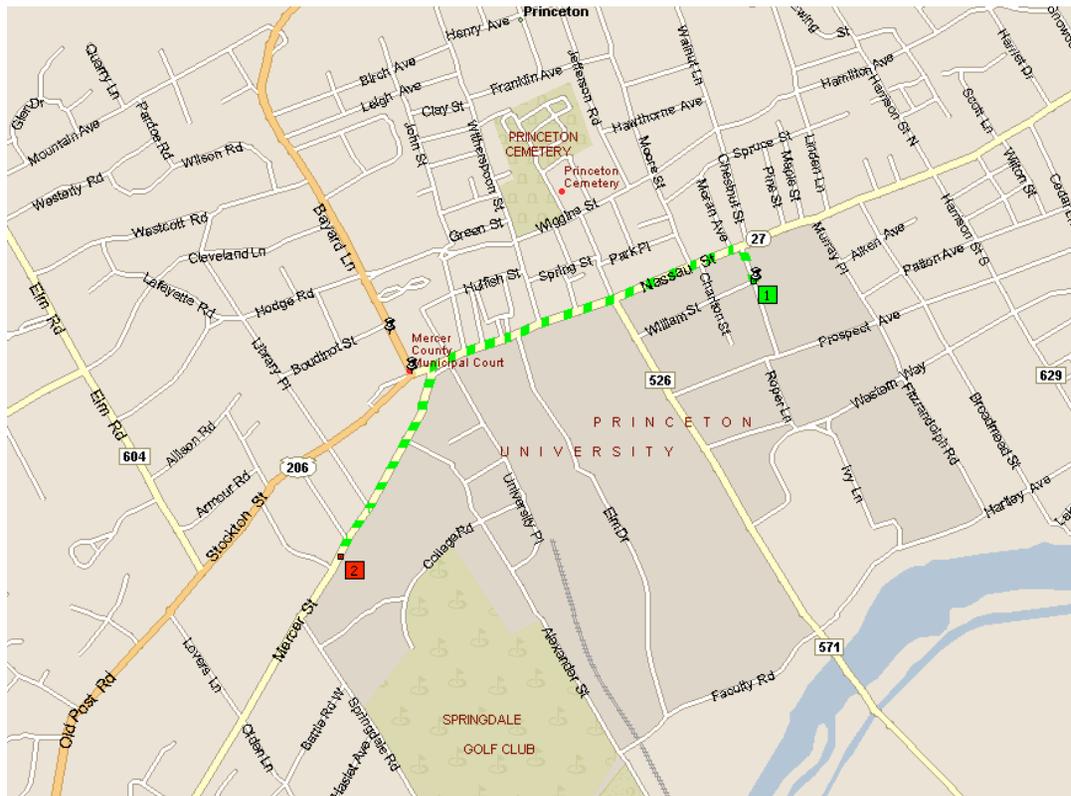


## 4.4 Shortest Paths in a Graph



shortest path from computer science department to Einstein's house

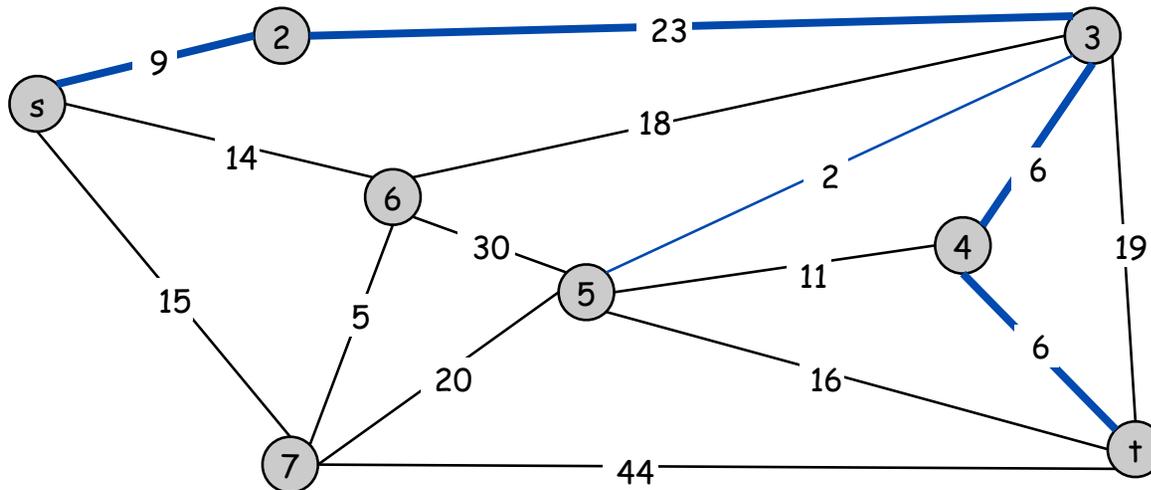
# Shortest Path Problem

## Shortest path network.

- Directed graph  $G = (V, E)$ .
- Source  $s$ , destination  $t$ .
- Length  $\ell_e =$  length of edge  $e$  ( $\ell_e \geq 0$ ).

Shortest path problem: find shortest directed path from  $s$  to  $t$ .

cost of path = sum of edge costs in path



Cost of path  $s-2-3-5-t$   
 $= 9 + 23 + 6 + 6$   
 $= 44.$

# Dijkstra's Algorithm

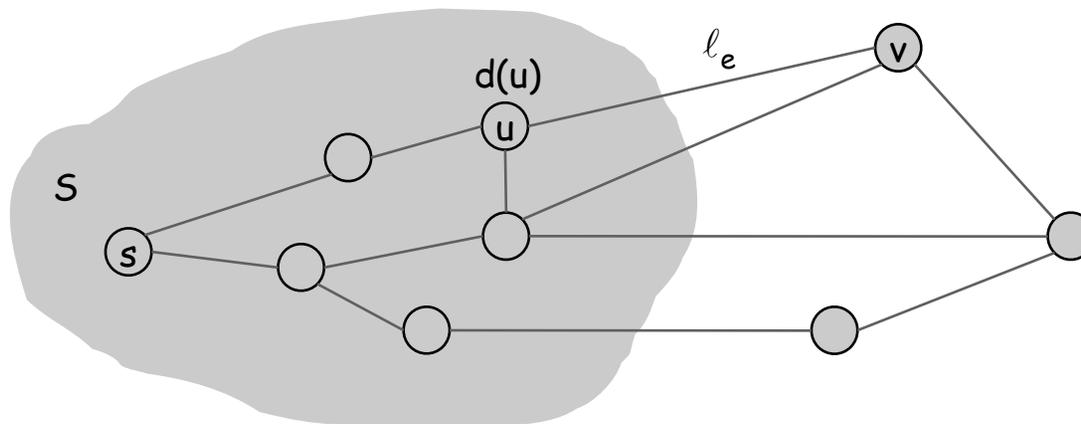
## Dijkstra's algorithm.

