DSC40B: Theoretical Foundations of Data Science II

Lecture 17: *Kruskal's algorithm for MST, and clustering*

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Previously

- Given a weighted undirected graph
  - Prim's algorithm to compute the minimum spanning tree (MST) in $\Theta((V+E)\lg V)$ time
    - It is a greedy algorithm

- Today:
  - Yet another greedy algorithm to compute MST, called Kruskal's algorithm
  - Relation to hierarchical clustering

Kruskal’s Algorithm for MST

Recall the general greedy idea:

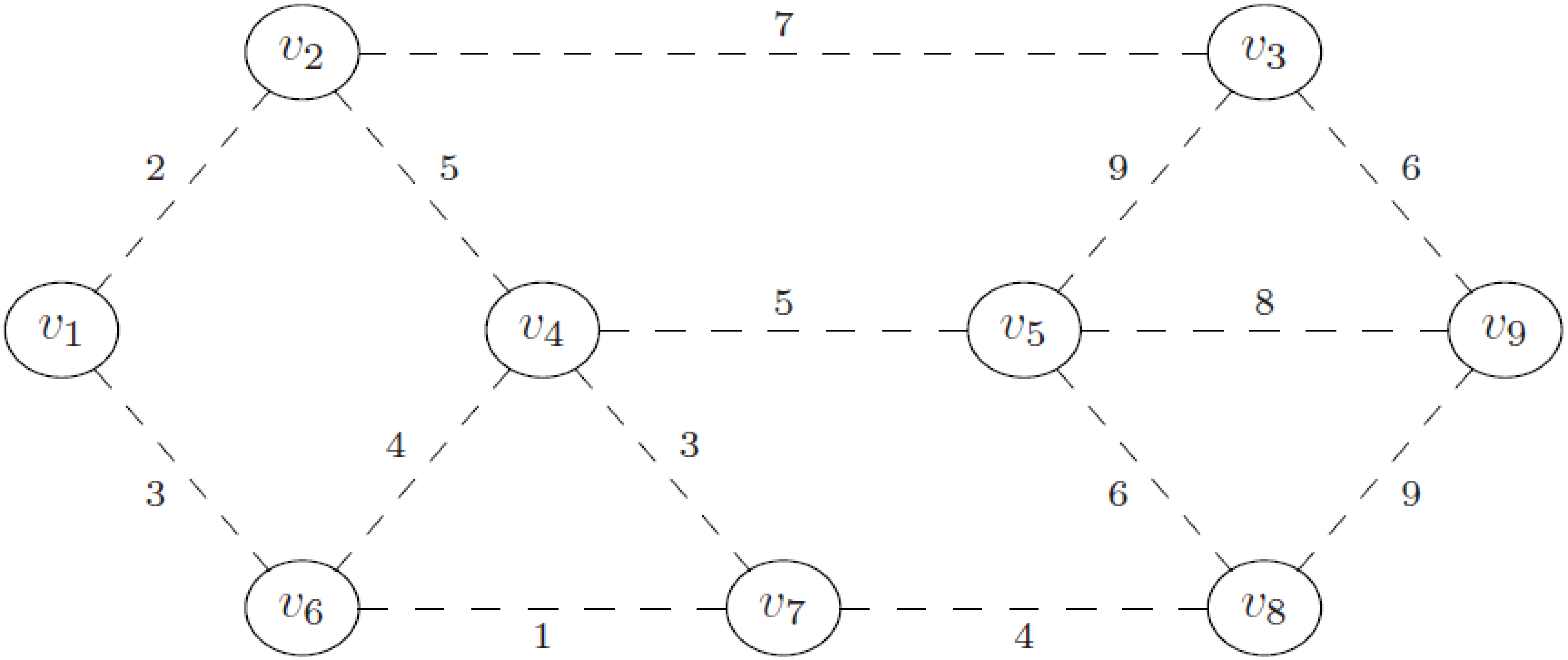
- Input:
  - a weighted undirected graph $G = (V, E)$, with $\omega: E \rightarrow R$
- Output:
  - the set of edges in a MST T of G

- A MST T is $V - 1$ number of edges that connect all nodes, with no cycle.
- Intuitively, we will choose "safe" edges greedily to incrementally build T
  - such that any time, the edges we choose will form a part of some MST

- Last time: Prim's algorithm
  - Starting from any node, it starts to grow a partial tree, by repeatedly choosing the minimum-weight edge to reach an unvisited node, till it connects all graph nodes

- Today: Kruskal's algorithm
  - We will choose the ``safe" edges in a different order, and still grow the tree edge by edge
    - However, during the intermediate stages, what we have may not be a partial tree, could be disconnected.

Example



- What is a "safe" edge to add first?
- What will be the next a "safe" edge to add?

Strategy

- We will add edges gradually in a greedy manner using smallest weights, while maintaining what we have so far does not have any cycle
  - add edges to tree in ascending order by weight
  - but if an edge creates a cycle, do not add it, and move on to next edge

- How do we check whether adding a new edge $e = (u, v)$ creates a cycle or not?
  - check whether nodes u, v are already connected.

