Design and Analysis of Algorithms

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Contents

1 Elementary Graph Algorithms

1.1 Basic Concepts on Graphs

Definitions

- Graph: Pair $G = (V, E)$ of a set V of vertices (nodes) and a set E of edges (u, v) with $u, v \in V$
- Edges imply direction: in (u, v) we go from u to v
- In general, graphs are **directed**
- **Undirected** graphs: $(u, v) \in E$ iff $(v, u) \in E$
- **Unweighted** graphs: we only consider edge structure
- **Weighted** graphs: edges (u, v) have weights w_{uv}

Storing an Unweighted Graph

- **Adjacency matrix:** Assume $V = \{1, \ldots, N\}$. Then if $(i, j) \in E$, $m_{ij} = 1$; else, $m_{ij} = 0$
  - By convention $m_{ii} = 1$ (although sometimes we may consider $m_{ii} = 0$)
- Cost: $\Theta(N^2)$
- **Adjacency list:** We work with pointer table $T[\ ]$ where $T[i]$ points to a linked list
  - If $(i, j) \in E$, then j is in one of nodes pointed by $T[i]$
- Cost: $\Theta(|V|) + \Theta(|E|)$
- In general $|E| \leq |V|(|V| - 1) = O(|V|^2)$

The Size of a Graph

- While $|V|$ and $|E|$ are in general independent, we may expect $|V| = O(|E|)$ for interesting graphs
  - $|E|$ will usually be G's size

- G is **dense** if $|E| = \Theta(|V|^2)$
- G is **sparse** if $\Omega(|V|) = |E| \ll |V|^2$
- If G s dense, the adjacency matrix storage is more efficient; if G is sparse, adjacency lists are better
- We will usually work with adjacency lists, using adjacency matrices for special algorithms

1.2 Minimum Distances on Graphs

Minimum Distance Problems

- **Path** from u to v: a subset $\pi = \{u = u_0, \ldots, u_K = v\}$ with $(u_i, u_{i+1}) \in E$
- **Length** of π: $|\pi| = K = \#$number of edges
- First problem: given u, find a **shortest path** (i.e., a path with the smallest number of edges) π from u to any other v
- First question: how to obtain such paths?
- First idea: get a tree like "descending representation" T of G starting from u and avoiding lower duplicate vertices

Minimum Distance Example

- Think of each vertex as a ball and of edges as equal lenght strings, and make G "hang" from u discarding "'repeated" edges
- **Example:**

$$\begin{tikzcd}
 & 1 \arrow[rr] \arrow[dl] \arrow[dr] & & 2 \arrow[dl] \arrow[dr] & \\
3 \arrow[dr] & & 4 \arrow[ll] \arrow[dl] \arrow[dr] & & 5 \arrow[ll] \arrow[dl] \\
 & 6 \arrow[rr] & & 7 &
\end{tikzcd}$$

- Once obtained, the tree layers give vertices at distances 1, 2, 3 and so on

Some Observations on Minimum Distance Problems

- If $d[v]$ is the depth of v in T, it is reasonable to expect $d[v]$ to be the minimum distance from u to v, but we have to prove it
- If $p[v]$ is the father of v in T, we can obtain a minimum length (backward) path from u to v with edges $(w = p[v], v)$, $(p[w], w)$, $\ldots$
- Notice that we have found all the minimum distance paths from u to **all** $v \in V$
- Q: how can we derive an algorithm for this?
- We can use a standard FIFO queue Q to process the different vertices and the tables $p[v]$ and $d[v]$
- In fact, this fits in the general framework of **Breadth First Search**

First Algorithm for Minimum Distances

- We need tables $p[v]$ for the vertex "previous" to v, $d[v]$ for the minimum distance from u to v and $v[v]$ to mark v as seen
- First, queue–based, pseudocode:

```
def distMin(u, G):
    s[ ] = F; p[ ] = NULL; d[ ] = inf
    Q = q()
    d[u] = 0; Q.put(u); s[u] = T
    while not Q.empty():
        v = Q.get()
        for all z adjacent to v:
            if not s[z]:  #first time z is seen
                d[z] = d[v] + c(v,z)
                p[z] = v; Q.put(z); s[z] = T
    return p, d
```

Some Observations on `distMin`

- The table $s[\,]$ is redundant: $s[v] == T$ if and only if $d[v] < \infty$ (exercise: update the psc)
- We can use $p[\,]$ to reconstruct the minimum paths from u to all v (exercise)
- We can use $p[\,]$ to reconstruct the minimum distance table $d[\,]$ (exercise), so $p[\,]$ is the table to return in, say, a C function

- A vertex enters Q only once $\Rightarrow$ the linked lists are traversed only once $\Rightarrow$ the cost of `distMin` is $O(|E|)$, i.e., linear on G's size
- `distMin` is a particular instance of the general **Breadth First Search** algorithm

Breadth First Search (BFS) v 1.0

- The pseudocode of the first, queue–based version of BFS is

```
def BFS(u, G):
    s[ ] = F; p[ ] = NULL
    Q = q()
    doSomething(u); Q.put(u)
    while not Q.empty():
        v = Q.get()
        for all z adjacent to v:
            if not s[z]:
                s[z] = T
                doSomething(z)
                p[z] = v; Q.put(z)
    return p
```

- Since we enter each list only once, if the cost of `doSomething` is $O(1)$, the cost of BFS is $O(|E|)$ (actually $\Theta(|E|)$, i.e., linear,
- If needed, we add a driver to restart `BFS` at unseen nodes

Minimum Distances on Weighted Graphs

- $G = (V, E)$ is a **weighted** graph if there is a function $c : E \to R$
  - We think of $c(i, j)$ as the cost of going from i to j (although sometimes $c(i, j)$ can be negative)
- **Cost** of path π: $c(\pi) = c(\{u_0, \dots, u_K\}) = \sum_1^K c(u_{j-1}, u_j)$
- Working with adjacency matrices we can store c as $m_{ij} = c_{ij}$ if $(i, j) \in E$ and $m_{ij} = \infty$ if not.
  - Now the convention is $m_{ii} = 0$
- Working with adjacency lists we can store c_{ij} in a second field of the same node of $T[i]$ that stores j

Problems . . .

- Observation: working with the tree like representation of G is now trickier

- **Example:**

$$\begin{tikzcd}
1 \arrow[rr, "10"] \arrow[dr, "1"] & & 2 \arrow[dl, "1"] & \\
& 3 \arrow[rr, "1"] & & 4 \arrow[ul, "1"]
\end{tikzcd}$$

- The node 2 gets out of Q too soon $\Rightarrow$ we have to change the ordering in Q
- We need a **priority queue** Q that orders vertices using the current value of $d[v]$
- Now v is seen when it **leaves** Q
  - We also need (again) a table $s[v]$ to check whether v has left Q and we do not consider it any longer
- This leads to Dijkstra's algorithm

Dijkstra's Algorithm

- Dijkstra's pseudocode is:

```
def Dijkstra(G, u):
    s[ ] = F; p[ ] = NULL; d[ ] = inf       # 1
    Q = pq()
    d[u] = 0; Q.put( (d[u], u) )
    while not Q.empty():                    # 2
        d[v], v = Q.get()                   # 3
        if not s[v]:
            s[v] = T
            for all z adjacent to v:        # 4
                if d[z] > d[v] + c(v, z):
                    d[z] = d[v] + c(v, z)
                    p[z] = v
                    Q.put( (d[z], z) )      # 5
    return p, d
```

Dijkstra's Algorithm II

- **Example**: First steps of Dijkstra's algorithm on the previous graph

	d	p	v	d	p	v	d	p	v
1	0	-	F	0	-	-	0	-	-
2	∞	-	F	10	1	F	10	1	F
3	∞	-	F	1	1	F	1	1	T
4	∞	-	F	∞	-	-	2	3	F
PQ	1_0			$3_1, 2_{10}$			$4_2, 2_{10}$		

Dijkstra's Cost

- The five commented numbers in the psc determine its cost
- The cost of (1) is clearly $O(N)$
- Q will contain at most all edges, so $|Q| = O(|E|)$
- Using a PQ over a binary heap the cost of `Q.put, Q.get` is $O(\log |Q|)$
  - Thus, the cost of (3) over all iterations in (2) is $O(|E| \log |E|)$
- The total number of joint iterations in (2) and (4) is $|E|$ and the cost of (5) over all iterations is thus $O(|E| \log |E|)$
- Since $|E| = O(|V|^2)$, the overall cost is

$$\begin{aligned} O(|V|) + O(|E| \log |E|) &= O(|V|) + O(|E| \log |V|^2) \\ &= O(|V|) + O(|E| \log |V|) \end{aligned}$$

- This will be $O(|E| \log |V|)$ for most graphs, i.e., log linear in a graph's size

Observations on Dijkstra's Algorithm

- We allow that several instances of the same v be in Q
- We can stop the algorithm earlier using a counter of seen vertices (exercise)
  - But have to clear Q, so ...
- Dijkstra **works**: at the end $d[v]$ contains the minimum distances from u to v and we can get the minimum paths using $p[v]$
  - But **this has to be proved**
- Dijkstra is an example of the general **breadth first search** graph algorithm

Breadth First Search (BFS) v 2.0

- The pseudocode for general, PQ based BFS, is

```
def BFS(u, G):
    s[ ] = F; p[ ] = NULL; Q = pq()
    d[u] = 0; Q.put( (d[u], u) )
    doSomething(u)
    while not Q.empty():
        d[v], v = Q.get()
        if not s[v]:
            s[v] = T
            for all z adjacent to v:
                doSomething(z)      #perhaps change d[z]
                if d[z] smaller afterwards:
                p[z] = v; Q.put( (d[z], z) )
    return p
```

- If needed, we add a driver to restart `BFS` at unseen nodes
- If the cost of `doSomething` is $O(1)$ and we work with a PQ over min heaps, the cost of BFS is $O(|E| \log |V|)$

1.3 All Pairs Shortest Paths

All Pairs Shortest Paths

- If (G, c) is a weighted directed graph, we can consider in principle three minimum distance problems:
  - For u, v fixed, find **only** the minimum distance between u and v
  - For u fixed, find the minimum distance between u and **all other** $v \in V$
  - For **all** $u, v \in V$, find the minimum distance between u and v
- While the first problem seems easier, no algorithm for general graphs is better than the best one for the second problem
  - Notice that a minimal path from u to v is also minimal for all vertices in between
- We can solve the third problem iterating an algorithm for the second one over all $u \in V$
- For instance, iterating Dijkstra over all $u \in V$ has a cost $|V| \times O(|E| \log |V|) = O(|V||E| \log |V|)$
  - If G is dense, the cost is then $O(|V|^3 \log |V|)$