- Maintain a set of **explored nodes**  $S$  for which we have determined the shortest path distance  $d(u)$  from  $s$  to  $u$ .
- Initialize  $S = \{s\}$ ,  $d(s) = 0$ .
- Repeatedly choose unexplored node  $v$  which minimizes

$$\pi(v) = \min_{e = (u,v) : u \in S} d(u) + \ell_e,$$

add  $v$  to  $S$ , and set  $d(v) = \pi(v)$ .

shortest path to some  $u$  in explored part, followed by a single edge  $(u, v)$



# Dijkstra's Algorithm

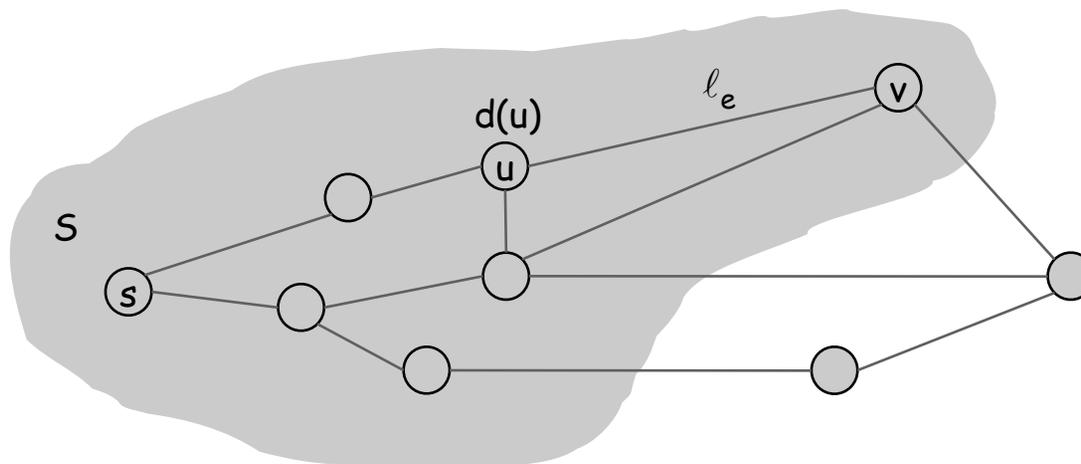
## Dijkstra's algorithm.

- Maintain a set of **explored nodes**  $S$  for which we have determined the shortest path distance  $d(u)$  from  $s$  to  $u$ .
- Initialize  $S = \{s\}$ ,  $d(s) = 0$ .
- Repeatedly choose unexplored node  $v$  which minimizes

$$\pi(v) = \min_{e = (u,v) : u \in S} d(u) + \ell_e,$$

add  $v$  to  $S$ , and set  $d(v) = \pi(v)$ .

shortest path to some  $u$  in explored part, followed by a single edge  $(u, v)$



## Dijkstra's Algorithm: Proof of Correctness

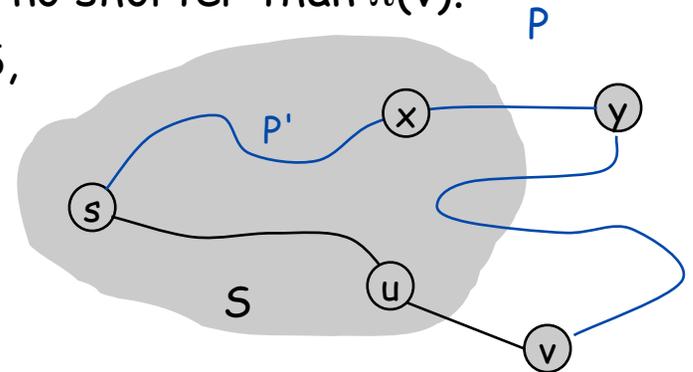
**Invariant.** For each node  $u \in S$ ,  $d(u)$  is the length of the shortest  $s$ - $u$  path.

**Pf.** (by induction on  $|S|$ )

**Base case:**  $|S| = 1$  is trivial.

**Inductive hypothesis:** Assume true for  $|S| = k \geq 1$ .

- Let  $v$  be next node added to  $S$ , and let  $u$ - $v$  be the chosen edge.
- The shortest  $s$ - $u$  path plus  $(u, v)$  is an  $s$ - $v$  path of length  $\pi(v)$ .
- Consider any  $s$ - $v$  path  $P$ . We'll see that it's no shorter than  $\pi(v)$ .
- Let  $x$ - $y$  be the first edge in  $P$  that leaves  $S$ , and let  $P'$  be the subpath to  $x$ .
- $P$  is already too long as soon as it leaves  $S$ .



$$\begin{array}{ccccccc}
 \ell(P) & \geq & \ell(P') + \ell(x, y) & \geq & d(x) + \ell(x, y) & \geq & \pi(y) \geq \pi(v) \\
 \uparrow & & \uparrow & & \uparrow & & \uparrow \\
 \text{nonnegative} & & \text{inductive} & & \text{defn of } \pi(y) & & \text{Dijkstra chose } v \\
 \text{weights} & & \text{hypothesis} & & & & \text{instead of } y
 \end{array}$$

## Dijkstra's Algorithm: Implementation

For each unexplored node, explicitly maintain  $\pi(v) = \min_{e=(u,v): u \in S} d(u) + \ell_e$ .