Kruskal’s algorithm (Pseudocode)

```
def kruskal(graph, weights):
    mst = UndirectedGraph()

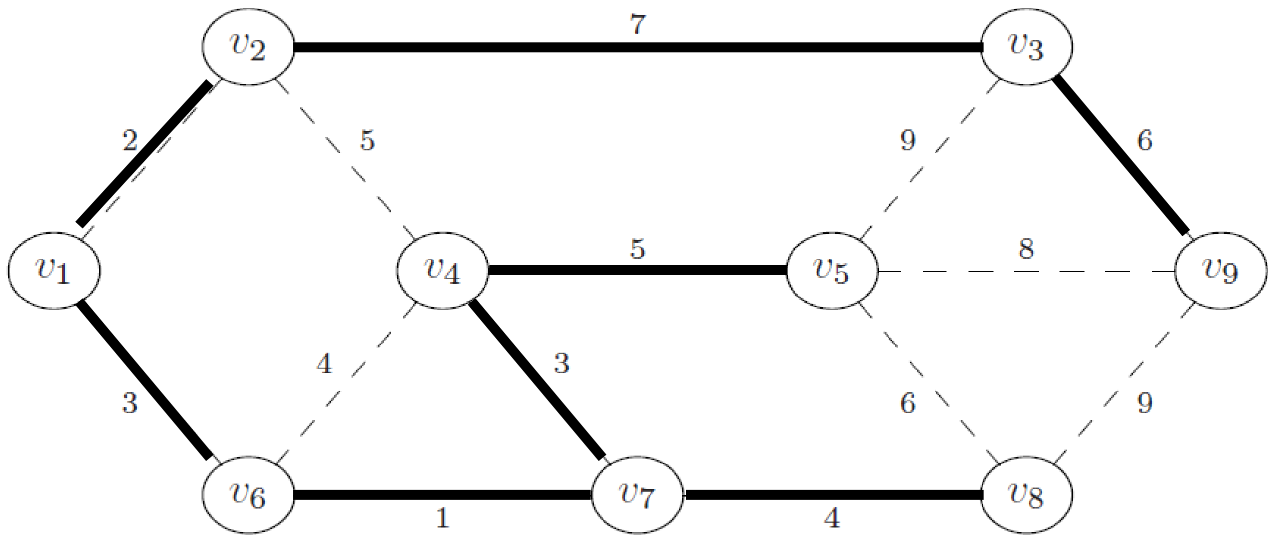
    # sort edges in ascending order by weight
    sorted_edges = sorted(graph.edges, key=weights)

    for (u, v) in sorted_edges:
        # if u and v are not already connected
        if ...:
            mst.add_edge(u, v)

            # (optional) if mst is now a spanning tree, break
            if len(mst.edges) == len(graph.nodes) - 1:
                break

    return mst
```

Example



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```

Checking for connectivity

- Each iteration: need to check if u and v are already connected in current $T = (V, E_{mst})$
- We can do a BFS/DFS on each iteration
  - $\Theta(V + E_{mst}) = \Theta(V)$ each time
  - Expensive!
- Again, remember:
  - If you're computing something once, use a fast algorithm
  - If you're computing it repeatedly, consider a data structure!

Disjoint Set Forests

- Represent a collection of disjoint sets over a set of elements
  - $\{\{1,5,6\},\{2,3\},\{0\},\{4\}\}$
- Two operations:
  - .union(x, y): Union the sets containing x and y
  - .in_same_set(x, y): return True/False if x and y are in the same set
    - Typically, this is implemented by an operation .find(x), which returns the representative of the set containing x.
- In the literature, this is also commonly referred to as the union-find data structure to maintain dynamic disjoint sets

Example

- \>>> *# create a DSF with {{0}, {1}, {2}, {3}, {4}, {5}}*
- \>>> dsf = DisjointSetForest([0, 1, 2, 3, 4, 5])
- \>>> dsf.union(0, 3)
- \>>> dsf.union(1, 4)
- \>>> dsf.union(3, 1)
- \>>> dsf.union(2, 5)
- \>>> *# dsf now represents {{0, 1, 3, 4}, {2, 5}}*
- \>>> dsf.in_same_set(0, 3)
- True
- \>>> dsf.in_same_set(0, 2)
- False

Disjoint Set Forests

- Each operation takes $\Theta(\alpha(n))$ time, where n is the number of objects in the collection

- $\alpha(n)$: inverse Ackermann function
  - It grows very very very slowly.
  - $\alpha(n) = o(\lg n)$
  - While asymptotically, it grows faster than a constant function, effectively in practice, for any number n we can imagine, $\alpha(n)$ is essentially a constant.

Disjoint Set Forest

- Can be used to keep track of connected components (CCs) of a dynamic graph

- Nodes of CCs are disjoint sets
  - Add an edge (u, v): .union(u, v)
  - Check if u and v are connected: .in_same_set(u, v)

- To check if u and v are already connected:
  - BFS/DFS: $\Theta(V)$ each time
  - Disjoin set forest: $\Theta(\alpha(V))$ each time (essentially like constant in practice, but not asymptotically!)

Kruskal’s Algorithm

```python
def kruskal(graph, weights):
    mst = UndirectedGraph()

    # place each node in its own disjoint set
    components = DisjointSetForest(graph.nodes)

    # sort edges in ascending order by weight
    sorted_edges = sorted(graph.edges, key=weights)

    for (u, v) in sorted_edges:
        if not components.in_same_set(u, v):
            mst.add_edge(u, v)
            components.union(u, v)

            # (optional) if mst is now a spanning tree, break
            if len(mst.edges) == len(graph.nodes) - 1:
                break

    return mst
```

Time complexity of Kruskal's algorithm

- Assume graph is connected. Then $E = \Omega(V)$

- Kruskal's algorithm takes $\Theta(E \lg E) = \Theta(E \lg V) time$
  - Dominated by sorting the edges

- Note: if graph is disconnected, then Kruskal's algorithm produces *a minimum spanning forest.*