Improving on Dijkstra I

- Assume $V = \{1, \dots, N\}$ and the cost c is nonnegative
- Denote by d_{ij} be the minimum distance between i and j
- We define d_{ij}^k be the minimum distance between i, j but where **the intermediate nodes are taken only from** $\{1, \dots, k\}$
- It is clear that
$$d_{ij}^0 = c(i,j), \quad d_{ij}^N = d_{ij}$$
- It is clear that **no vertex is repeated on the optimal path** that gives d_{ij}^k

Improving on Dijkstra II

- Obvioulsy, an optimal path between i and j with $\{1, \dots, k\}$ as intermediate nodes may or may not contain k
- If it doesn't, we have
$$d_{ij}^k = d_{ij}^{k-1}$$
- If it does, we have
$$d_{ij}^k = d_{ik}^{k-1} + d_{kj}^{k-1}$$
- A path from i to j **is optimal iff the partial subpaths** between i and k and k and j **are optimal**, i.e.,
$$d_{ij}^k = d_{ik}^k + d_{kj}^k$$
- A path **having another** k between i and k or between k and j **cannot be optimal**: we can remove the subpath from k to k
- But then obviously
$$d_{ik}^k = d_{ik}^{k-1}, d_{kj}^k = d_{kj}^{k-1}$$

Floyd–Warshall Algorithm

- We can conclude $d_{ij}^k = \min\{d_{ij}^{k-1}, d_{ik}^{k-1} + d_{kj}^{k-1}\}$ and $d_{ij} = d_{ij}^N$
- Working with adjacency matrices, this suggest the following (quite bad) pseudocode

```
def FW_0(m_c):
    n = m_c.shape[0]
    d = np.empty( (n, n, n+1) )
    d[:, :, 0] = m_c
    for k in range(n):
        for i in range(n):
            for j in range(n):
                t = d[i, k, k] + d[k, j, k]
                d[i, j, k+1] = min(d[i, j, k], t)
    return d[:, :, n]
```

- The algorithm is $\pm$ obviously correct

Floyd–Warshall Cost

- The time cost is $O(N^3)$, better than iterated Dijkstra for dense graphs
- The space cost is a first sight also $O(N^3)$ as we use N matrices $N \times N$; but in fact a single matrix D is enough, for
  - We first "retain" d_{ik}, d_{kj}
  - Then for i or $j \neq k$ we set $c = d_{ik} + d_{kj}$, and we can overwrite d_{ij} as $d_{ij} = \min\{d_{ij}, c\}$
- Exercise (easy): rewrite FW taking advantage of this
  - Is it now a good algorithm?
- Exercise (more difficult): how can we recover the optimal paths?
- Observation: FW is our first example of a problem solvable by a **DP** algorithm
  - An optimization problem with an **optimal substructure** (obvious: any optimization problem has it) that we are able to make **explicit**
  - The explicit substructure formula also shows FW to be correct

Applying Floyd–Warshall

- Example:

$$\begin{tikzcd}
1 \arrow[r, "2"] \arrow[dr, "2"] & 2 \arrow[d, "3"] \\
3 \arrow[u, "4"] & 4 \arrow[l, "2"]
\end{tikzcd}$$

2 Minimum Spanning Trees

2.1 The Algorithms of Prim and Kruskal

Trees

- An undirected graph $G = (V, E)$ is **connected** if for every pair $u, v \in V$ there is a path π in E from u to v
- A **cycle** π in a graph $G = (V, E)$ is a path that starts and ends at the same point
- A **tree** is an undirected connected graph that is also **acyclic**, i.e., there are no cycles in E
- A tree T is a **spanning tree** (ST) for $G = (V, E)$ if $T = (V, E_T)$ with $E_T \subset E$
- If G is weighted, the **cost** of an ST T is

$$c(T) = \sum_{(u,v) \in E_T} c(u, v)$$

- $T = (V, E_T)$ is a **minimum spanning tree** (MST) for the undirected graph $G = (V, E)$ if for any other ST $T' = (V, E'_T)$ we have $c(T) \leq c(T')$

Prim's Algorithm

- Changing slightly Dijktsra's gives **Prim's** algorithm for finding MSTs

```
def prim(G, u):
    s[ ] = F; p[ ] = NULL; c_t[ ] = inf          # 1
    Q = pq()
    c_t[u] = 0; Q.put( (c_t[u], u) )
    while not Q.empty():                         # 2
        _, v = Q.get()                           # 3
        if not s[v]:
            s[v] = T
            for all z adjacent to v:             # 4
                if not s[z] and c_t[z] > c(v, z):
                    c_t[z] = c(v, z)
                    p[z] = v
                    Q.put( (c_t[z], z) )         # 5
    return p, c_t
```

- The second `if not s[z]` didn't appear in Dijkstra; do we need it here?

Observations on MSTs

- There may be several minimum spanning trees in a graph
- We have $c(T) = \sum_{v \neq u} c(p[v], v)$
- The cost of Prim is $O(|E| \log |V|)$ if the PQ is built over a min heap
- **Prim works**: at the end $p[v]$ gives the edges $(p[v], v)$ of a MST E_T and $cE[v]$ its costs
  - But again this has to be proved
  - And we do not need to check `s[v] == T` (although it saves time) for if `z` already seen,
    `c_t[z] <= c(v, z)`,
    since it is correct,
- Prim and Dijkstra are examples of a **greedy** algorithms

Greedy Algorithms

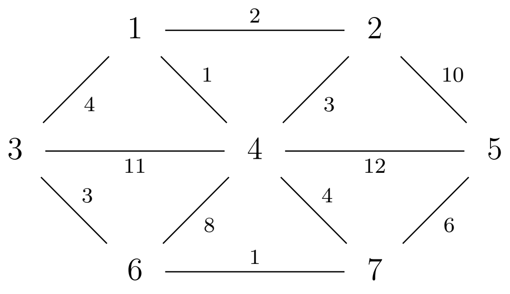
- A greedy algorithm tries to solve a **global optimization problem** by making **locally optimal choices** at each of its steps
- Simple example: the Nearest Neighbor algorithm for the **Traveling Salesman Problem** (TSP)
- Dijkstra maintains a table $d[v]$ of locally minimum distances from u to v computed over a partial subset of all paths from u to v
- Prim maintains a table $c_t[v]$ of locally minimum edge costs of a partial spanning subtree that is progressively grown from a starting node u
- The greedy strategy is quite natural, but Dijkstra and Prim are not obviously correct algorithms
  - It often results on wrong algorithms, with greedy TSP an example
- **Kruskal's** is another, clearer example of a greedy algorithm to obtain a MST

A First Look at Kruskal's Algorithm

- Main idea: sort the edges of E in a PQ by increasing costs and build a forest of partial STs
  - Starting from single node trees $T_u = (\{u\}, \emptyset)$ and

- Adding edges from the PQ that do not produce cycles

- **Example:**



Elements of Kruskal's Algorithm

- To implement Kruskal we need a PQ, a way of storing the selected edges and a way to maintain the forest of partial subtrees and to detect cycles
- No problem with the PQ and we can store the edges on a linked list (or simply build the graph of the final MST)
- At first sight maintaining trees and detecting cycles in them looks complicated and costly
- However, observe that (u, v) **gives a cycle iff** u **and** v **are in the same subset** $V_{T'}$ of the vertices of a tree T' in the Kruskal forest
  - Thus we do not need to work with trees but with **subsets**
- We do this with a new abstract data type, the **Disjoint Set**

2.2 The Disjoint Set Abstract Data Type

Disjoint Set

- A **Disjoint Set** (DS) S over a universal set U is a dynamic family of disjoint subsets of U (i.e., a **partition** of U), each of which is **represented** by a certain element x and that has the following primitives:
  - `init_DS(U, S)`: receives the universal set U and returns the initial S as the famility of atomic subsets $\{\{u\} : u \in U\}$

  - `find(x, S)`: receives an element $x \in U$ and returns the representative of the subset S_x of S that contains x
  - `union(x, y)`: receives two representatives x, y, computes their union $S_x \cup S_y$ and returns the representative of the subset $S_x \cup S_y$

Observations on the Disjoint Set

- The subsets of a Disjoint Set are never split; they can only change to bigger subsets
  - The Disjoint Set is never empty
- After `init_DS` we start with a partition with $|U|$ subsets;
  - Thus, the maximum number of unions is $|U| - 1$
- Even if we don't have yet a data structure for DS, its primitives allow us to write a first pseudocode for Kruskal

Kruskal's Algorithm

```
def kruskal(G):
    L = []                              #we save the MST in L
    init_DS(V, S)                       # 1

    Q = pq()
    for all (u, v) in E:
        Q.put( (c(u, v), (u, v)))       # 2

    while not Q.empty:                  # 3
        _, (u, v) = Q.get()             # 4
        x = find(u, S)
        y = find(v, S)                  # 5
        if x != y:
            L.append( (u, v) )          # 6
            union(x, y, S)              # 7

    return L
```

Observations on Kruskal's Algorithm

- We simply store E_T on a list L
- The algorithm may return a faulty ST, for instance if G is not connected
  - We can control this introducing a counter c and increasing it when a new edge is added to L

  - c should have the value $|V| - 1$ when the PQ is empty
  - Python exercise: add it

- The maximum number of unions is $|V| - 1$
- Even if we achieve a efficient implementation of `union` and `find`, the cost of Kruskal will be at least $O(|E| \log |V|)$ because of (1)

A First Data Structure for DS

- We assume $V = \{1, \ldots, N\}$
- A simple idea is keep each subset in a list with the representative in the first node
- We also construct a pointer (dict?) table `T[ ]` where `T[i]` points to the list that contains `i`
- The cost of `find` is clearly $O(1)$
- To implement `union(x, y, S)` we can concatenate the list `T[y]` after the list `T[x]` and then make sure that for each `j in T[y]` we have `T[j] = T[x]`
- However this is not satisfactory as the cost of the union is then
  - `|T[x]|` (to find the end point) plus
  - `|T[y]|` (to reset the pointers of $V_{T(y)}$)

