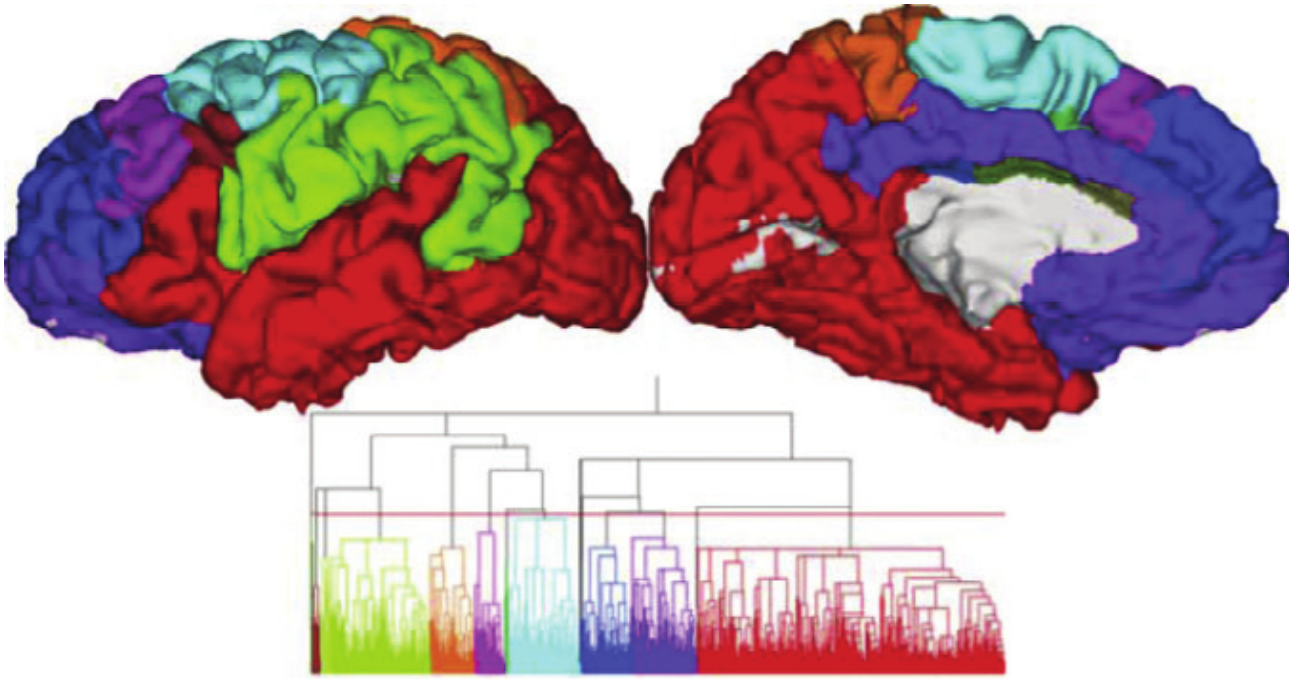
CS 6824: Modules

T. M. Murali

February 22, 27, and March 1, 2018



Student Presentations

- Wiring cost optimisation and cost-efficiency trade-offs
  Scott Clark, Omar Faruqi, Cameron Rader
- Degree-based measures of centrality
  Branden Arnold, Mostafa Elmary, Madison Wilkins
- Betweenness centrality
  Aidan Barton, Jose Canahui, Jordan Kuhn
- Rich clubs
  Team Valkyrie: Shane Davies, Heidi Tubbs, Tianna Woodson
- Overlapping modules
  Team Wildcards: Kavin Aravind, Tom Evans, Rishi Pulluri
- Growth connectomics: generative models for brain networks
  William Edmisten, Ethan Gallagher, Sophia Sheikl

Schedule of Meetings and Presentations

- Each group meets me for 60–90 minutes one week before practice presentation.
  - Goal is to discuss details of presentation.
  - Come prepared: read your section, find relevant papers, have a talk outline, ask me quesitons.
- Each group meets me for 60–90 minutes about one week before actual presentation.
- Office hours for these meetings: 10am-12pm on Tuesdays and Thursdays, after Spring break, and by appointment.

Schedule of Meetings and Presentations

- Each group meets me for 60–90 minutes one week before practice presentation.
  - Goal is to discuss details of presentation.
  - Come prepared: read your section, find relevant papers, have a talk outline, ask me quesitons.
- Each group meets me for 60–90 minutes about one week before actual presentation.
- Office hours for these meetings: 10am-12pm on Tuesdays and Thursdays, after Spring break, and by appointment.

Topic	First meeting	Practice	Second meeting	Present
Wiring cost optimisation	Mar 13	Mar 20	Apr 3	Apr 10
Degree-based centrality	TBD	Mar 22	Apr 5	Apr 12
Betweenness	Mar 20	Mar 27	Apr 10	Apr 17
Rich clubs	Mar 22	Mar 29	Apr 12	Apr 19
Overlapping Modules	Mar 27	Apr 3	Apr 17	Apr 24
Growth connectomics	Mar 29	Apr 5	Apr 19	Apr 26

Plan after Spring Break

- Invited presentation by Heidi Theussen from Smith Career Center (March 13)
- No class on March 15
- Practice presentations (March 20 to April 5)
- Presentations (April 10 to Apr 26)
- No class on May 1

Summary of Course Thus Far

- Clustering coefficient is a local measure of graph density.
- Small world property captures global features of graph density.

Summary of Course Thus Far

- Clustering coefficient is a local measure of graph density.
- Small world property captures global features of graph density.

Are there intermediate notions of graph density?

- We have already considered components, shortest paths, cliques, and cores.
- We have also seen two specific types of modules: cliques and k-cores.

Why Modules?

Why should (brain) networks be modular?
Do modules exist in brain networks?
How do we define modules and find them?

Why Modules?

Why should (brain) networks be modular?
Do modules exist in brain networks?
How do we define modules and find them?

- Do E-R graphs contain modules?

Why Modules?

Why should (brain) networks be modular?
Do modules exist in brain networks?
How do we define modules and find them?

- Do E-R graphs contain modules? No, because all nodes have roughly the same degree.

Why Modules?

Why should (brain) networks be modular?
Do modules exist in brain networks?
How do we define modules and find them?

- Do E-R graphs contain modules? No, because all nodes have roughly the same degree.
- Do W-S graphs contain modules?

Why Modules?

Why should (brain) networks be modular?
Do modules exist in brain networks?
How do we define modules and find them?

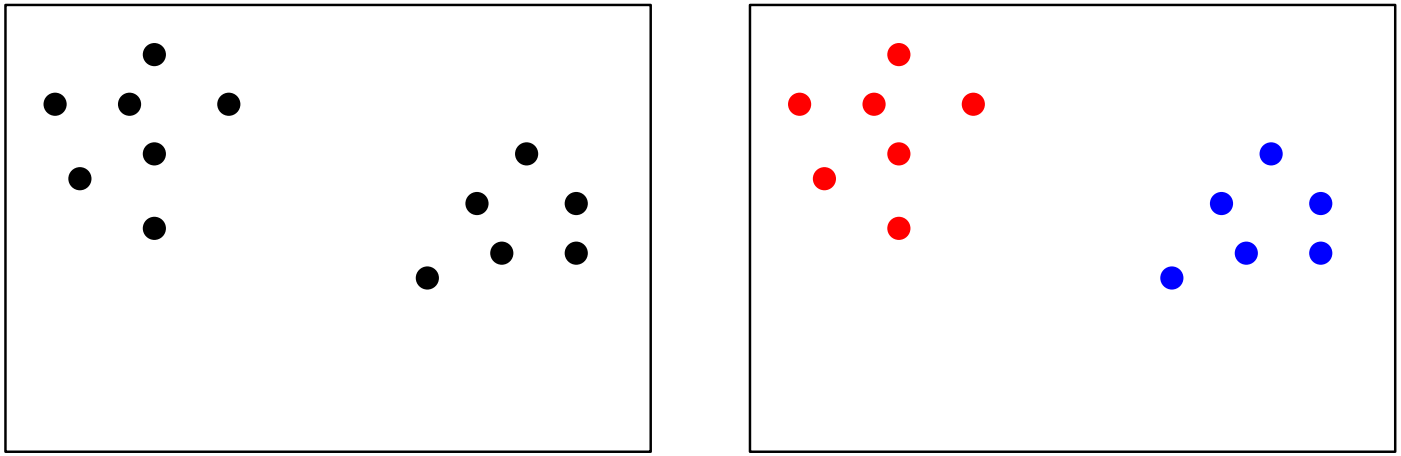
- Do E-R graphs contain modules? No, because all nodes have roughly the same degree.
- Do W-S graphs contain modules? No, although other small-world networks can contain modules.
- But the brain is indeed modular: organ, hemispheres, coarse divisions, lobes, cytoarchitectural areas, nuclei, etc.

- Modularity and hierarchical organisation offer several advantages: evolvability, flexibility, adaptability, and complexity.

Modules and Clustering

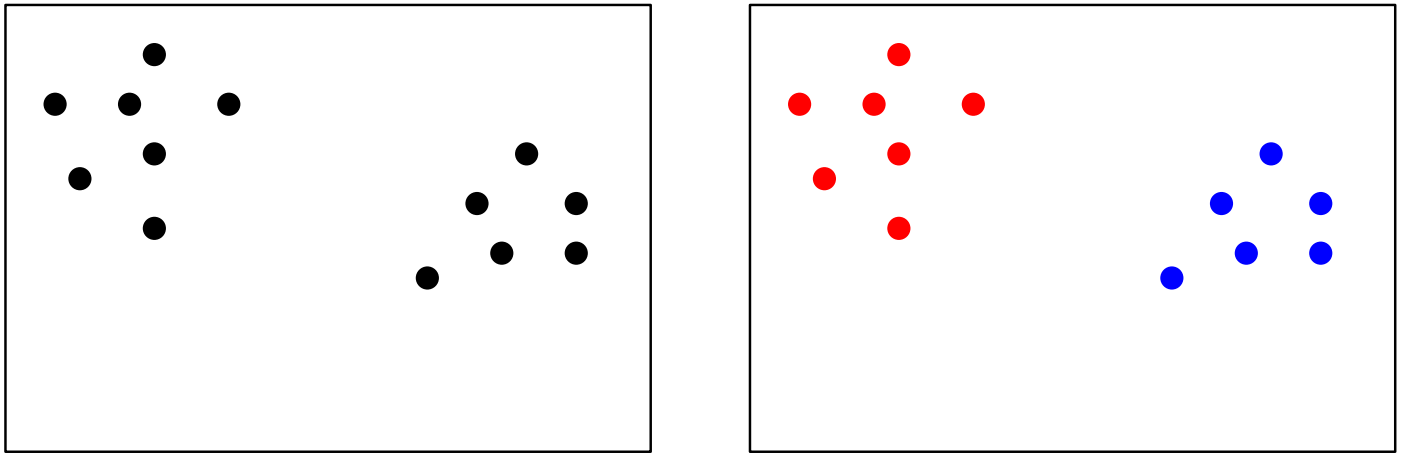
- Finding modules or clusters formed by a set of objects is a widely studied problem.
- Long history in mathematics, statistics, and computer science.
- Module $\equiv$ Cluster $\equiv$ Community.

Definition of Clustering



Given a set of n objects, find the best partition of the objects into subsets such that each subset contains objects that are similar/close to each other.

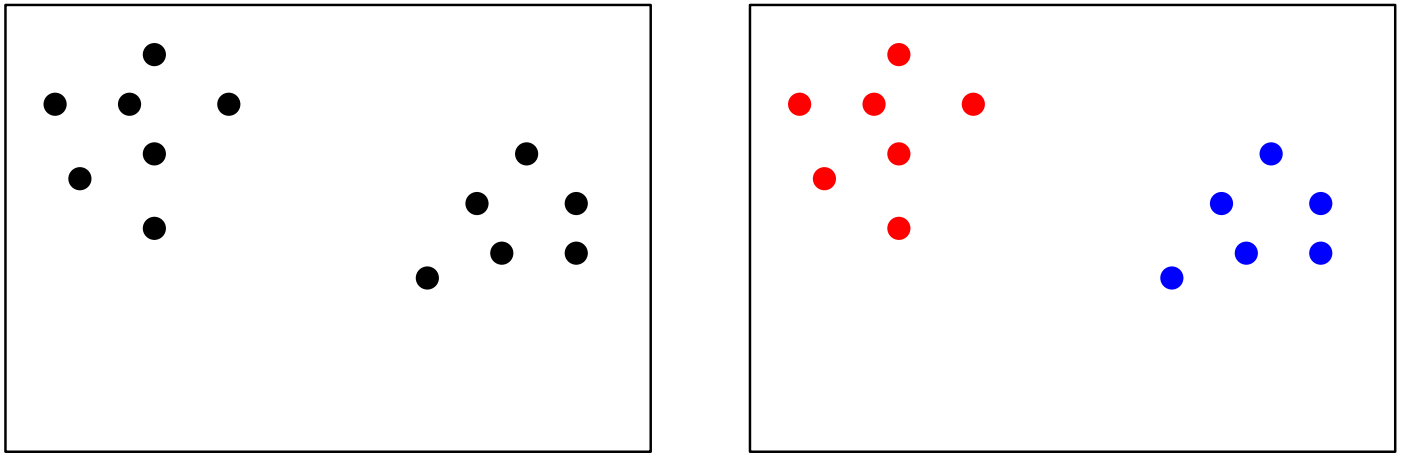
Definition of Clustering



Given a set of n objects, find the best partition of the objects into subsets such that each subset contains objects that are similar/close to each other.

- How do we measure how similar or close two objects are?

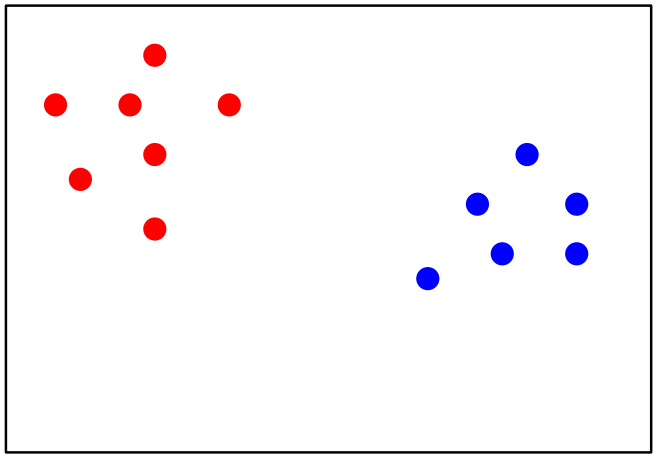
Definition of Clustering

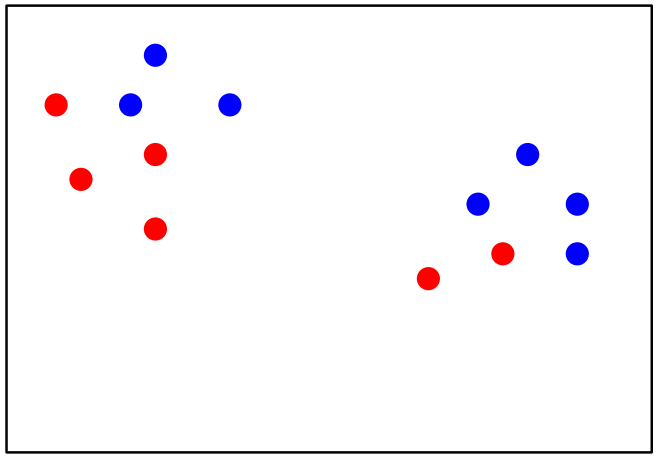


Given a set of n objects, find the best partition of the objects into subsets such that each subset contains objects that are similar/close to each other.

- How do we measure how similar or close two objects are?
- How many subsets?

Definition of Clustering





Given a set of n objects, find the best partition of the objects into subsets such that each subset contains objects that are similar/close to each other.

- How do we measure how similar or close two objects are?
- How many subsets?
- How do we compare two different partitions?

Measuring Similarity of Objects

- Assume each object specified by a list of values, e.g., x, y, z coordinates indicating voxel position in an fMRI image.

Measuring Similarity of Objects

- Assume each object specified by a list of values, e.g., x, y, z coordinates indicating voxel position in an fMRI image.
- Distance between two objects p and q is $d(p, q)$.
- Euclidean metric: $d(p, q) = \sqrt{\sum_i (p_i - q_i)^2}$.

Measuring Similarity of Objects

- Assume each object specified by a list of values, e.g., x, y, z coordinates indicating voxel position in an fMRI image.
- Distance between two objects p and q is $d(p, q)$.
- Euclidean metric: $d(p, q) = \sqrt{\sum_i (p_i - q_i)^2}$.
- Manhattan metric: $d(p, q) = \sum_i |p_i - q_i|$.

Measuring Similarity of Objects

- Assume each object specified by a list of values, e.g., x, y, z coordinates indicating voxel position in an fMRI image.
- Distance between two objects p and q is $d(p, q)$.
- Euclidean metric: $d(p, q) = \sqrt{\sum_i (p_i - q_i)^2}$.
- Manhattan metric: $d(p, q) = \sum_i |p_i - q_i|$.
- Other distances: normalised dot product, K-L divergence, relative entropy, Pearson's correlation.

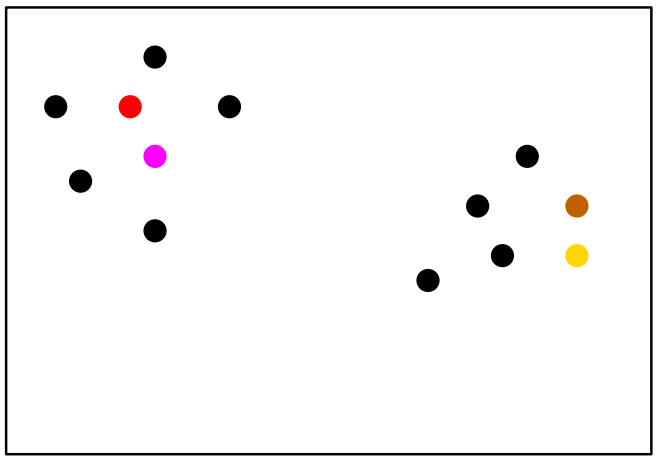
Measuring Similarity of Objects

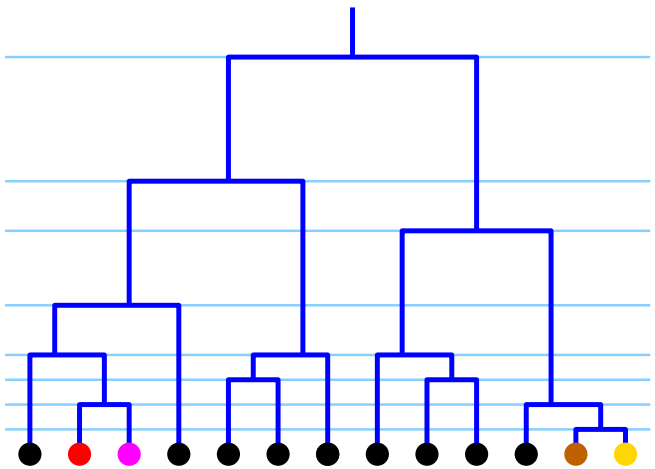
- Assume each object specified by a list of values, e.g., x, y, z coordinates indicating voxel position in an fMRI image.
- Distance between two objects p and q is $d(p, q)$.
- Euclidean metric: $d(p, q) = \sqrt{\sum_i (p_i - q_i)^2}$.
- Manhattan metric: $d(p, q) = \sum_i |p_i - q_i|$.
- Other distances: normalised dot product, K-L divergence, relative entropy, Pearson's correlation.

- Metrics obey triangle inequality: $d(p, q) + d(q, r) \geq d(p, r)$.
  - Euclidean, Manhattan distances are metrics.
  - Correlation, dot product are not metrics.

Hierarchical Clustering

- Attempt to recursively find sub-modules within modules.
- Natural way to "zoom into" areas of interest.
- Represent using a tree or dendrogram.