Kruskal's vs. Prim's

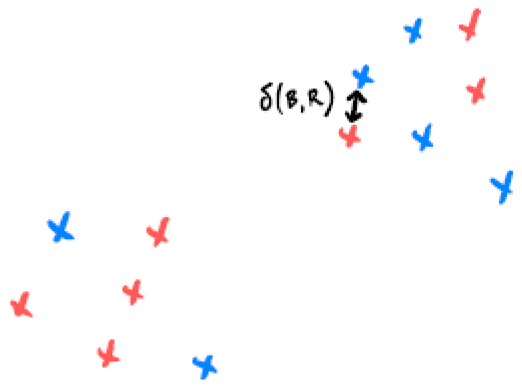
- Time complexity:
  - Prim's:
    - Binary heap: $\Theta(V \lg V + E \lg V)$ (= $\Theta(E \lg V)$ if graph is connected)
    - Fibonacci heap: $\Theta(V \lg V + E)$
  - Kruskal's:
    - $\Theta(V + E \lg V)$(= $\Theta(E \lg V)$ if graph is connected)
  - If graph is dense (e.g, $E = \Theta(V^2)$), then Prim's with Fibonacci heap "wins" in asymptotic time complexity
  - In practice, Fibonacci heaps are hard to implement with high overhead.
    - Kruskal's may be faster for smaller dense graphs

MSTs and (hierarchical) clustering

Clustering problem

- Identify the groups in data
- We frame clustering as a loss minimization problem
  - Input: n data points in R^d
  - Goal: assign each data point a color (red or blue, which is class labels) so that the distance between the closest pair of red and blue points is maximized

input points



bad clustering

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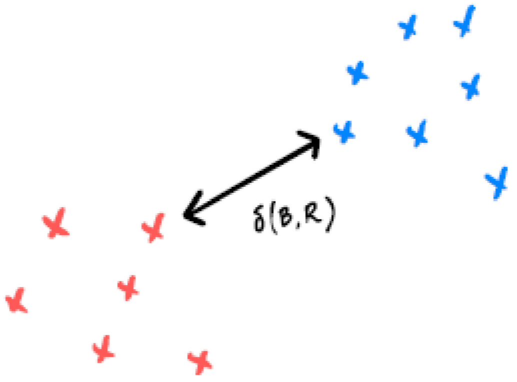


good clustering

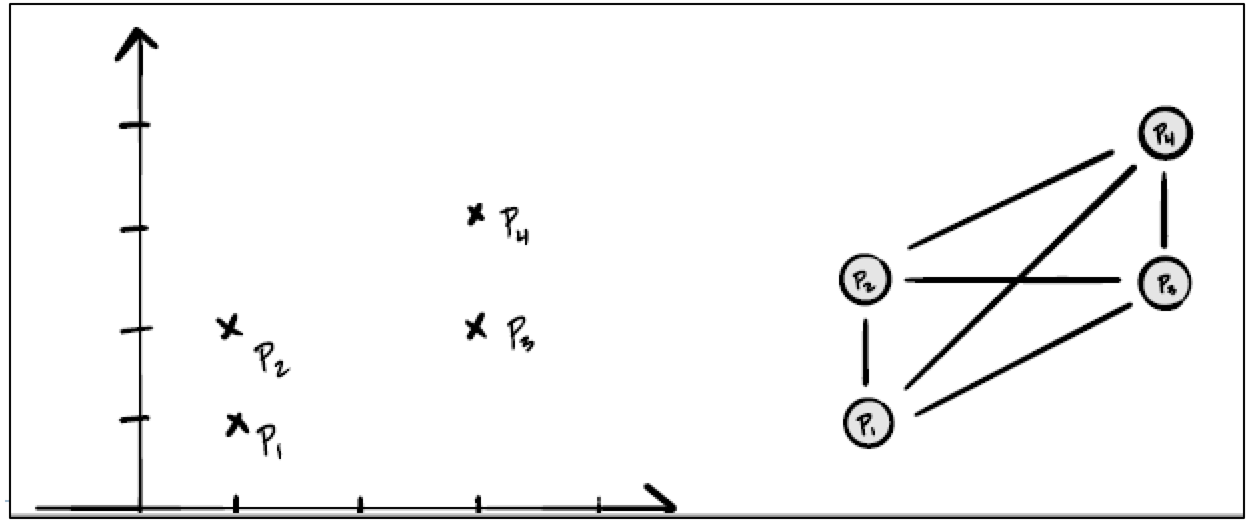
Recall the brute-force solution

- Try all possible assignments
  - there are 2^n possible assignments! (n is the number of input points)
  - highly not efficient!

- Instead, we will convert it to a graph problem

Distance graph

- Given n data points $V = \{ p_1, p_2, \dots, p_n\}$
  - create a complete undirected graph $G = (V, E)$ such that for any $p_i \neq p_j$, there is an edge $(p_i, p_j) \in E$
  - the weight of an edge (p_i, p_j) is $\omega(p_i, p_j) = dist(p_i, p_j)$
- We call this resulting weighted graph the distance graph spanned by V



Clustering

- Given n data points $V = \{ p_1, p_2, \ldots, p_n\}$
- Create distance graph G
- Run either Prim's or Kruskal's Algorithm to compute MST of G, T:

- Delete largest edge in MST, and we obtain two components => clusters!
- In general, if we remove largest $k - 1$ edges in MST
  - then we obtain k clusters (components)

Single linkage clustering

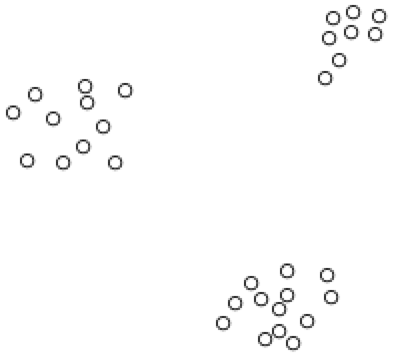
- Alternatively, we can perform Kruskal's algorithm, adding edges in ascending order by weights without forming cycles, and stop till we have a target k number of components (clusters)
  - That is, we terminate early in the Kruskal's algorithm
- Time complexity
  - $\Theta(E \lg V) = \Theta(V^2 \lg V)$ as $E = \Theta(V^2)$ in this case

- This is called the single-linkage clustering algorithm
  - One of the most well-known clustering algorithm.
  - It is popular, although it suffers from the so-called chaining-effect in practice.
  - Variants of it, e.g., average-linkage clustering algorithm and complete-linkage clustering algorithm, are popular as a simple clustering algorithm.