- Next node to explore = node with minimum  $\pi(v)$ .
- When exploring  $v$ , for each incident edge  $e = (v, w)$ , update

$$\pi(w) = \min \{ \pi(w), \pi(v) + \ell_e \}.$$

**Efficient implementation.** Maintain a priority queue of unexplored nodes, prioritized by  $\pi(v)$ .

PQ Operation	Dijkstra	Array	Binary heap	d-way Heap	Fib heap †
Insert	$n$	$n$	$\log n$	$d \log_d n$	1
ExtractMin	$n$	$n$	$\log n$	$d \log_d n$	$\log n$
ChangeKey	$m$	1	$\log n$	$\log_d n$	1
IsEmpty	$n$	1	1	1	1
Total		$n^2$	$m \log n$	$m \log_{m/n} n$	$m + n \log n$

† Individual ops are amortized bounds

## Edsger W. Dijkstra

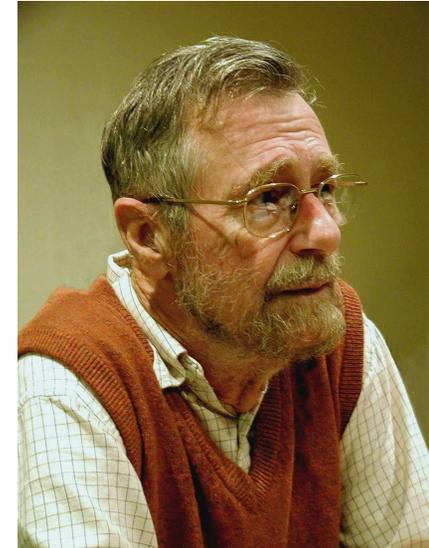
The question of whether computers can think is like the question of whether submarines can swim.

Do only what only you can do.

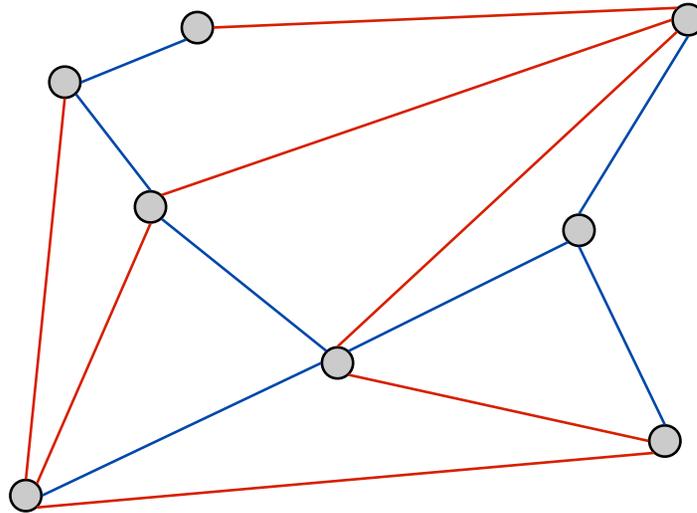
In their capacity as a tool, computers will be but a ripple on the surface of our culture. In their capacity as intellectual challenge, they are without precedent in the cultural history of mankind.

The use of COBOL cripples the mind; its teaching should, therefore, be regarded as a criminal offence.

APL is a mistake, carried through to perfection. It is the language of the future for the programming techniques of the past: it creates a new generation of coding bums.

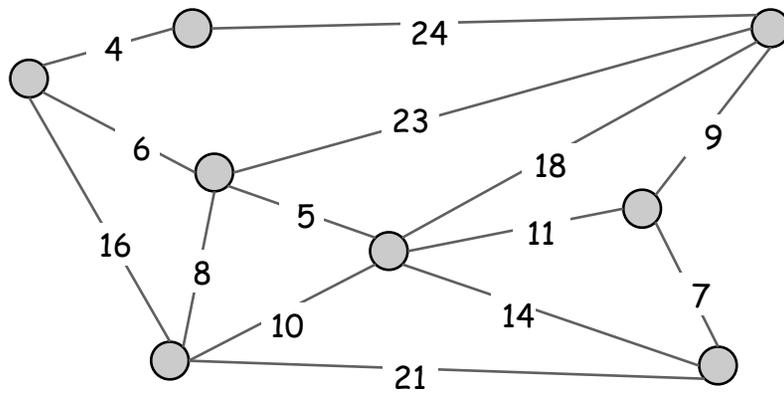


## 4.5 Minimum Spanning Tree

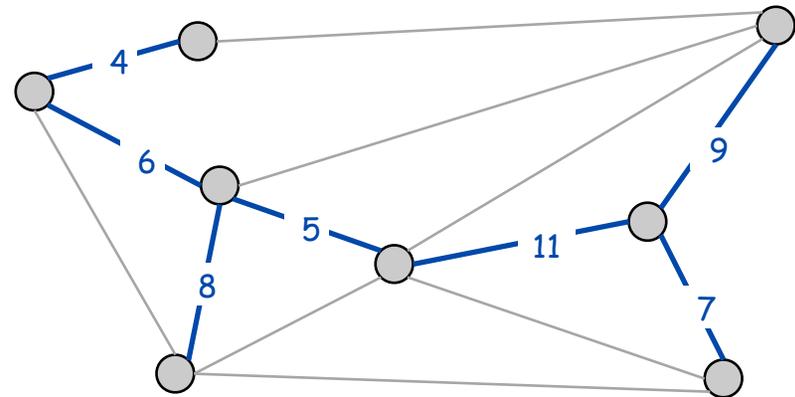


## Minimum Spanning Tree

**Minimum spanning tree.** Given a connected graph  $G = (V, E)$  with real-valued edge weights  $c_e$ , an MST is a subset of the edges  $T \subseteq E$  such that  $T$  is a spanning tree whose sum of edge weights is minimized.



$G = (V, E)$



$T, \sum_{e \in T} c_e = 50$

**Cayley's Theorem.** There are  $n^{n-2}$  spanning trees of  $K_n$ .

↑  
can't solve by brute force

# Applications

MST is fundamental problem with diverse applications.

- Network design.
  - telephone, electrical, hydraulic, TV cable, computer, road
- Approximation algorithms for NP-hard problems.
  - traveling salesperson problem, Steiner tree
- Indirect applications.
  - max bottleneck paths
  - LDPC codes for error correction
  - image registration with Renyi entropy
  - learning salient features for real-time face verification
  - reducing data storage in sequencing amino acids in a protein
  - model locality of particle interactions in turbulent fluid flows
  - autoconfig protocol for Ethernet bridging to avoid cycles in a network
- **Cluster analysis.**

## Greedy Algorithms

**Kruskal's algorithm.** Start with  $T = \phi$ . Consider edges in ascending order of cost. Insert edge  $e$  in  $T$  unless doing so would create a cycle.

**Reverse-Delete algorithm.** Start with  $T = E$ . Consider edges in descending order of cost. Delete edge  $e$  from  $T$  unless doing so would disconnect  $T$ .

**Prim's algorithm.** Start with some root node  $s$  and greedily grow a tree  $T$  from  $s$  outward. At each step, add the cheapest edge  $e$  to  $T$  that has exactly one endpoint in  $T$ .