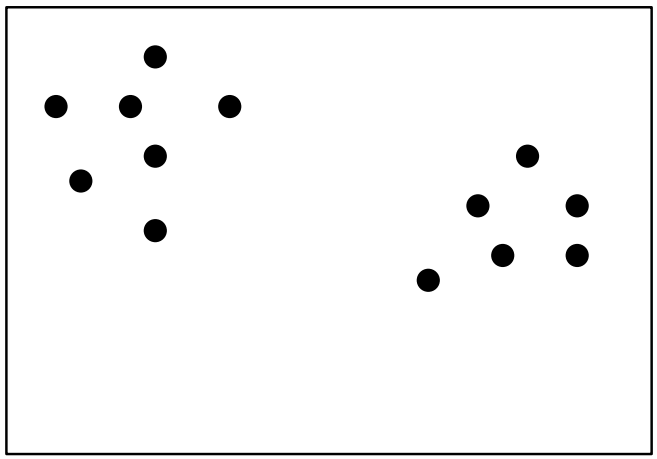
Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

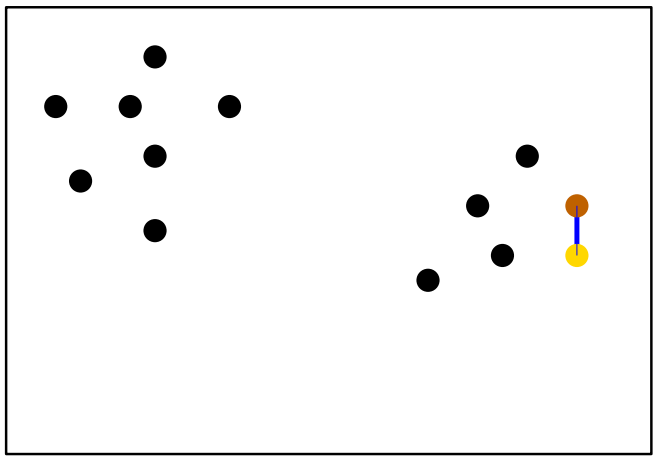
1. Start with every object in its own cluster.



Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

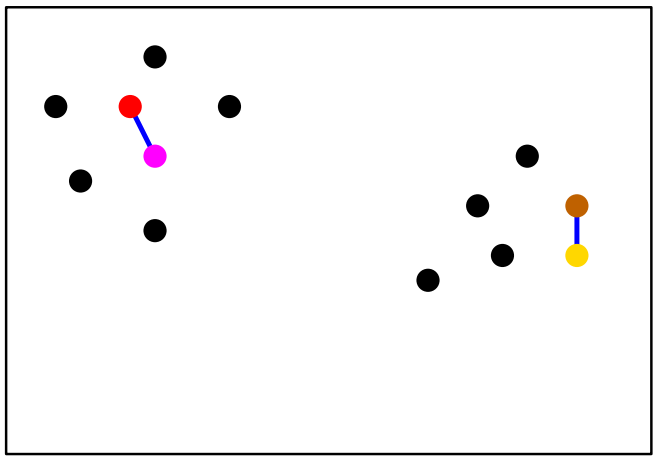
1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.



Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

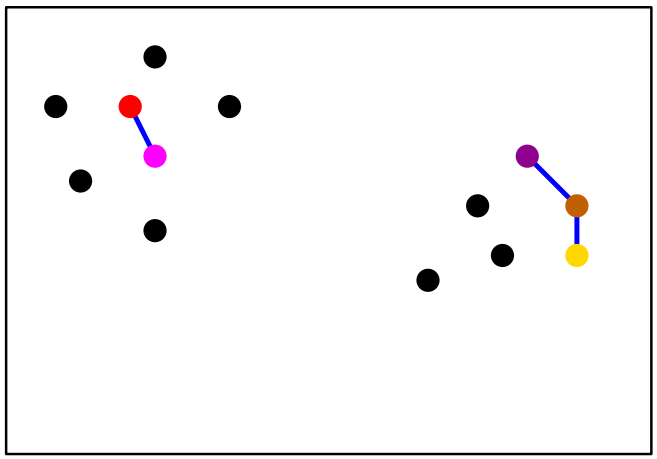
1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.



Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

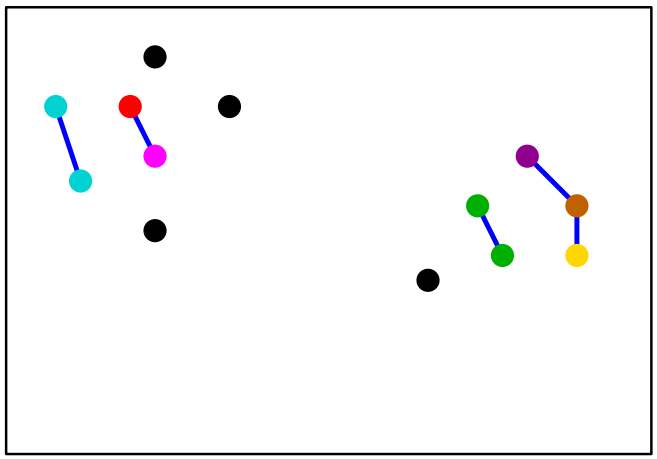
1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.

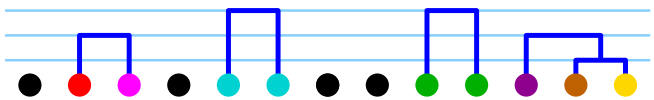


Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.

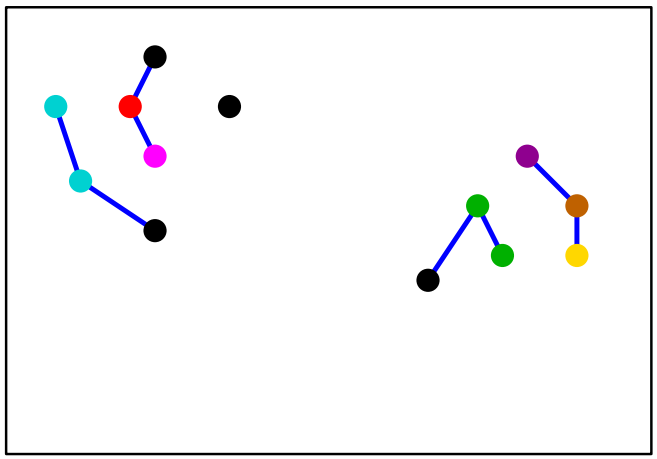


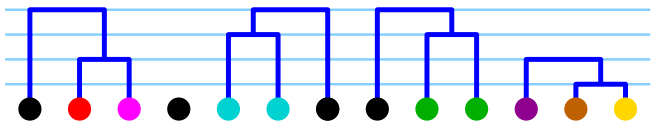


Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.

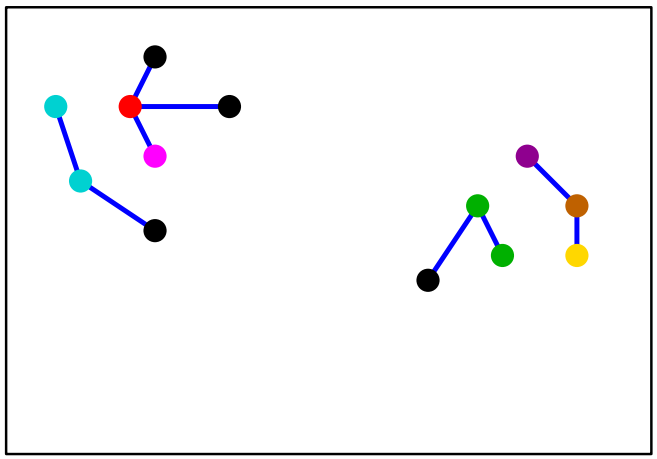


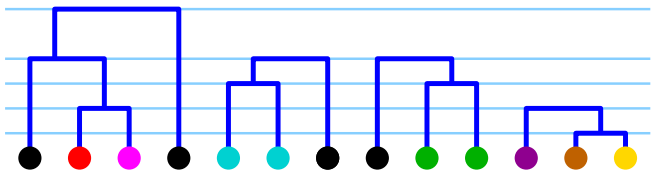


Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.

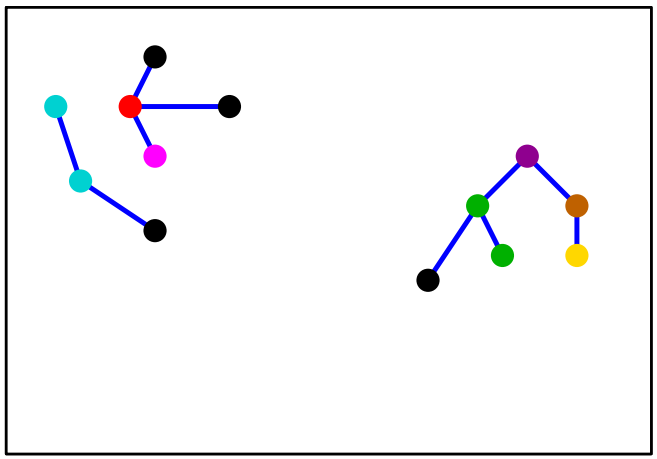


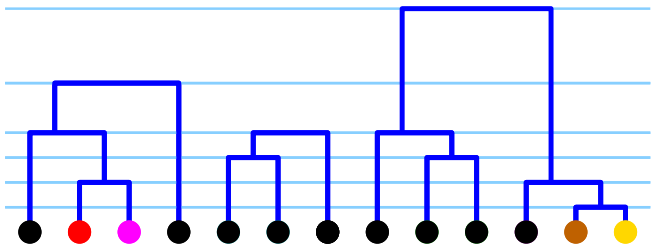


Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.

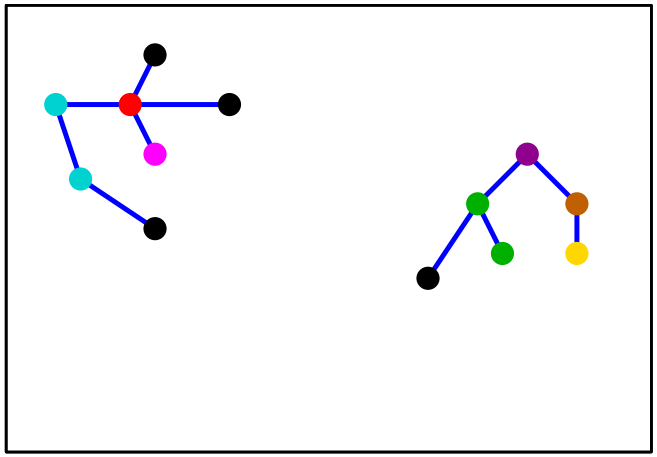


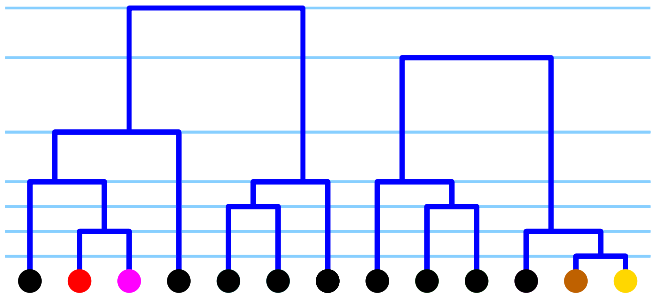


Hierarchical Clustering Algorithm

- Bottom-up clustering algorithm.

1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.

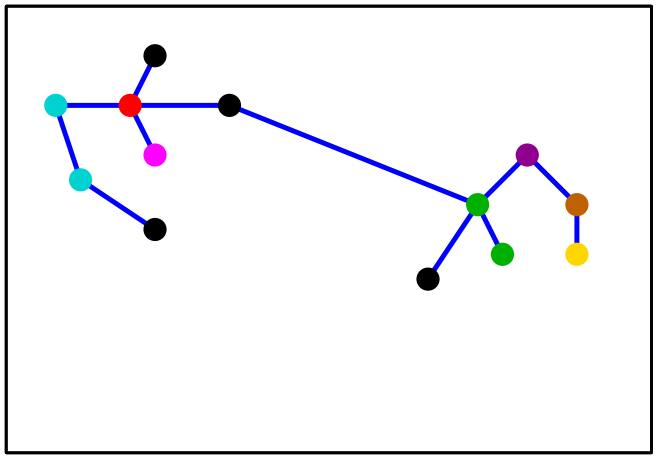


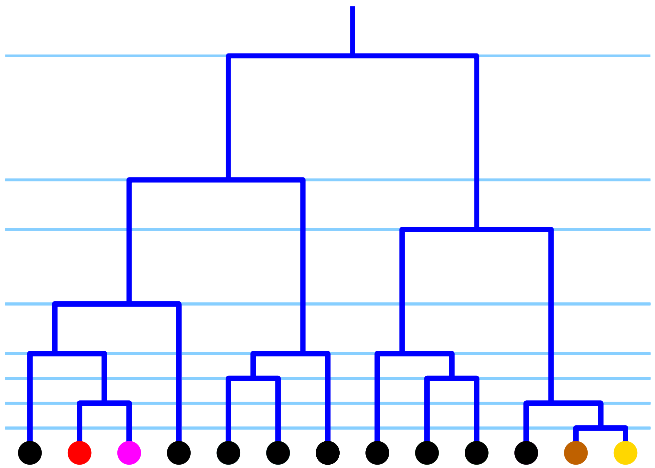


Hierarchical Clustering Algorithm

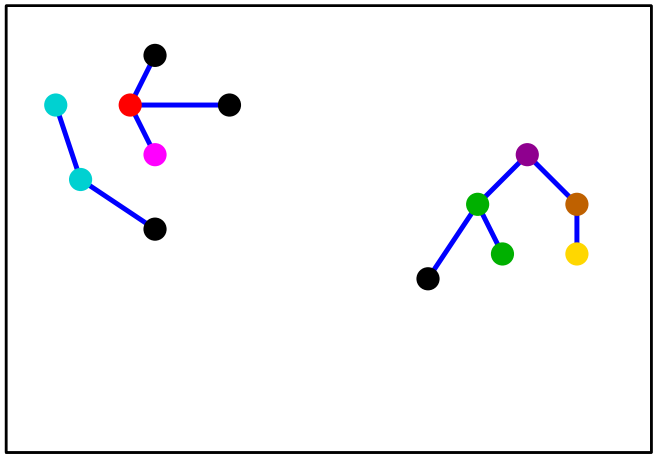
- Bottom-up clustering algorithm.

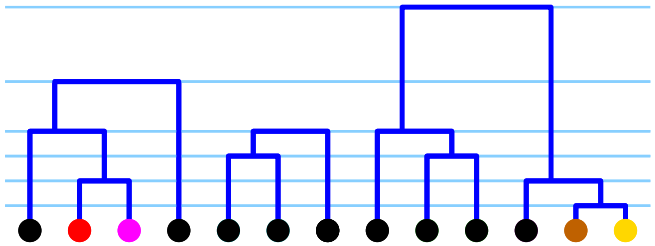
1. Start with every object in its own cluster.
2. Repeat
   - Let C_i and C_j be the clusters "nearest" each other.
   - Merge C_i and C_j.
3. until all the objects are in one cluster.





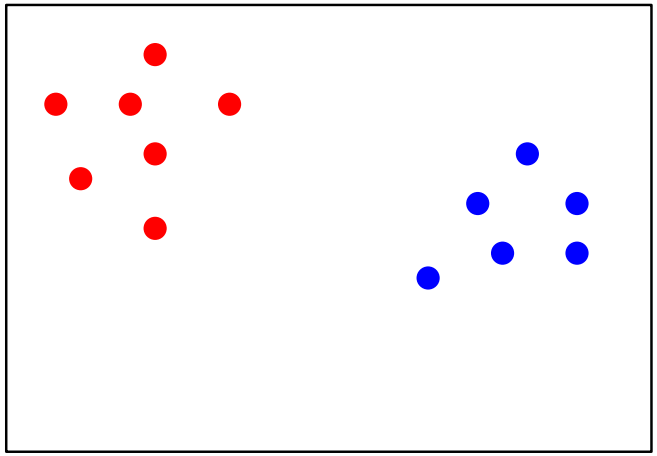
Measuring Distance between Clusters





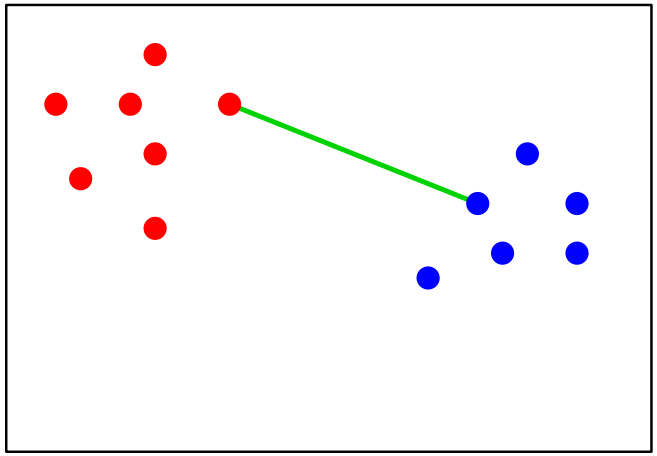
- How do we measure distance between two clusters C_i and C_j?

Measuring Distance between Clusters



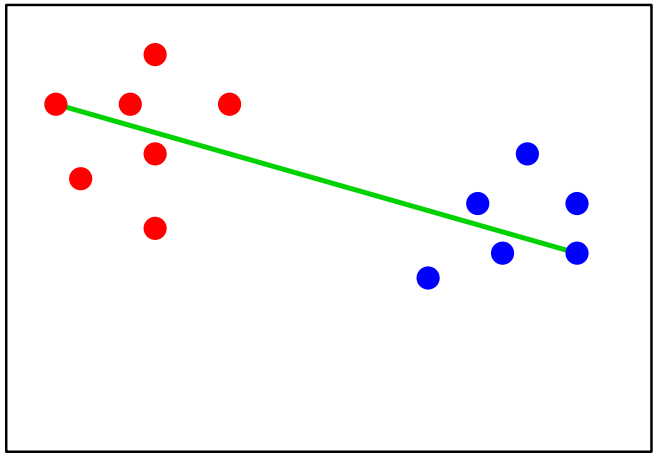
- How do we measure distance between two clusters C_i and C_j?

Measuring Distance between Clusters



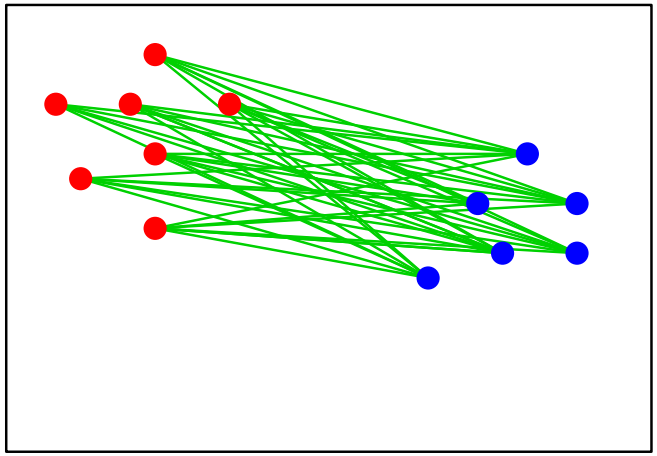
- How do we measure distance between two clusters C_i and C_j?
- $d_{min}(C_i, C_j)$ = distance between closest pair of objects.

Measuring Distance between Clusters



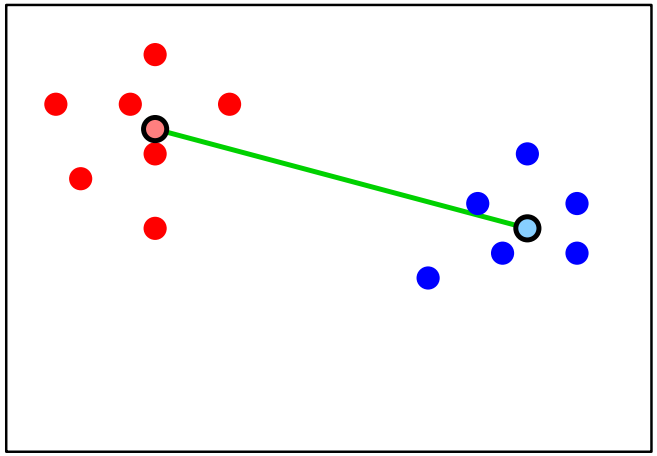
- How do we measure distance between two clusters C_i and C_j?
- $d_{min}(C_i, C_j)$ = distance between closest pair of objects.
- $d_{max}(C_i, C_j)$ = distance between farthest pair of objects.

Measuring Distance between Clusters



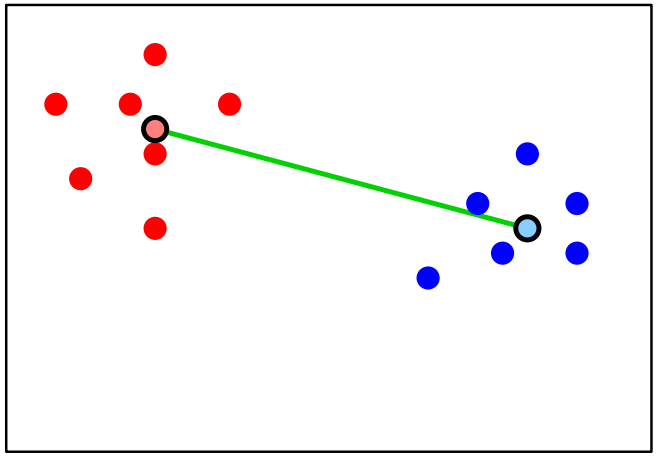
- How do we measure distance between two clusters C_i and C_j?
- $d_{min}(C_i, C_j)$ = distance between closest pair of objects.
- $d_{max}(C_i, C_j)$ = distance between farthest pair of objects.
- $d_{mean}(C_i, C_j)$ = average of distances between all pairs of objects.

