Upper Bound

Sometime the exact order is unknown.

Matrix Multiplication

We have seen an \( \Theta(n^3) \) algorithm.

But since there may be a faster algorithm, we say that the problem of matrix multiplication is \( O(n^3) \).

\- A lower bound of \( \Theta(n^2) \) is known.
\- Strassen 1969: \( O(n^{\log_27}) = O(n^{2.807}) \)
\- Coppersmith-Winograd 1987: \( O(n^{2.376}) \)
\- Stothers 2010: \( O(n^{2.373}) \)
\- Williams 2012: \( O(n^{2.3729}) \)
\- Le Gall 2014: \( O(n^{2.3728639}) \)
**Exercise**

List the following from lowest to highest order, indicating any which have the same order:

- \( n^3/2 \)
- \( \log n \)
- \( 2^n \)
- \( n^2 - n^3 + n^5/2 \)
- \( \log(n^2) \)
- \( 2^{n-1} \)
- \( n/5 \)
- \( 6n + \log n \)
- \( 2^{\sqrt{n}} \)

**Strassen’s Algorithm**

Assume we are multiplying two \( n \times n \) matrices:

\[
AB = C
\]

Start with \( n = 2 \).

Then

\[
C = \begin{pmatrix}
    a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\
    a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22}
\end{pmatrix}
\]

This takes 8 multiplications (and 4 additions).

Suppose that \( n = 2^h \).

Divide up matrices into four quadrants each \( n/2 \times n/2 \):

\[
\begin{pmatrix}
    A_{11} & A_{12} \\
    A_{21} & A_{22}
\end{pmatrix}
\begin{pmatrix}
    B_{11} & B_{12} \\
    B_{21} & B_{22}
\end{pmatrix} =
\begin{pmatrix}
    C_{11} & C_{12} \\
    C_{21} & C_{22}
\end{pmatrix}
\]

Compute \( C_{ij} \) using the formulas for \( c_{ij} \).

Recursively compute each multiplication by further subdivision until bottom out at \( n = 2 \).
**Strassen’s Algorithm**

Need to add/subtract 18 matrices of dimension $n/2 \times n/2$. Recursively perform 7 multiplications of $n/2 \times n/2$ matrices.

Number of arithmetic operations $A(k)$ for $n = 2^k$:

- $A(0) = 1$
- $A(k) = 7A(k - 1) + 18(n/2)^2$

Can solve by repeated expansion and then summing the resulting geometric progression.

Solution:

$$A(k) = 7.7^k - 6.4^k = 7.7^{\log n} - 6n^2 = 7n^{\log 7} - 6n^2 \approx 7n^{2.807} - 6n^2$$

So Strassen’s matrix multiplication is $\Theta(n^{2.807})$.

What if $n \neq 2^k$?

Can add extra row and column to keep the dimension even to allow subdivision.

**Divide and Conquer Algorithms**

Strassen’s algorithm is an example of a divide and conquer algorithm.

- Divide problem into $a$ subproblems of size $n/b$ (here $a = 7$ and $b = 2$):
  - May take work to set up the subproblems (here matrix addition).
- Solve each subproblem recursively.
- Then combine to get the result.
  - Again, this may take work (here matrix addition).

We shall see further examples: MergeSort, QuickSort.

**Sorting**

1. Measure time complexity of sorting algorithms.
2. Obtain lower bounds for the amount of work required.

**Techniques**

1. Recurrence relations
2. Decision trees
3. Finding orders of functions

**Insertion Sort**

1. Measure time complexity of sorting algorithms.
2. Obtain lower bounds for the amount of work required.

Insert $L[i]$ into $L[0..i-1]$ in correct position.

Then $L[0..i]$ is sorted.

Insertion performed by letting $L[i]$ filter downwards by successive swaps.

This takes between 1 and $i$ comparisons.

- worst case when $L[i]$ below $L[0]$

Perform insertion for $i = 1$ to $n - 1$:

$$W(n) = \sum_{i=1}^{n-1} i$$
**Solution**

**Fact**

\[ \sum_{i=1}^{n} i = \frac{n(n + 1)}{2} \]

Hence

\[ W(n) = \frac{n(n - 1)}{2} \]

The worst case actually arises when the list is in reverse order.

\[ W(n) \text{ is } \Theta(n^2). \]

We wish to see if this can be improved upon.

**Example: Algorithm 3-Sort**

Sorts a list of length 3.

Simply given by a decision tree.

Each leaf is a possible permutation of \( L \).

Worst-case number of comparisons is 3.

**Lower Bounds**

Idea: express sorting algorithm as decision tree.

The internal nodes are the comparisons.

The leaves are the results (the rearranged lists).

We then argue that to have a certain number of leaves, the tree must have sufficient depth.

Depth = worst-case number of comparisons

**Exercise**

Find a decision tree for Insertion Sort on \( n = 3 \).
Optimality for \( n = 3 \)

Any decision tree for sorting a list of length 3 must have \( 3! = 6 \) leaves.
Cannot have depth \( \leq 2 \), as all binary trees of depth \( \leq 2 \) have \( \leq 4 \) leaves.
So depth at least 3.
Worst-case number of comparisons at least 3.
Hence 3-Sort (and Insertion Sort) are optimal for \( n = 3 \).

General Case

Sorting a list of length \( n \).
There are \( n! \) permutations.
So the decision tree must have \( n! \) leaves (at least).
How deep must a binary tree be to have \( n! \) leaves?
e.g. \( n = 4? \)

Bound on Leaves

**Proposition**

*If a binary tree has depth \( d \) then it has \( \leq 2^d \) leaves.*

Proof: By induction on \( d \).
\( d = 0 \): \( 2^0 = 1 \). Checked.
Assume if depth \( d \) then \( \leq 2^d \) leaves.
Consider a tree of depth \( d + 1 \):

Subtrees have depth \( \leq d \) and so \( \leq 2^d \) leaves.
So tree of depth \( d + 1 \) has \( \leq 2^d + 2^d = 2^{d+1} \) leaves.

Lower Bound for Sorting

Decision tree has \( \geq n! \) leaves and depth \( d \).
So
\[
2^d \geq n!
\]
\[
d \geq \log(n!)
\]
\[
d \geq \lceil \log(n!) \rceil
\]

**Lower bound for sorting in worst case**

Any algorithm for sorting by comparisons must perform at least
\[
\lceil \log(n!) \rceil
\]
comparisons in worst case.
How Good is Insertion Sort?

We compare the lower bound \(\lceil \log(n!) \rceil\) with \(W(n)\) for Insertion Sort.