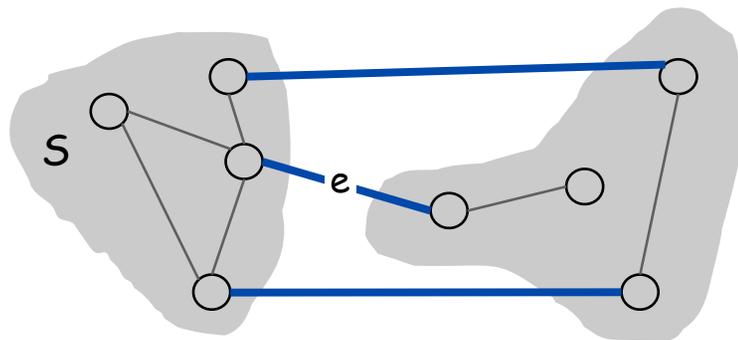
**Remark.** All three algorithms produce the MST.

## Greedy Algorithms

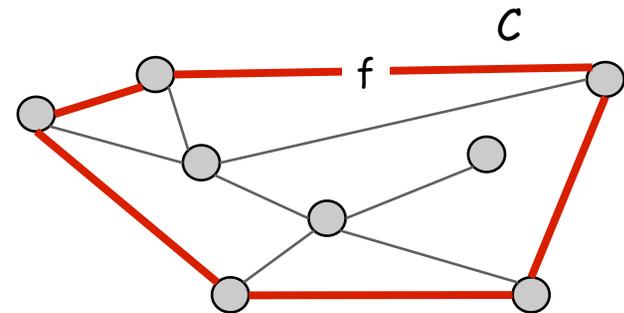
**Simplifying assumption.** All edge costs  $c_e$  are distinct.

**Cut property.** Let  $S$  be any subset of nodes, and let  $e$  be the min cost edge with exactly one endpoint in  $S$ . Then the MST contains  $e$ .

**Cycle property.** Let  $C$  be any cycle, and let  $f$  be the max cost edge belonging to  $C$ . Then the MST does not contain  $f$ .



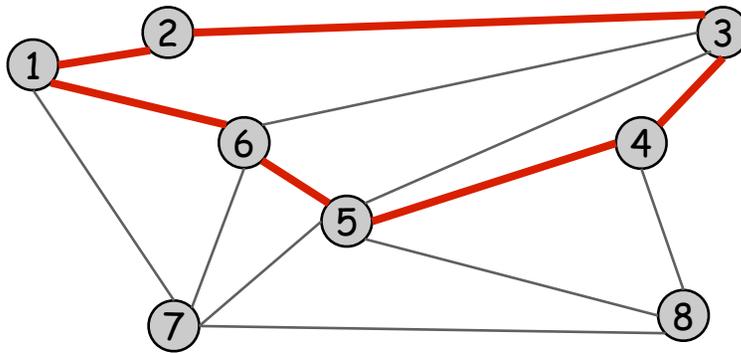
$e$  is in the MST



$f$  is not in the MST

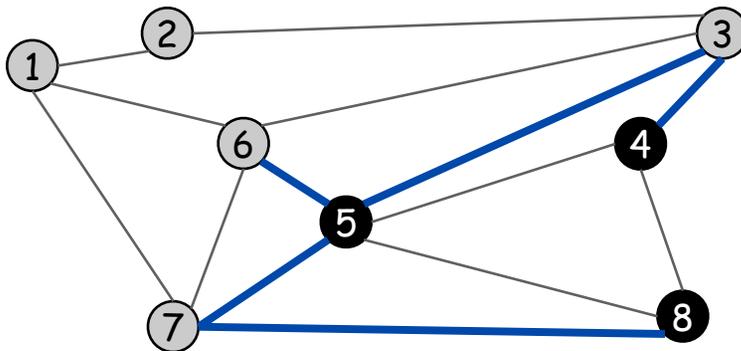
## Cycles and Cuts

**Cycle.** Set of edges the form  $a-b, b-c, c-d, \dots, y-z, z-a$ .



Cycle  $C = 1-2, 2-3, 3-4, 4-5, 5-6, 6-1$

**Cutset.** A cut is a subset of nodes  $S$ . The corresponding cutset  $D$  is the subset of edges with exactly one endpoint in  $S$ .

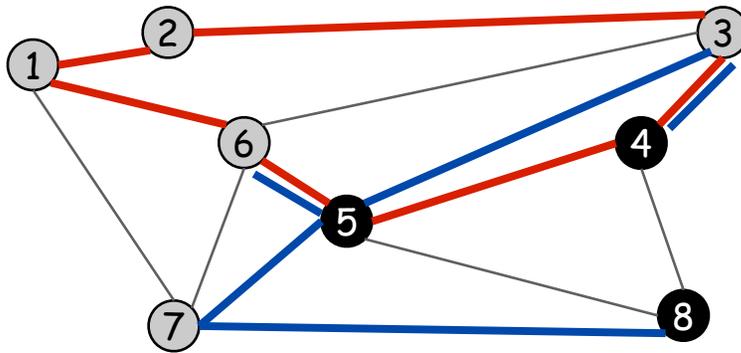


Cut  $S = \{4, 5, 8\}$

Cutset  $D = 5-6, 5-7, 3-4, 3-5, 7-8$

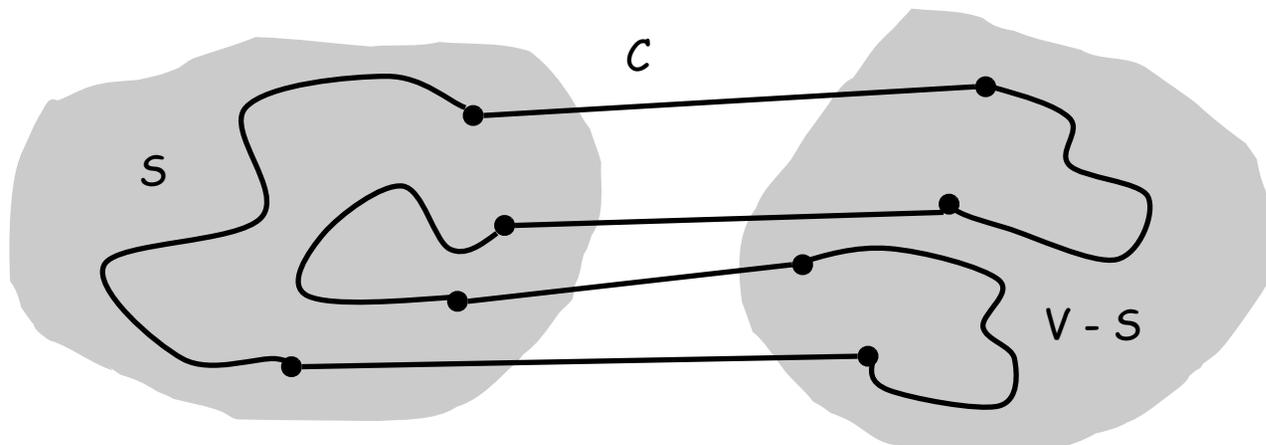
## Cycle-Cut Intersection

**Claim.** A cycle and a cutset intersect in an even number of edges.



Cycle  $C = 1-2, 2-3, 3-4, 4-5, 5-6, 6-1$   
Cutset  $D = 3-4, 3-5, 5-6, 5-7, 7-8$   
Intersection =  $3-4, 5-6$