Example of chaining effect

Hierarchical clustering, and single linkage clustering algorithm (Optional)

Clustering



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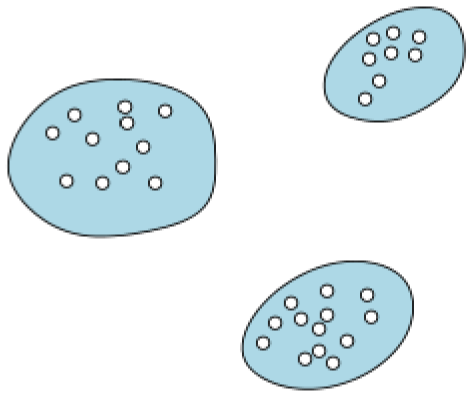
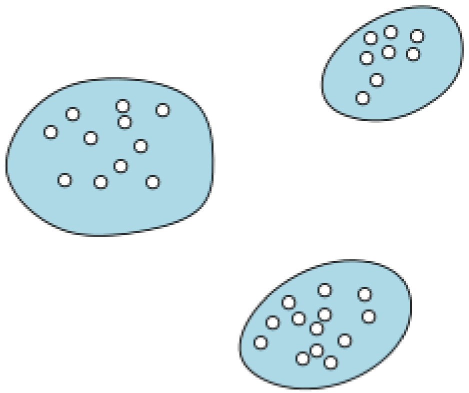
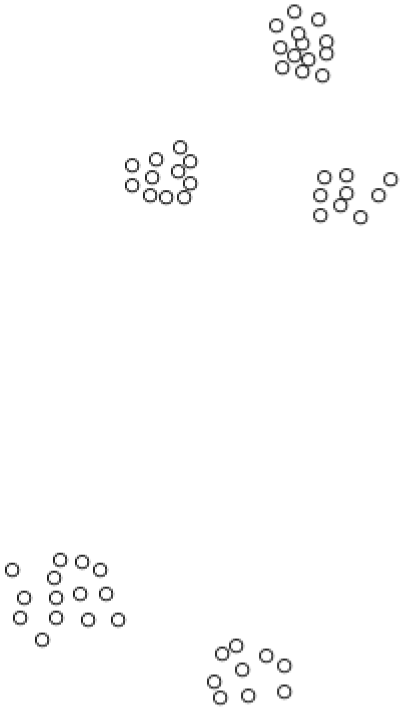


Hierarchical Clustering





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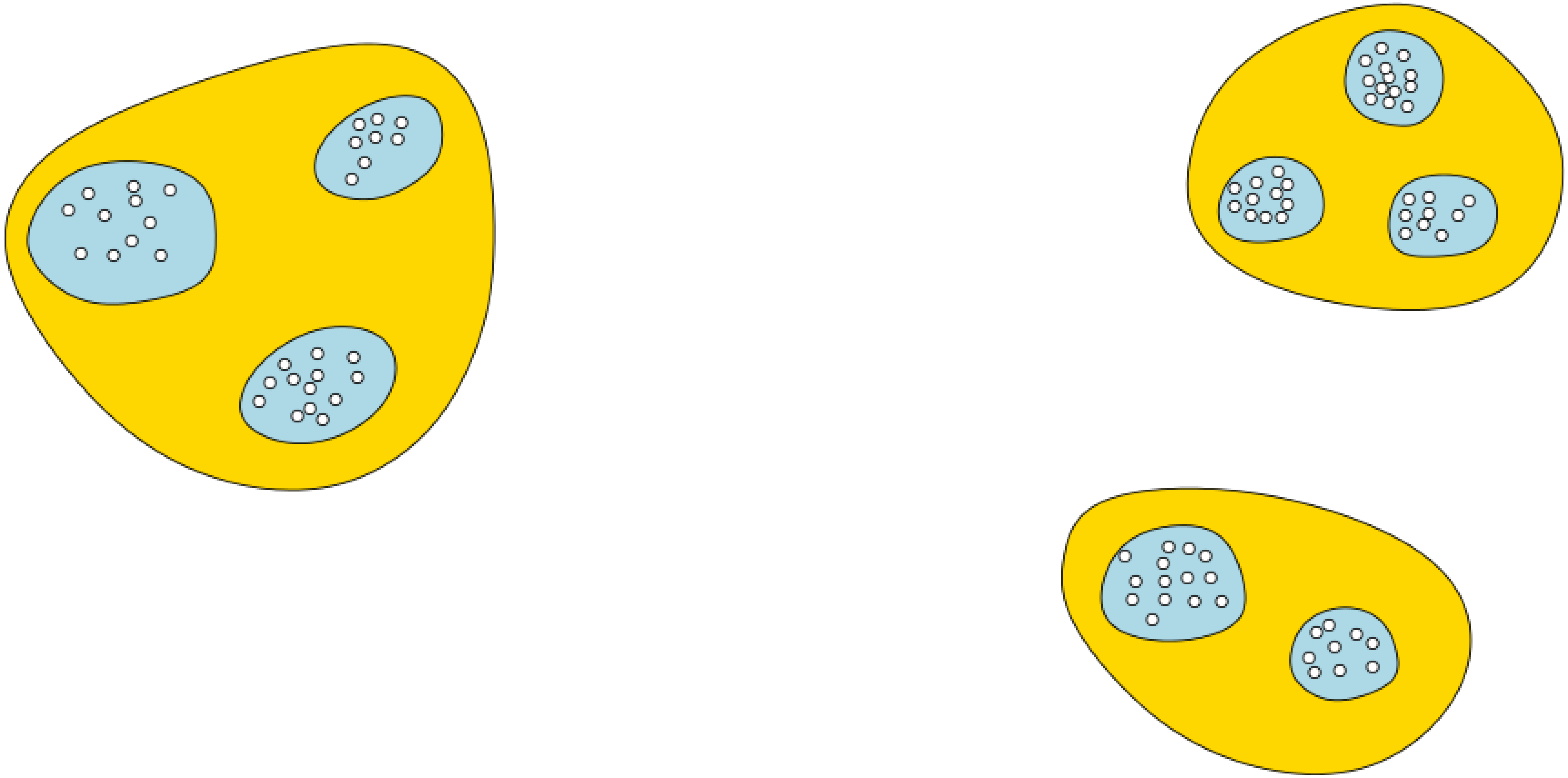