Measuring Distance between Clusters



- How do we measure distance between two clusters C_i and C_j?
- $d_{min}(C_i, C_j)$ = distance between closest pair of objects.
- $d_{max}(C_i, C_j)$ = distance between farthest pair of objects.
- $d_{mean}(C_i, C_j)$ = average of distances between all pairs of objects.
- $d_{centroid}(C_i, C_j) = d(\mu_i, \mu_j)$, where μ_i is the centroid of C_i.

Measuring Distance between Clusters



- How do we measure distance between two clusters C_i and C_j?
- $d_{min}(C_i, C_j)$ = distance between closest pair of objects.
- $d_{max}(C_i, C_j)$ = distance between farthest pair of objects.
- $d_{mean}(C_i, C_j)$ = average of distances between all pairs of objects.
- $d_{centroid}(C_i, C_j) = d(\mu_i, \mu_j)$, where μ_i is the centroid of C_i.
- Methods are called minimum linkage, maximum linkage, mean linkage, and centroid linkage clustering, respectively.

- Computing $d_{min}, d_{max}, d_{avg}$ takes $O(n_i n_j)$ time.
- Computing d_{mean} takes $O(n_i + n_j)$ time.

Running Time of Hierarchical Clustering

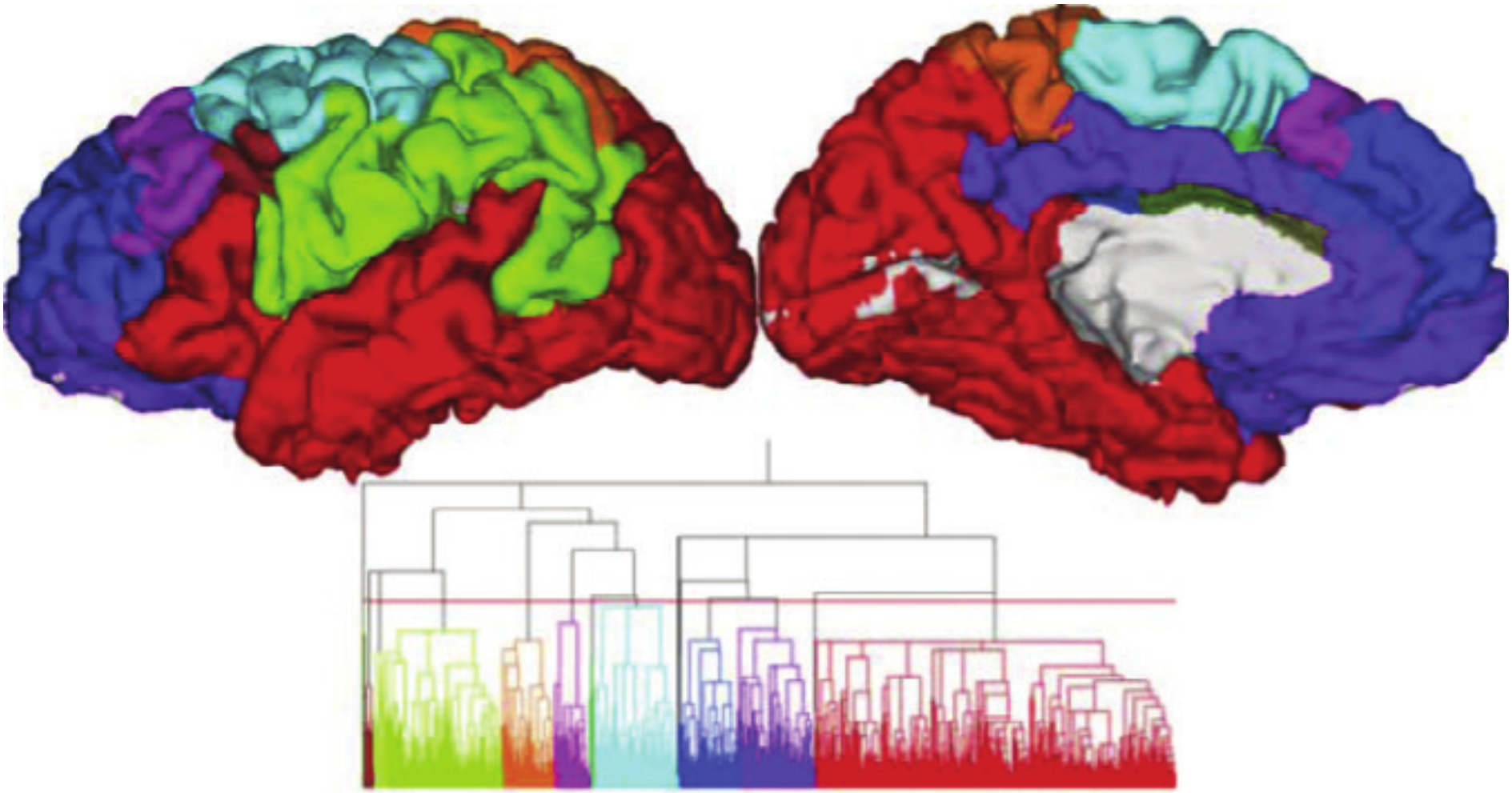
1. Start with every object in its own cluster.
2. Repeat
   - Let D_i and D_j be the clusters "nearest" each other.
   - Merge D_i and D_j.
3. until all the objects are in one cluster.

Running Time of Hierarchical Clustering

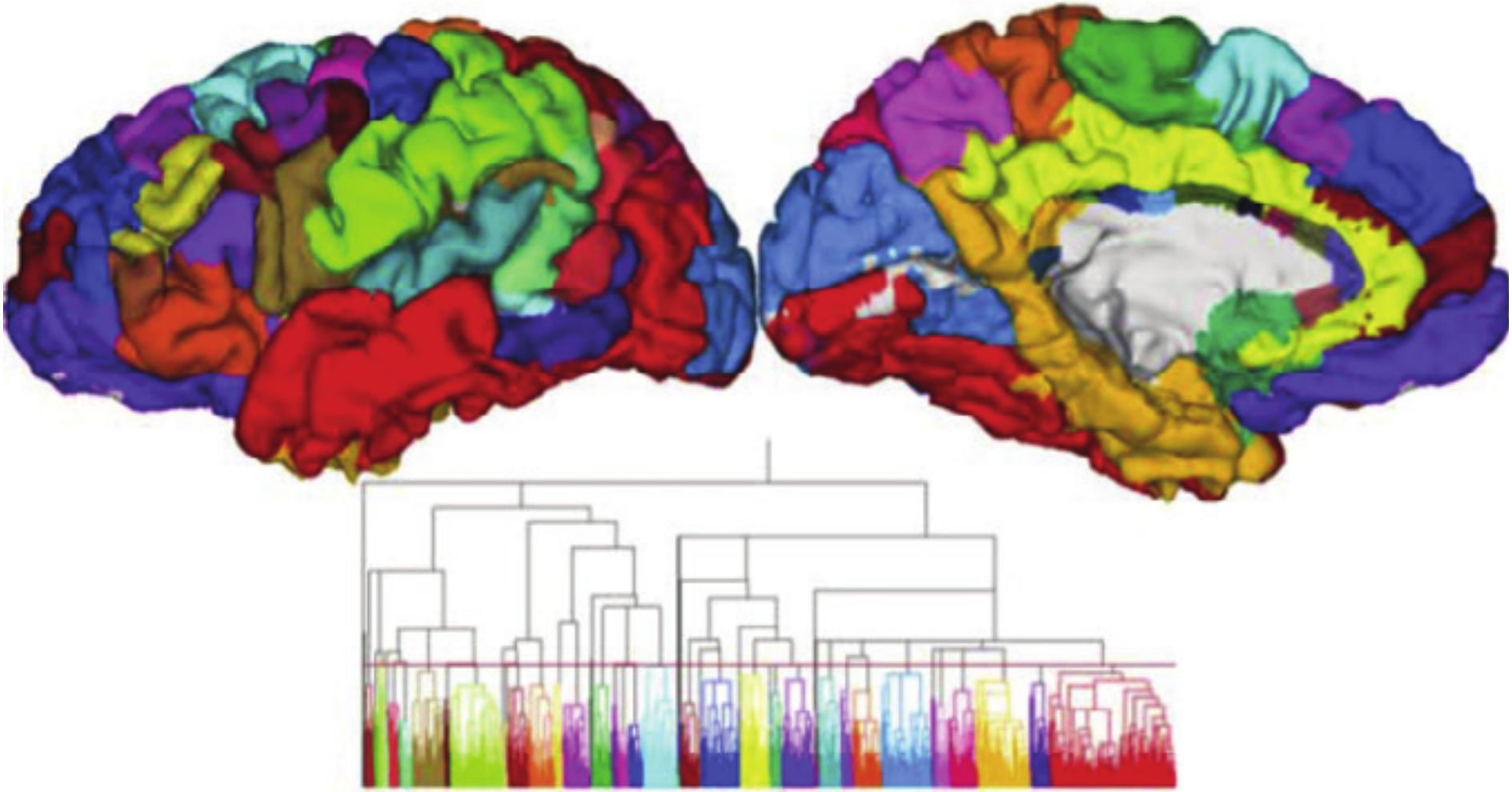
1. Start with every object in its own cluster.
2. Repeat
   - Let D_i and D_j be the clusters "nearest" each other.
   - Merge D_i and D_j.
3. until all the objects are in one cluster.

- Assume computing distance between two objects takes $O(1)$ time.
- Store all $O(n^2)$ inter-object distances.
- At each iteration, compute distance between every pair of clusters: takes $O(n^2)$ time in total.
- There are n iterations, so overall running time is $O(nn^2) = O(n^3)$.

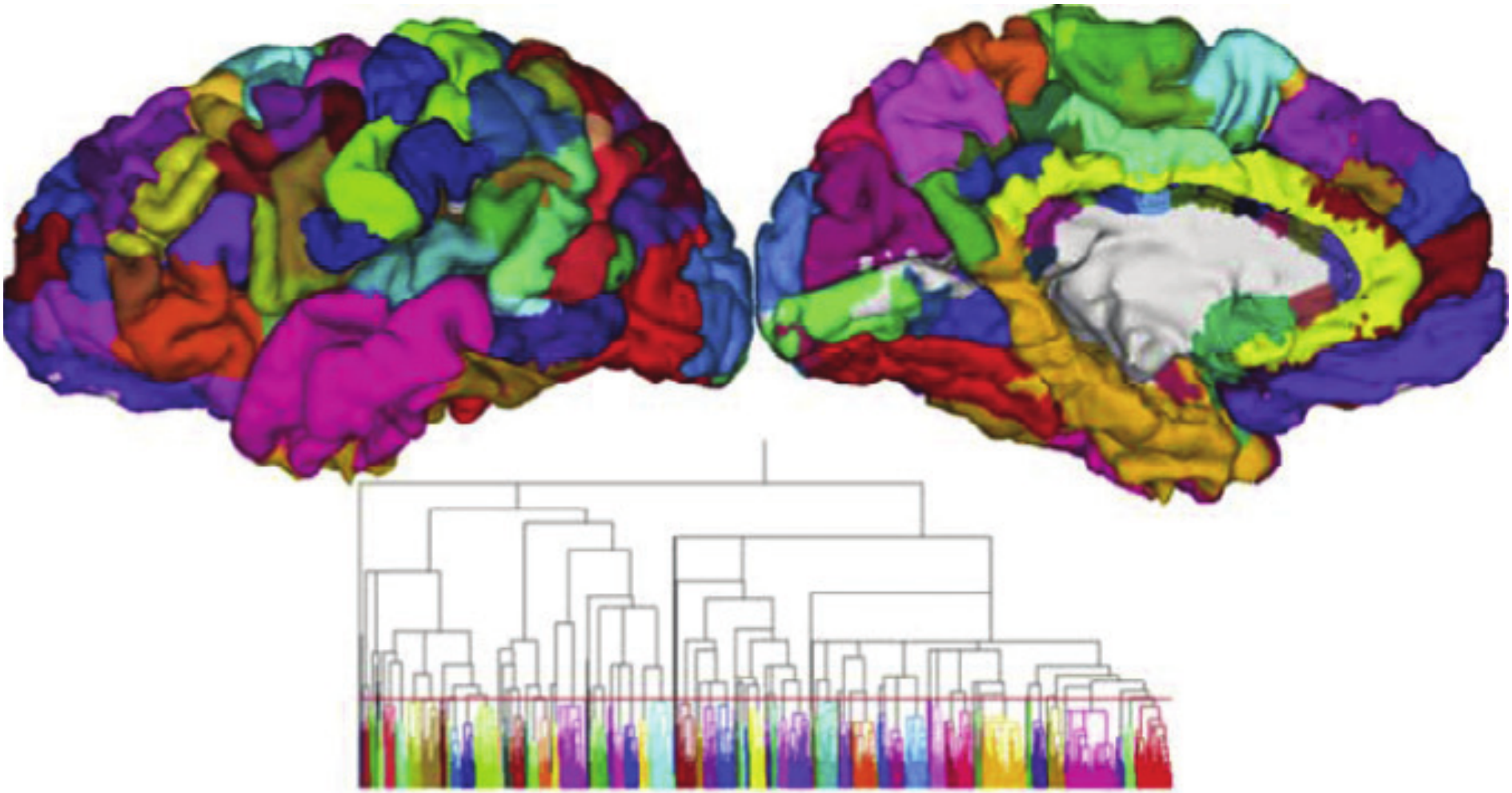
Hierarchical Clustering Result



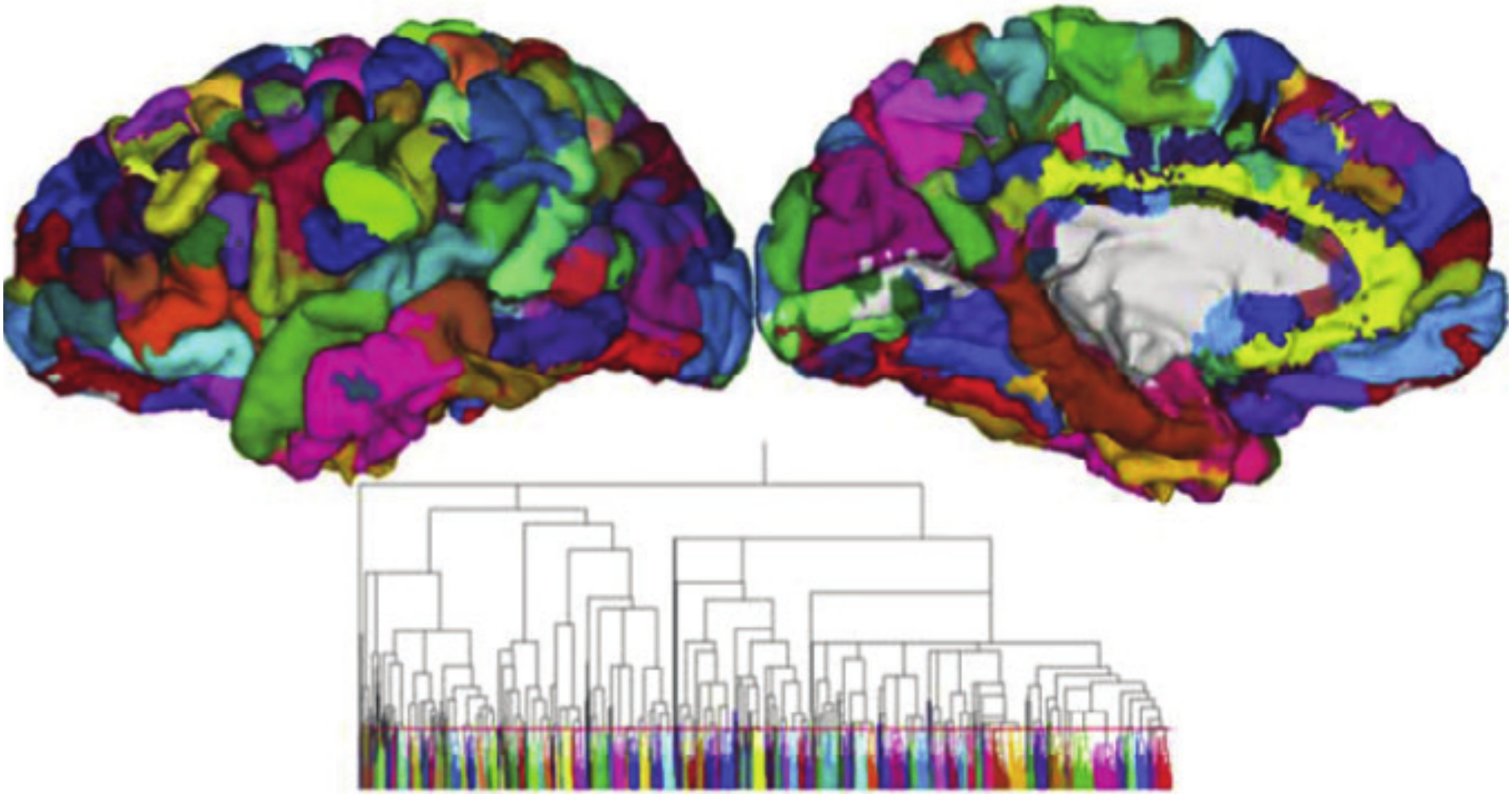
Hierarchical Clustering Result



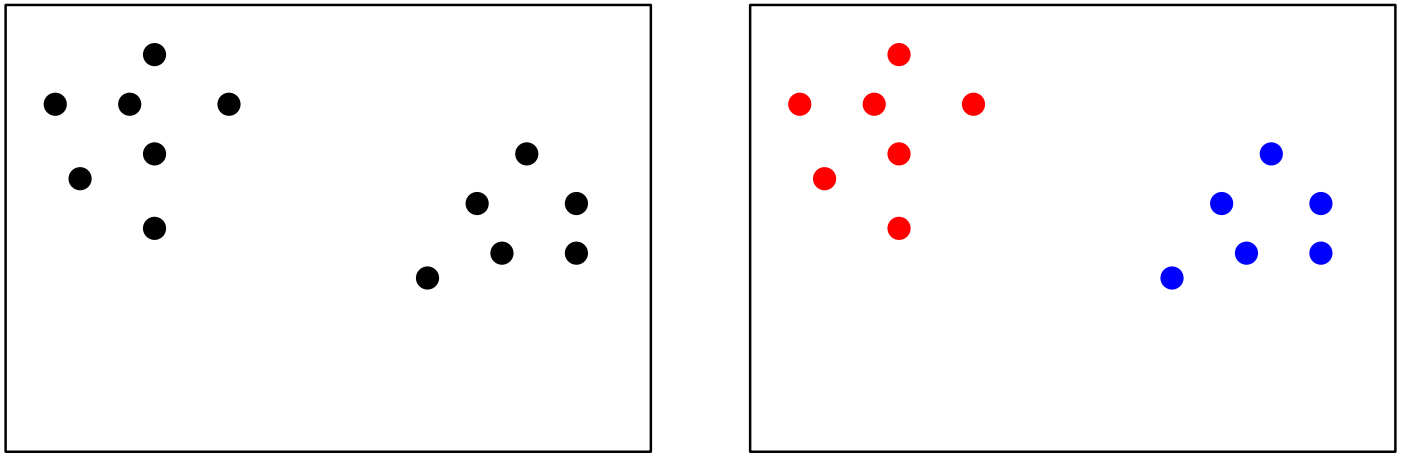
Hierarchical Clustering Result



Hierarchical Clustering Result



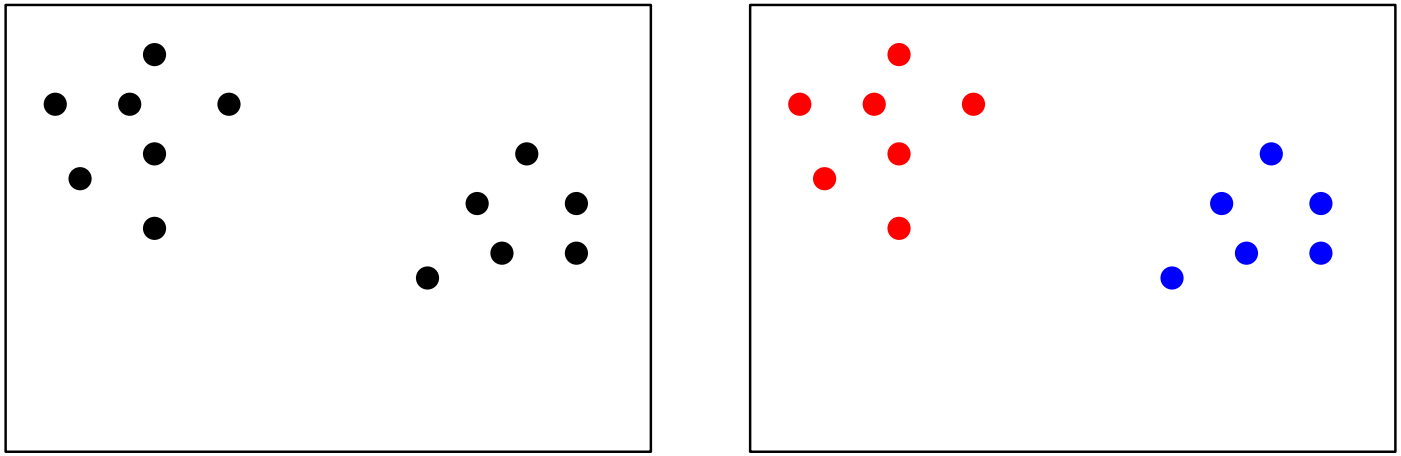
Definition of Clustering



Given a set of n objects, find the best partition of the objects into subsets such that each subset contains objects that are similar/close to each other.