**Pf.** (by picture)



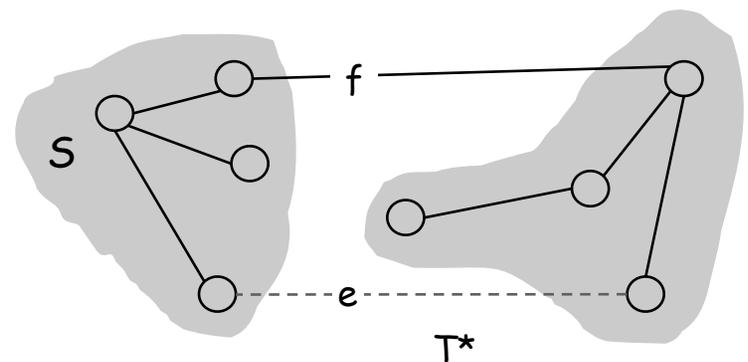
## Greedy Algorithms

**Simplifying assumption.** All edge costs  $c_e$  are distinct.

**Cut property.** Let  $S$  be any subset of nodes, and let  $e$  be the min cost edge with exactly one endpoint in  $S$ . Then the MST  $T^*$  contains  $e$ .

Pf. (exchange argument)

- Suppose  $e$  does not belong to  $T^*$ , and let's see what happens.
- Adding  $e$  to  $T^*$  creates a cycle  $C$  in  $T^*$ .
- Edge  $e$  is both in the cycle  $C$  and in the cutset  $D$  corresponding to  $S$   
 $\Rightarrow$  there exists another edge, say  $f$ , that is in both  $C$  and  $D$ .
- $T' = T^* \cup \{e\} - \{f\}$  is also a spanning tree.
- Since  $c_e < c_f$ ,  $\text{cost}(T') < \text{cost}(T^*)$ .
- This is a contradiction. ■



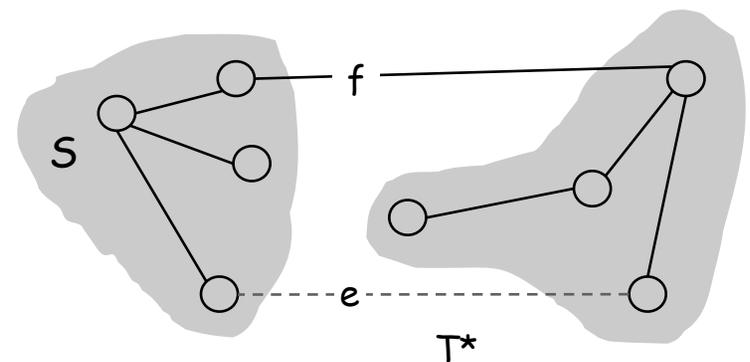
## Greedy Algorithms

**Simplifying assumption.** All edge costs  $c_e$  are distinct.

**Cycle property.** Let  $C$  be any cycle in  $G$ , and let  $f$  be the max cost edge belonging to  $C$ . Then the MST  $T^*$  does not contain  $f$ .

**Pf.** (exchange argument)

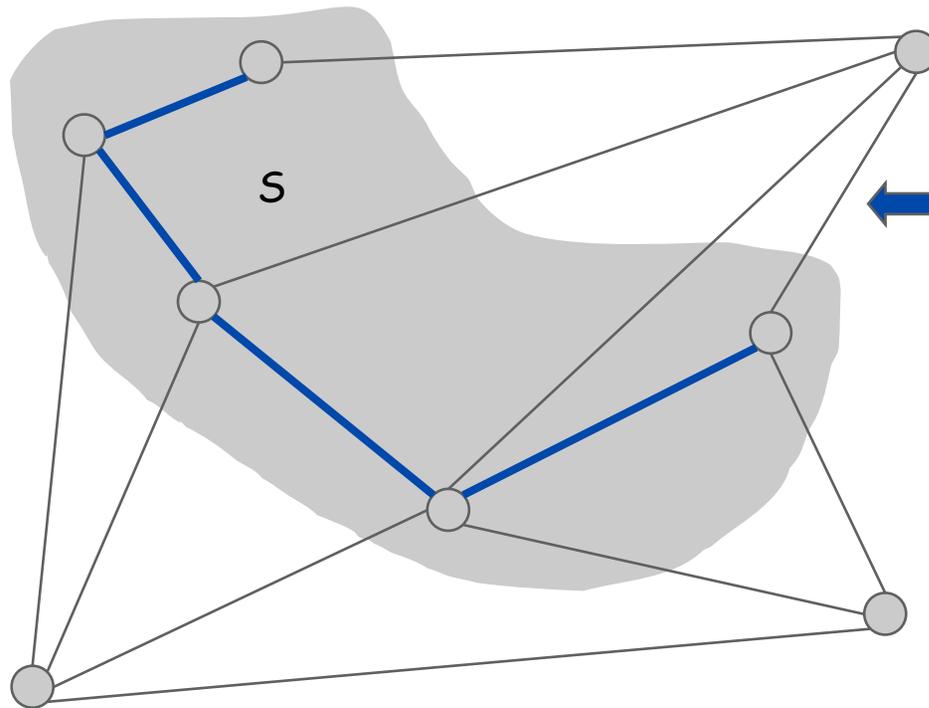
- Suppose  $f$  belongs to  $T^*$ , and let's see what happens.
- Deleting  $f$  from  $T^*$  creates a cut  $S$  in  $T^*$ .
- Edge  $f$  is both in the cycle  $C$  and in the cutset  $D$  corresponding to  $S$   
 $\Rightarrow$  there exists another edge, say  $e$ , that is in both  $C$  and  $D$ .
- $T' = T^* \cup \{e\} - \{f\}$  is also a spanning tree.
- Since  $c_e < c_f$ ,  $\text{cost}(T') < \text{cost}(T^*)$ .
- This is a contradiction. ■



## Prim's Algorithm: Proof of Correctness

Prim's algorithm. [Jarník 1930, Dijkstra 1957, Prim 1959]

- Initialize  $S =$  any node.
- Apply cut property to  $S$ .
- Add min cost edge in cutset corresponding to  $S$  to  $T$ , and add one new explored node  $u$  to  $S$ .