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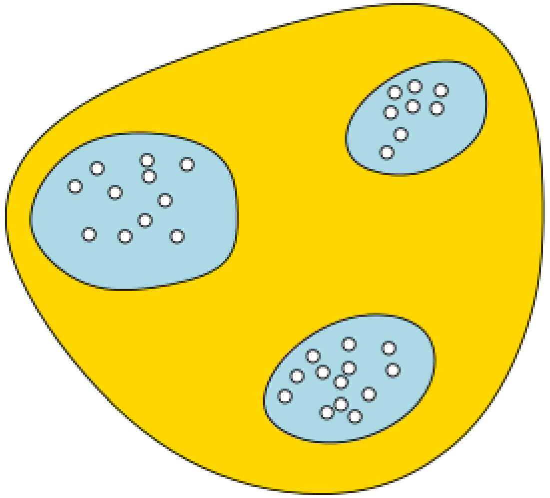
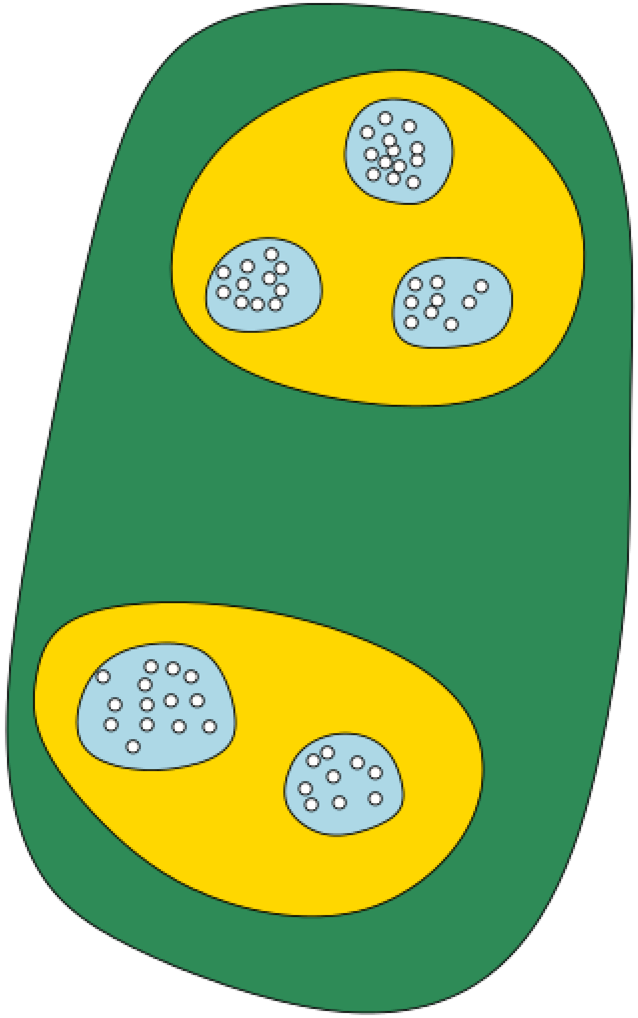
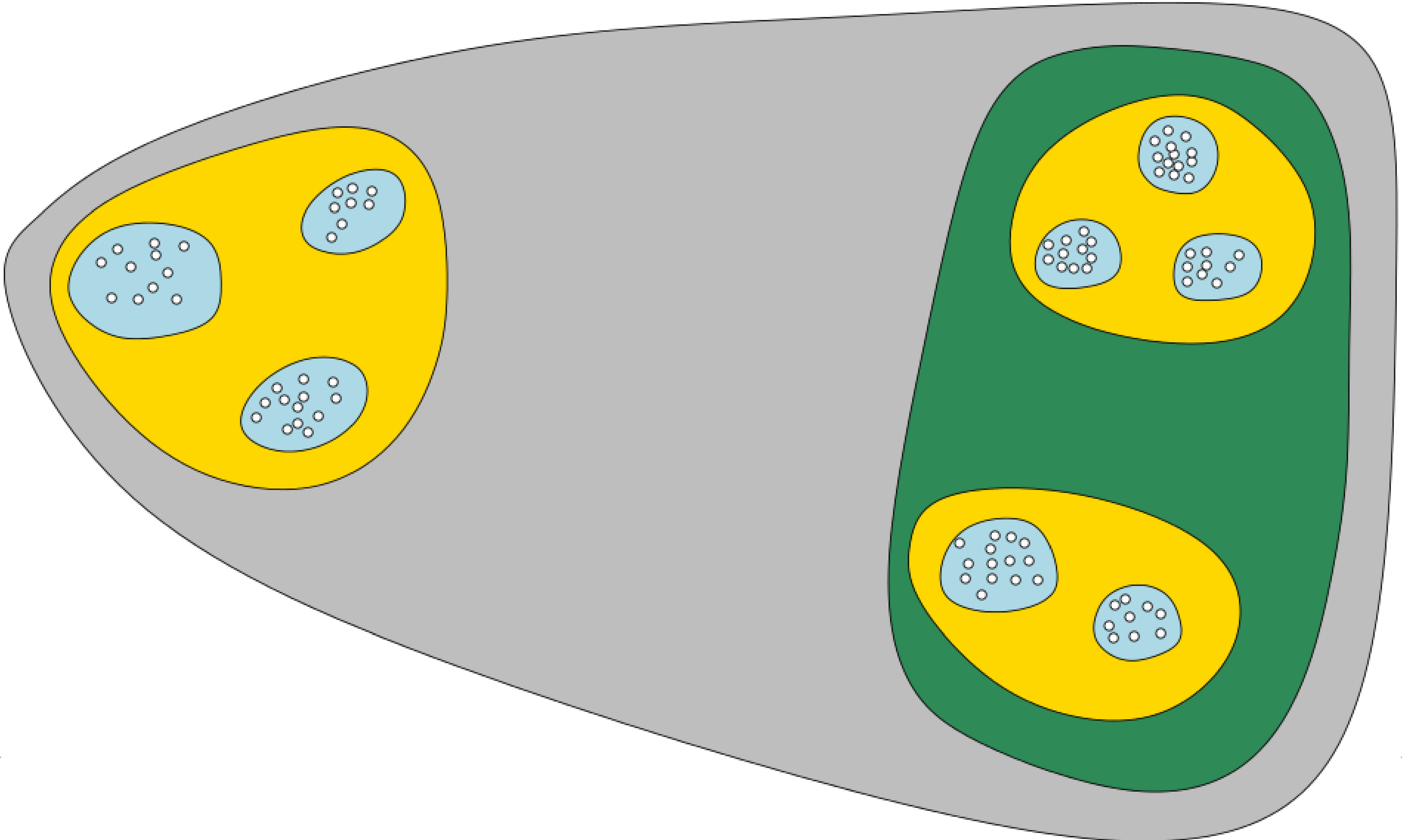
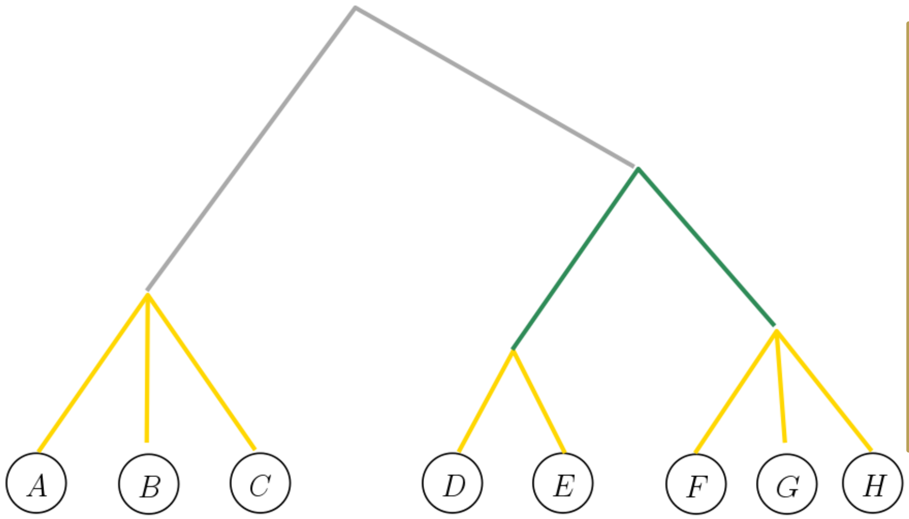