- How do we measure how similar or close two objects are?

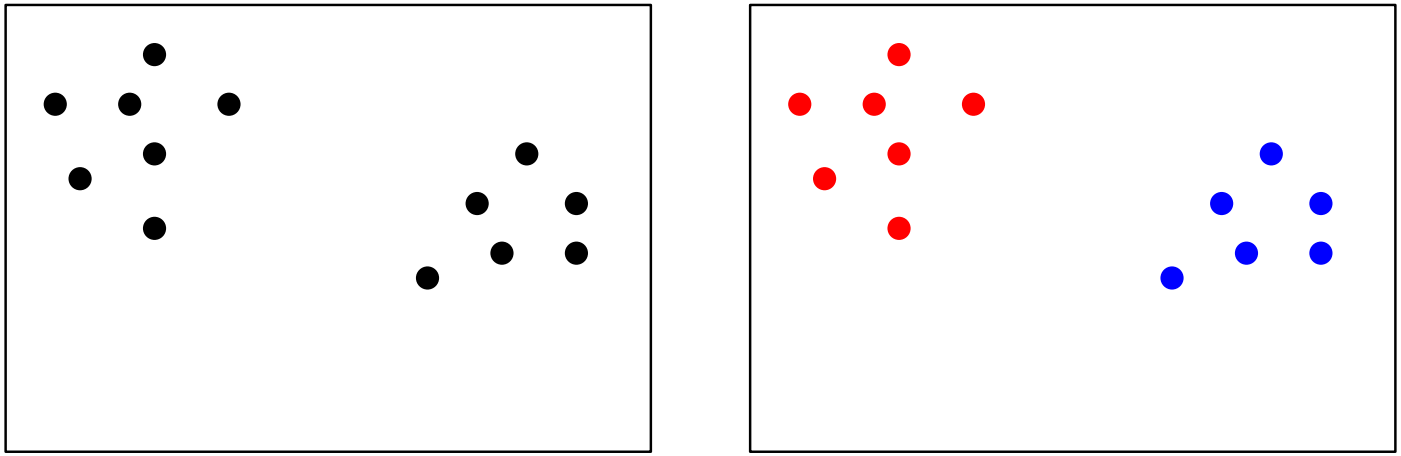
Definition of Clustering



Given a set of n objects, find the best partition of the objects into subsets such that each subset contains objects that are similar/close to each other.

- How do we measure how similar or close two objects are?
- How many subsets?

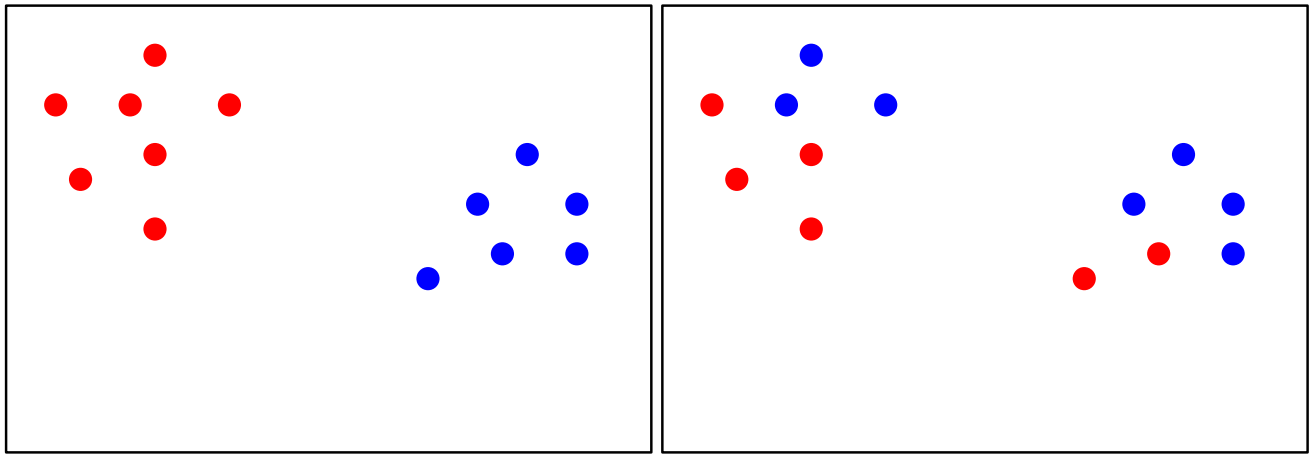
Definition of Clustering



Given a set of n objects, find the best partition of the objects into subsets such that each subset contains objects that are similar/close to each other.

- How do we measure how similar or close two objects are?
- How many subsets? Not specified in hierarchical clustering.

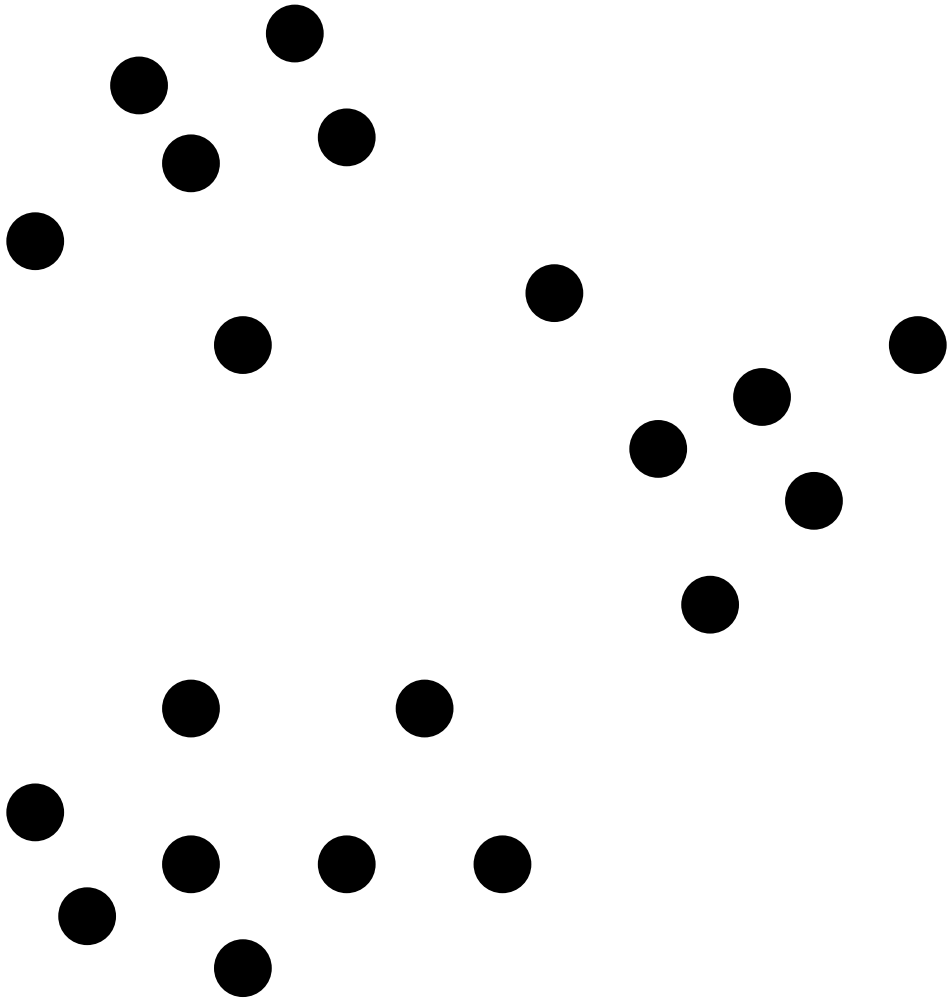
Definition of Clustering



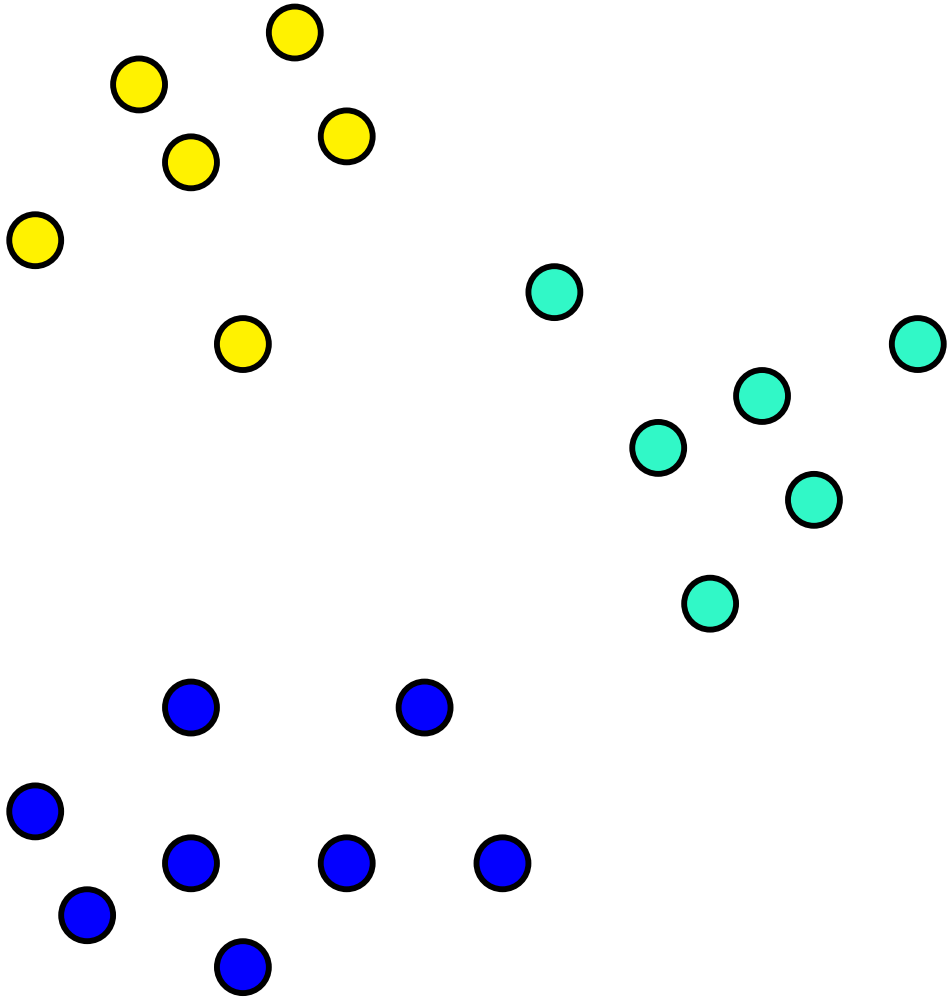
Given a set of n objects, find the best partition of the objects into subsets such that each subset contains objects that are similar/close to each other.

- How do we measure how similar or close two objects are?
- How many subsets? Not specified in hierarchical clustering.
- How do we compare two different partitions?

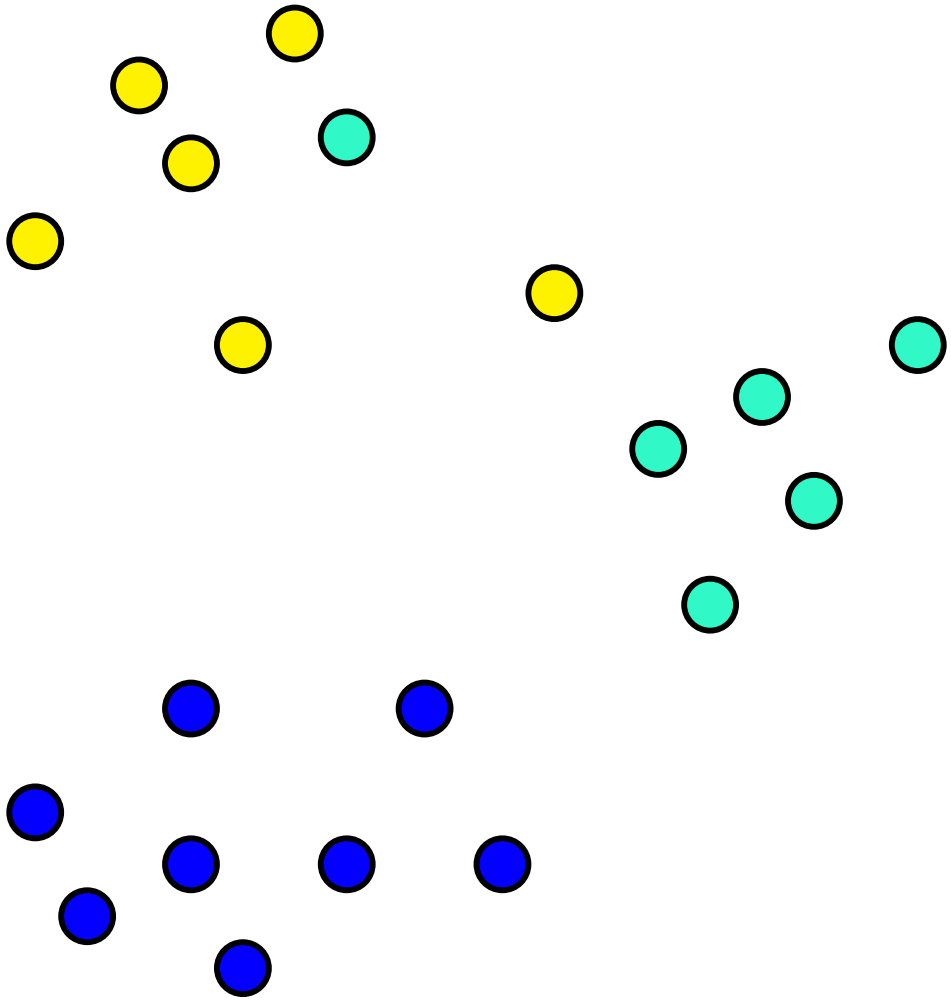
Example of Clustering



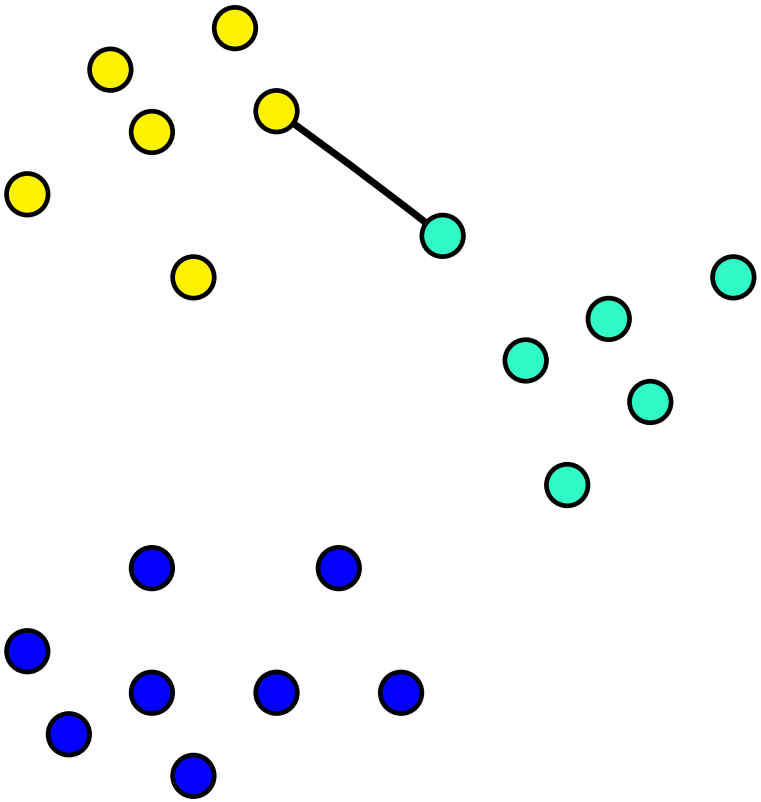
Example of Clustering

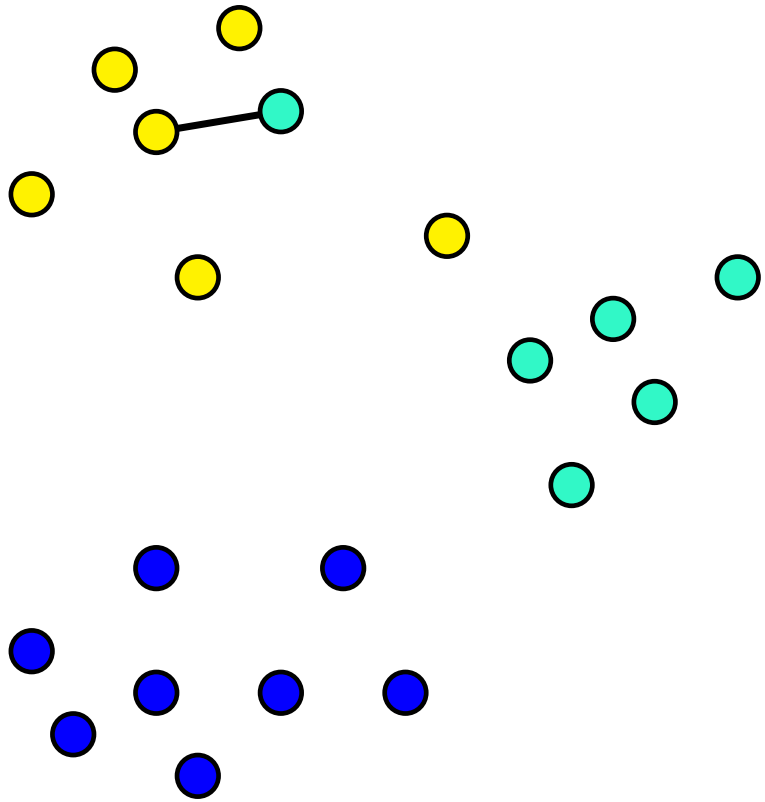


Example of Clustering



Example of Clustering





Formalising the Clustering Problem

- Let U be the set of n objects labelled $p_1, p_2, \ldots, p_n$.
- For every pair p_i and p_j, we have a distance $d(p_i, p_j)$.
- We require $d(p_i, p_i) = 0$, $d(p_i, p_j) > 0$, if $i \neq j$, and $d(p_i, p_j) = d(p_j, p_i)$

Formalising the Clustering Problem

- Let U be the set of n objects labelled $p_1, p_2, \ldots, p_n$.
- For every pair p_i and p_j, we have a distance $d(p_i, p_j)$.
- We require $d(p_i, p_i) = 0$, $d(p_i, p_j) > 0$, if $i \neq j$, and $d(p_i, p_j) = d(p_j, p_i)$
- Given a positive integer k, a *k-clustering* of U is a partition of U into k non-empty subsets or "clusters" $C_1, C_2, \ldots C_k$.