Improving the First Data Structure

- We can improve things if we keep track of the last node of each `T[i]` and also on the sizes `|T[x]|`.
- This way we find the last element of `T[x]` with cost $O(1)$ and then join the smaller subset to the largest one
- Working with pure linked lists, notice that we have to keep track of the size and the last element only at the first node of `T[x]`
  - The extra cost is then $O(1)$
- The cost of `union(x, y, S)` is then `min (|T[x]|, |T[y]|)` and
  - If done well, we'll see in the exercises it is always $O(\log N)$

- But we need to work with 3–field nodes in the lists, which in most nodes just keep outdated information
  - Although things are much simpler in Python
- We try to do something better

A Second Data Structure for DS

- Our second data structure stores DS as trees (not to be confused with the conceptual subtrees that Kruskal builds)
- The representative x of a subset S is at the root of the subset tree T_S
- The cost of `union(x, y, S)` is then just $O(1)$, as we simply make, say, T_{S_y} a child subtree of the x root
- To implement `find(u, S)` we need a fast way to first locate the tree of u and then to go from the u node to the root
- This can be easily done if we place the subsets on a table `p[ ]`:
  - `p[u]` is the index of the father of `u`
  - `p[x]=-1` for a root `x`, i.e., a representative

Union and Find over Trees

- To initialize the DS we simply need `p[i]=-1` for all i
- The simplest pseudocode for `find` is

```
def find(u, p):
    while p[u] != -1:
        u = p[u]
    return u
```

- The pseudocode for `union` is

```
def union(x, y, p):
    p[y] = x    #join second tree to first
    return x
```

Improving Union

- Since the cost of `find` is $O(\ height\ (T_x))$ it is clear that we should join the shorter tree into the taller one

- For this we need to keep a tree's height h
  - We simply can change $p[x]$ at the root x from -1 to $-h$
- We then change the pseudocode for `union` as

```
def union_height(x, y, p):
    if p[y] < p[x]:         #T_y is taller
        p[x] = y; return y
    elif p[y] > p[x]:       #T_x is taller
        p[y] = x; return x
    else:                   #T_x, T_y have the same lenght
        p[y] = x; p[x] -= 1; return x
```

- We also change the while condition on `find` to

```
while p[u] >= 0:
```

The Cost of Find

- **Proposition.** *If $prof(T)$ denotes the depth of a DS tree T, we have $prof(T) \leq \lg |T|$*
- **Proof Sketch:**
  - Use induction on $|T|$, with an obvious base case $|T| = 1$
  - Assume it true for $|T'| < |T|$ and that we join T_y into T_x
  - If $prof(T_y) < prof(T_x)$,

$$prof(T_x \cup T_y) = prof(T_x) \leq \lg |T_x| \leq \lg |T_x \cup T_y|$$

  - If $prof(T_y) = prof(T_x)$ and $|T_y| \leq |T_x|$,

$$\begin{aligned} prof(T_x \cup T_y) &= 1 + prof(T_y) \leq 1 + \lg |T_y| = \lg\ 2|T_y| \\ &\leq \lg |T_x \cup T_y| \end{aligned}$$

Improving Find

- Thus, the cost of `find(x, p)` is also $O(\log |S_x|) = O(\log N)$
- We thus get the same cost as before but with a much simpler data structure.
- Moreover, we can further improve on this
- Observe that when finding the representative of u we also find the **representative of all the v between u and the root of its tree**

- We can thus change `find` to update `p[v]` for al v between u and the root
- In other words, we can **compress the path** from u to the root

Path Compression

- Recall that after finding the representative of u, we also know it for all the other nodes between u and the root of the tree
- We thus improve `find` as follows:

```
def find_cc(u, p):
    # find the representative
    z=u
    while p[z] >= 0:
        z = p[z]

    # compress the path from u to the root
    while p[u] >= 0:
        y= p[u]
        p[u] = z
        u = y
    return z;
```

Path Compression and Union by Rank

- The problem is now that, after `find`, we no longer have in $-p[x]$ the tree's height
- We do nothing about this other than calling $-p[x]$ the tree's **rank**
- We change nothing on `union` although it is no longer a union by height but a **union by rank**
- However the joint cost of unions and finds considerably improves
- **Proposition:** *If on a DS with N elements we do L unions by rank and $M = \Omega(N)$ path compression finds, the overall cost is*

$$O(L + M \lg^* N)$$

The $\lg^*$ Function

- We define $\lg^* H = K$ if K is the smallest integer such that after K binary logs we have

$$\lg(\ldots \lg(\lg H)\ldots) \leq 1$$

- For instance $\lg^* 65536 = \lg^* 2^{16} = 4$, but then

$$\lg^* 2^{65536} = 1 + \lg^* 2^{16} = 5$$

- Now 2^{65536} is a huge number:
  - Find out how many digits its decimal expression has (easy)
  - Then try to write it using millions, billions, googols and so on! ;-)
- For practical purposes $\lg^* H = O(1)$

Back to Kruskal's Algorithm

- Assume we work with union by rank and path compression and go back to Kruskal's pseudocode

```
def kruskal(G):
    l_mst = []                          # we save the MST in L
    p = init_DS(V)                      # 1
    Q = pq()

    for all (u, v) in E:
        Q.put( (c(u, v), (u, v)))       # 2

    while not Q.empty:                  # 3
        _, (u, v) = Q.get()             # 4

        x = find(u, p)                  # 5
        y = find(v, p)

        if x != y:
            l_mst.append( (u, v) )      # 6
            union(x, y, p)              # 7

    return l_mst
```

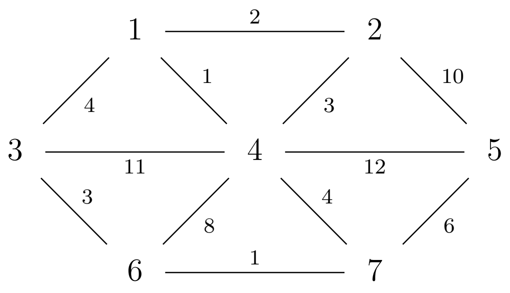
The Cost of Kruskal's Algorithm

- Clearly the cost of (1) is $O(|E| \log |V|)$ and that of (2) is $O(|V|)$
- The cost of (4) accumulated over (3) is again $O(|E| \log |V|)$
- Since the single cost of (6) and (7) is $O(1)$ and only happens when `x!=y`, their accumulated costs are $O(|V|)$
- Finally, since we must do at least one `findPC` for each node, the total number is $\Omega(N)$ and, therefore, the cost of (5) accumulated over (3) is $O(|E| \lg^* |V|)$, that is, essentially $O(|E|)$

- Summing things up, the cost of Kruskal is $O(|E| \lg |V|)$, dominated by the PQ operations
- In particular the DS operations do not penalize the algorithm

Applying Kruskal's Algorithm

- **Example:**



2.3 Correctness of Prim and Kruskal

Cuts and Minimal Crossings

- Assume we have an undirected weighted graph $G(V, E)$ with cost c
- A **cut** P of G is a partition of V into two disjoint subsets $P = (S, V - S)$
- An edge (u, v) **crosses** P if either $u \in S$ and $v \in V - S$ or viceversa
- A subset $A \subset E$ **preserves** P if no edge in A crosses P
- An edge (u, v) that crosses P is **minimal** w.r. to P if $c(u, v) \leq c(w, z)$ for any other edge (w, z) that crosses P

A Meta MST Algorithm

- Consider the following meta–algorithm to find MSTs

```
def metaMST(G, c):
    L = [ ]                 #we see L as a subset of E

    while len(L) < |V|:
        find a cut P that preserves L
        select (u, v) minimal w.r. to P
        L.append( (u,v) )

    return L
```

- Notice that `metaMST` is also a kind of greedy meta–algorithm
  - At each step a minimal edge is added to the MST list

Prim as an Example of metaMST

- Recall that Prim works with a table $v[\,]$ of nodes "seen" and that the nodes still in Q are ordered by their cost at insertion
- Assume that a node v has been extracted from Q just before is marked as seen, and take
  - $P = (\{seen\ nodes\}, \{others\})$
  - $L = \{(p[w], w) : w \in \{seen\ nodes\}\}$
- Then we have
  1. L preserves P for if $(p[w], w) \in L$, both w and $p[w]$ are seen
  2. $(p[v], v)$ crosses P, for v is unseen but $p[v]$ was processed when v entered Q, i.e., it is seen by now
  3. If other (w, z) crosses P we have $v[w] = T$, $v[z] = F$ and, hence, $z \in Q$ since it is adjacent to the already seen node w
  4. Since we extract v but not z, $c(p[v], v) \leq c(w, z)$ and, thus, $(p[v], v)$ is minimal
- Hence, Prim is a particular case of metaMST

Kruskal as an Example of metaMST

- Assume that we are about to add the edge (u, v) and let
  - $L = \{(w, z)\}$ be the edges already selected
  - $P = (S_u, V - S_u)$ where S_u is the subset of the tree T_u that contains u
- Then we have
  1. L preserves P for the subtrees are disjoint and if $(w, z) \in L$, they are in the same subtree T, which cannot happen if $w \in S_u$ and $z \in V - S_u$
  2. (u, v) crosses P: if not, it would make a cycle in T_u

3. If (w, z) also crosses P, it must connect different subtrees and cannot make a cycle
4. Thus (w, z) must still be in Q: it can only be been discharged if w and z were in the same subtree
5. Thus, $c(u, v) \leq c(w, z)$ and (u, v) is minimal w.r. P

- Hence, Kruskal is a particular case of metaMST

Correctness of metaMST I

- Thus, if metaMST is correct, Prim and Kruskal will also be correct
- **Proposition.** *Let $G = (V, E)$ be a undirected, connected, weighted graph and assume $A \subset E$ verifies $A \subset E_T$ for some MST T.*
  Then, if A preserves some P and (u, v) is minimal w.r. to P, we have $A \cup \{(u, v)\} \subset E_{T'}$ for some MST T'
- **Proof sketch:**
  - Assume $T = (V, E_T)$; then $\pi = E_T \cup \{(u, v)\}$ is a cycle with an edge (w, z) that crosses P
  - Define $T' = (V, E_{T'})$ with $E_{T'} = (E_T - \{(w, z)\}) \cup \{(u, v)\}$; clearly $c(T') \leq c(T)$ and to prove T' a tree we have to check it connected
  - Assume x, y at different sides of P; since T is connected, there is a path π from x to y in E_T and it crosses P at (w, z) (if two edges of T cross P, T would be a cycle)
  - We can decompose π as $\pi = \pi_{x,w} \cup \{(w, z)\} \cup \pi_{z,y}$
  - Then $\pi' = \pi_{x,w} \cup \pi_{w,u} \cup \{(u, v)\} \cup \pi_{v,z} \cup \pi_{z,y}$ is a path on $E_{T'}$