<table>
<thead>
<tr>
<th>(n)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\lceil \log(n!) \rceil)</td>
<td>0</td>
<td>1</td>
<td>3</td>
<td>5</td>
<td>7</td>
<td>10</td>
<td>13</td>
<td>16</td>
<td>19</td>
<td>22</td>
<td>26</td>
<td>29</td>
</tr>
<tr>
<td>(\frac{n(n-1)}{2})</td>
<td>0</td>
<td>1</td>
<td>3</td>
<td>6</td>
<td>10</td>
<td>15</td>
<td>21</td>
<td>28</td>
<td>36</td>
<td>45</td>
<td>55</td>
<td>66</td>
</tr>
</tbody>
</table>

Average Case

Example: 3-Sort.

Total Path Length

Consider this tree:

6 leaves.
Depths are \(2, 2, 3, 4, 4, 2\)
Average depth
\[\frac{1}{6}(2 + 2 + 3 + 4 + 4 + 2)\]

Definition
The total path length of a tree is the sum of the depths of all leaf nodes.

Minimising Total Path Length

Suppose \(T\) is a decision tree for sorting a list of length \(n\).
Suppose \(T\) has \(n!\) leaves and total path length \(b\).
Then average number of comparisons is
\[\frac{b}{n!}\]
Given a fixed number of leaves (\(n!\)) we want to find a lower bound on the total path length.
It turns out that the total path length is lowest when leaves are at roughly equal depth.
Balanced Trees

**Definition**
A tree of depth $d$ is balanced if every leaf is at depth $d$ or $d - 1$.

**Proposition**
If a tree is unbalanced then we can find a balanced tree with the same number of leaves without increasing the total path length.

Has the total path length reduced?

---

Lower Bound for Average Case

So when looking for a lower bound on total path length, we can just consider balanced trees. But in a balanced tree of depth $d$, average is between $d$ and $d - 1$. Hence:

**Lower bound for average case**
Any algorithm for sorting a list of length $n$ must perform at least $\lceil \log(n!) \rceil$ comparisons in average case.

---

Room for Improvement

We have a lower bound on the number of comparisons needed in worst/average case to sort a list of length $n$.

- e.g. for $n = 10$ require:
  - worst case 22
  - average case 21.84

A good sorting algorithm will use not much more than this number. Insertion Sort is poor, since it uses 45 comparisons in worst case. So we look for a better sorting algorithm.

---

MergeSort

1. Divide roughly into two.
2. Sort each half separately (by recursion)
3. Merge the two halves.

We need to know how many comparisons must be done to merge the two halves.

**The merging will be done by comparing the current least elements of the lists, and outputting the smaller.**
Examples

How many comparisons?

1. $L_1 : [2, 3, 5, 7]$ with $L_2 : [4, 6, 9, 11]$
2. $L_3 : [2, 4, 6, 8]$ with $L_4 : [3, 5, 7, 9]$

Worst-Case Analysis

Adding an element to the merged list takes one comparison until one of the lists is exhausted.

In the worst case, only the last element is transferred “for free”. So worst case is $n - 1$ comparisons.

$x \geq 1$

$\frac{n}{2}$

$\frac{n}{2}$

$W(1) = 0$

$W(n) = n - 1 + W\left(\left\lceil \frac{n}{2} \right\rceil \right) + W\left(\left\lfloor \frac{n}{2} \right\rfloor \right)$

MergeSort Performs Well

We compare the lower bound $\lceil \log(n!) \rceil$ with $W(n)$ for MergeSort.

<table>
<thead>
<tr>
<th>$n$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
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<td>16</td>
<td>19</td>
<td>22</td>
<td>26</td>
<td>29</td>
</tr>
<tr>
<td>$W(n)$</td>
<td>0</td>
<td>1</td>
<td>3</td>
<td>5</td>
<td>8</td>
<td>11</td>
<td>14</td>
<td>17</td>
<td>21</td>
<td>25</td>
<td>29</td>
<td>33</td>
</tr>
</tbody>
</table>

Does MergeSort remain close to optimal as $n$ gets large?

Solving the Recurrence Relation

$W(1) = 0$

$W(n) = n - 1 + W\left(\left\lceil \frac{n}{2} \right\rceil \right) + W\left(\left\lfloor \frac{n}{2} \right\rfloor \right)$

Assume $n = 2^k$.

$W(n) = n - 1 + 2W(n/2)$

Use repeated expansion.

$W(n) = kn - n + 1$

This is $\Theta(n \log n)$.

How does $n \log(n) - n + 1$ compare with $\lceil \log(n!) \rceil$?
Recurrence relations

Worst case comparisons for Binary Search:

\[ W(1) = 1 \]
\[ W(n) = W(n/2) + 1 \]

Worst case comparisons for MergeSort:

\[ W(1) = 0 \]
\[ W(n) = 2W(n/2) + (n - 1) \]

Number of arithmetic operations for Strassen’s Algorithm:

\[ A(1) = 1 \]
\[ A(n) = 7A(n/2) + 18(n/2)^2 \]

All examples of Divide and Conquer algorithms.

Divide and Conquer

General form for Divide and Conquer

Work \( T(n) \) for input size \( n \)

Split into \( a \) sub-problems of size \( n/b \).

Non-recursive work (split and combine) is \( f(n) \).

\[ T(n) = aT(n/b) + f(n) \]

(plus base cases)

We shall show how to solve such a recurrence relation up to \( \Theta \).
Recursion Trees

Example:

\[ T(1) = 1 \]
\[ T(n) = aT(n/2) + n \]

(like MergeSort if \( a = 2 \))

Create a recursion tree:

• Start with input of size \( n \)
• Each unfolding of the recursion takes us down one level to a subproblem with size halved
• Each node of the tree records size and non-recursive work done

Suppose \( n = 2^k \).

\[ n + a(n/2) + a^2(n/2^2) + \cdots + a^{k-1}n/(2^{k-1}) + a^k = n + (a/2)n + (a/2)^2n + \cdots + (a/2)^{k-1}n + a^k \]

Geometric series.

Geometric Series

Proposition

\[ \sum_{i=0}^{k} ar^i = \frac{a(r^{k+1} - 1)}{r - 1} \]

provided \( r \neq 1 \).

Clearly sum is \( (k+1)a \) if \( r = 1 \).

Corollary

Let \( t(n) \) be the largest term in the geometric progression

\[ a, ar, ar^2, \ldots, ar^k \]

where \( r \) is non-negative, \( r \neq 1 \) and \( r \) does not depend on \( n \) (though \( a \) and \( k \) can depend on \( n \)). Then

\[ \sum_{i=0}^{k} ar^i = \Theta(t(n)) \]

Three cases

Apply Corollary to

\[ n + (a/2)n + (a/2)^2n + \cdots + (a/2)^{k-1}n + a^k \]

Here \( r = a/2 \).

• If \( a < 2 \) greatest term is \( n \).

\[ T(n) = \Theta(n) \]

Non-recursive work at level 0 dominates.