Formalising the Clustering Problem

- Let U be the set of n objects labelled $p_1, p_2, \ldots, p_n$.
- For every pair p_i and p_j, we have a distance $d(p_i, p_j)$.
- We require $d(p_i, p_i) = 0$, $d(p_i, p_j) > 0$, if $i \neq j$, and $d(p_i, p_j) = d(p_j, p_i)$
- Given a positive integer k, a *k-clustering* of U is a partition of U into k non-empty subsets or "clusters" $C_1, C_2, \ldots C_k$.
- The *spacing* of a clustering is the smallest distance between objects in two different subsets:

$$\text{spacing}(C_1, C_2, \ldots C_k) = \min_{\substack{1 \leq i,j \leq k \\ i \neq j, \\ p \in C_i, q \in C_j}} d(p, q)$$

Formalising the Clustering Problem

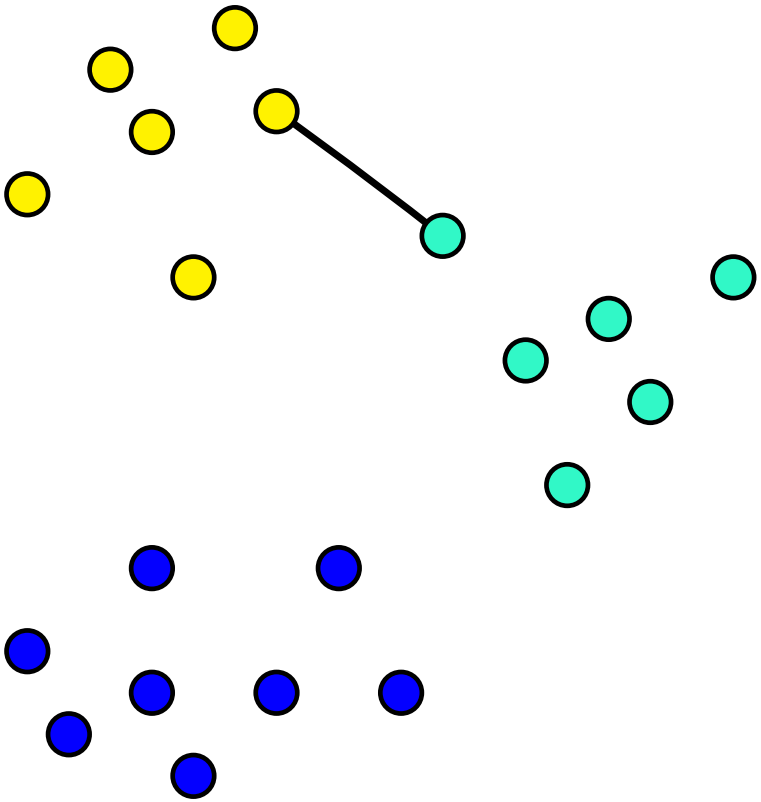
- Let U be the set of n objects labelled $p_1, p_2, \ldots, p_n$.
- For every pair p_i and p_j, we have a distance $d(p_i, p_j)$.
- We require $d(p_i, p_i) = 0$, $d(p_i, p_j) > 0$, if $i \neq j$, and $d(p_i, p_j) = d(p_j, p_i)$
- Given a positive integer k, a *k-clustering* of U is a partition of U into k non-empty subsets or "clusters" $C_1, C_2, \ldots C_k$.
- The *spacing* of a clustering is the smallest distance between objects in two different subsets:

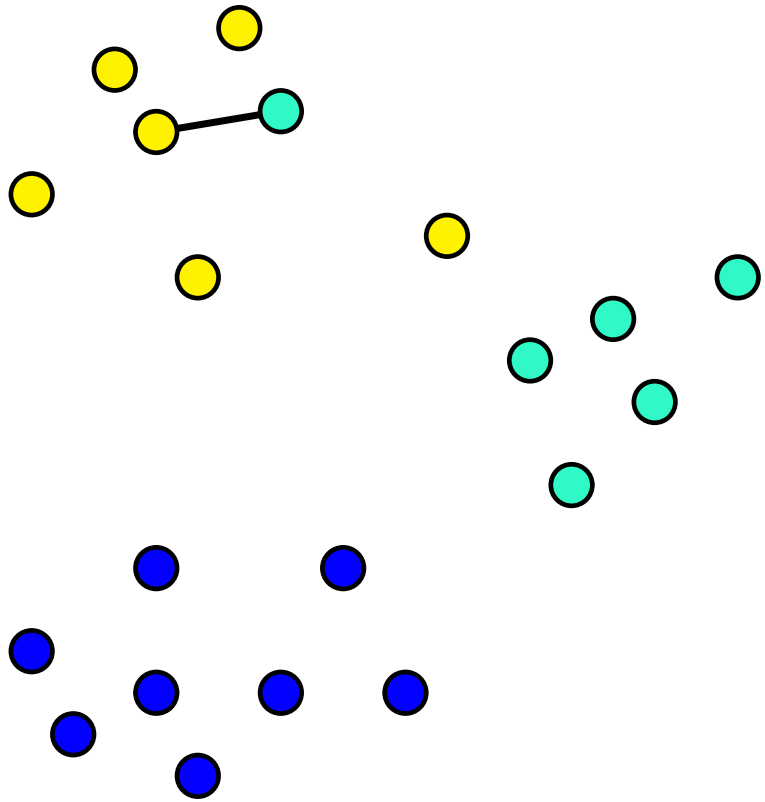
$$\text{spacing}(C_1, C_2, \ldots C_k) = \min_{\substack{1 \leq i,j \leq k \\ i \neq j, \\ p \in C_i, q \in C_j}} d(p, q)$$

Clustering of Maximum Spacing

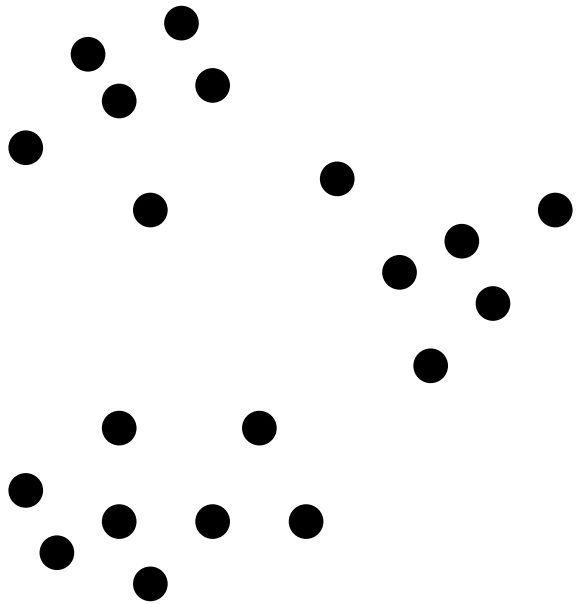
Given a set U of objects, a distance function $d : U \times U \to \mathbb{R}^+$, and a positive integer k,
compute a k-clustering of U whose spacing is the largest over all possible k-clusterings.

Example of Clustering

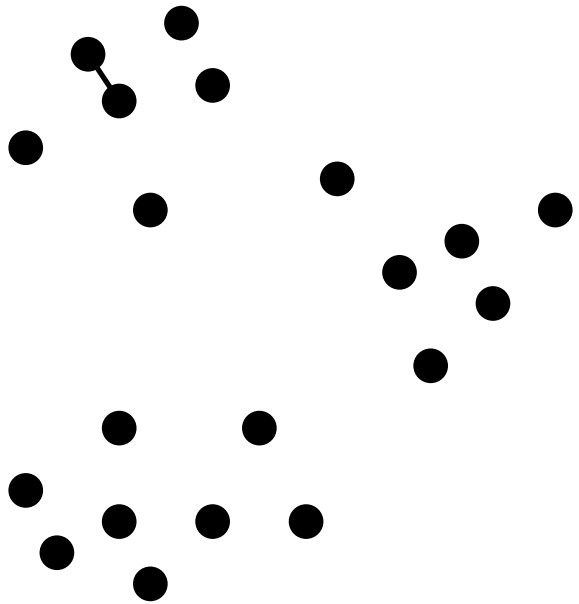




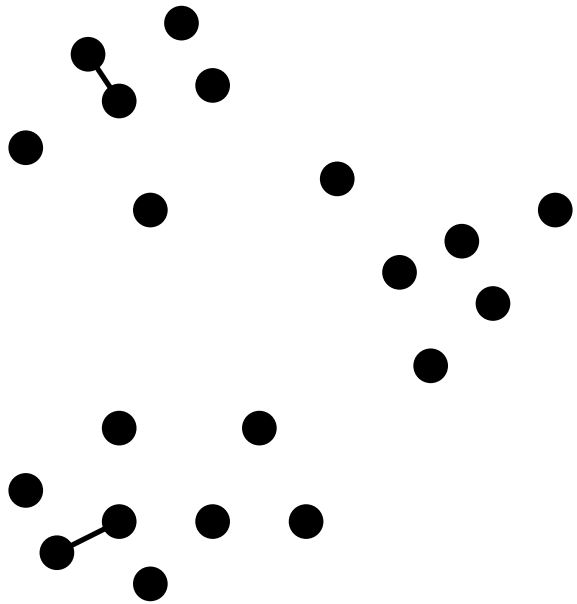
Algorithm for Clustering of Maximum Spacing



Algorithm for Clustering of Maximum Spacing

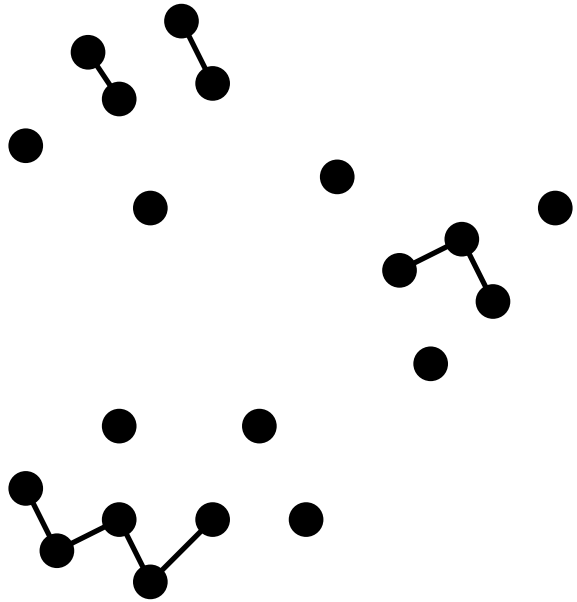


Algorithm for Clustering of Maximum Spacing



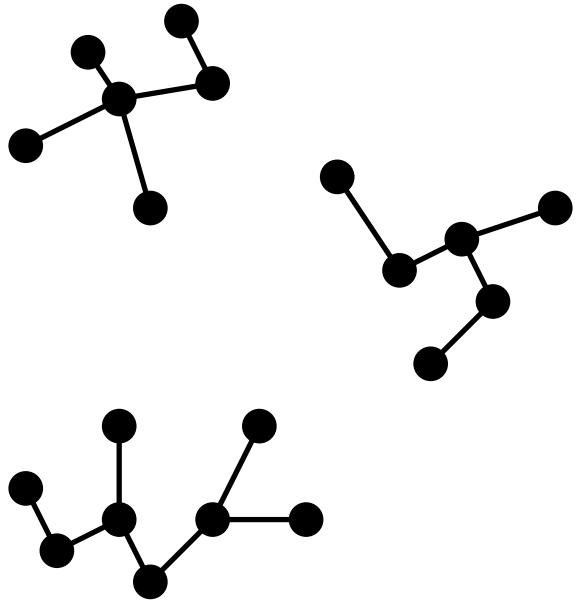
- Intuition: greedily cluster objects in increasing order of distance.

Algorithm for Clustering of Maximum Spacing



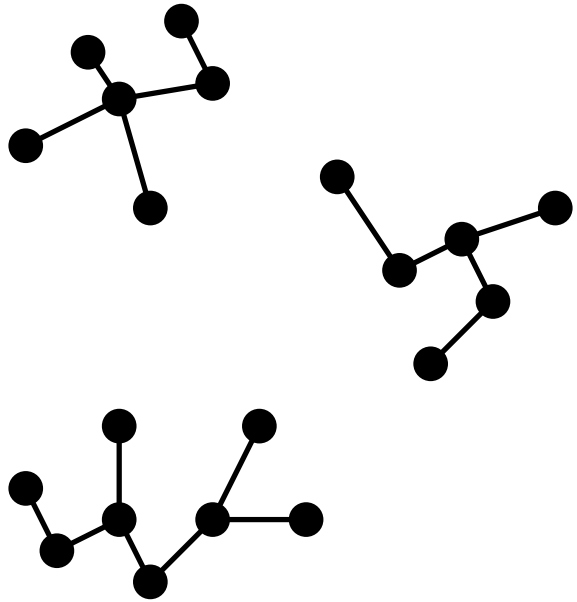
- Intuition: greedily cluster objects in increasing order of distance.

Algorithm for Clustering of Maximum Spacing



- Intuition: greedily cluster objects in increasing order of distance.
- Let $\mathcal{C}$ be a set of n clusters, with each object in U in its own cluster.
- Process pairs of objects in increasing order of distance.
  - Let (p, q) be the next pair with $p \in C_p$ and $q \in C_q$.
  - If $C_p \neq C_q$, add new cluster $C_p \cup C_q$ to $\mathcal{C}$, delete C_p and C_q from $\mathcal{C}$.
- Stop when there are k clusters in $\mathcal{C}$.

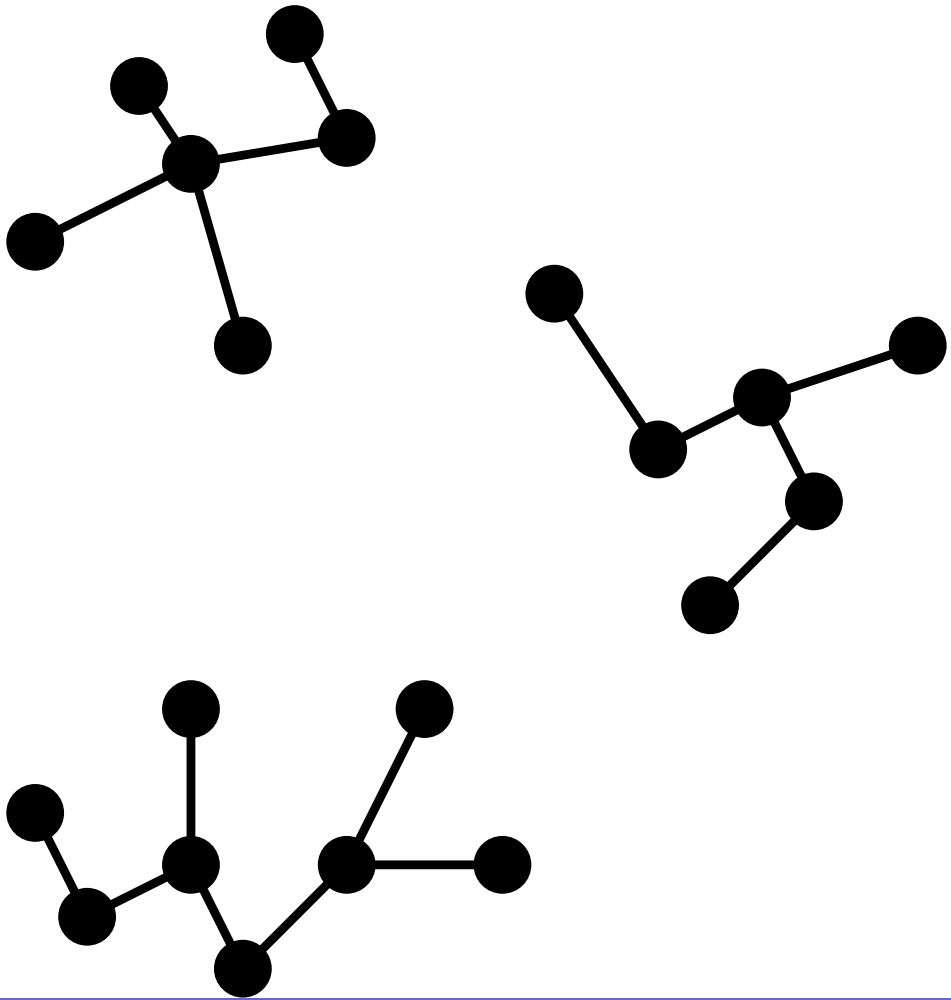
Algorithm for Clustering of Maximum Spacing



- Intuition: greedily cluster objects in increasing order of distance.
- Let $\mathcal{C}$ be a set of n clusters, with each object in U in its own cluster.
- Process pairs of objects in increasing order of distance.
  - Let (p, q) be the next pair with $p \in C_p$ and $q \in C_q$.
  - If $C_p \neq C_q$, add new cluster $C_p \cup C_q$ to $\mathcal{C}$, delete C_p and C_q from $\mathcal{C}$.
- Stop when there are k clusters in $\mathcal{C}$.
- Same as Kruskal's algorithm but do not add last $k-1$ edges in MST.

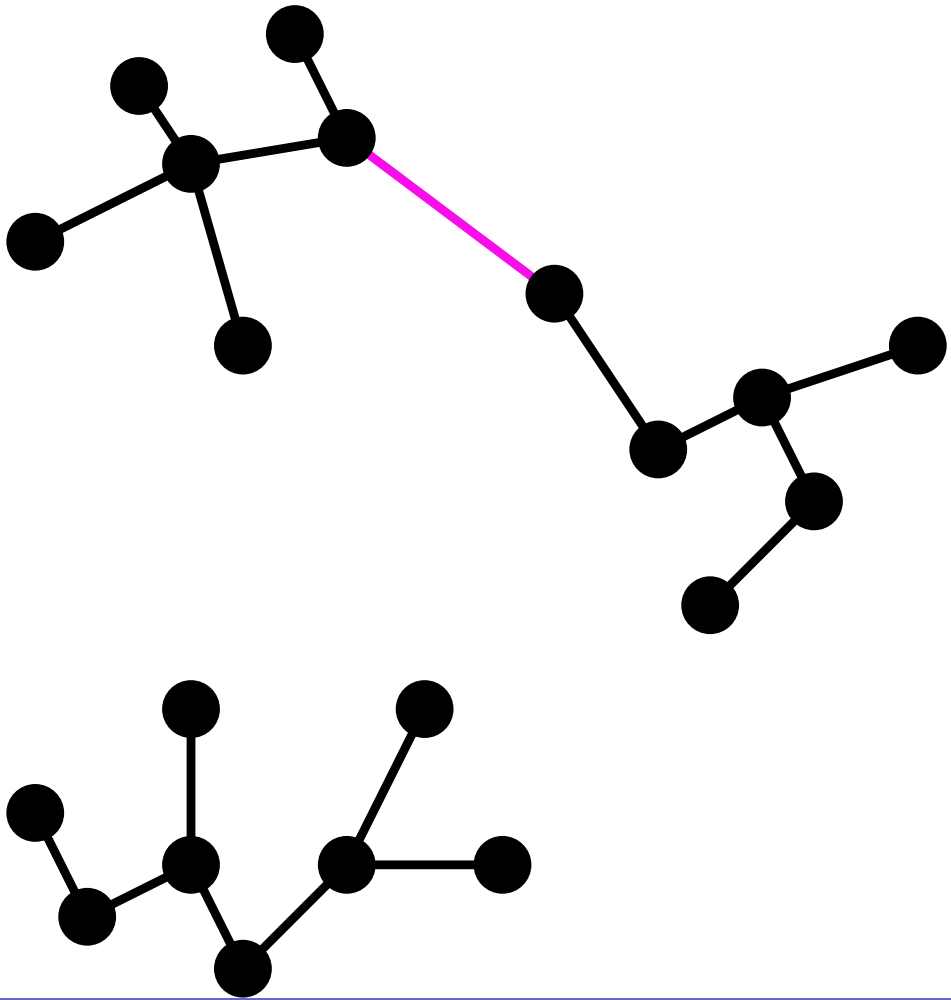
What is the spacing of the Algorithm's Clustering?

- Let $\mathcal{C}$ be the clustering produced by the algorithm.
- What is spacing($\mathcal{C}$)?

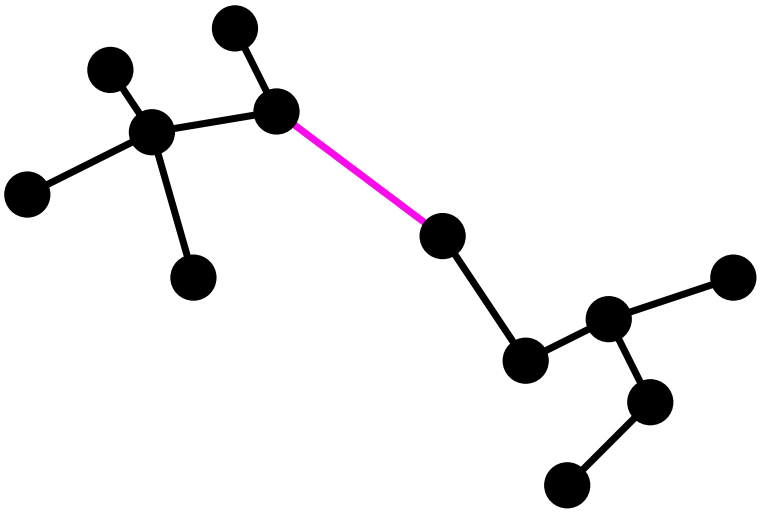


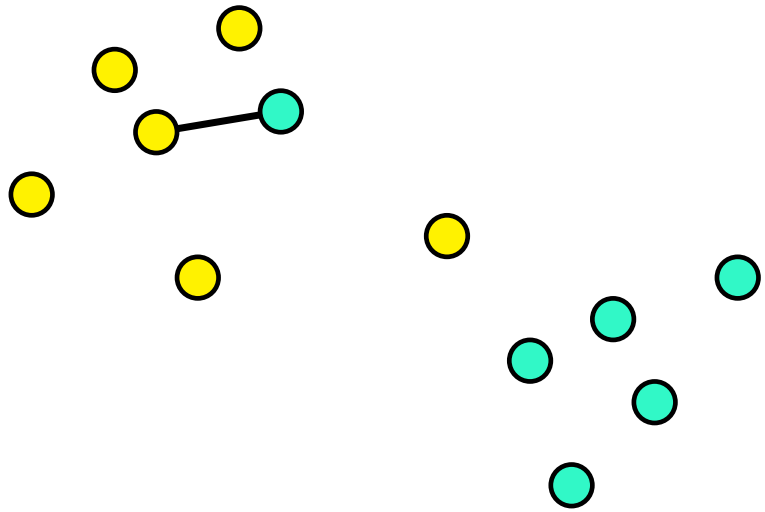
What is the spacing of the Algorithm's Clustering?