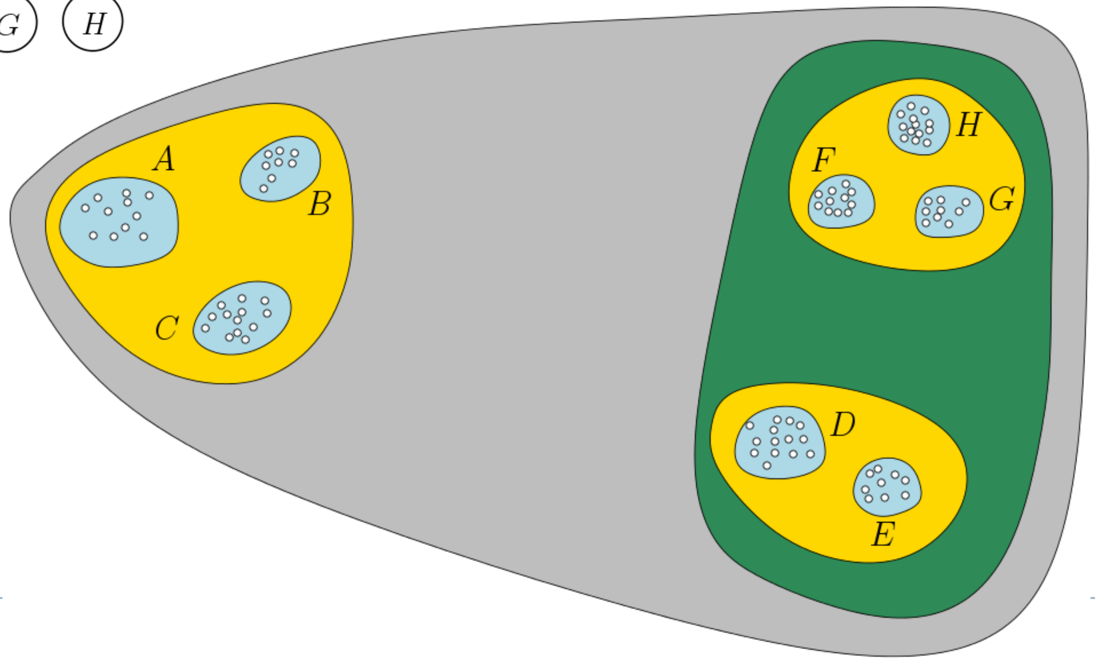
Hierarchical Clustering



Hierarchical Clustering Tree (HCT)