Loop Invariants

- The proposition says that at each iteration the selected edges are part of a MST
- This is an example of a **loop invariant**:

  A condition that remains true after each loop and that “leads” the algorithm towards a correct solution
- The standard way to prove the correctness of an iterative algorithm is to find an adequate loop invariant for its iterations

- Example: loop invariants for InsertSort or BubbleSort
  - InsertSort: after iteration i, $i = p+1, \ldots, u$, the subtable $T[p], \ldots, T[i]$ is sorted
  - BubbleSort: after iteration i, $i = u, \ldots, p+1$, the subtable $T[i], \ldots, T[u]$ is sorted

Correctness of metaMST II

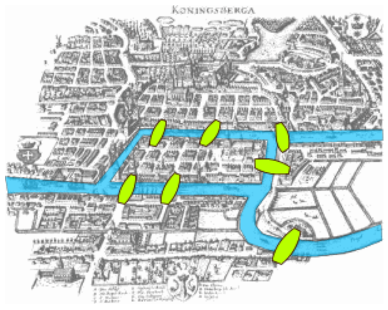
- **Corollary.** `metaMST` *returns a MST*
- **Proof sketch:**
  - We just exploit the loop invariant provided by the previous proposition
  - Let $L_0 = \emptyset \subset L_1 \subset \ldots \subset L_{N-1}$ be the successive subsets `metaMST` produces
  - If L_j is a subset of some MST, the proposition shows that so is L_{j+1}
  - But obviously L_0 is a subset of some MST and, thus, so is L_{N-1} and since it has $N-1$ edges, (V, L_{N-1}) is a MST
- **Corollary** *Prim and Kruskal also return MSTs*

3 Eulerian and Hamiltonian Circuits

3.1 Eulerian Circuits

The Bridges of Königsberg

- The bridges of Königsberg (East Prussia) over the Pregel river circa 1700:

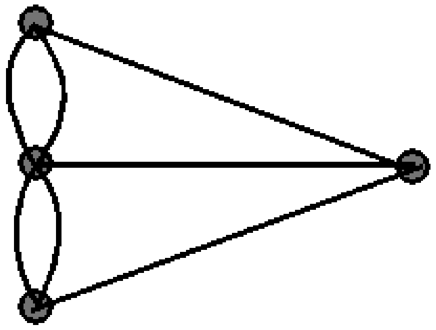


- The problem: find a promenade that crosses all bridges but only once

- Exercise: google `pregel graph`

The Bridges of Königsberg as a Graph Problem

- We can depict the bridges of Königsberg as a multigraph (i.e., we allow for multiple edges between two nodes)



- The problem: find a circuit that passes **through all edges but only once**
- Such a circuit in a multigraph is called an **Eulerian circuit** (EC)

Euler's Insight

- Leonhard Euler showed in 1736 (*Solutio problematis ad geometriam situs pertinentis*) that such a circuit is not possible
- If G is an udirected graph, we define the **degree** $deg(w)$ of a node w as the number of edges that leave w (or that enter w or simply the size of $T[w]$)
- Assume that $\pi = \{(u = u_0, u_1), \ldots, (u_{K-1}, u_K = u)\}$ is an EC for G
- If $w \neq u$ is a node in π, each time we enter w we substract 1 from $deg(w)$ and also when we leave w
  - Since at the end we have passed by all the edges of w, **we must have at the beginning** $deg(w)$ **even**
- Similarly each time we enter u inside π we substract 1 from $deg(u)$ and also when we leave u; moreover, when we start and end π we also substract 1 from $deg(u)$

- Thus, **we must also have** $deg(u)$ **even**

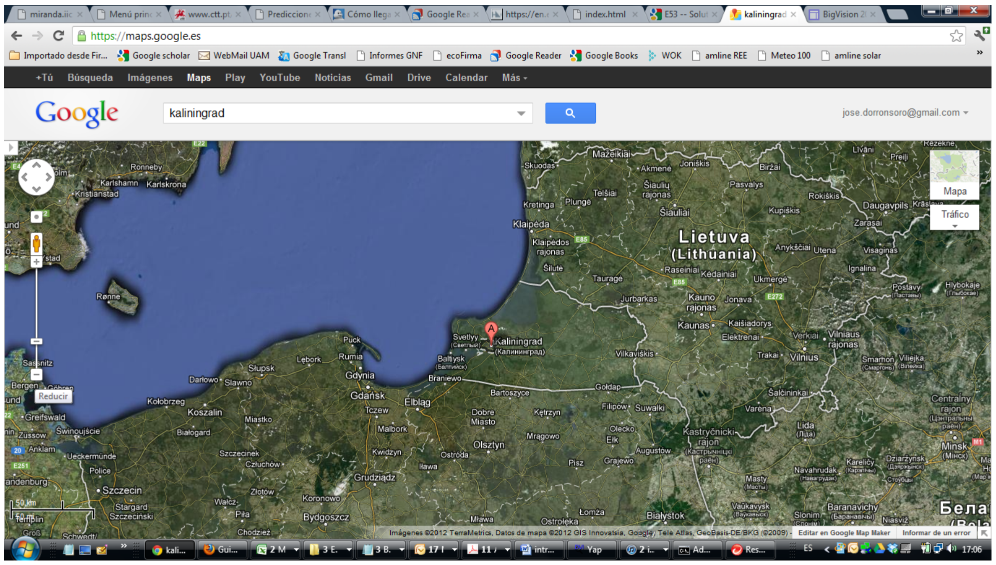
There Are No ECs in Königsberg

- It follows from the previous analysis that a necessary condition to have an EC is that $deg(v)$ is even for all $v \in V$
- Since all the nodes in the previous multigraph have odd degrees, Euler concluded that no Eulerian circuit is possible in Königsberg
- As we shall see later, Euler also proved that the condition is sufficient:

  If $deg(v)$ is even for all nodes v of an undirected graph G, then there is an Eulerian circuit in G

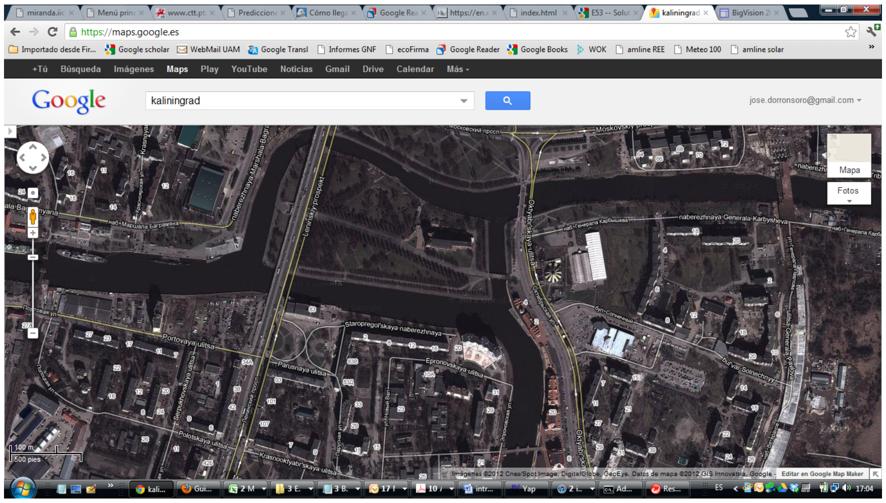
The Bridges of Kaliningrad

- After World War II Königsberg becomes Kaliningrad (Russia)



The Bridges of Kaliningrad II

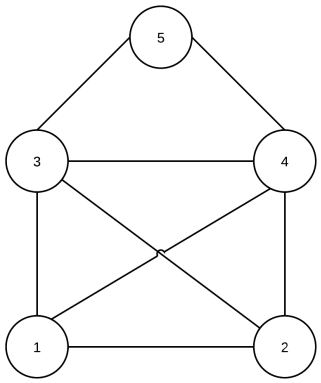
- And there only remain five bridges of the initial seven (and some more modern ones)



- But still, there is no EC

Drawing Houses Without Lifting the Pen

- A child's game is to try to draw the house below without lifting the pen from the sheet



- It is very easy if we start at nodes 1 or 2 but impossible if we start from 3, 4 or 5

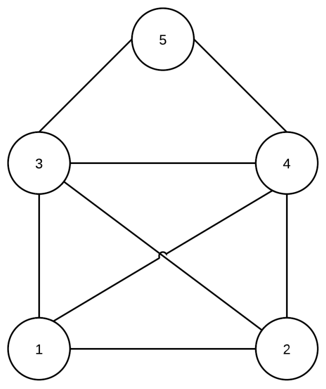
Euler's Insight Again

- Now we want to find an **Eulerian path** (EP) and not a circuit
- Let $\pi = \{(u = u_0, u_1), \ldots, (u_{K-1}, u_K = v \neq u)\}$ be such an EP

- If $w \neq u, v$ is a node in π, each time we enter w we substract 1 from $deg(w)$ and also when we leave w;
  - Since at the end we have passed through all the edges of w, we must have at the beginning $deg(w)$ even
- Similarly each time we enter u inside π we substract 1 from $deg(u)$ and also when we leave u; moreover, since we start π at u, we also substract 1 from $deg(u)$
  - Thus, we must also have $deg(u)$ odd
- Similarly each time we enter v inside π we substract 1 from $deg(v)$ and also when we leave v; moreover, since we end π at v, we also substract 1 from $deg(v)$
  - Thus, we must also have $deg(v)$ odd
- Thus, **a necessary condition to have an EP is that $deg(w)$ is even for all w except the first node u and the final one v of π**

Back to Drawing Houses

- Since $deg(1) = deg(2) = 3$ we can find an EP for the house drawing if we start at either 1 or 2



- But since $deg(3) = deg(4) = deg(5)$ even, it is impossible to draw an EP for the house starting at them

Euler's Theorem for Circuits

- **Theorem.** *If $G = (V, E)$ is a connected undirected* **multigraph***, there is an EC in G iff $deg(u)$ is even for all $u \in V$*