## Implementation: Prim's Algorithm

**Implementation.** Use a priority queue ala Dijkstra.

- Maintain set of explored nodes  $S$ .
- For each unexplored node  $v$ , maintain attachment cost  $a[v]$  = cost of cheapest edge  $v$  to a node in  $S$ .
- $O(n^2)$  with an array;  $O(m \log n)$  with a binary heap.

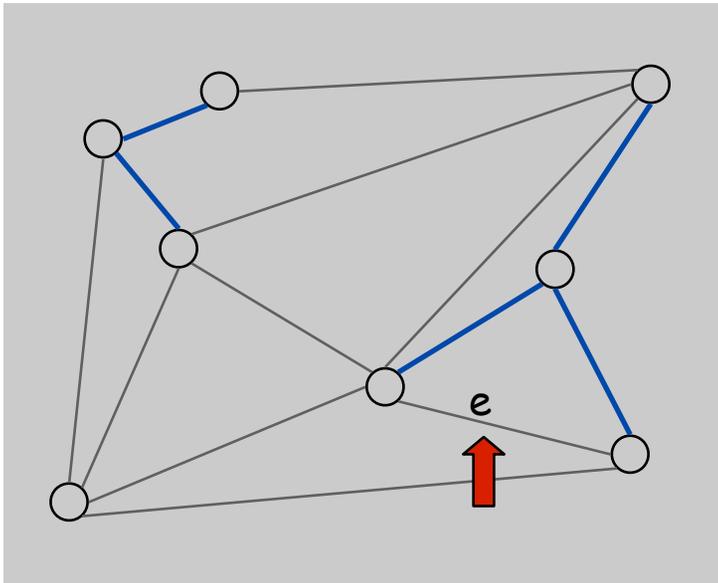
```
Prim(G, c) {
  foreach (v ∈ V) a[v] ← ∞
  Initialize an empty priority queue Q
  foreach (v ∈ V) insert v onto Q
  Initialize set of explored nodes S ← ∅

  while (Q is not empty) {
    u ← delete min element from Q
    S ← S ∪ { u }
    foreach (edge e = (u, v) incident to u)
      if ((v ∉ S) and (ce < a[v]))
        decrease priority a[v] to ce
  }
```

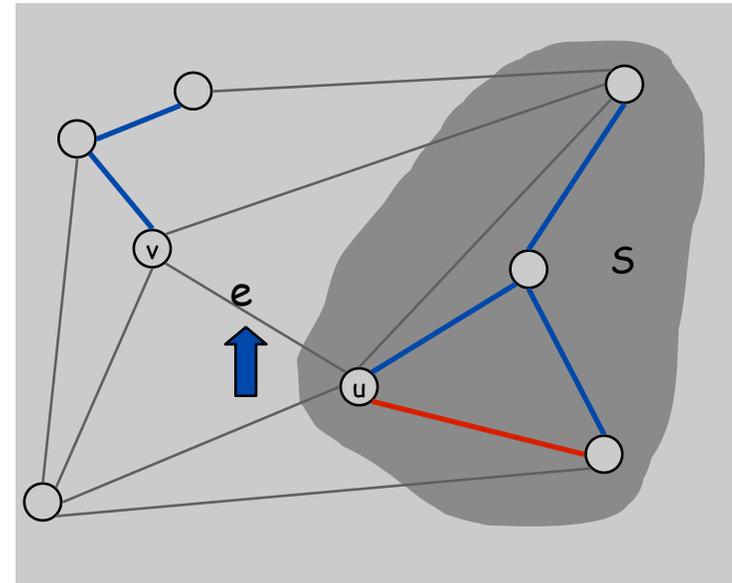
## Kruskal's Algorithm: Proof of Correctness

Kruskal's algorithm. [Kruskal, 1956]

- Consider edges in ascending order of weight.
- Case 1: If adding  $e$  to  $T$  creates a cycle, discard  $e$  according to cycle property.
- Case 2: Otherwise, insert  $e = (u, v)$  into  $T$  according to cut property where  $S$  = set of nodes in  $u$ 's connected component.



Case 1



Case 2

## Implementation: Kruskal's Algorithm

**Implementation.** Use the **union-find** data structure.

- Build set  $T$  of edges in the MST.
- Maintain set for each connected component.
- $O(m \log n)$  for sorting and  $O(m \alpha(m, n))$  for union-find.

```
Kruskal(G, c) {  
  Sort edges weights so that  $c_1 \leq c_2 \leq \dots \leq c_m$ .  
   $T \leftarrow \phi$   
  
  foreach ( $u \in V$ ) make a set containing singleton  $u$   
  
  for  $i = 1$  to  $m$       are u and v in different connected components?  
    ( $u, v$ ) =  $e_i$       ↙  
    if ( $u$  and  $v$  are in different sets) {  
       $T \leftarrow T \cup \{e_i\}$   
      merge the sets containing  $u$  and  $v$   
    }  
  return  $T$       ↙ merge two components  
}
```

## Lexicographic Tiebreaking

To remove the assumption that all edge costs are distinct: perturb all edge costs by tiny amounts to break any ties.

**Impact.** Kruskal and Prim only interact with costs via pairwise comparisons. If perturbations are sufficiently small, MST with perturbed costs is MST with original costs.

↑  
e.g., if all edge costs are integers,  
perturbing cost of edge  $e_i$  by  $i / n^2$

**Use implementation detail.** Can handle arbitrarily small perturbations implicitly by breaking ties lexicographically, according to index.

```
boolean less(i, j) {  
    if      (cost(ei) < cost(ej)) return true  
    else if (cost(ei) > cost(ej)) return false  
    else if (i < j)                 return true  
    else                             return false  
}
```

## MST Algorithms: Theory

### Deterministic comparison based algorithms.

- $O(m \log n)$  Jarník, Prim, Dijkstra, Kruskal, Boruvka
- $O(m \log \log n)$ . Cheriton-Tarjan (1976), Yao (1975)
- $O(m \beta(m, n))$ . Fredman-Tarjan (1987)
- $O(m \log \beta(m, n))$ . Gabow-Galil-Spencer-Tarjan (1986)
- $O(m \alpha(m, n))$ . Chazelle (2000)

Holy grail.  $O(m)$ .