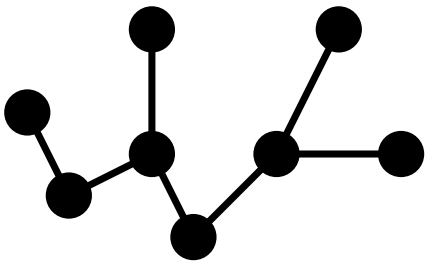
- Let $\mathcal{C}$ be the clustering produced by the algorithm.
- What is spacing($\mathcal{C}$)? It is the cost of the $(k-1)$st most expensive edge in the MST. Let this cost be d^*.

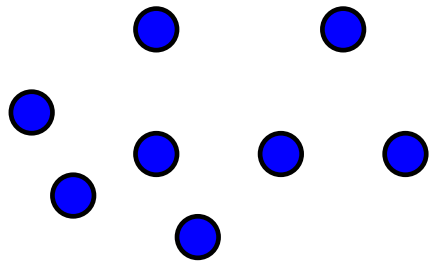


Why does the Algorithm Work?



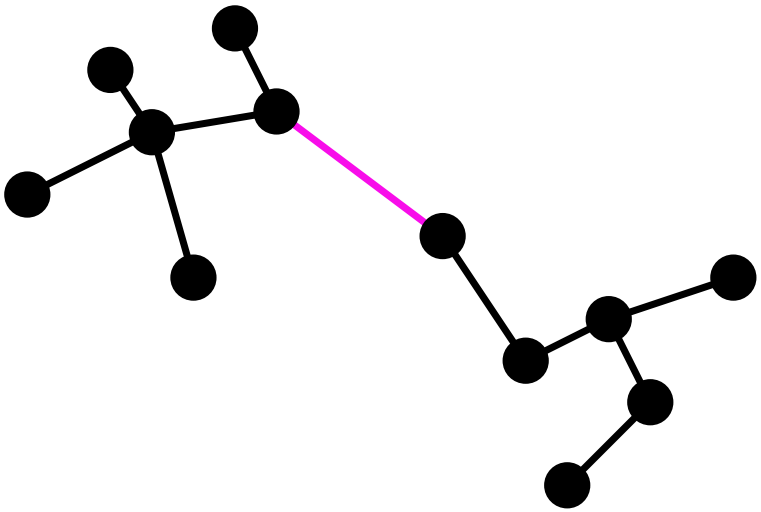


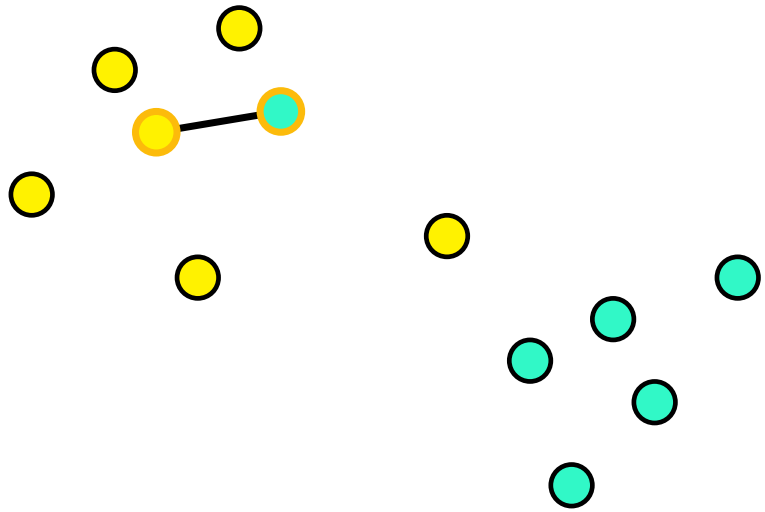


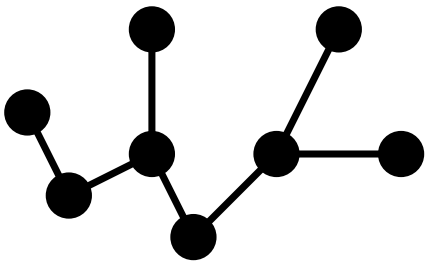


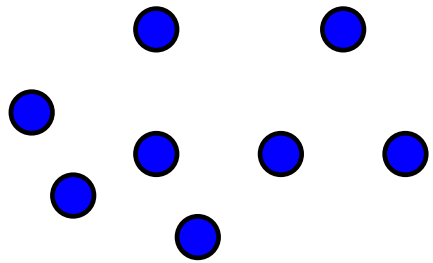
- Let $\mathcal{C}'$ be any other clustering.
- We will prove that spacing$(\mathcal{C}') \leq d^*$.

Why does the Algorithm Work?



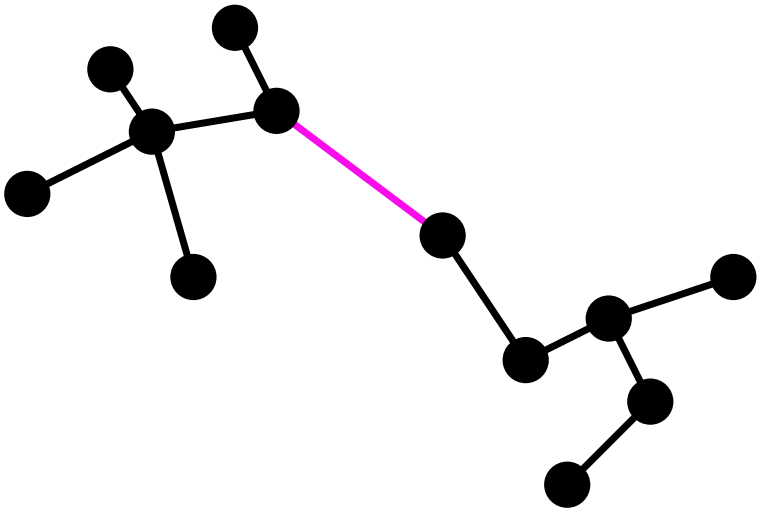


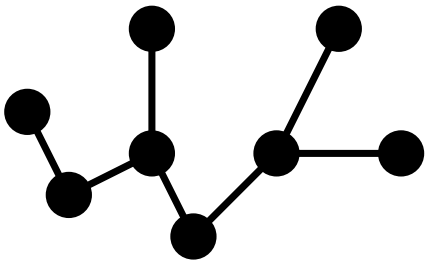


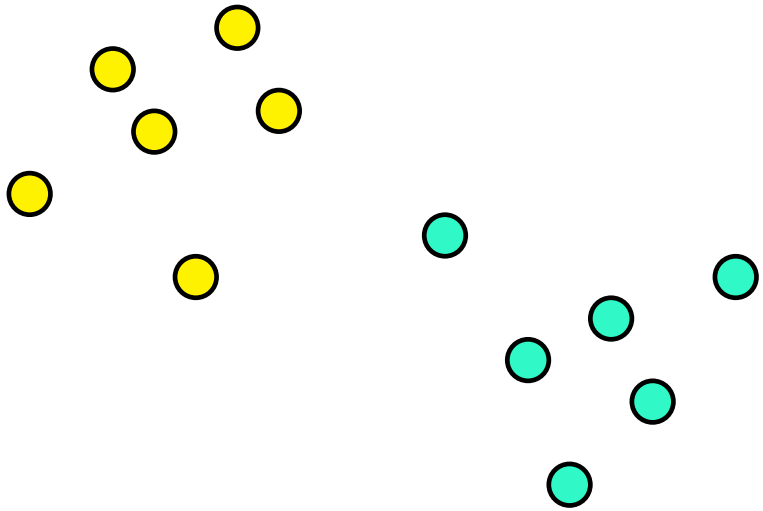


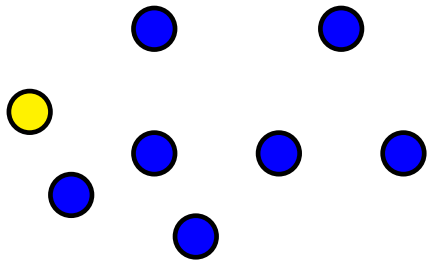
- Let $\mathcal{C}'$ be any other clustering.
- We will prove that spacing$(\mathcal{C}') \leq d^*$.

spacing$(\mathcal{C}') \leq d^*$: Intuition

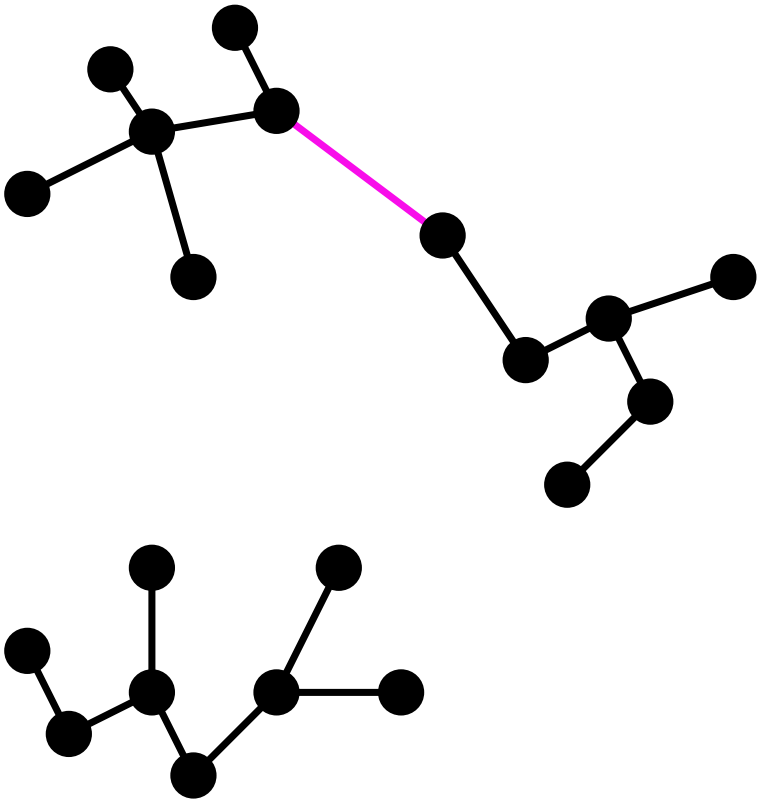


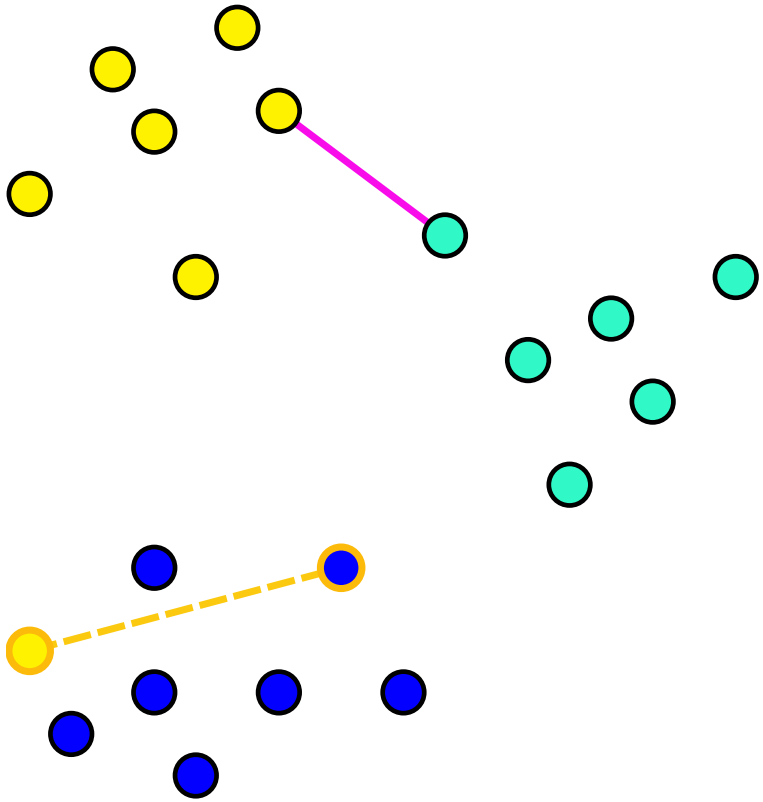




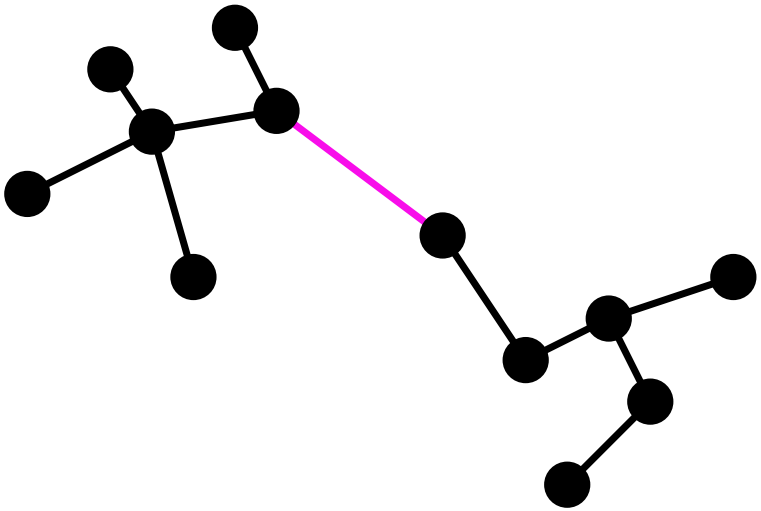


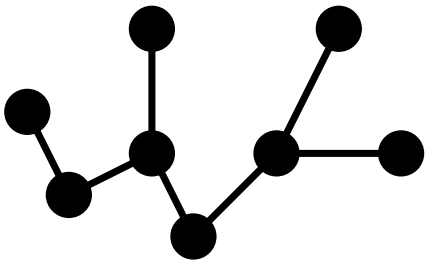
spacing$(\mathcal{C}') \leq d^*$: Intuition

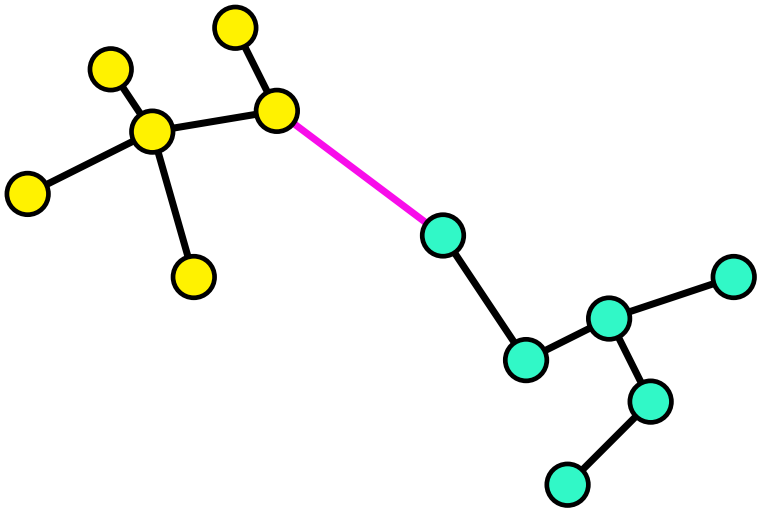


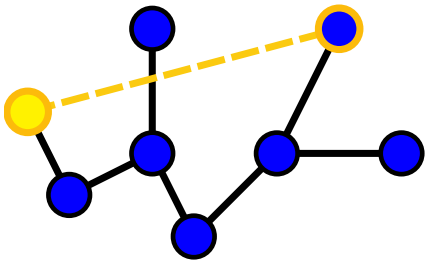


spacing$(\mathcal{C}') \leq d^*$: Intuition

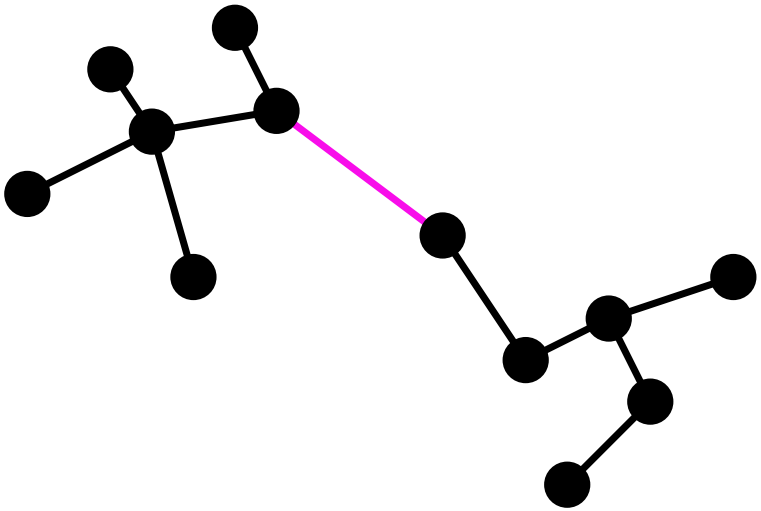


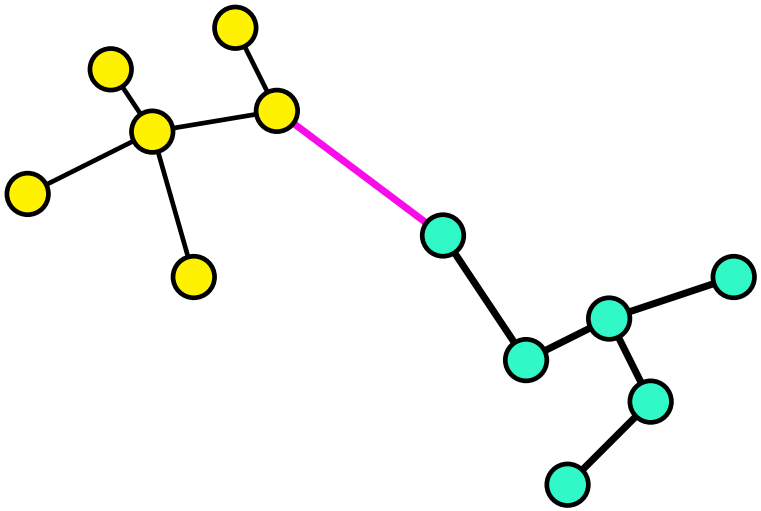


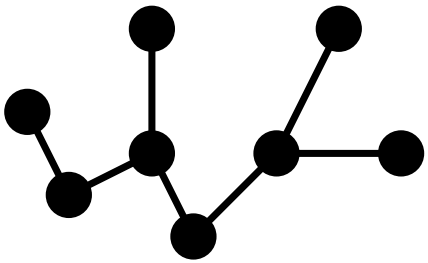


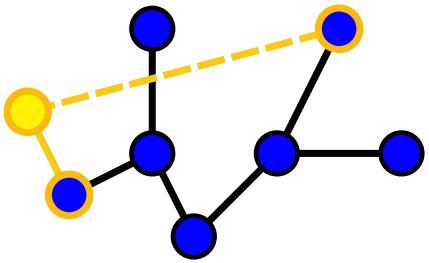


spacing$(\mathcal{C}') \leq d^*$: Intuition









$\textbf{spacing}(\mathcal{C}') \leq d^*$

- There must be two objects p_i and p_j in U in the same cluster C_r in $\mathcal{C}$ but in different clusters in $\mathcal{C}'$:

spacing$(\mathcal{C}') \leq d^*$

- There must be two objects p_i and p_j in U in the same cluster C_r in $\mathcal{C}$ but in different clusters in $\mathcal{C}'$: spacing$(\mathcal{C}') \leq d(p_i, p_j)$.

spacing$(\mathcal{C}') \leq d^*$

- There must be two objects p_i and p_j in U in the same cluster C_r in $\mathcal{C}$ but in different clusters in $\mathcal{C}'$: spacing$(\mathcal{C}') \leq d(p_i, p_j)$. But $d(p_i, p_j)$ could be $> d^*$.
- Suppose $p_i \in C'_s$ and $p_j \in C'_t$ in $\mathcal{C}'$.

spacing$(\mathcal{C}') \leq d^*$

- There must be two objects p_i and p_j in U in the same cluster C_r in $\mathcal{C}$ but in different clusters in $\mathcal{C}'$: spacing$(\mathcal{C}') \leq d(p_i, p_j)$. But $d(p_i, p_j)$ could be $> d^*$.
- Suppose $p_i \in C'_s$ and $p_j \in C'_t$ in $\mathcal{C}'$.
- All edges in the path Q connecting p_i and p_j in the MST have length $\leq d^*$.
- In particular, there is an object $p \in C'_s$ and an object $p' \notin C'_s$ such that p and p' are adjacent in Q.
- $d(p, p') \leq d^* \Rightarrow$ spacing$(\mathcal{C}') \leq d(p, p') \leq d^*$.