• If \( a = 2 \) then

\[ T(n) = (k+1)n = \Theta(n \log n) \]

Work is (roughly) evenly spread at all levels. (cf. MergeSort)

• If \( a > 2 \) greatest term is \( a^k = a^{\log n} = n^{\log a} \).

\[ T(n) = \Theta(n^{\log a}) \]

Base cases (leaves of recursion tree) dominate.

Three cases depending on \( a \).
Towards the general case

$$T(n) = aT(n/b) + f(n)$$

(plus base cases) Recursion tree will have $1 + \log_b n$ levels.

- **Level 0**: work $f(n)$
- **Level 1**: work $af(n/b)$
- **Level 2**: work $a^2f(n/b^2)$
  
  $\vdots$
  
  - **Level $\log_b n$**: work $\Theta(a^{\log_b n})$

For the bottom level we just need to know the number of leaves, as the work for each is constant.

Suppose that $f(n) = n^c$.

Then ratio $r = a/b^c$.

Let the critical exponent be $E = \log_b a = \log a / \log b$.

Then $r > 1$ iff $a > b^c$ iff $\log_b a > c$ iff $E > c$.

Three cases

- **$E < c$**:
  
  $$T(n) = \Theta(f(n))$$

- **$E = c$**:
  
  $$T(n) = \Theta(f(n) \log_b n) = \Theta(f(n) \log n)$$

- **$E > c$**:
  
  $$T(n) = \Theta(a^{\log_b n}) = \Theta(n^{\log_b a}) = \Theta(n^E)$$

Master Theorem

$$T(n) = aT(n/b) + f(n)$$

has solutions as follows, where $E = \log_b a / \log b$ is the critical exponent:

1. If $n^{E+\epsilon} = O(f(n))$ for some $\epsilon > 0$ then $T(n) = \Theta(f(n))$.
2. If $f(n) = \Theta(n^E)$ then $T(n) = \Theta(f(n) \log n)$.
3. If $f(n) = O(n^{E-\epsilon})$ for some $\epsilon > 0$ then $T(n) = \Theta(n^E)$. 
Examples

Worst case comparisons for Binary Search:

\[ W(n) = W(n/2) + 1 \]

Here \( a = 1 \) and \( b = 2 \) and \( f(n) = \Theta(n^0) \).

Then \( E = \log a / \log b = 0 \). So

\[ W(n) = \Theta(n^0 \log n) = \Theta(\log n) \]

Worst case comparisons for MergeSort:

\[ W(n) = 2W(n/2) + (n - 1) \]

Here \( a = 2 \) and \( b = 2 \) and \( f(n) = \Theta(n^1) \).

Then \( E = \log a / \log b = 1 \). So

\[ W(n) = \Theta(n \log n) \]

Number of arithmetic operations for Strassen’s Algorithm:

\[ A(n) = 7A(n/2) + 18(n/2)^2 \]

Here \( a = 7 \) and \( b = 2 \), \( f(n) = \Theta(n^2) \).

Then \( E = \log a / \log b = \log 7 > 2 \). So

\[ A(n) = \Theta(n^{\log 7}) \]

Note that any improvement to \( f(n) \) here will not help with the order of \( A(n) \).

QuickSort

Split the list around the first element.
e.g.

\[ L = [7, 2, 10, 12, 3, 1, 8] \]

Split around 7.
Get

\[ [3, 2, 1, 7, 12, 8, 10] \]

Now sort the two sides recursively.
The list is then sorted:

\[ [1, 2, 3, 7, 8, 10, 12] \]

• Clearly split takes \( n - 1 \) comparisons.

QuickSort may well not split \( L \) evenly.

Split

Algorithm Split(left,right):

\# pre-condition: left < right
\n\[ d = L[left] \] # pivot
\n\[ i = left + 1; j = right \]
\n\# Invariant:
\n\# left < i ≤ j + 1
\n\# j ≤ right
\n\# if left < k < i then L[k] ≤ d
\n\# if j < k ≤ right then L[k] > d
\n\# while i ≤ j:
\n\# if L[i] ≤ d:
\n\# \quad i = i + 1
\n\# else:
\n\# \quad Swap(i,j); j = j - 1
\n\# \quad i = j + 1
\n\# Swap(left,j)
\nreturn j
Worst Case Analysis

Suppose \( L \) was \([1, 7, 2, 10, 12, 3, 8]\).
Split around 1.
The list becomes \([1, 2, 10, 12, 3, 8, 7]\).
Must then sort \([2, 10, 12, 3, 8, 7]\).
A particularly bad case is when \( L \) is already sorted, e.g. \([1, 2, 3, 7, 8, 10, 12]\).
This is in fact the worst case.

\[
W(1) = 0 \\
W(n) = n - 1 + W(n-1)
\]

So

\[
W(n) = 1 + 2 + \cdots + (n-1) = \frac{n(n-1)}{2}
\]

No better than Insertion Sort.

Analysis

After splitting, the “split position” can be anywhere from 1 to \( n \).

Then call QuickSort on lists of length \( s - 1 \) and \( n - s \),
taking \( A(s - 1) + A(n - s) \) comparisons.

\[
A(n) = n - 1 + \frac{1}{n} \sum_{s=1}^{n} (A(s - 1) + A(n - s))
\]

(assuming each position equally likely)

Average Case

But QuickSort is good in practice.
This is because the split is unlikely to occur at one end.
The average number of comparisons \( A(n) \) is of lower order than \( W(n) \).
We calculate \( A(n) \).

\[
A(n) = n - 1 + \frac{1}{n} \sum_{s=1}^{n} (A(s - 1) + A(n - s))
\]

After simplifying:

\[
A(1) = 0 \\
A(n) = n - 1 + \frac{2}{n} \sum_{i=2}^{n-1} A(i)
\]

Fact

\( A(n) \) is \( \Theta(n \log n) \).
**Performance**

QuickSort gives good performance in average case.

- \( n = 10 \):
  - Average case lower bound 21.84
  - \( A(n) \) for QuickSort 24.44

For comparison:

- Worst case lower bound 22
- \( W(n) \) for MergeSort 25

It might seem that MergeSort is better than QuickSort. However:

- Can improve chances of a good split.
- QuickSort uses less space
  (merging requires extra space).

**Heapsort**

We now discuss Heapsort.

A **heap structure** is a left-complete binary tree.

Left-complete means that if the tree has depth \( d \) then

- all nodes are present at depth \( 0, 1, \ldots, d - 1 \)
- and at depth \( d \) no node is missing to the left of a node which is present.

Call the rightmost node at depth \( d \) the **last** node.

**Min Heap**

- A tree \( T \) is a **minimising partial order tree** if the key at any node \( \leq \) the keys at each child node (if any).
- A **min heap** is a heap structure with the min partial order tree property.