  Proof sketch: We argue by induction on $|V|$

  - The theorem is obviously true if $|V| = 2$ and assume it also to be true for any $G' = (V`, E')$ such that $|V'| < |V|$
  - We start walking from a node u substracting from deg at each node until we arrive at v such that $deg(v) = 0$ after we enter v and, thus, cannot leave it
  - It is easy to see that $v = u$ and we have found a cycle π
  - We remove E_π from E and from V the nodes w whose deg π has exhausted and let $G' = (V', E')$ be the resulting graph
  - Since $|V'| \leq |V| - 1$ and $deg_{G'}(w) = deg_G(w) - deg_\pi(w)$ is even, we can apply induction on the connected components $G_1, \ldots, G_K$ of G'
  - By induction there are ECs π_k in the G_k that start at nodes from π and we get an EC on G "collating" π and the π_k

Euler's Theorem for Paths

- **Corollary.** *If G is a connected undirected graph, there is an EP π in G iff $deg(w)$ is even for all $w \in V$ except for two vertices u and v. Moreover, then π starts at u and ends at v or viceversa*

  Proof sketch: We just show the condition to be sufficient:

  - Consider $G' = (V, E' = E \cup \{(u, v)\})$, i.e., we add an extra edge (u, v) to E
  - Since $deg_{G'}(u) = deg_G(u) + 1$, $deg_{G'}(v) = deg_G(v) + 1$ and $deg_{G'}(w) = deg_G(w)$ for all other w, all the G' degrees are even and there is an EC π' in G'
  - Let's write π' as $\pi' = \{(v, z), \ldots, (w, u), (u, v)\}$, with the last edge the one we added to get G'.
  - Then removing this edge we get the EP $\pi = \{(v, z), \ldots, (w, u)\}$.

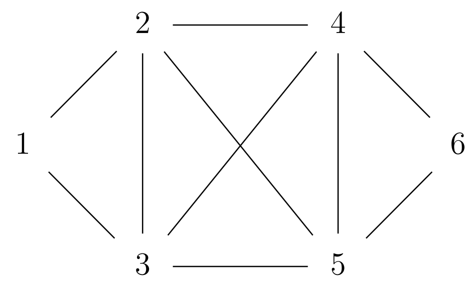
How to Find an EC

- Assuming an EC exists, the basic idea is simply to follow the proof's argument

- We start at any u_1 and build $\pi_1 = \{(u_1, v_2), \ldots, (v_{K-1}, v_K)\}$ substacting 1 from $deg(w)$ each time we enter or leave w and where we stop because after entering v_K we have $deg(v_K) = 0$
  - It is then clear that $u_1 = v_K$, and
- Let $G_1 = (V_1, E_1)$ the graph obtained after removing π_1 from E and all the $w \in V$ for which $deg(w) = 0$ after π, i.e., for which $deg_\pi(w) = deg_G(w)$
  - Clearly u_1 at least will be removed, i.e., $|V_1| < |V|$
  - If $|V_1| = 0$, clearly π_1 is an EC in G
  - If however $|V_1| > 0$, there is a first u_2 in π_1 such that $deg_{G_1}(u_2) > 0$
  - We can thus **restart the above process on** G_1 obtaining a new circuit π_2 and a "remaining" graph G_2
- If we repeat the preceeding and find circuits $\pi_1, \ldots, \pi_M$ until $V_M = \emptyset$, then we can "collate" the π_j circuits to get an EC π for G

How to Find an EC II

- **Example:**



- We do not write a pseudocode (good exercise!) but it is clear that its cost will be $O(|E|)$

3.2 Hamiltonian Circuits and an Excursion on Complexity Theory

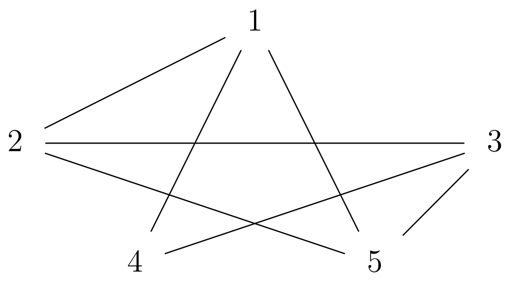
Hamiltonian Circuits

- If G is an undirected connected graph, a **Hamiltonian circuit** (HC) is a circuit on G that visits **only once each node** other than the initial

- Finding HCs may be trivial in some cases, such as complete graphs
- There are also sufficient conditions for special graphs
- But for general graphs, while finding ECs has an $O(|E|)$ cost, finding HCs is much costlier
- In fact, essentially the only general algorithm is an exhaustive search with backtracking

Hamiltonian Circuits II

- **Example:**



- Since the number of node orderings is $N!$, the search's cost can be very high
- Actually, finding HCs in general graphs is an example of an **NP–complete** problem

P and NP I

- We will make a brief (and light) excursion on Complexity Theory
- We consider **decision problems** $\mathcal{P}$ for which there is a set of solution inputs $S_\mathcal{P}$, i.e., the decision on an input I is 1 iff $I \in S_\mathcal{P}$ otherwise
  - To decide whether a graph has an EC or HC is a decision problem but notice that an algorithm does not have to actually find an EC or HC to solve them
  - Optimization problems can be partially reduced to decision problems using a bound C: change *find the optimum* by *find a solution with cost* $\leq C$
- For an input I we can consider its size $|I|$ to be the number of bits needed to store it

- We say that $\mathcal{P}$ **is in the class** P if there is an algorithm A with cost polynomial on $|I|$ that solves $\mathcal{P}$, i.e., $A(I) = 1$ iff $I \in S_\mathcal{P}$
  - Note that to be in class P does not mean that A is efficient: if its cost is $O(|I|^{1000})$, $\mathcal{P}$ is in P

P and NP II

- Decision–EC is in P: we check in linear time whether or not there are ECs in G by counting degrees and checking that they are even
- An algorithm $C(I, t)$ is a **certifier** for $\mathcal{P}$ if
  - For every input $I \in S_\mathcal{P}$ there is another, different input $t = t(I)$ to C such that $C(I, t) = 1$
  - If $I \notin S_\mathcal{P}$, then $C(I, t) = 0$ no matter which t is used
- t is a kind of certificate (solution?) that the certifier validates
  - For the EC or HC problems, t can just be a possible EC or HC
- We say that $\mathcal{P}$ **is in the class** NP if there is a certifier C that runs in polynomial time on the sizes $|I|$ and $|t|$
  - For instance, if $I = G$ and t is a possible CH, we can check it in polynomial time;
  - Thus HC belongs to NP

P and NP III

- Clearly $P \subset NP$: if $\mathcal{P} \in P$ and A solves it, set $C(I, t) = A(I)$; then
  - If $I \in S_\mathcal{P}$, we can simply use an empty certificate and set $C(I, \emptyset) = A(I)$
  - If $I \notin S_\mathcal{P}$, we will have $C(I, t) = A(I) = 0$ no matter the t presented
- Big question: $P = NP$?
- If yes, there would be a polynomial time algorithm for HC
- It is one of the Millenium Problems of the Clay Mathematics Institute with a 1M \$ prize

  - For more details see http://www.claymath.org/millennium/P_vs_NP

- General opinion: $P \neq NP$
- Reason: NP**–complete problems**

NP–complete Problems

- We say that $\mathcal{P}_1$ is **reducible** to $\mathcal{P}_2$ if there is a map
$$T : \{\,inputs\ of\ \mathcal{P}_1\} \to \{\,inputs\ of\ \mathcal{P}_2\}$$
such that I_1 has a solution for $\mathcal{P}_1$ iff $T(I_1)$ has a solution for $\mathcal{P}_2$
- Thus, **if** A **is an algorithm that solves** $\mathcal{P}_2$**, then** $A \circ T$ **solves** $\mathcal{P}_1$:
$$I \in S_{\mathcal{P}_1} \ \text{ iff } \ T(I) \in S_{\mathcal{P}_2} \ \text{ iff } \ A(T(I)) \equiv A \circ T(I) \equiv 1$$
- If T has polynomial cost, we say that $\mathcal{P}_1$ is **polynomially reducible** to $\mathcal{P}_2$
- We say that problem $\mathcal{P}$ is NP**–complete** if any other $\mathcal{P}' \in NP$ is polynomially reducible to $\mathcal{P}$
- Notice that **if we show for just one** NP**–complete problem** $\mathcal{P}$ **that** $\mathcal{P} \in P$**, then we have proved that** $P = NP$

Is There Any NP–complete Problem?

- At first sight the NP–complete definition seems very strict so a natural question is whether there any such problem
- Answer: yes, and in fact many!! HC is such a problem
- The first (basically) NP–complete problem found is 3–SAT
- Given a Boolean expression B written using only AND, OR, NOT operators, and parentheses, the **satisfiability problem (SAT)** is to decide whether there is some assignment of T and F to the variables that will make B true
- The k–SAT problem deals with expressions in **conjunctive normal form** (i.e., as a sequence of OR clauses joined by AND) with k variables or their negation per clause

Cook's Theorem

- Example: 3–SAT deals with expressions like

  ```
  (x11 OR !x12 OR x13)AND (!x21 OR x22 OR !x23)AND
  (x31 OR !x32 OR x33)AND ...
  ```

- **Cook's Theorem (1971)**: 3–SAT is NP–complete
  - However, 2-SAT $\in P$
- More to read: Chapter 5 of H. Wilff's book **Algorithms and Complexity**
- Much more to read: M.R. Garey and D.S. Johnson. **Computers and Intractability: A Guide to the Theory of NP-Completeness**. W.H. Freeman, 1979.
- But are P, NP and NP–complete problems just academic curiosities?