- Each internal tree node indicates a cluster, containing all leaves in subtree
- Ancestor/descendent indicates containment relation
- Height at each tree node corresponds to certain *cost* of the corresponding cluster (e.g, tightness of cluster)



Single Linkage Clustering

- One of the family of agglomerative clustering methods

- Input: A discrete n-point metric (P, d_P)
- Output: A hierarchical clustering tree T, with points in P being leaves

- Starting with each data point as a single cluster
- Keep merging clusters based on nearest distance between points from their members

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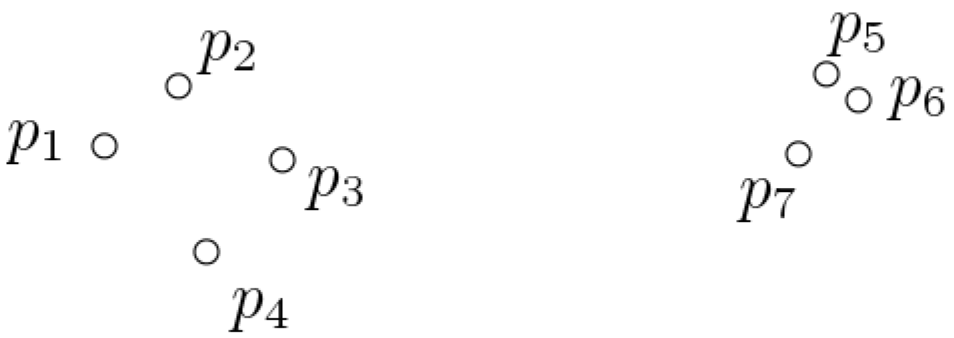

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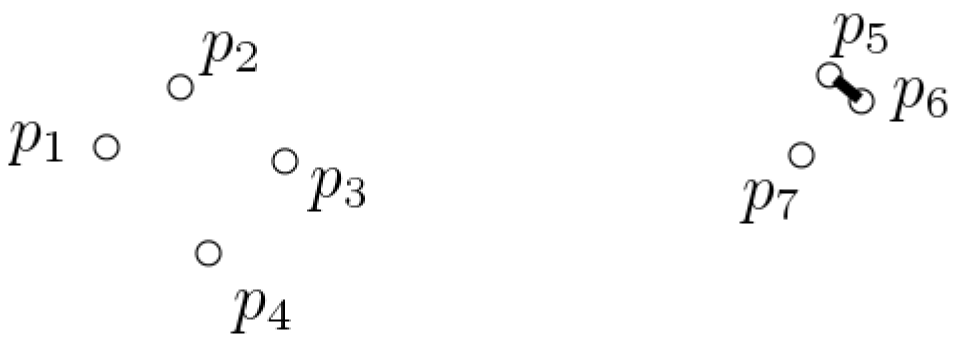

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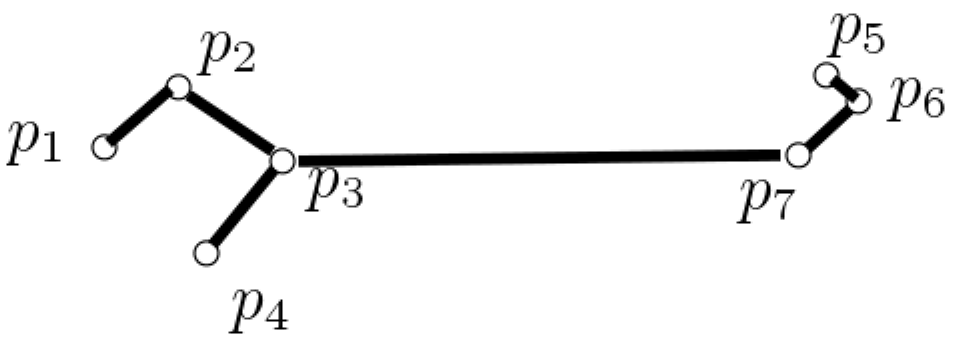