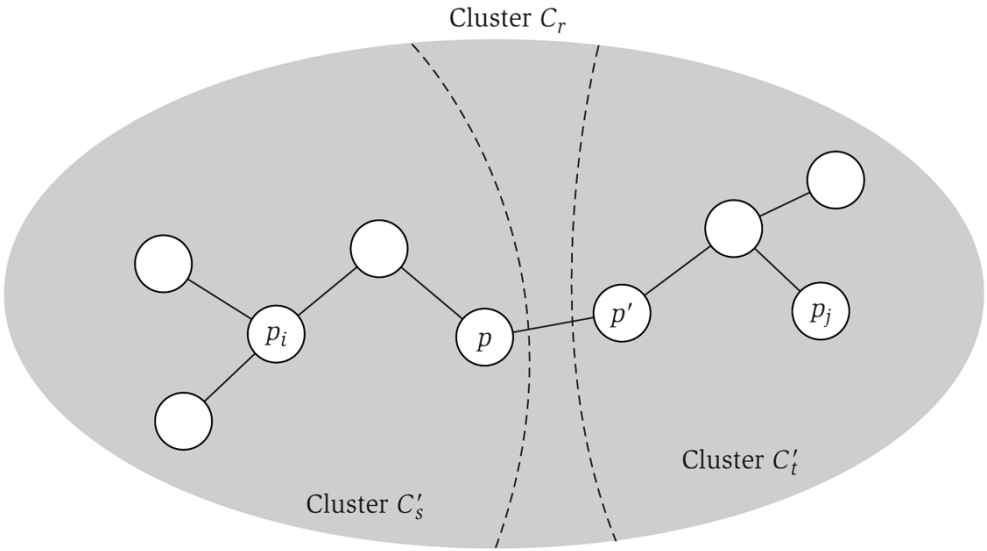
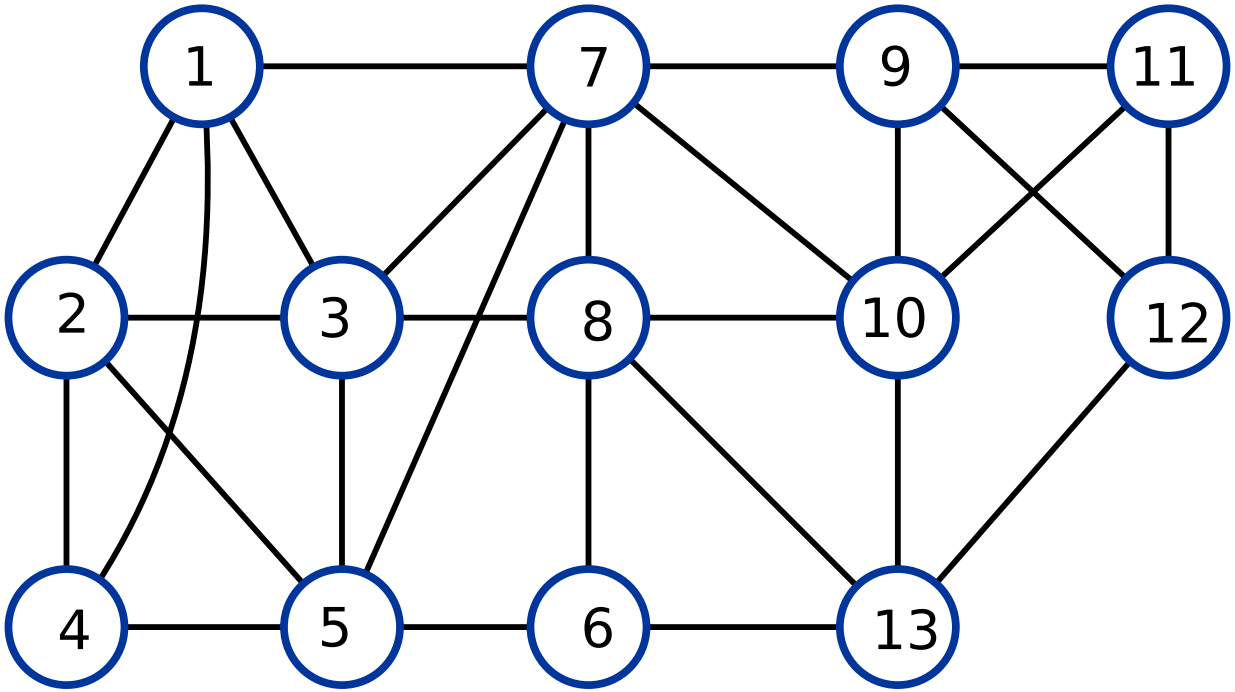


Figure 4.15 An illustration of the proof of (4.26), showing that the spacing of any other clustering can be no larger than that of the clustering found by the single-linkage algorithm.

Disadvantages of Hierarchical Clustering

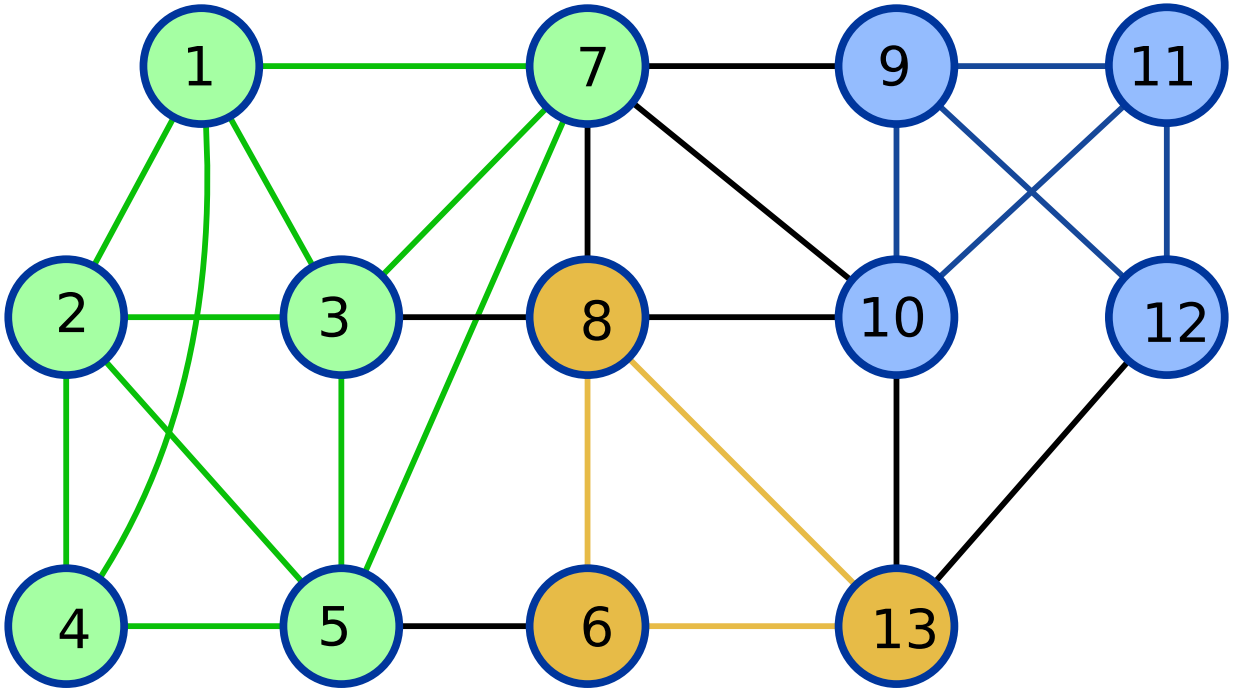
- To get a set of modules, at which level do we cut the dendrogram?
- Optimality due to spacing argument applies only to single linkage clustering.
- We need a different definition of module quality that captures connectivity within and across modules.

Motivation



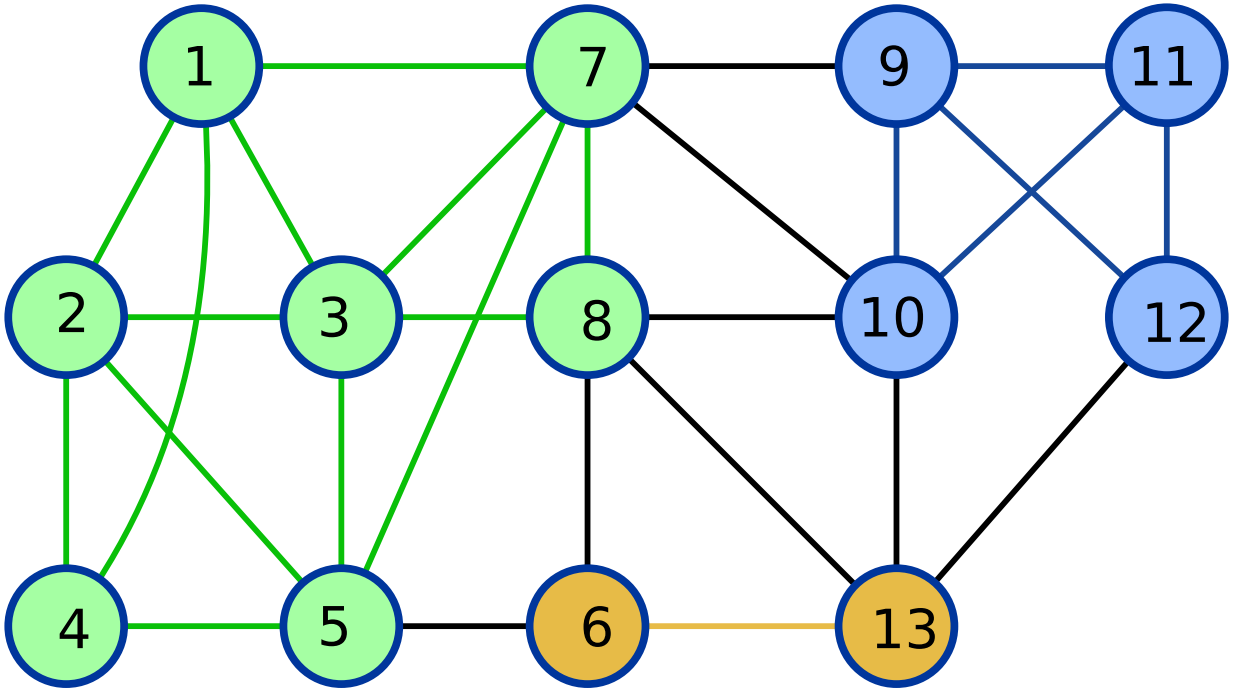
- Given an undirected, unweighted graph $G = (V, E)$ suppose we partition the nodes into k modules $\mathcal{C} = C_1, C_2, \ldots C_k$.
- How do we measure the "quality" of $\mathcal{C}$?
- Intuition: many more edges within modules than among modules.

Motivation



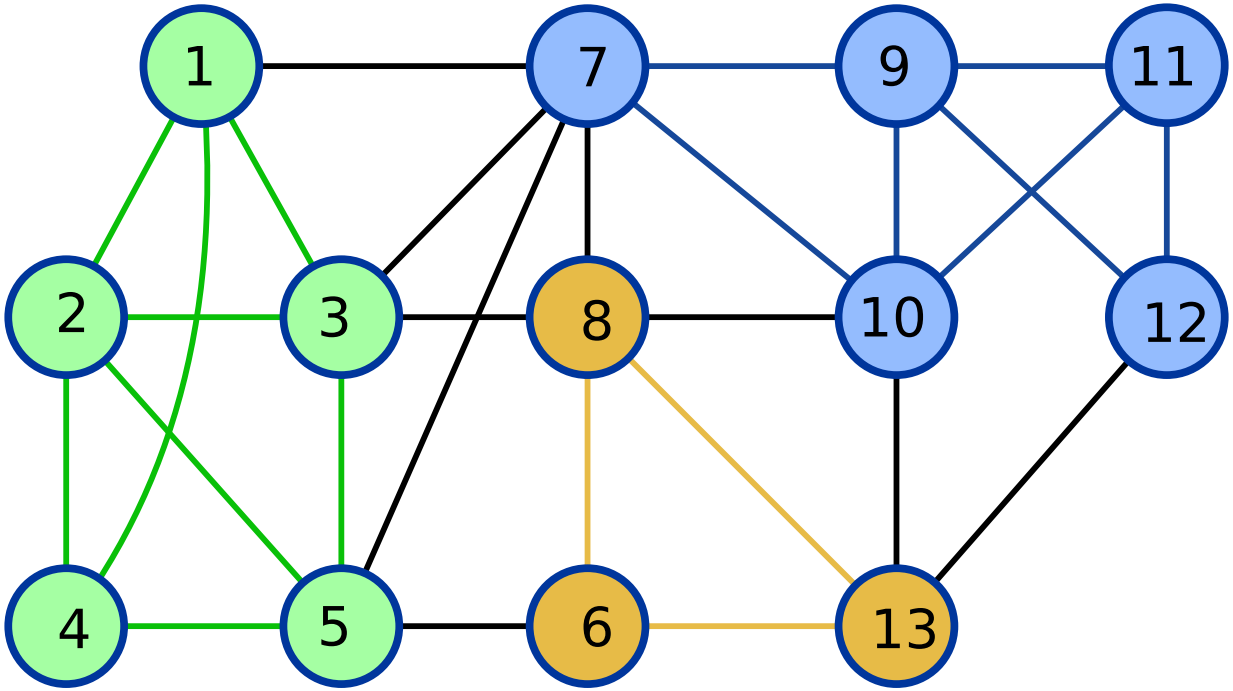
- Given an undirected, unweighted graph $G = (V, E)$ suppose we partition the nodes into k modules $\mathcal{C} = C_1, C_2, \ldots C_k$.
- How do we measure the "quality" of $\mathcal{C}$?
- Intuition: many more edges within modules than among modules.

Motivation



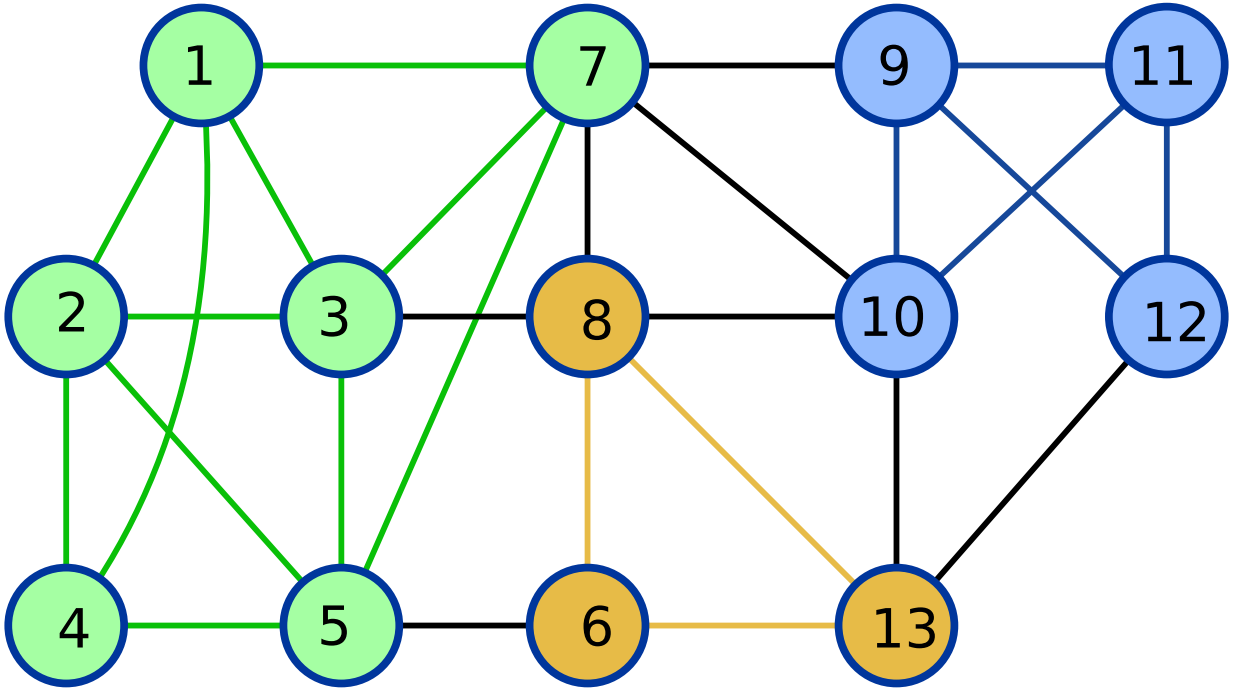
- Given an undirected, unweighted graph $G = (V, E)$ suppose we partition the nodes into k modules $\mathcal{C} = C_1, C_2, \ldots C_k$.
- How do we measure the "quality" of $\mathcal{C}$?
- Intuition: many more edges within modules than among modules.

Motivation



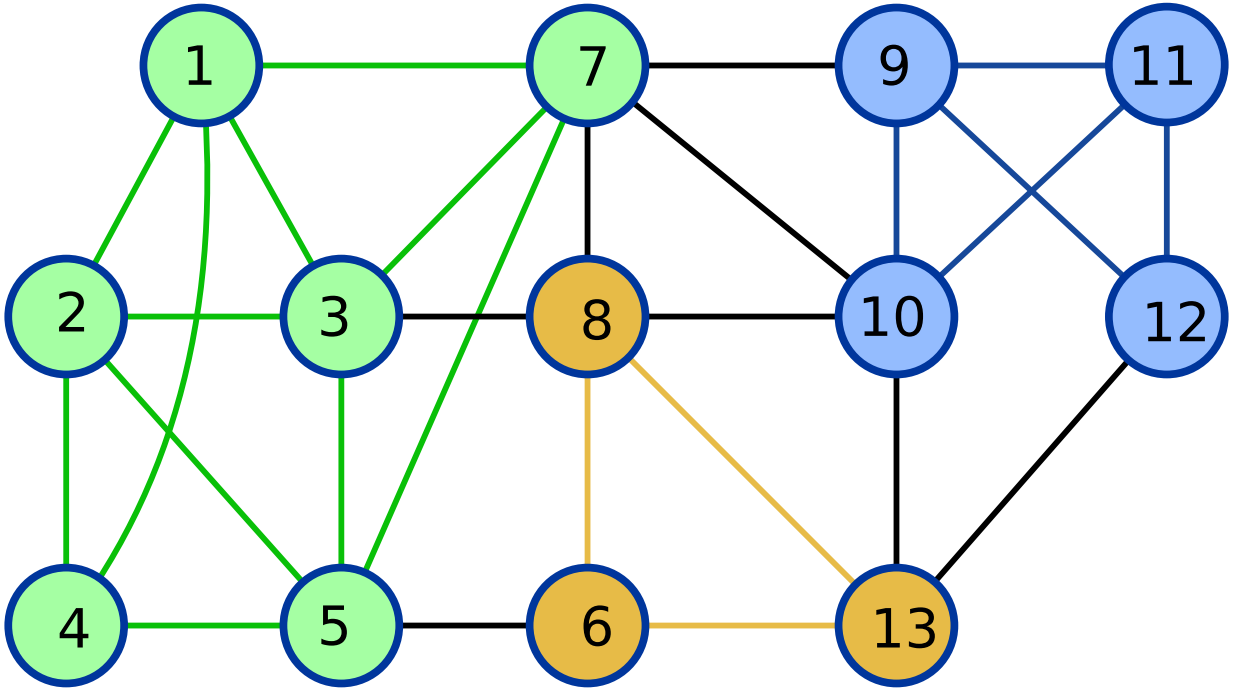
- Given an undirected, unweighted graph $G = (V, E)$ suppose we partition the nodes into k modules $\mathcal{C} = C_1, C_2, \ldots C_k$.
- How do we measure the "quality" of $\mathcal{C}$?
- Intuition: many more edges within modules than among modules.

Initial Definition of Modularity



- How do we count the number of edges within modules?