3.3 The Traveling Salesman Problem

The Traveling Salesman Problem

- TSP: Given a weighted complete graph G, find a HC (trivial) with minimum cost
- It is an optimization problem with obvious practical interest: many persons have to solve it every morning
  - Decision version: given a weighted complete graph G and a bound C, is there a HC π such that $c(\pi) \leq C$?
- TSP is **NP–hard**: every problem in NP can be polynomically reduced to TSP
  - A NP–hard problem may not have to be in NP or to be a decision problem
  - Also, TSP–decision for general graphs is NP–complete
- But TSP–decision is also NP–complete for "real world" problem versions, such as for cities in the plane with Euclidean distances
- Many related problems of great practical interest in planning, logistics or DNA sequencing are also NP–complete

From TSP to HC

- Fact: **HC is polynomially reducible to TSP**
- Assume `tsp(V, c)` is a routine that returns the TSP solution for G with cost c and consider the following routine for HC:

```
def tsp_2_hc(V, E):
    for any u, v in V:
        if (u, v) in E:
            c(u, v) = 1
        else:
            c(u, v) = 2

    p = tsp(V, c)
    if cost(p) == |V|:
        return p
```

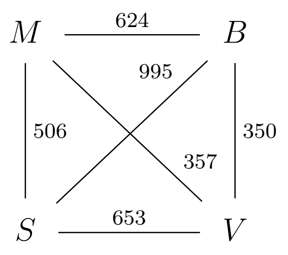
- `tsp_2_hc` solves HC for π is a HC on G iff $c(\pi) = |V|$
- Thus TSP has not only practical but also theoretical interest

A TSP Example

- Simple example:

```
cities = ["madrid", "barcelona", "sevilla", "valencia"]
```

- The (complete) graph is



- And distances given by a 4×4 Numpy matrix

A Greedy TSP Solution

- Simple greedy approach: Nearest–Neighborhood (NN) TSP, that simply visits the nearest unseen city

```
def nn_tsp_circuit(distance_matrix, node_ini=0):

    num_cities = distance_matrix.shape[0]
    circuit = [node_ini]

    while len(circuit) < num_cities:
        current_city = circuit[-1]

        # sort cities in ascending distance from current
        options = list(np.argsort(distance_matrix[ current_city ]))

        # add first city in sorted list not visited yet
        for city in options:
            if city not in circuit:
                circuit.append(city)
                break

    return circuit + [node_ini]
```

What Can We Do About TSP?

- On average, NN gives a path that is about 25% longer than the optimum
- But one can set up special instances of TSP where NN gives the worst route
- If c satisfies the triangle inequality $c(u,v) \leq c(u,z) + c(z,v)$ for any z, we have

  $$c(\pi_{NN}) = O(\log |V|) \times c^*,$$

  with π_{NN} the NN solution and c^* the optimal cost
- TSP has great practical importance, but there is no cost effective **exact** algorithm for general graphs
- So, it may be very hard to find the best route to, say, deliver mail (at least in big cities)

Approximation Algorithms

- Alternative: **approximate** algorithms
- **Definition:** Given an optimization problem $\mathcal{P}$, an **approximate algorithm** for $\mathcal{P}$ **with bound** $\lambda \geq 1$ is an algorithm A that for every input I returns a solution $s_A(I)$ such that

  $$c^*(I) \leq c(s_A(I)) \leq \lambda c^*(I)$$

  with $c^*(I)$ the optimal cost for $\mathcal{P}$ on I

- NN is not exactly an approximate algorithm for TSP, since its bound is $O(\log |V|)$ and depends on $|V|$

Approximation Algorithms for TSP

- **Proposition:** *If the cost function is Euclidean, i.e., it verifies*

$$c(u, v) \leq c(u, w) + c(w, v) \ for \ all \ u, v, w \in V,$$

then there is an approximate algorithm for TSP with $\lambda = 2$

- Algorithm:

```
def euclideanTSP(g, c):
  find a MST t on g
  duplicate its edges to obtain a graph g_1

  #now each node in g_1 has degree 2 and there is an EC
  find a EC p_1 in g_1

  short--cut seen edges in p_1 to get HC p
  return p
```

Approximation Algorithms for TSP

- **Proof sketch:** Let T_1, p_1 and p be the MST, the Eulerian and the returned circuits in the previous algorithm

  Let p^* be an optimal HC and remove an edge on p^* to get a spanning tree T^*

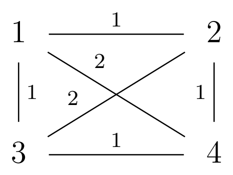
  - Since T_1 is an MST, we have $c(T_1) \leq c(T^*) \leq c(\pi^*)$
  - And using the Euclidean distance property, we then we conclude that

$$c(\pi) \leq c(\pi_1) = 2c(T_1) \leq 2c(\pi^*)$$

- The **Christofides** algorithm improves this to $\lambda = 1.5$
- To learn more: Johnson, McGeoch, The Traveling Salesman Problem: A Case Study in Local Optimization
  - Or the movie The Travelling Salesman

Approximation Algorithms for TSP II

- **Example**



4 An Excursion on DNA Sequencing

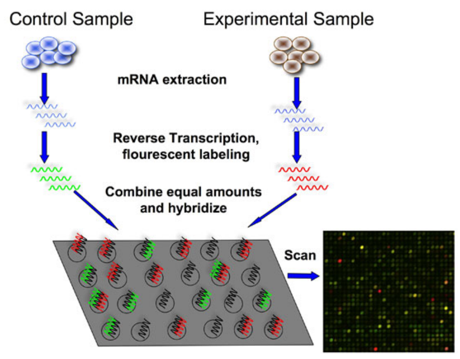
4.1 Hamilton, Euler and DNA Sequencing

DNA Sequencing

- **Note:** this is a very, very light description of DNA Sequencing
- Goal: decompose a gene into a sequence of four letters $\{A, C, G, T\}$ that correspond to DNA **bases**
- **Shotgun sequencing** follows a four step process:
  - Blast the gene into random short fragments ("reads") of 100–500 bases
  - Identify read subsequences by hybridizing them on a DNA microarray
  - Reconstruct each read from these subsequences
  - Reconstruct the entire gene from the reads
- First two steps: biochemistry
- Third step: Hamiltonian or (better) Eulerian circuits
- Fourth step: compute the Shortest Superstring Problem solving TSP (plus more algorithms and a lot of biochemistry)

Sequencing by Hybridization II

- Scheme of the process:


Control Sample
Experimental Sample
mRNA extraction
Reverse Transcription, flourescent labeling
Combine equal amounts and hybridize
Scan

From *bitesizebio.com/7206/introduction-to-dna-microarrays*

Microarray Hybridization

- Put all the posible lenght ℓ probes, i.e., DNA subsequences of a fixed lenght ℓ, into the spots of a microarray
- Put a drop of fluorescently labeled DNA into each microspot of the array
- The DNA fragment hybridizes with those microspots that are complementary to a certain substring of length ℓ of the fragment
- This way we get all possible lenght ℓ subsequences that make the fragment but they are **unordered**

ℓ–mers and the Spectrum

- We call the sequence on each one of the probes an **ℓ–mer**
- The **ℓ–spectrum** $sp(S, \ell)$ of a sequence S is the set of all the ℓ–mers from S
- For instance, `S = [TATGGTGC]` we have

  ```
  sp(S, 3)= {TAT, ATG, TGG, GGT, GTG, TGC}
  ```
- We have $|sp(S, \ell)| \leq |S| - \ell + 1$
- After hybridization, the hybridized probes in the microarray give us **an unordered version of** $sp(S, \ell)$ that we have to correct to recover S
- The overlap $\omega(s_1, s_2)$ between two ℓ–mers s_1, s_2 is the longest leght of a suffix of s_1 that is also a prefix of s_2

- We clearly have $\omega(s_1, s_2) \leq \ell - 1$ and if s_2 follows s_1 in S, we must have $\omega(s_1, s_2) = \ell - 1$

Sequencing by Hamiltonian Paths

- We can reconstruct the sequence S by finding an ordering $s_{i_1}, \ldots, s_{i_K}$ of $sp(S, \ell)$ such that $\omega(s_{i_j}, s_{i_{j+1}}) = \ell - 1$
- This suggests to define the graph $G_\ell(S) = (V_\ell, E_\ell)$ where
  - $V_\ell = sp(S, \ell)$ and
  - $(s, s') \in E_\ell$ iff $\omega(s, s') = \ell - 1$
- Notice that reconstructing S is equivalent to pass once through all the nodes of $G_\ell(S)$
- In other words, we can reconstruct S by finding a Hamiltonian path in $G_\ell(S)$

Sequencing by Hamiltonian Paths II

- **Example:** consider `S = [TATGGTGC]` and the unordered 3–spectrum

```
sp(S, 3)= {GGT, TAT, TGG, TGC, ATG, GTG}
```

Sequencing by Eulerian Paths

- The obvious problem of HP sequencing is the lack of efficient algorithms to solve the HP problem
- The alternative is to try to have ℓ–mers on the edges instead of on nodes
- If $s \in sp(S, \ell)$ and s_1 is its $\ell - 1$ prefix and s_2 its $\ell - 1$ suffix, we can consider s as the edge connecting nodes s_1 and s_2

  - Now we have $\omega(s_1, s_2) = \ell - 2$

- We define now the graph $G_{\ell-1} = (V_{\ell-1}, E_{\ell-1})$ where
  - $V_{\ell-1} = sp(S, \ell - 1)$ and
  - $(s, s') \in E_{\ell-1}$ iff they are respectively prefix and suffix of an $s \in sp(S, \ell)$
- Notice that now reconstructing S is equivalent to pass once over all the edges of $G_{\ell-1}$
- In other words, we can reconstruct S by finding a EP in $G_{\ell-1}$

Eulerian Circuits on Directed Graphs

- However, notice that $G_{\ell-1}$ is a **directed** graph and we have to adapt the Eulerian circuit/path theory to these graphs
- In an directed graph $G(V, E)$ we have to distinguish between incident and adjacent edges
- For any $u \in V$, we say that (u, v) is an **adjacent** (outgoing) edge and (w, u) an **incident** (incoming) edge
- The **indegree** $in(u)$ of u is the number of incoming edges to u
- The **outdegree** $out(u)$ is the number of outgoing edges from u

Eulerian Circuits on Directed Graphs II

- Assume that $\pi = \{(u = u_0, u_1), \ldots, (u_{K-1}, u_K = u)\}$ is an Eulerian circuit on G
- If $w \neq u$ is a node in π, each time we enter w we substract 1 from $in(w)$ and also from $out(w)$ when we leave w
- Since at the end we have passed through all the edges of w, we must have at the beginning $in(w) = out(w)$
- Similarly each time we enter u inside π we substract 1 from $in(u)$ and also from $out(u)$ when we leave it

  Moreover, when we start we substract 1 from $out(u)$ and also substract 1 we substract 1 from $in(u)$ when we finish