Note that for any node of a heap, the left and right subtrees below the node are also heaps.

**Max Heap**

- A tree \( T \) is a **maximising partial order tree** if the key at any node \( \geq \) the keys at each child node (if any).
- A **max heap** is a heap structure with the max partial order tree property.
Heapsort

**Heapsort scheme**
Build max heap $H$ out of an array $E$ of elements
for $i = n$ to 1:
  - max = getMax($H$)
  - deleteMax($H$)
  - $E[i] = \text{max}$

getMax($H$) - just read the root node of $H$

**deleteMax($H$) scheme**
- copy element at last node into root node
- remove last node
- fixMaxHeap($H$)

We use fixMaxHeap($H$) to restore the heap property.

Building a heap

Starting from a heap structure $H$ that does not necessarily have the partial order property, build a heap.

**buildMaxHeap($H$) scheme**
- if $H$ not a leaf:
  - buildMaxHeap(left subtree of $H$)
  - buildMaxHeap(right subtree of $H$)
  - fixMaxHeap($H$)

Divide and conquer algorithm.

FixMaxHeap

Starting from a heap structure $H$ where the left and right subtrees of the root are heaps, make $H$ into a heap (again).

**fixMaxHeap($H$) scheme**
- if $H$ not a leaf:
  - largerSubHeap = the left or right subheap with the larger root
  - if root($H$).key < root(largerSubHeap).key:
    - swap elements at root($H$) and root(largerSubHeap)
    - fixMaxHeap(largerSubHeap)

If the heap has depth $d$ we see that fixMaxHeap takes at most $2d$ comparisons.

Since a heap with $n$ elements has depth $\lfloor \log n \rfloor$, fixMaxHeap takes $O(\log n)$ comparisons.

Analysis of buildMaxHeap

Suppose for simplicity $n = 2^k - 1$ so that the heap structure is a complete binary tree with depth $k - 1$.

Let $W(n)$ be the worst-case number of comparisons for buildMaxHeap.

$$W(n) = 2W((n - 1)/2) + 2 \log n$$

Apply Master Theorem with $a = 2$, $b = 2$ and $f(n) = 2 \log n$.

Critical exponent $E = 1$, and so

$$W(n) = \Theta(n^E) = \Theta(n)$$

So can build the heap in linear time.
Analysis of Heapsort

Heapsort scheme
Build max heap \( H \) out of an array \( E \) of elements \( O(n) \)
for \( i = 1 \) to \( n \):
- \( \text{max} = \text{getMax}(H) \) \( O(1) \)
- \( \text{deleteMax}(H) \) \( O(\log n) \)
- \( E[i] = \text{max} \)

Overall \( O(n \log n) \) comparisons.

Heaps as arrays
We can implement heaps using arrays.
Store the heap level by level in an array starting at index 1.
Left and right children of node \( i \) are at \( 2i \) and \( 2i + 1 \).
Parent node is at \( \lfloor i/2 \rfloor \).
No need for pointers.
It turns out that Heapsort can be carried out entirely in place (like Quicksort).

Algorithm Heapsort(\( E, n \))
- \# perform Heapsort on elements 1..\( n \) of an array \( E \) of elements
- BuildMaxHeap(\( n \))
- \( \text{heapsize} = n \)
- \# Invariant:
- \# max heap in \( E[1..\text{heapsize}] \) of first \( \text{heapsize} \)-many elements
- \# of sorted list
- \# elements in \( \text{heapsize} + 1 \) to \( n \) are correctly sorted
- while \( \text{heapsize} > 1 \):
  - swap(1,\( \text{heapsize} \))
  - \( \text{heapsize} = \text{heapsize} - 1 \)
  - fixMaxHeap(1,\( \text{heapsize} \))
Heaps as arrays

**Algorithm fixMaxHeap(root, heapsize)**

```plaintext
left = 2*root
right = 2*root + 1
if left ≤ heapsize:
    # root is not a leaf
    if left = heapsize:
        # no right subheap
        largerSubHeap = left
    elif E[left].key > E[right].key:
        # favours right subheap if equal
        largerSubHeap = left
    else:
        largerSubHeap = right
    if E[root].key < E[largerSubHeap].key:
        swap(root, largerSubHeap)
    fixMaxHeap(largerSubHeap, heapsize)
```

Heaps and priority queues

Priority queues can be implemented as binary heaps.

Min PQ as used for Prim's algorithm:

- Each item \( x \) of the queue has a priority \( \text{key}[x] \)
- Items removed lowest key first.

Operations:

- \( Q = \text{PQcreate()} \)
- \( \text{isEmpty}(Q) \)
- \( \text{insert}(Q, x) \)
- \( \text{getMin}(Q) \)
- \( \text{deleteMin}(Q) \)
- \( \text{decreaseKey}(Q, x, \text{newkey}) \) — updates \( \text{key}[x] = \text{newkey} \)

Plainly we should use a min binary heap.

Insert

**insert(Q, x)**

```plaintext
heapsize = heapsize + 1
E[heapsize] = x
# allow x to percolate towards the root until heap property is restored
percolateup(heapsize)
```

**procedure percolateup(c):**

```plaintext
if c > 1:
    parent = ⌊c/2⌋
    if E[c].key < E[parent].key:
        swap(c, parent)
    percolateup(parent)
```

Time \( O(\log n) \).

It may be possible to build the queue in one go (time \( O(n) \)) rather than inserting elements individually (time \( O(n \log n) \).
**Decrease Key**

```plaintext
decreaseKey(Q, x, newkey)
If we know the location c of x in the heap then we can change its key to newkey and use percolateup(c) to restore the heap.
The problem is to locate x efficiently – time $O(\log n)$ rather than $O(n)$.
Solution:
Suppose that each element has an identifier id.
Suppose that identifiers are integers in a compact range [1..maxid]
Use a supplementary array xref to store the location of id:
xref[id] = k means that element is at location k in heap.
Need to add code to percolateup to keep xref up to date as swaps occur.
```

**Dynamic Programming**

We have seen several examples of dynamic programming.
We now consider an example to illustrate:
- top-down versus bottom-up solutions
- memoisation

---

**Word break problem**

As an example consider the following problem:
Given a string of characters s, can s be split into words occurring in a dictionary?
Example: s = ‘windown’ can be split as ‘win down’ (or ‘wind own’)
But ‘trcarlenz’ cannot be split into (English) words.
Looking at all possible splits would take too long—exponentially many.