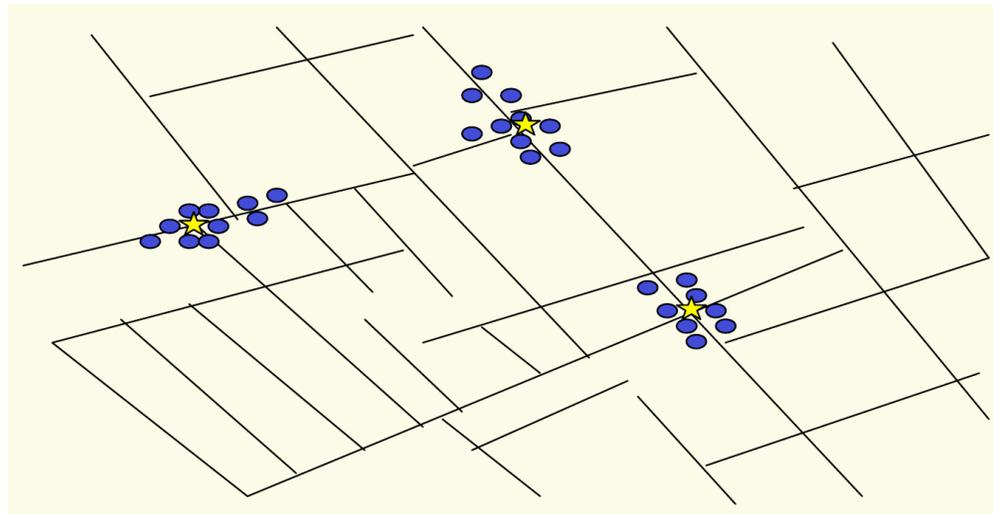
### Notable.

- $O(m)$  randomized. Karger-Klein-Tarjan (1995)
- $O(m)$  verification. Dixon-Rauch-Tarjan (1992)

### Euclidean.

- 2-d:  $O(n \log n)$ . compute MST of edges in Delaunay
- k-d:  $O(k n^2)$ . dense Prim

## 4.7 Clustering



Outbreak of cholera deaths in London in 1850s.  
Reference: Nina Mishra, HP Labs

# Clustering

**Clustering.** Given a set  $U$  of  $n$  objects labeled  $p_1, \dots, p_n$ , classify into coherent groups.

↑  
photos, documents, micro-organisms

**Distance function.** Numeric value specifying "closeness" of two objects.

↑  
number of corresponding pixels whose intensities differ by some threshold

**Fundamental problem.** Divide into clusters so that points in different clusters are far apart.

- Routing in mobile ad hoc networks.
- Identify patterns in gene expression.
- Document categorization for web search.
- Similarity searching in medical image databases
- Skycat: cluster  $10^9$  sky objects into stars, quasars, galaxies.

## Clustering of Maximum Spacing

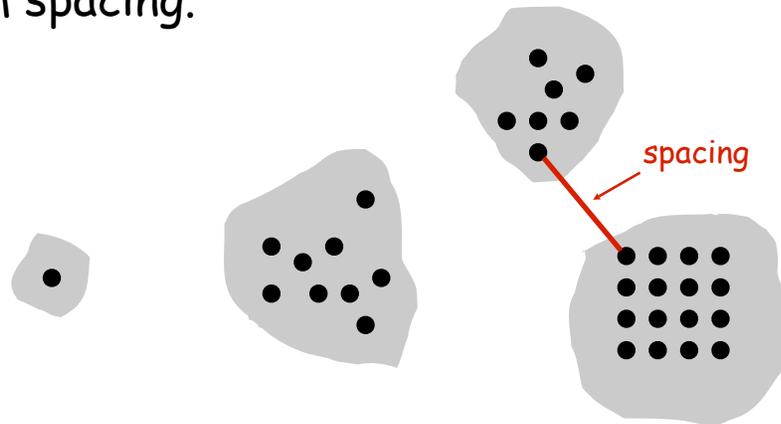
**k-clustering.** Divide objects into  $k$  non-empty groups.

**Distance function.** Assume it satisfies several natural properties.

- $d(p_i, p_j) = 0$  iff  $p_i = p_j$  (identity of indiscernibles)
- $d(p_i, p_j) \geq 0$  (nonnegativity)
- $d(p_i, p_j) = d(p_j, p_i)$  (symmetry)