- Thus, we must also have $in(u) = out(u)$

Euler‘s Theorem for Directed Graphs

- **Euler’s Theorem.** *A neccesary and sufficient condition to have an EC in a directed G is that $in(v) = out(v)$ for all $v \in V$*
- **Corollary.** *A neccesary and sufficient condition to have an Eulerian path $\pi = \{(u = u_0, u_1), \ldots, (u_{K-1}, u_K = v\}$ in a directed graph G is that we have $in(w) = out(w)$ for all $w \in V$ different from u and v and also $in(v) = out(v) + 1$, $in(u) = out(u) - 1$*
- Essentially the same $O(|E|)$ algorithm we saw for undirected graphs can be applied to directed ones
- Thus we can efficiently sequence genomic reads

Eulerian Sequencing

- **Example:** consider again `S = [TATGGTGC]` and

```
sp(S, 2)= {TA, AT, TG, GG, GT, GC}
```

4.2 From Reads to the Genome

The Shortest Superstring Problem (SSP)

- Given a string set $\{s_1, \ldots, s_M\}$, find the **shortest superstring S that contains the M substrings s_j**
- Recall that the **overlap** $\omega_{i,j}$ between strings s_i, s_j is the lenght of the longest suffix of s_i that is also a prefix of s_j

- Notice that the lenght of the shortest string containing first s_i and then s_j is $|s_i| + |s_j| - \omega_{i,j}$ where $|s|$ denotes the lenght of s
- If we add another string s_k after s_j, the extra added lenght is $|s_k| - \omega_{j,k}$
- Thus, if we get S' collating the ordering $\{s_{i_1}, \dots, s_{i_M}\}$ then

$$\begin{aligned} |S'| &= |s_{i_1}| + |s_{i_2}| - \omega_{i_1,i_2} + |s_{i_3}| - \omega_{i_2,i_3} + \dots \\ &= \sum_1^M |s_j| - \sum_1^{M-1} \omega_{i_j,i_{j+1}} \end{aligned}$$

The Longest Path Problem (LPP)

- As an example, if we collate this way the strings
  `'ATGGTAG'` , `'GTAGACTA'` , `'CTAGGTATT'`
  we get the sequence `'ATGGTAGACTAGGTATT'` of lenght $17 = 7 + 8 + 9 - 4 - 3$
- Clearly $|S'|$ will be minimal iff $\sum_1^{M-1} \omega_{i_j,i_{j+1}}$ is maximal
- Consider the complete graph G over $V = \{s_1, \dots, s_M\}$ and with cost $\omega_{i,j}$
- Solving the Shortest Superstring Problem is thus equivalent to solving the **Longest Path Problem(LPP)** in (G, ω): to find a cycle–free path of maximal lenght

LPP and Hamiltonian Paths

- A Hamiltonian path (HP) is a path that passes over all the $|V|$ vertices once
- It can be shown that HC reduces polynomially to HP (the argument is easy but not totally obvious)
- Consider LPP–d, the decision version of LPP: given a graph G and c, to decide whether there is an acyclic path in G with lenght $\geq c$
- It is easy to see that LPP–d is in NP
- It is also easy to see that HP reduces to LPP–d: there is a HP in G iff LPP–d over $(G, |V| - 1)$ returns 1
- As a consequence, if HC is NP–complete, so is HP and so is LPP–d
- In general, if P_1 is NP–complete and it reduces polinomially to P_2, P_2 is also NP–complete

How to Create New NP–complete Problems

- Assume T is the reduction operator from P_1 to P_2 with cost $O(|I|^p)$ when applied to an input I of P_1
- If P' is another problem that reduces polinomially to P_1 via T', $T \circ T'$ **reduces P' to P_2 with polynomial cost**
- In fact, if $I = T'(I')$ with I' an input of P' with size n and T' has cost $O(n^q)$, we have $|I| = O(n^q)$, for the size of the ouputs of T' cannot be larger than the cost of computing them
- But the cost of applying $T \circ T'$ to I' is $O(n^q + (n^q)^p) = O(n^{pq})$
- Thus, if a NP problem reduces polynomically to P_1, so it does to P_2
- Thus, if P_1 is NP–complete, so is P_2
- Thus, if we manage to prove HC to be NP–complete, so is HP and so is LPP–d. And so is TSP–d

Another Look at SSP

- Alternatively, assume we decompose two sequences s and t as

$$s = pre_{st} + over_{st}; \quad t = over_{st} + suf_{st}$$

  with pre, $over$ and suf the prefix, overlap and suffix of s and t and $+$ the concatenation operator
- For instance, for `s = ATGGTAG`, `t = GTAGACTA`, we have `tpre_s = ATG`, `tover_s= GTAG`, `tsuf_s = ACTA`
- Then the shortest superstring $s \circ t$ of s and t is

$$pre_{st} + over_{st} + suf_{st} = s + suf_{st} = pre_{st} + t$$

- Now, concatenating s_i, s_j, s_k to get s_{ijk}, we have $s_{ijk} = s_i \circ (s_j \circ s_k) = s_i \circ s_{jk}$, i.e.,

$$s_{ijk} \quad = \quad s_i \circ s_{jk} = pre_{ij} + s_{jk} = pre_{ij} + pre_{jk} + s_k$$

- But $s_k = pre_{k\ell} + over_{k\ell}$ for any other s_ℓ

SSP and TSP

- Thus, choosing $\ell = i$, $s_{ijk} = s_i \circ (s_j \circ s_k) = pre_{ij} + pre_{jk} + pre_{ki} + over_{ki}$
- Therefore, setting $\rho_{i,j} = |pre_{ij}|$ and $\omega_{i,j} = |over_{ij}|$ we have

$$|s_{ijk}| = \rho_{i,j} + \rho_{j,k} + \rho_{k,i} + \omega_{k,i}$$

- Therefore, collating $\{s_{i_1}, \ldots, s_{i_M}\}$ to get a possible SS S', we have

$$|S'| = \sum_1^{M-1} \rho_{i_j,i_{j+1}} + \rho_{i_M,i_1} + \omega_{i_M,i_1}$$

- Consider the complete graph G defined by the M sequences s_k with cost ρ_{ij}
- Then, if ρ^* is the optimal cost of TSP on G we have

$$\begin{aligned} |S'| &= \sum_1^{M-1} \rho_{i_j,i_{j+1}} + \rho_{i_M,i_1} + \omega_{i_M,i_1} \geq \rho^* + \omega_{i_M,i_1} \\ &\geq \rho^* + \min_j \{\omega_{i_j,i_{j+1}}\} \geq \rho^* \end{aligned}$$

Solving SSP and LPP

- Thus, the solution of TSP on the complete graph over the s_j with cost $c(i,j) = \rho_{i,j}$ gives a lower bound on the lenght of the shortest superstring
- The relationship between SPP and TSP hints that SPP–d is also NP–complete (and it is so)
- Both SSP and LPP are NP–hard
- There are approximation algorithms for SSP with a 2.5 bound
- But LPP is much harder to approximate
- For directed acyclic graphs (DAGs) LPP can be solved in linear time using the Topological Order algorithm

Back to Genome Sequencing

- Recall the four steps of the process:
  - Blast the gene into individual short fragments ("reads")
  - Identify read subsequences by hybridizing them on a DNA microarray
  - Reconstruct each read from these subsequences
  - Reconstruct the gene from the reads
- Biochemistry provides the first two and Computer Science (CS) can be applied to the last two steps and will give a plausible genome
- But: is it the one we started with?
- Not obvious in principle: much more Biochemistry needed!!

5 Depth First Search and Connectivity

5.1 Depth First Search

Breadth First Search (BFS)

- Recall the general pseudocode for BFS

```
def BFS(u, G):
    s[ ] = False; p[ ] = NULL; Q = pq()
    d[u] = 0; Q.put( (d[u], u) )
    do_something(u)
    while not Q.empty():
        (d, v) = Q.get()
        if not s[v]:
            s[v] = True
            for all z adjacent to v:
                do_something(z) #perhaps change d[z]
                if d[z] smaller:
                    p[z] = v; Q.put( (d[z], z) )
    return p
```

- If the cost of `do_something` is $O(1)$ and we work with a PQ, the cost of BFS is $O(|E| \log |V|)$ (which can be improved using more sophisticated PQ implementations)
- If we only need simple queue, we get a linear cost $O(|E|)$
- If needed, we add a driver to restart BFS at unseen nodes

Depth First Search (DFS)

- The alternative to BFS is recursive DFS

```
def DFS(u, G):
    s[u] = True
    do_something_before_DFS(u)
    for all w adjacent to u:
        if s[w] == False:
            p[w] = u
            DFS(w, G)
    do_something_after_DFS(u)
```

- The table `p[ ]` defines the DFS tree (or forest)

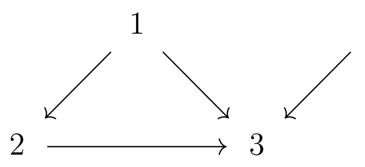
Depth First Search II

- We may have to restart DFS if not all nodes have been processed

- We need a driver for DFS

```
def driver_DFS(G):
    v[ ] = F; p[ ] = NULL
    for all u in V:
        if v[u] == F:
            DFS(u,G)
```

- An example:



- If doing something has cost $O(1)$, the joint cost of `driver_DFS` and `DFS` is clearly $O(|E|)$

Edge Classification by DFS

- DFS induces a classification on the edges of G

  - **Tree edges**: (u, v) where $u = p[v]$
  - **Back (ascending) edges**: (u, v) where $v = p[\dots p[u] \dots]$ (one or more p)
  - **Forward (descending) edges**: (u, v) where $u = p[\dots p[v] \dots]$ (with at least 2 p)

  - **Cross edges**: any other $(u, v) \in E$

- If G is undirected and (u, v) is a forward edge, then (v, u) is a back edge
  - Thus, we will not distinguish then between forward and back edges
- We prove next that if G is undirected there are no cross edges

Parenthesis Theorem

- Assume we have a counter c in DFS and consider 2 time–stamps:
  - **Discovery**: $d_u = c; c+ = 1$, updated when DFS **starts** on u
  - **Finish**: $f_u = c; c+ = 1$, updated when DFS **ends** on u
- Obviously $d_u < f_u$
- **Parenthesis Theorem.** *For a graph G and $u, v \in V$, consider the intevals $I_u = (d_u, f_u)$, $I_v = (d_v, f_v)$. Assuming $d_u < d_v$ we either have $I_v \subset I_u$, or $I_u \cap I_v = \emptyset$*
- **Proof sketch:** Assume $d_u < d_v$;
  - If $f_u < d_v$, obviously $I_u \cap I_v = \emptyset$
  - And if $f_u > d_v$, DFS recursively started on v before finishing with u; thus the recursion on v must finish before that of u and $f_v < f_u$
  - Thus, $I_v \subset I_u$