**Recursive solution**

‘top down’

```plaintext
procedure wb1(s)
if len(s) == 0:
  return true
else:
  for i = 0 to len(s) – 1:
    if indict(s[i :]):
      if wb1(s[i:]):
        return true
  return false
```

indict checks if a string is a word in the dictionary.
Slice notation:
- $s[i : j]$ string s from index i to index $j – 1$
- $s[: i]$ string s from start index 0 to index $i – 1$
- $s[i :]$ string s from index $i$ to the end index len(s) – 1
**Recursive solution**

Recurrence relation for worst case on strings of length $n$:

\[
W_0 = 0 \\
W_i(n) = n + W_0 + \cdots + W_i(n-1) \quad (n \geq 1)
\]

Solution

\[W_1(n) = 2^n - 1\]

Exponential!

Inefficiency from computing $wb(s[i:])$ repeatedly.

**Memoised recursive solution**

Use memo to store previously computed results of recursive calls.

```
memo = {} # empty associative array

procedure wb2(s)
    if len(s) == 0:
        return true
    else:
        for i = 0 to len(s) - 1:
            if indict(s[i:]):
                if memo[s[i:]] undefined:
                    memo[s[i:]] = wb2(s[i:])
                if memo[s[i:]]:
                    return true
        return false
```

Note that the transformation is generic.

**Recursion tree**

Recursion tree now cut off at depth two (red nodes removed).

```
Worst case on strings of length $n$:
\[
\sum_{i=0}^{n-1} i = n(n+1)/2
\]

Complexity is $O(n^2)$.
```
Non-recursive solution

‘bottom up’
Idea: solve increasing sub-problems culminating in main problem:

\[s[:0], s[:1], \ldots, s[:n] = s\]

Note that these problems overlap.
Store result for \(s[:i]\) in array \(wb[i]\).

Non-recursive solution

Algorithm \(wb_3(s)\)

\[
\begin{align*}
\text{n} &= \text{len}(s) \\
\text{wb}[0] &= \text{true} \\
\text{if} \ \text{n} > 0: \\
\text{for} \ i = 1 \ \text{to} \ n: \\
&\quad \text{wb}[i] = \text{false} \\
&\quad \text{for} \ j = 0 \ \text{to} \ i - 1: \\
&\quad \quad \text{if} \ \text{wb}[j] \ \text{and} \ \text{indict}(s[j:i]): \\
&\quad \quad \quad \text{wb}[i] = \text{true} \\
&\quad \quad \text{break} \\
\text{return} \ \text{wb}[n]
\end{align*}
\]

Complexity is again \(O(n^2)\).

Comparison

Which is better?
Top-down with memoisation:
- perhaps easier to develop
- may be faster if not all subproblems need computing

Bottom-up non-recursive
- avoids overheads due to recursion

Discussion

Dynamic programming typically involves taking a problem with exponentially large solution space and finding a path to a solution in polynomial time.

Find whether a solution exists (Hamiltonian Circuit, Word Break) or (very often) find best solution (TSP).

Overlapping subproblems (contrast with divide and conquer)
Storing the results of computations of subproblems

Here ‘programming’ means planning a suitable order/plan of computation.
In many cases the subproblems to consider will depend on the previously obtained results (hence ‘dynamic’).
Part IV

Introduction to Complexity

Overview

Tractable problems and P

NP

Problem reduction

NP-completeness

Outline

Tractable problems and P

NP

Problem reduction

NP-completeness

Tractability

We wish to identify which problems are tractable (aka feasible)

• efficiently computable, i.e. can be computed in a reasonable amount of time

We focus on worst-case:
We want $W(n)$ to be not too large, where $n$ is the input size.

Sorting a list by comparisons

We have seen $W(n) = n \log n$ comparisons where $n$ is the length of the list (MergeSort).

We can agree that sorting is tractable, since comparing two elements in a list can be done easily.
Euler path

**Problem EulerPath**
Given a graph $G$, does $G$ have a Euler path?

Suppose $G$ has $n$ nodes and $m$ arcs. Input size $|G|$ depends on the representation of $G$:
- adjacency matrix has size $O(n^2)$
- linked list has size $O(n + m)$

$G$ has Euler path iff $G$ has 0 or 2 nodes of odd degree.
This is tractable, since we can count the odd degree nodes by making a single pass through either representation, keeping track of the degree count for the current node and the number of odd degree nodes found so far.

Hamiltonian path

By contrast:

**Problem HamPath**
Given a graph $G$, does $G$ have a Hamiltonian path?

To see whether a graph with $n$ nodes has a Ham path seems to require $O(n/2^n)$ time - this takes too long.

Decision problems

Decision problems are those which have a yes/no answer, e.g. EulerPath, HamPath.

**Definition**
- A decision problem $D$ is decided by an algorithm $A$ if for any input $x$, $A$ returns 'yes' or 'no' depending on whether $D(x)$ (and in particular $A$ always terminates).
- A decision problem $D$ is decidable in polynomial time iff it is decided by some algorithm $A$ which runs within polynomial time, i.e. on all inputs of size $n$, $A$ takes $\leq p(n)$ steps for some $p(n)$.

We abbreviate polynomial time to poly time or p-time.

E.g. EulerPath is decidable in p-time, but HamPath (apparently) not.

Note: We use $D$ rather than $P$ to range over decision problems as $P$ will be the class of polynomial-time problems.

Tractability

**Cook-Karp Thesis**
A problem is tractable iff it can be computed within polynomially many steps in worst case ($W(n) \leq p(n)$ for some polynomial $p(n)$).

More succinctly

**Slogan**
Tractable = polynomial time.

According to the thesis, sorting a list is tractable, as is EulerPath, but HamPath is (apparently) not.
Different models
We have been talking about $p(n)$ steps in a computation on input size $n$. Clearly

- input size
- computation step

have different meanings depending on the model we are using.

- For sorting a list, we took input size to be the number of list items, and we counted comparisons, ignoring other computation steps (swaps, copying, recursive procedure calls, etc.).
- For EulerPath we measured input size either using adjacency matrices or adjacency lists, and computation steps would involve inspecting the input and incrementing counters.

However it turns out that all reasonable models of computation and measures of input size give essentially the same results.

Polynomial Invariance Thesis
If a problem can be solved in polynomial time $p(n)$ in some model, then if we change the model the problem can still be solved in p-time $q(n)$.

We may get a different polynomial, but the concept of p-time is robust.

Polynomial invariance thesis
If a problem can be solved in p-time in some reasonable model of computation, then it can be solved in p-time in any other reasonable model of computation.

Thus for sorting a list, a different model would be to take the sizes of the items to be sorted into account in measuring input length, and to take into account the fact that comparisons can take different amounts of time depending on the sizes of the items and the length of the list.

We would still get p-many steps but not necessarily $O(n \log n)$.

P and reasonable models
Definition
A decision problem $D(x)$ is in the complexity class $P$ (polynomial time) if it can be decided within time $p(n)$ in some reasonable model of computation, where $n$ is the input size $|x|$.

By the Invariance Thesis this definition is model-independent.