**Spacing.** Min distance between any pair of points in different clusters.

**Clustering of maximum spacing.** Given an integer  $k$ , find a  $k$ -clustering of maximum spacing.

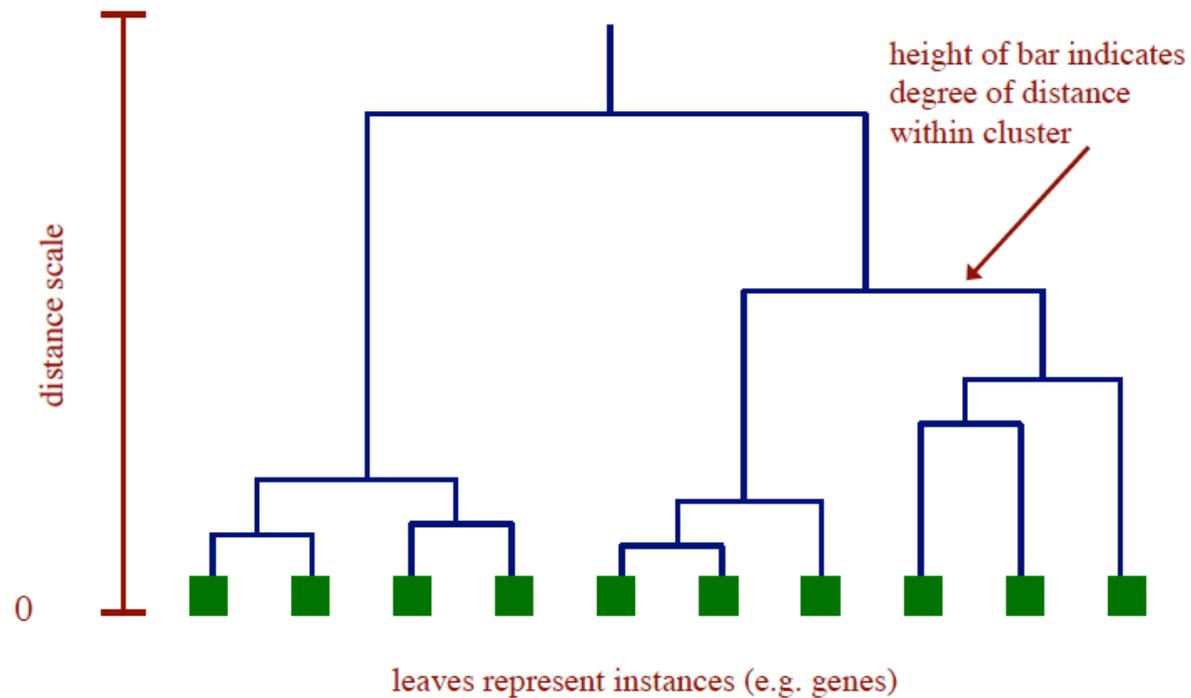


$k = 4$

# Dendrogram

**Dendrogram.** Scientific visualization of hypothetical sequence of evolutionary events.

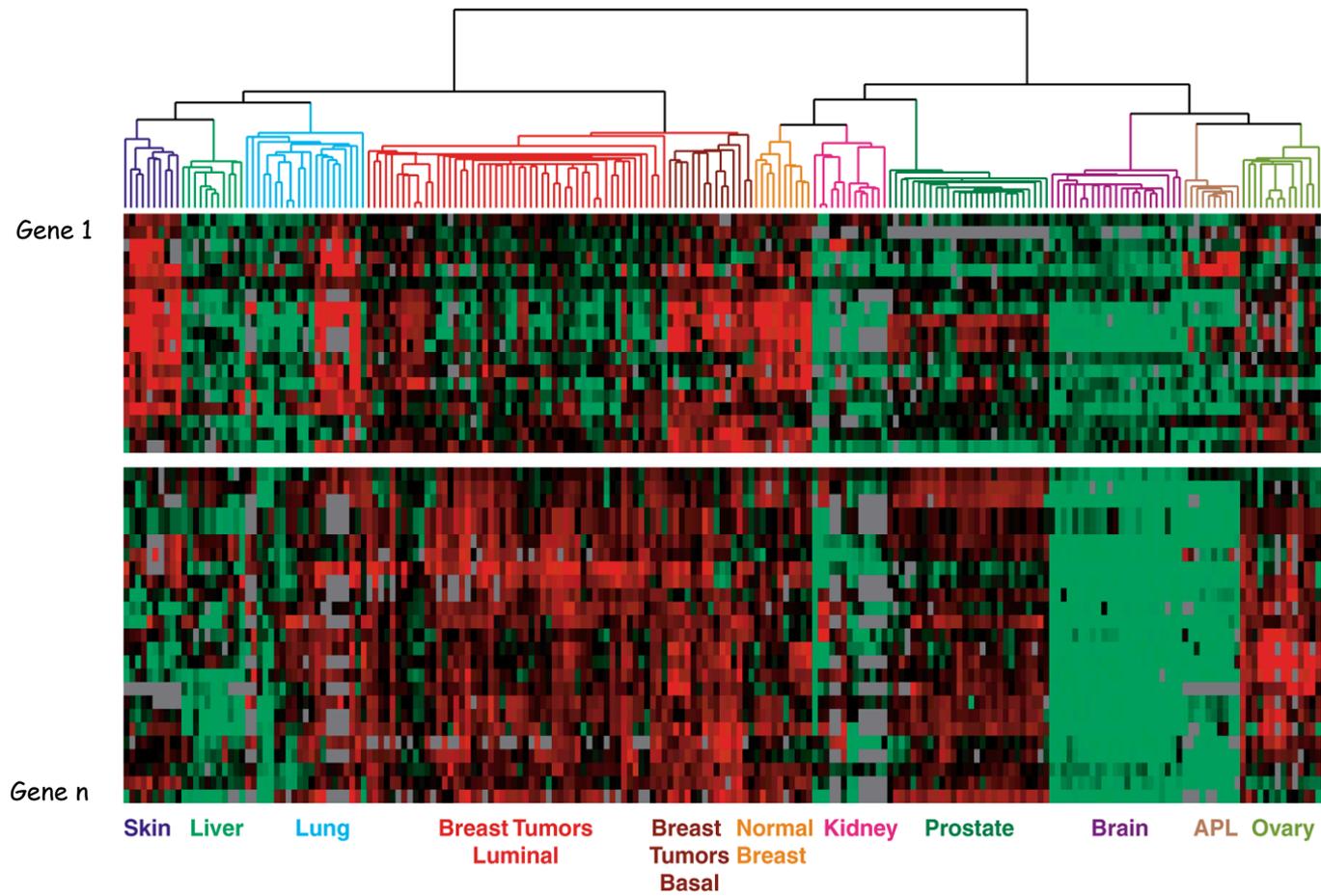
- Leaves = genes.
- Internal nodes = hypothetical ancestors.



Reference: <http://www.biostat.wisc.edu/bmi576/fall-2003/lecture13.pdf>

# Dendrogram of Cancers in Human

Tumors in similar tissues cluster together.



Reference: Botstein & Brown group

■ gene expressed  
■ gene not expressed

## Greedy Clustering Algorithm

### Single-link k-clustering algorithm.

- Form a graph on the vertex set  $U$ , corresponding to  $n$  clusters.
- Find the closest pair of objects such that each object is in a different cluster, and add an edge between them.
- Repeat  $n-k$  times until there are exactly  $k$  clusters.

**Key observation.** This procedure is precisely Kruskal's algorithm (except we stop when there are  $k$  connected components).

**Remark.** Equivalent to finding an MST and deleting the  $k-1$  most expensive edges.

## Greedy Clustering Algorithm: Analysis

**Theorem.** Let  $C^*$  denote the clustering  $C^*_1, \dots, C^*_k$  formed by deleting the  $k-1$  most expensive edges of a MST.  $C^*$  is a  $k$ -clustering of max spacing.

**Pf.** Let  $C$  denote some other clustering  $C_1, \dots, C_k$ .

- The spacing of  $C^*$  is the length  $d^*$  of the  $(k-1)^{\text{st}}$  most expensive edge.
- Let  $p_i, p_j$  be in the same cluster in  $C^*$ , say  $C^*_r$ , but different clusters in  $C$ , say  $C_s$  and  $C_t$ .
- Some edge  $(p, q)$  on  $p_i$ - $p_j$  path in  $C^*_r$  spans two different clusters in  $C$ .
- All edges on  $p_i$ - $p_j$  path have length  $\leq d^*$  since Kruskal chose them.
- Spacing of  $C$  is  $\leq d^*$  since  $p$  and  $q$  are in different clusters. ■