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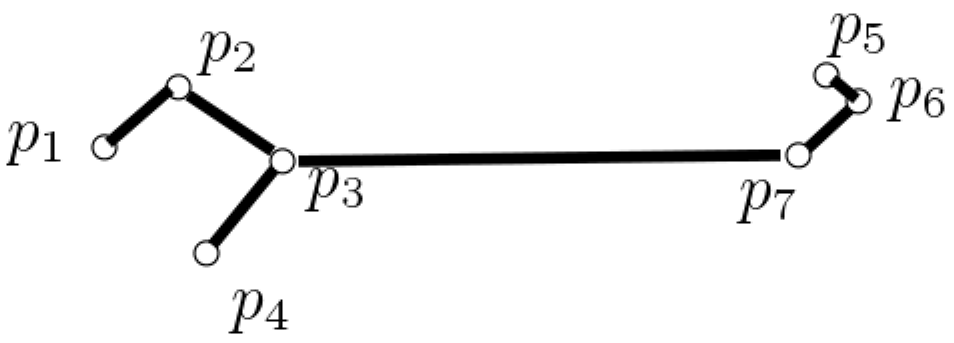
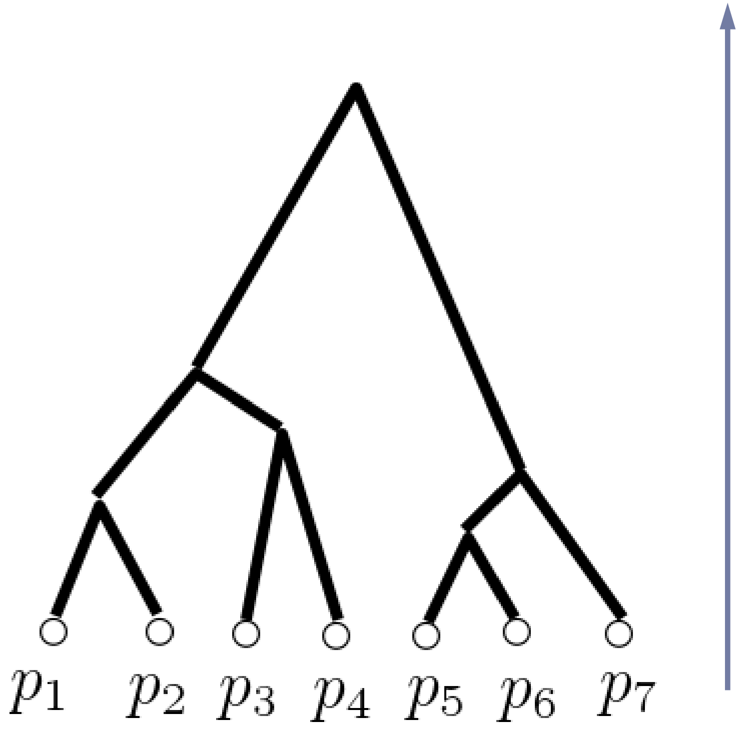
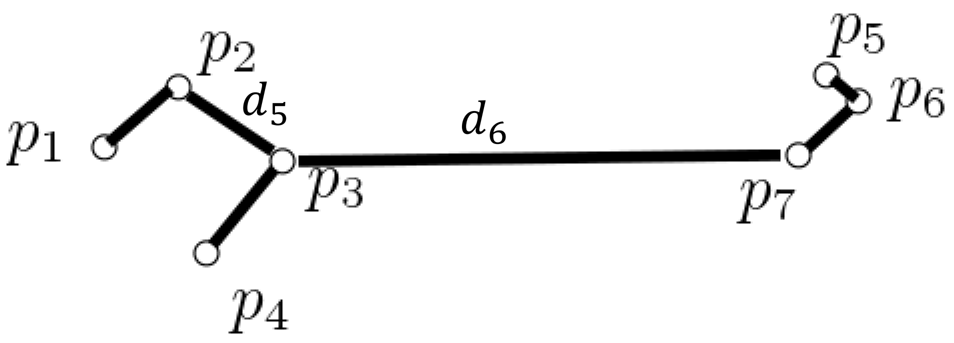


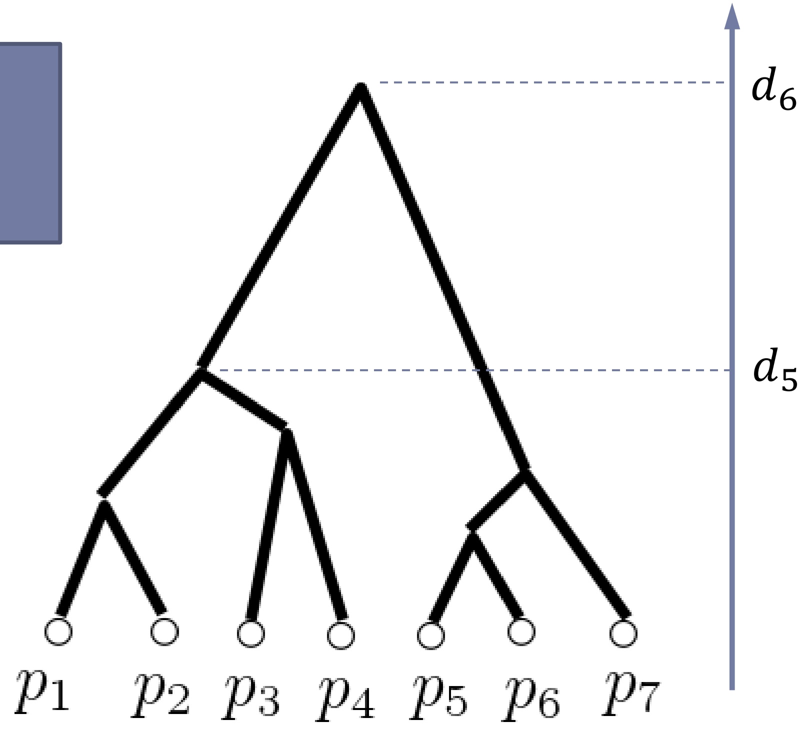


One Example: Single Linkage Clustering

- Starting with each data point as a single cluster
- Keep merging clusters based on nearest distance between points from their members

This procedure is exactly Kruskal's algorithm!





Summary

- MST for weighted undirected graphs
  - Prim's algorithm
  - Kruskal's algorithm
  - Both $\Theta\big((V+E)\lg V\big)$ (which is $\Theta(E\lg V)$ for connected graphs)

  - Kruskal's algorithm can be used to produce single linkage clustering

FIN