Note that sorting a list does not belong to the class $P$, since it is not a decision problem.

It is technically convenient to define complexity classes for decision problems only, at least to start with.

What models would be unreasonable?

Unreasonable models
- Superpolynomial parallelism is unreasonable. If we could carry out more than polynomially many operations in parallel in a single step, then we might be able to solve exponential time problems in p-time. So this model is unreasonable.
- Unary numbers (writing $\text{one.osf/one.osf/one.osf/one.osf/one.osf}$ for $\text{five.osf}$) are unreasonable. When dealing with numbers we do not allow unary representation (use base 2 or greater). This is because unary gives input size which is exponentially larger than binary, and so an exponential time algorithm can appear to be p-time.

Example
With unary we can check whether a number $n$ is prime by looking at all $m < n$ and seeing whether $m$ divides $n$. This takes $n$ divisions. This is p-time if input size is $n$.

However the true input size $|n|$ is actually $\log n$ and so we have an exp-time algorithm.
Arithmetical operations

Arithmetical operations (addition, subtraction, multiplication, division) are p-time
i.e. they are polynomial in $|n| = \log n$ rather than in $n$.

**Function Composition**

The next result shows that poly time is well-behaved.
It will be useful when discussing reduction and NP-completeness.

**Proposition**
Suppose that $f$ and $g$ are functions which are p-time computable. Then the composition $g \circ f$ is also p-time computable.

Suppose

- $f(x)$ is computed by algorithm $A$ within time $p(n)$ where $n = |x|$
- $g(y)$ is computed by algorithm $B$ within time $q(m)$ where $m = |y|$

**Function Composition (continued)**

Take input $x$ with $|x| = n$.

We compute $g(f(x))$ by first running $A$ on $x$ to get $f(x)$ and then running $B$ on $f(x)$ to get $g(f(x))$.

Running $A$ on $x$ takes $\leq p(n)$ steps.

To see how long running $B$ takes we need a bound on the size of the input $f(x)$.

But $A$ runs for $\leq p(n)$ steps to build $f(x)$. So $|f(x)|$ must be poly bounded in $n$ - there is no time to build a larger output.

Say $|f(x)| \leq p'(n)$ for some polynomial $p'(n)$.

Then $B$ runs within $q(p'(n))$ steps.

Total running time (A followed by B) is $p(n) + q(p'(n))$.

This is polynomial in $n$. Hence result.
**Outline**

Tractable problems and \( P \)

**NP**

Problem reduction

NP-completeness

---

**Guessing a certificate**

Consider the HamPath problem. Given a graph \( G \), if we guess a list \( \pi \) then it is easy to check whether \( \pi \) is a Ham path of \( G \).

- check that the items of \( \pi \) are a permutation of \( \text{nodes}(G) \);
- check that successive nodes of \( \pi \) are adjacent in \( G \).

It is pretty clear that these checks can be carried out in \( p \)-time. Thus HamPath becomes easy (\( p \)-time) if we guess the path.

The Ham path \( \pi \) acts as a certificate that \( \text{HamPath}(G) \).

Of course if we guess \( \pi \) and we discover that \( \pi \) is not a Ham path of \( G \), then we are none the wiser, since it might be that \( G \) has a (different) Ham path, or that \( G \) has no Ham path.

Nevertheless, it remains the case that if \( G \) has a Ham path then some guess will prove correct.

---

**Problem** Ver-HamPath

Given a graph \( G \) and a list \( \pi \), is \( \pi \) a Ham path of \( G \)?

Note that the verification problem \( \text{Ver-HamPath}(G, \pi) \) is in \( P \).

Clearly \( \text{HamPath}(G) \iff \exists \pi. \text{Ver-HamPath}(G, \pi) \).

**Definition**

A decision problem \( D(x) \) is in \( \text{NP} \) (non-deterministic polynomial time) if there is a problem \( E(x, y) \) in \( P \) and a polynomial \( p(n) \) such that

- \( D(x) \iff \exists y. E(x, y) \)
- if \( E(x, y) \) then \( |y| \leq p(|x|) \) (\( E \) is poly balanced)

We require that the certificate \( y \) is poly bounded in \( x \) since otherwise it would take too long to guess \( y \).

Clearly the guess for the Ham path can be p-bounded in size of \( G \).

---

**Slogan**

- \( P \) class of decision problems which can be efficiently solved
- \( \text{NP} \) class of decision problems which can be efficiently verified
Satisfiability

A formula \( \phi \) of propositional logic is in conjunctive normal form (CNF) if it is of the form
\[
\bigwedge \left( \bigvee a_{ij} \right)
\]
where each \( a_{ij} \) is either a variable \( x \) or its negation \( \neg x \).

- Terms \( a_{ij} \) are called literals
- Terms \( \bigvee a_{ij} \) are called clauses

### Problem SAT
Given a formula \( \phi \) in CNF, is \( \phi \) satisfiable? (i.e. is there an assignment \( v \) to the variables of \( \phi \) which makes \( \phi \) true?)

SAT \( \in \) NP

It seems that SAT is not decidable in p-time: we have to try all possible truth assignments.

If \( \phi \) has \( m \) variables there are \( 2^m \) assignments - exponential.

We can let \( |\phi| \) be the number of symbols in \( \phi \) and \( |v| \) be \( m \) (size of the domain of \( v \)).

Notice that \( m \) can be of similar size to \( |\phi| \) - every literal could be a different variable.

However SAT does belong to NP:

- guess a truth assignment \( v \)
- verify in p-time that \( v \) satisfies \( \phi \)

Let \( \text{Ver-SAT}(\phi, v) \) iff \( \phi \) is in CNF and \( v \) satisfies \( \phi \).

Then:

- \( \text{SAT}(\phi) \) iff \( \exists v. \text{Ver-SAT}(\phi, v) \)
- if \( \text{Ver-SAT}(\phi, v) \) then \( |v| \leq |\phi| \) (Ver-SAT is p-balanced)

P \( \subseteq \) NP

### Proposition
If a decision problem is in P then it is in NP, i.e. \( P \subseteq NP \).

**Proof.**
Suppose that problem \( D \) is in P.

Idea: to verify that \( D(x) \) holds we don’t need to guess a certificate \( y \) - we can decide \( D(x) \) directly.

More formally, we define \( E(x, y) \) iff \( D(x) \) and \( y = \epsilon \) (the empty string - a dummy guess). Then clearly
\[
D(x) \iff \exists y. E(x, y) \text{ and } |y| \leq p(|x|)
\]

The \( P = NP \) question

It remains unknown whether \( P = NP \) despite many researchers’ attempts.

This is the most important open problem in computer science. It is arguably one of the most important open problems in mathematics.

The Clay Mathematics Institute has offered a prize of one million dollars for a solution (either equal or not equal).