No Cross Edges in Undirected Graphs

- **Corollary.** *If G is undirected there are no cross edges*
- **Proof sketch:** Take $(u, v) \in E$:
  - Assume $d_u < d_v$; then we have $f_v < f_u$ for v is adjacent to u
  - If $s[v] = F$ when we arrive at v, then (u, v) is a tree edge
  - And if $s[v] = T$ when we arrive at v, we have processed $L[v] \Rightarrow$ we have processed (v, u), that must be a back edge
  - Thus, (u, v) is a forward edge
- Thus, in no case is (u, v) a cross edge

5.2 Biconnected Graphs

Undirected Graph Connectivity

- Recall that an undirected graph $G = (V, E)$ is connected if for every pair $u, v \in V$ there is a path π in E from u to v
- **Connected component**: a maximal connected subgraph of G
- If $G_i = (V_i, E_i)$ are the connected components of G, the V_i are a **partition** of V and the E_i of E
- If we order the vertices of G as $V = V_1 \cup \ldots \cup V_K$, then the adjacency matrix M is **block diagonal** with the blocks M_k being the adjacency matrices of the G_k
- BFS can be used to give the connected components of G through the table $p[\ ]$ just counting how many nodes u verify $v[u] = V$ and restarting BFS if it is $< |V|$
- DFS and its driver can also be used to give the connected components of G through the table $p[\ ]$

An Aside: Directed Graph Connectivity

- A directed graph $G = (V, E)$ is **weakly connected** if its extension to an undirected graph is connected
- A directed graph $G = (V, E)$ is **strongly connected** if for every pair $u, v \in V$ there is a path π in E from u to v
- DFS is also used in **Tarjan's Algorithm** to obtain the strong components of a graph
- Tarjan's algorithm basically obtains the strong components computing DFS's ending times on G and applying again DFS to the transpose graph G^τ in the order inverse to the ending times

Articulation Points

- If G is undirected and connected, a **cut vertex** or **articulation point (AP)** is a vertex u such that

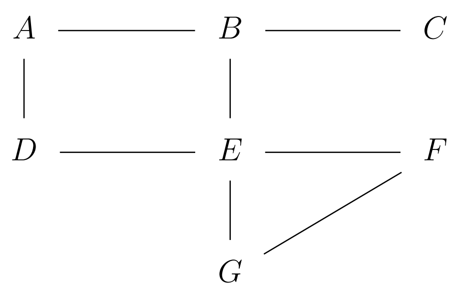
$$G' = (V - \{u\}, E - \{(u, z) \in E\})$$

  is no longer connected

- An undirected and connected graph G is **biconnected** if it has no articulation points
- Biconnected graphs are desirable in computer networks, as they are more robust against router failures
- Q: how we detect APs?

How to Detect APs?

- An example: the graph below has two APs, B and E



- If we apply DFS ...

DFS and Articulation Points

- The example shows that the DFS tree gives a "top–bottom" view of a graph in which
  - APs other than the root disconnect lower parts of the graph
  - An AP at the root disconnects subtrees
- We can use two auxiliary tables to detect articulation points that can be computed by DFS
  - The **order** table $o[\,]$ that contains the order in which DFS arrives at a node u.
  - The **ascent** table $a[\,]$ which is defined as $a[u] = \min\{o[v]\}$ where v is any node that can be accessed from u by
    * Going "down" through 0, 1 o more tree edges, and then

- Going“up” through a single back edge

Detecting Articulation Points

- Clearly if we remove a non root node u from the DFS tree, it will disconnect one of its children v unless v can go “above” $o[u]$ using back edges,
- In other words, u **will be an AP if for some child** v **we have** $o[u] \leq a[v]$
  - Notice that a larger number means a “lower” node
- Since there are no cross edges on the DFS tree, **the root node will be an AP if it has two or more children**
- It is also clear that these sufficient conditions are also neccessary
  - A single root node cannot be an AP
  - If all children of u bypass it, u cannot be an AP

Computing $o[\,]$ and $a[\,]$

- We compute $o[u]$ **before** DFS explores u’s adjacency list
- We can use two auxiliary tables to compute the table $a[\,]$
- The **direct ascent** table $o'[u]$ that contains the order of highest node accessible from u by an ascending edge

$$o'[u] = \min\{o[v] : (v, u) \text{ is a back edge}\}$$

  $o'[u]$ can be computed **before** DFS looking at the w adjacent to u s.t. $v[w] == T$

- The **ascent by children** table $a'[u]$ that contains the order of highest node accessible from any of the children of u

$$a'[u] = \min\{a[v] : u = p[v]\}$$

  $a'[u]$ can be computed **after** the recursive call to DFS returns

- We then have $a[u] = \min\{o[u], o'[u], a'[u]\}$

Computing $o[\,]$ and $a[\,]$ II

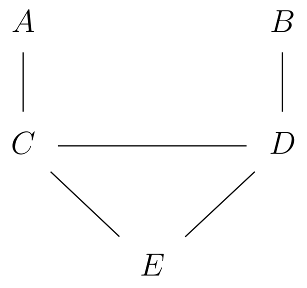
- Assume the DFS driver has initialized $o[\,]$ and $a[\,]$ to ∞ and a counter c to 0
- We compute $o[\,]$ and $a[\,]$ recursively as follows

```
def ap_tables(u, G):
    s[u] = True; o[u] = c; a[u] = o[u]; c += 1
    for all w adjacent to u: # direct ascent
        if s[w] == True and w != p[u] and o[w] < a[u]:
            a[u] = o[w]
    for all w adjacent to u:
        if s[w] == False:
            p[w] = u; ap_tables(w, G)
    for all w adjacent to u: # ascent by children
        if p[w] == u and a[u] > a[w]:
            a[u] = a[w]
```

- The cost of `ap_tables` is clearly $O(|E|)$

Algorithm Application

- An example:



5.3 DAGs, Topological Sort and Project Graphs

Directed Acyclic Graphs

- A **directed acyclic graph** (DAG) is a directed graph without cycles
- **Proposition:** G is a DAG iff there are no ascending edges in G
  - If (v, u) is ascending, there is a path from u to v in the DFS forest, and adding (v, u) results in a cycle
  - Assume π is a cycle and let $u \in V_\pi$ be the first node processed in DFS and assume (v, u) in E_π

Then it can be shown that v descends from u in the DFS forest and, thus, (v, u) is ascending

- DFS can be used to detect cycles in a graph modifying our previous AP algorithm
- DAGs can be used to model many problems of interest

Topological Sort

- Recall: $\leq$ is a **total order** if either $u \leq v$ or $v \leq u$ or both
- A **topological sort** in a DAG $G = (V, E)$ is a total ordering of its vertices s.t. if $(u, v) \in E$, then $u \leq v$
- If G is a DAG, a topological sort can be obtained
  - Applying DFS starting at u with $inc[u] = 0$ (there is always one) and
  - Adding a vertex u at the beginning of a linked list after DFS ends its process
- We end up with a topological sort of G:
  - Since DFS ended at v **after** processing of the vertices w adjacent to v, then these w are in the list **after** v
- The cost of TS on DAGs is thus $O(|E|)$

Applying Topological Sort

- An example:

$$\begin{tikzcd}
1 \arrow[rr] & & 2 & \\
& 3 \arrow[ul] \arrow[ur] \arrow[dl] \arrow[dr] & & 6 \arrow[ul] \\
4 \arrow[uu] \arrow[rr] & & 5 \arrow[uu] \arrow[ur] &
\end{tikzcd}$$

Single Source Shortest Paths in DAGs

- A source in a DAG is a node with incidence 0

- TS can be used to find shortest paths in a weighted single source DAG with linear cost, i.e., better than Dijkstra's
- The psc is

```
def dist_min_DAG(G):
    L = OT(G)
    d[ ] = np.inf; p[ ] = NULL
    d[ L[0] ] = 0 #the source is the first node in L
    while L not empty:
        u = L.pop(0)
        for all v adjacent to u:
            if d[v] > d[u] + c(u,v):
                d[v] = d[u] + c(u,v); p[v] = u
    return d, p
```

- Easy exercise: change `dist_min_DAG` to another `dist_max_DAG` that computes **longest paths**

Finding Shortest Paths in a DAG

- An example:

$$\begin{tikzcd}
1 \arrow[rr, "4"] & & 2 & \\
& 3 \arrow[ul, "2"'] \arrow[ur, "6"] \arrow[dl, "1"] \arrow[dr, "1"] & & 6 \arrow[ul, "1"'] \\
4 \arrow[uu, "0"] \arrow[rr, "1"] & & 5 \arrow[uu, "4"] \arrow[ur, "1"] &
\end{tikzcd}$$

Project Graphs

- A **project graph** (PG) is a DAG P
  - With a single node S with $inc[S] = 0$ and a single F with $adj(F) = 0$
  - The other nodes u correspond to tasks and have associated a time cost $t(u)$
  - Edges denote task dependences
- As such they are not weighted graphs
- A **milestone graph** is a weighted DAG version P_M of a PG P where if several tasks $u, v, \ldots$ converge in another z
  - An extra node z' and edge (z', z) with cost $t(z)$ is added

  - The edges $(u, z), (v, z), \dots$ are converted to $(u, z'), (v, z'), \dots$ with weights $c(w, z') = 0$

- If only task u incides in v, we have $c(u, v) = t(v)$

Critical Paths in Project Graphs

- The quantity of interest is $T(F)$, the **minimum time** needed to arrive at F, i.e., to complete the project
- $T(F)$ coincides with the length of the **longest path** from S to F in the milestone graph P_M
- Such a path is a **critical path**: any delay in any milestone node implies a delay in the project
- We can define for a milestone node v
  - Its **minimum arrival time** $T_{min}(v)$: the length of the longest path from S to v
  - Its **maximum departure time** $T_{max}(v)$: the latest time at which v can be completed without delaying the project
  - Its **slack** time $S(v) = T_{max}(v) - T_{min}(v)$
- Any node w in a critical path verifies $S(w) = 0$.
- Solving LPP on DAGs is at the core of the **Program Evaluation and Review Technique (PERT)** for project management