It is fair to say that most researchers believe that \( P \neq NP \).
Outline

Tractable problems and P

NP

Problem reduction

NP-completeness

Motivation

Since P ⊆ NP, if we show that a problem such as HamPath belongs to NP we do not know whether it is tractable (in P) or not.

We want to identify the hard (high complexity) problems in NP.

We start by saying what it means for one problem to be harder than another, using the concept of reduction.

Many-one reduction

Suppose that D and D' are two decision problems. We say that D (many-one) reduces to D' (D ≤ D') if there is a p-time computable function f such that

D(x) iff D'(f(x))

Note that f can be a many-one function (hence the name).

The idea is that we reduce a question about D (the easier problem) to a question about D' (the harder problem).

P and reduction

Suppose that we have an algorithm A' which decides D' in time p'(n). Then if D ≤ D' via reduction function f running in time p(n) we have an algorithm A to decide D:

Algorithm A (input x)
1. Compute f(x)
2. Run A' on input f(x) and return the answer (yes/no)

Now A runs in p-time - same argument as when composing p-time functions.

Step 1 takes p(n) steps.

|f(x)| ≤ q(n) for some poly q. Step 2 takes p'(q(n)) steps.

Hence:

Proposition
Suppose D ≤ D' and D' ∈ P. Then D ∈ P.
NP and reduction

**Proposition**

Suppose \( D \leq D' \) and \( D' \in \text{NP} \). Then \( D \in \text{NP} \).

Assume that \( D \leq D' \) and \( D' \in \text{NP} \).

Then there is \( E'(x, y) \in \text{P} \) and a \( p'(n) \) such that

\[
D'(x) \iff \exists y. E'(x, y)
\]

and if \( E'(x, y) \) then \( |y| \leq p'(|x|) \).

Also we have \( D(x) \iff D'(f(x)) \).

Combining:

\[
D(x) \iff \exists y. E'(f(x), y)
\]

Define \( E(x, y) \iff E'(f(x), y) \).

Then \( D(x) \iff \exists y. E(x, y) \).

Also \( E \in \text{P} \) (same argument as previous slide).

Properties of reduction

The reduction order is reflexive and transitive:

- \( D \leq D \)
- if \( D \leq D' \leq D'' \) then \( D \leq D'' \)

The proofs are left as an exercise.

If both \( D \leq D' \) and \( D' \leq D \) we write \( D \sim D' \). Here \( D \) and \( D' \) are as hard as each other.

Outline

Tractable problems and \( \text{P} \)

NP

Problem reduction

NP-completeness
### NP-completeness

We want to identify problems in NP which are unlikely to be in P.

**Definition**

A decision problem $D$ is **NP-hard** if for all problems $D' \in \text{NP}$ we have $D' \leq D$.

- Note that NP-hard problems do not necessarily belong to NP. They could be harder.
- If $D$ is NP-hard and $D \leq D'$ then $D'$ is also NP-hard (consequence of transitivity of reduction)

**Definition**

A decision problem $D$ is **NP-complete** (NPC) if

1. $D \in \text{NP}$
2. $D$ is NP-hard

NP-complete problems are the hardest problems in NP.

### Cook-Levin Theorem

It is not clear from the definition that NPC problems exist. However:

**Theorem (Cook-Levin 1971)**

SAT is NP-complete.

Many other problems have been shown to be NPC.

Rather than proving this directly as for SAT, we use reduction as follows:

**Method**

To see that $D$ is NPC show:

1. $D \in \text{NP}$
2. $D' \leq D$ for some known NPC problem $D'$

It is clear that item 2 establishes that $D$ is NP-hard, since $D'$ is NP-hard.

### HamPath ∈ NP

As an example take HamPath. We have already seen that HamPath ∈ NP by guessing and verifying in p-time.

If we can show SAT $\leq$ HamPath then we can conclude that HamPath is NPC.

It is indeed possible to show SAT $\leq$ HamPath but we omit the reduction as it is long and difficult.

So HamPath is NP-complete.

### Intractability via NP-completeness

**Proposition**

*Suppose $P \neq \text{NP}$. If $D$ is NP-hard then $D \not\in P$.*

**Proof.**

Assume $P \neq \text{NP}$ and $D$ is NP-hard.

Suppose for a contradiction that $D \in P$. We show that $\text{NP} \subseteq P$.

Take $D' \in \text{NP}$. Since $D$ is NP-hard, we have $D' \leq D$.

Hence $D' \in P$.

We have shown that $\text{NP} \subseteq P$.

But we know $P \not\subseteq \text{NP}$. Hence $P = \text{NP}$ which contradicts our assumption.

Thus if we can show that a problem is NPC, we know that it is intractable (assuming that $P \neq \text{NP}$, as is generally believed).
Complexity classes

- **NPC**
- **NP**
- **P**

The Travelling Salesman Problem (TSP) is a fundamental problem in combinatorial optimization. Given a (complete) weighted graph \((G, W)\), the goal is to find a tour of \(G\) of minimum weight which visits each node exactly once and returns to the start node.

We first define a decision version of TSP:

**Problem TSP(D)**

Given a weighted graph \((G, W)\) and a bound \(B\), is there a tour of \(G\) with total weight \(\leq B\)?

TSP(D) is NP-complete

We show that TSP(D) is NP-complete using the Method:

1. **TSP(D) \(\in\) NP:**
   - If we guess a path \(\pi\), we can check in p-time that \(\pi\) is a Hamiltonian circuit of \(G\) and that \(W(\pi) \leq B\). Clearly \(|\pi| \leq |G|\).
   - More formally define \(\text{Ver-TSP(D)}(\langle G, W, B, \pi \rangle)\) iff \(\pi\) is a Hamiltonian circuit of \((G, W)\) and \(W(\pi) \leq B\).
   - Then \(\text{TSP(D)}(\langle G, W, B \rangle)\) iff \(\exists \pi. \text{Ver-TSP(D)}(\langle G, W, B, \pi \rangle)\).
   - Also if \(\text{Ver-TSP(D)}(\langle G, W, B, \pi \rangle)\) then \(|\pi| \leq |G|\) under reasonable definitions of size.

2. **\(D' \leq TSP(D)\) for some known NPC problem \(D'\):**
   - We choose HamPath as the known NPC problem and show HamPath \(\leq TSP(D)\).

HamPath \(\leq TSP(D)\)

We need to define a p-time function \(f\) which transforms a graph \(G\) into a weighted graph \((G', W)\) together with a bound \(B\) so that

\(\text{HamPath}(G)\) iff \(\text{TSP(D)}(\langle G', W, B \rangle)\).

Given \(G\) we construct \((G', W)\) as follows:

- **Set nodes** \((G') = \text{nodes}(G)\).
- **Given any two distinct nodes** \(x, y\) of \(G\):
  - If \((x, y)\) is an arc of \(G\) then \((x, y)\) is also an arc of \(G'\), with \(W(x, y) = 1\).
  - If \((x, y)\) is not an arc of \(G\) then \((x, y)\) is an arc of \(G'\), with \(W(x, y) = 2\).

Thus we add in the missing arcs of \(G\) but with higher weight.

Finally we let \(B = n + 1\) where \(G\) has \(n\) nodes.

Not hard to see that \(f(G) = (\langle G', W, B \rangle)\) is p-time — easiest to see using the adjacency matrix representation.
We now check $\text{HamPath}(G)$ iff $\text{TSP}(D)((G', W), B)$.

Suppose $G$ has Ham path $\pi$ with endpoints $x$ and $y$.
The same path in $G'$ has weight $n - 1$.
We get a TS tour by adding in arc $(x, y)$ with $W(x, y) \leq 2$.
Thus we have a tour of weight $\leq n + 1 = B$.

Conversely, suppose $(G', W)$ has a tour of weight $\leq B = n + 1$.
This has $n$ arcs.
So at most one arc can have weight 2.
Suppose this arc has endpoints $x, y$.
Then omitting arc $(x, y)$ gives us a Ham path in $G$.
We conclude that $\text{TSP}(D)$ is NP-complete.

Finally we can show that TSP is intractable (assuming $P \neq NP$):
Suppose that TSP can be solved by a $p$-time algorithm.
We compute the optimal value $O$ in $p$-time.
Then we can also solve $\text{TSP}(D)$ in $p$-time — simply check whether $O \leq B$.
But this is impossible since $\text{TSP}(D)$ is NP-complete and we assume $P \neq NP$.

We look at further examples of NP-complete problems:
- Metric TSP MTSP
- Vehicle routing problem with capacities VRPC

Further examples
The **metric TSP (MTSP)** is the TSP restricted to graphs \((G, W)\) satisfying the **triangle inequality**

\[ W(x, z) \leq W(x, y) + W(y, z) \quad \text{for all } x, y, z \in \text{nodes}(G) \]

A very natural condition, since if does not hold we would choose to travel from \(x\) to \(z\) via \(y\) rather than directly.

Decision version: **MTSP** - can we find a tour not exceeding given bound \(B\)?

We want to show: **MTSP** is **NP-complete**.

By Method:

1. **MTSP** \(\in\) **NP**: Ver-**MTSP**\((G, W), B, T) holds if \(T\) is a TS tour of \(G\) with weight \(\leq B\).
   
   Easy to check in p-time.

Instead we look at the reduction **HamPath** \(\leq\) **TSP**\((D)\).

- If \((x, y)\) is an arc of \(G\) then \((x, y)\) is also an arc of \(G'\), with \(W(x, y) = 1\).
- If \((x, y)\) is not an arc of \(G\) then \((x, y)\) is an arc of \(G'\), with \(W(x, y) = 2\).

Clearly

\[ W(x, z) \leq W(x, y) + W(y, z) \quad \text{for all } x, y, z \in \text{nodes}(G') \]

since \(1 \leq W(x, y) \leq 2\) for all \(x \neq y\).

So we actually constructed an instance of **MTSP**\((D)\).

Conclude **HamPath** \(\leq\) **MTSP**\((D)\).

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**Vehicle Routing Problem**

Suppose we have a depot, some vehicles and some deliveries to be made to various addresses.

Want to find the smallest cost set of routes for the vehicles.

Can model the network as a (complete) graph:

- nodes are the depot plus customer addresses
- \(W(x, y)\) is cost of shortest path from \(x\) to \(y\).
- will satisfy triangle inequality

Give the vehicles a capacity and ensure that the total size of the packages transported on each trip is within the capacity.

Assume that each vehicle performs at most one trip.
Vehicle Routing Problem

Vehicle routing problem with capacities VRPC(D)

Given
- a complete weighted graph \((G, W)\) satisfying the triangle inequality,
- a distinguished node \(\text{start} \) (the depot),
- \(k\) vehicles with capacity \(C\),
- a set of packages with sizes \(s_1, \ldots, s_n\) to be delivered to nodes \(x_1, \ldots, x_n\) respectively,
- and a budget \(B\):

Can the packages be delivered within total cost \(B\), subject to total size of the packages on each vehicle being within the capacity \(C\)?

Thus we are looking for an assignment of packages to vehicles, plus an itinerary for each vehicle that takes it to each of its addresses.

(2) We need \(D'\) such that \(D' \leq \text{VRPC}(D)\).

TSP(D) is the most obvious, but because of the triangle inequality we use MTSP(D) instead and show

\[
\text{MTSP}(D) \leq \text{VRPC}(D)
\]

Idea: convert an instance of MTSP(D) into a simple case of VRPC(D) via reduction \(f\).

Given \((G, W)\) with \(n\) nodes satisfying triangle inequality and \(B\):
- keep \((G, W)\) and \(B\) the same
- make one node into the \text{start} node (depot)
- assign one package with size 1 to each of the remaining nodes
- create just one vehicle with capacity \(n - 1\)

Clearly \(f\) is \(p\)-time.

Then a yes instance of \(f((G, W), B)\) means that it is possible to visit all nodes at least once and return to the start within bound \(B\).

We want to show: \(\text{VRPC}(D)\) is \(NP\)-complete.

By Method:

(1) \(\text{VRPC}(D) \in NP\): Plainly given an assignment of packages to vehicles and itineraries for each vehicle we can check in \(p\)-time that:
- all packages are assigned to exactly one vehicle
- the total size of packages does not exceed \(C\) for each vehicle
- the itinerary for each vehicle takes it from the depot to each delivery address assigned to it and back to the depot
- the total cost does not exceed \(B\)

We check

\[
\text{MTSP}(D)((G, W), B) \iff \text{VRPC}(D)(f((G, W), B))
\]

Suppose \(\text{MTSP}(D)((G, W), B)\): then we can start at \text{start} and visit each node exactly once returning to \text{start} all within cost \(B\).

We can do the same in \(f((G, W), B)\) since the graph is unaltered. Also we do not exceed the vehicle capacity.

Hence \(\text{VRPC}(D)(f((G, W), B))\).

Conversely, assume \(\text{VRPC}(D)(f((G, W), B))\): then we have a route starting at the depot which delivers packages to each node and returns to the depot within cost \(B\).

This is a TS tour except that we might visit a node more than once.

But since graph satisfies triangle inequality we can remove repeats by taking short cuts, without increasing the total cost.

Hence \(\text{MTSP}(D)((G, W), B)\).
We have seen that the following problems are NP-complete:

- TSP(D)
- VRPC(D)
- MTSP(D)
- HamPath
- SAT

Therefore MTSP, TSP, VRPC are intractable (if P ≠ NP).