Initial Definition of Modularity

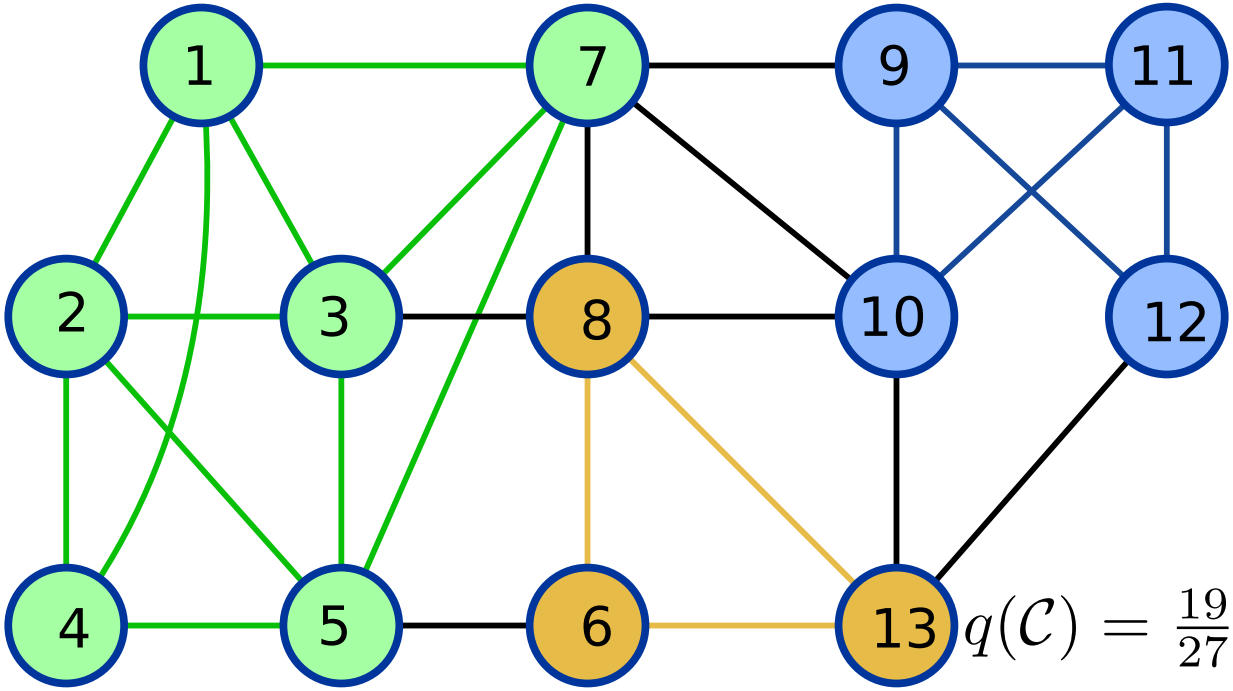


- How do we count the number of edges within modules?
- For every node $u \in V$, define $c(u)$ as the index of u's module.

$$q(\mathcal{C}) = \frac{1}{m} \sum_{(u,v)\in E} \delta(c(u), c(v)), \text{ where } \delta \text{ is the Kronecker delta function}$$

$$= \frac{1}{2m} \sum_{u,v\in V} a(u,v)\delta(c(u), c(v)), \text{ where } a(u,v) = 1 \text{ iff } (u,v) \text{ is an edge}$$

Initial Definition of Modularity

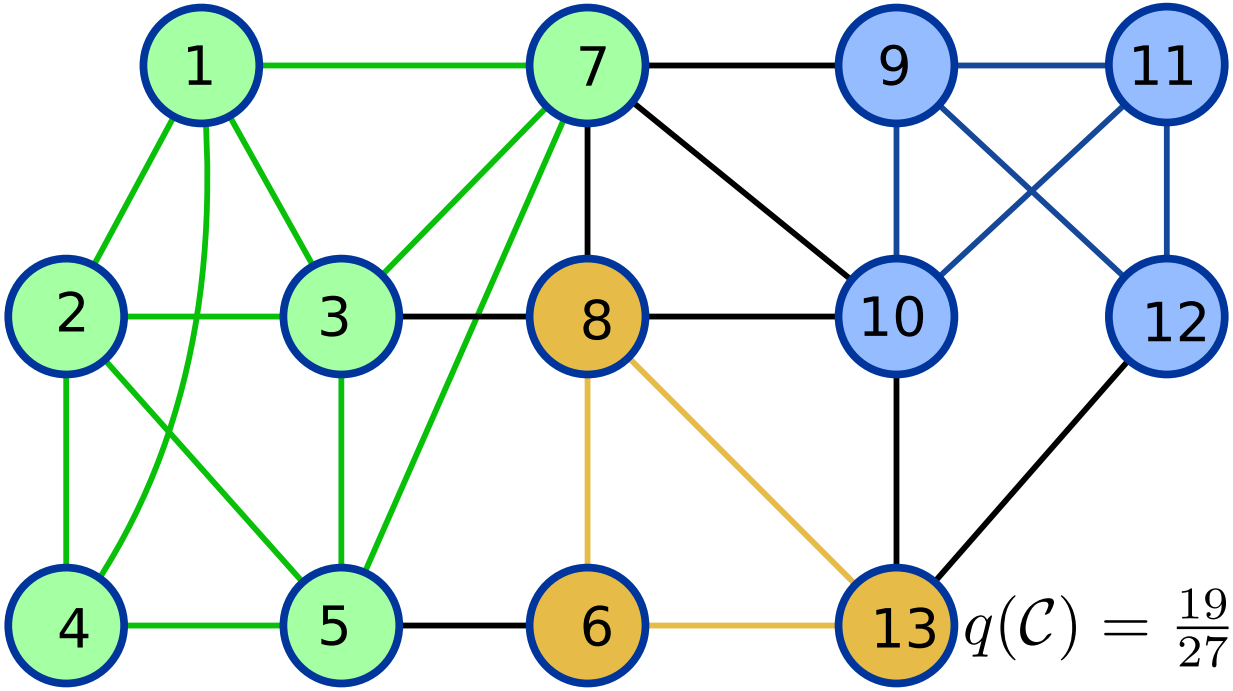


- How do we count the number of edges within modules?
- For every node $u \in V$, define $c(u)$ as the index of u's module.

$$q(\mathcal{C}) = \frac{1}{m} \sum_{(u,v) \in E} \delta(c(u), c(v)), \text{ where } \delta \text{ is the Kronecker delta function}$$

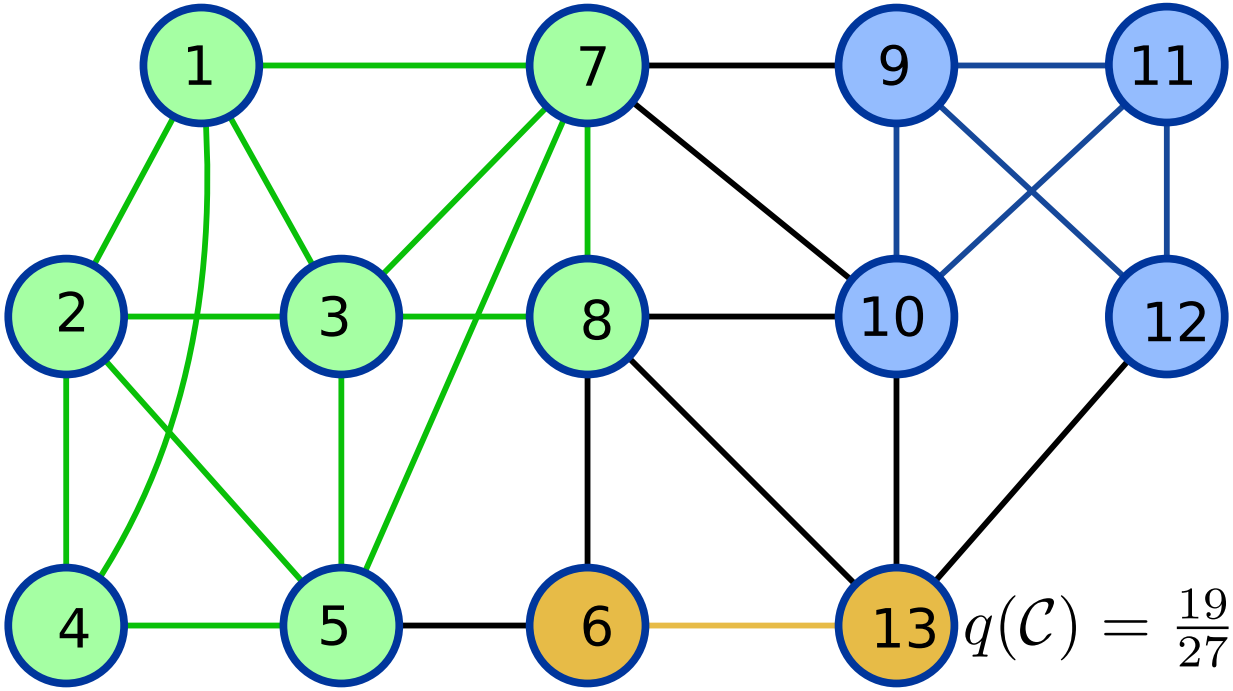
$$= \frac{1}{2m} \sum_{u,v \in V} a(u,v)\delta(c(u), c(v)), \text{ where } a(u,v) = 1 \text{ iff } (u,v) \text{ is an edge}$$

Optimising Modularity



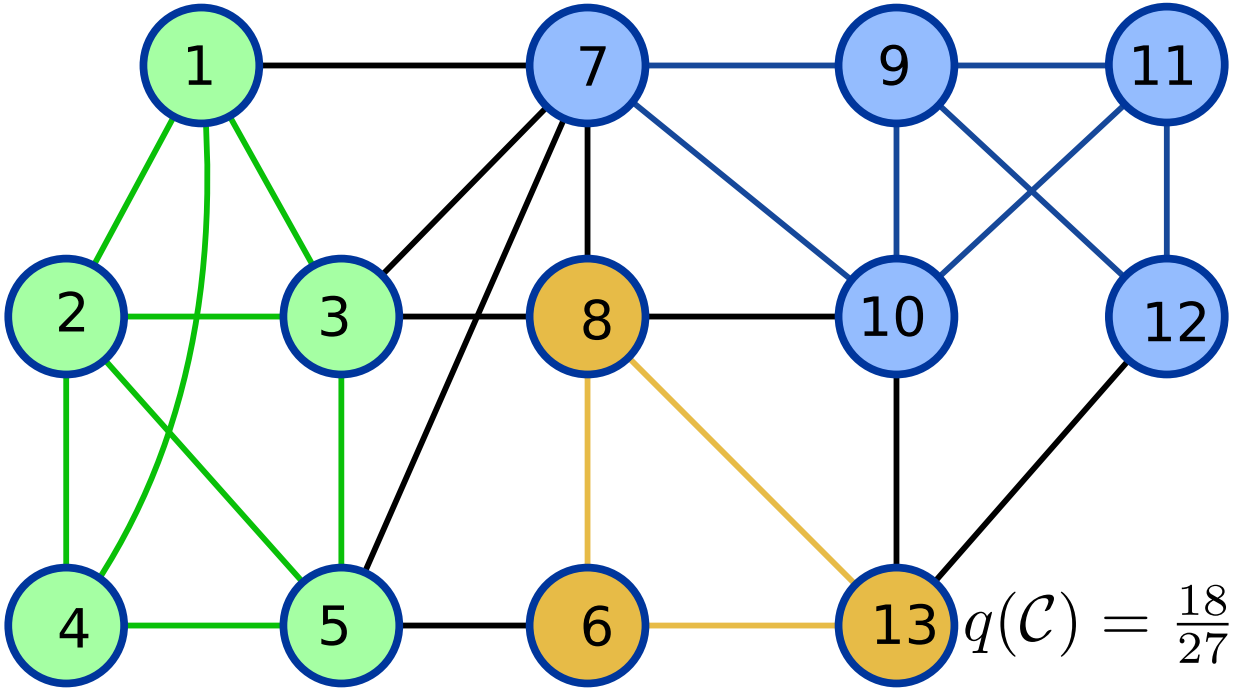
$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} a(u,v)\delta(c(u),c(v))$$

Optimising Modularity



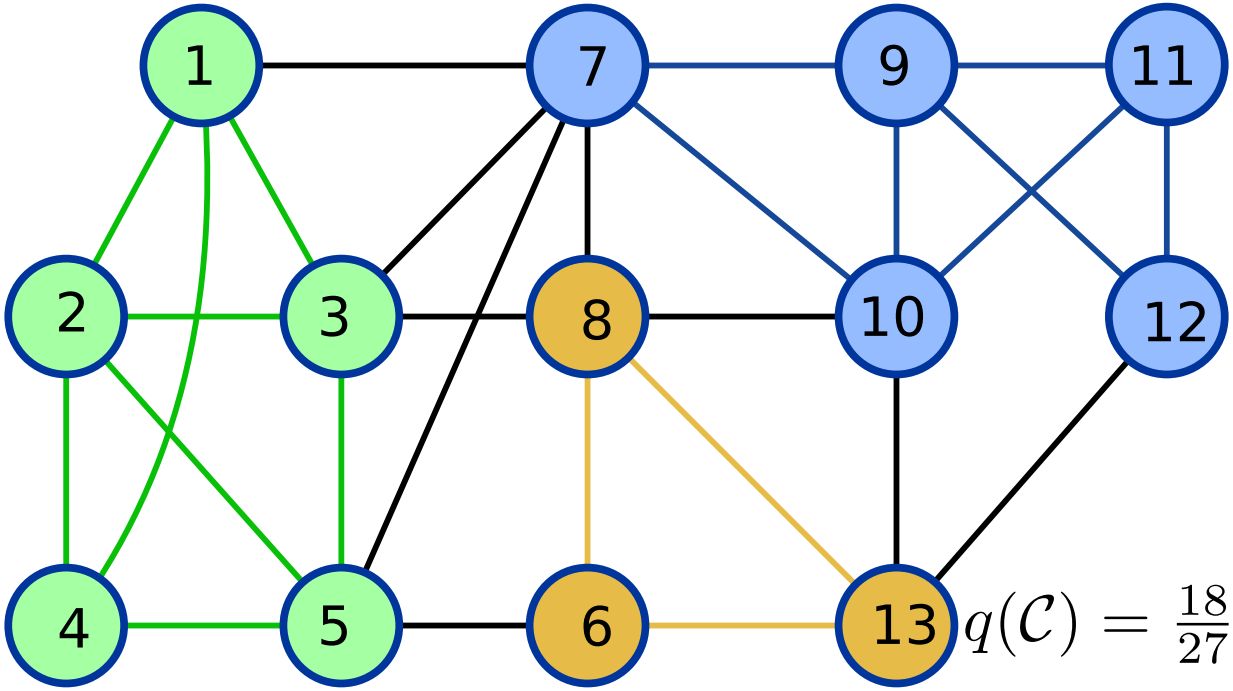
$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} a(u,v)\delta(c(u),c(v))$$

Optimising Modularity



$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} a(u,v)\delta(c(u),c(v))$$

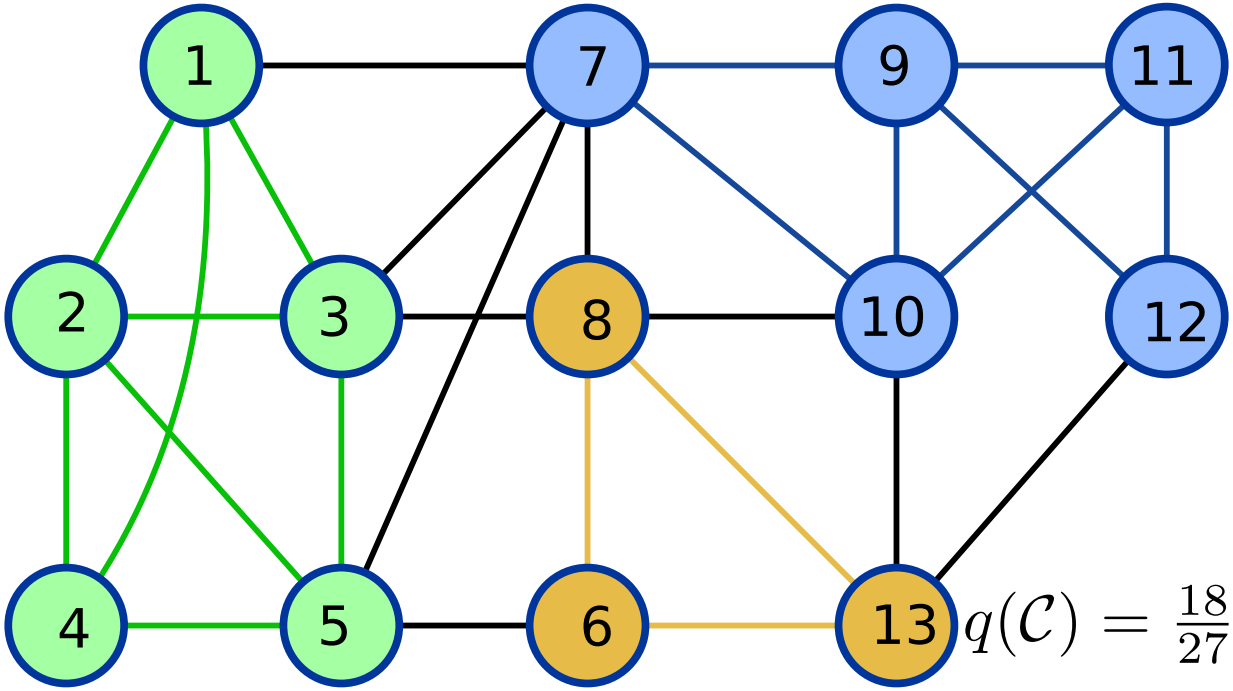
Optimising Modularity



$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} a(u,v)\delta(c(u),c(v))$$

- Should we maximise or minimise $q(\mathcal{C})$?

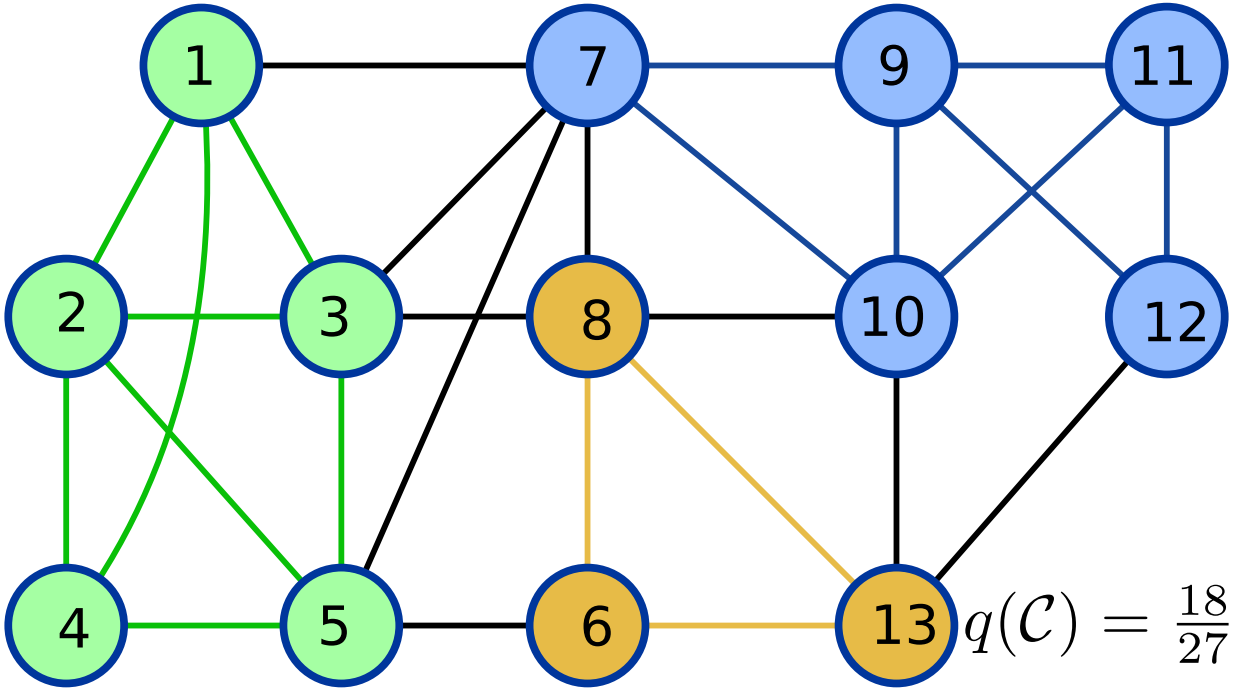
Optimising Modularity



$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} a(u,v)\delta(c(u),c(v))$$

- Should we maximise or minimise $q(\mathcal{C})$? Maximise it.
- What is the value of $q(\mathcal{C})$ if we place all nodes in G in a single cluster?

Optimising Modularity



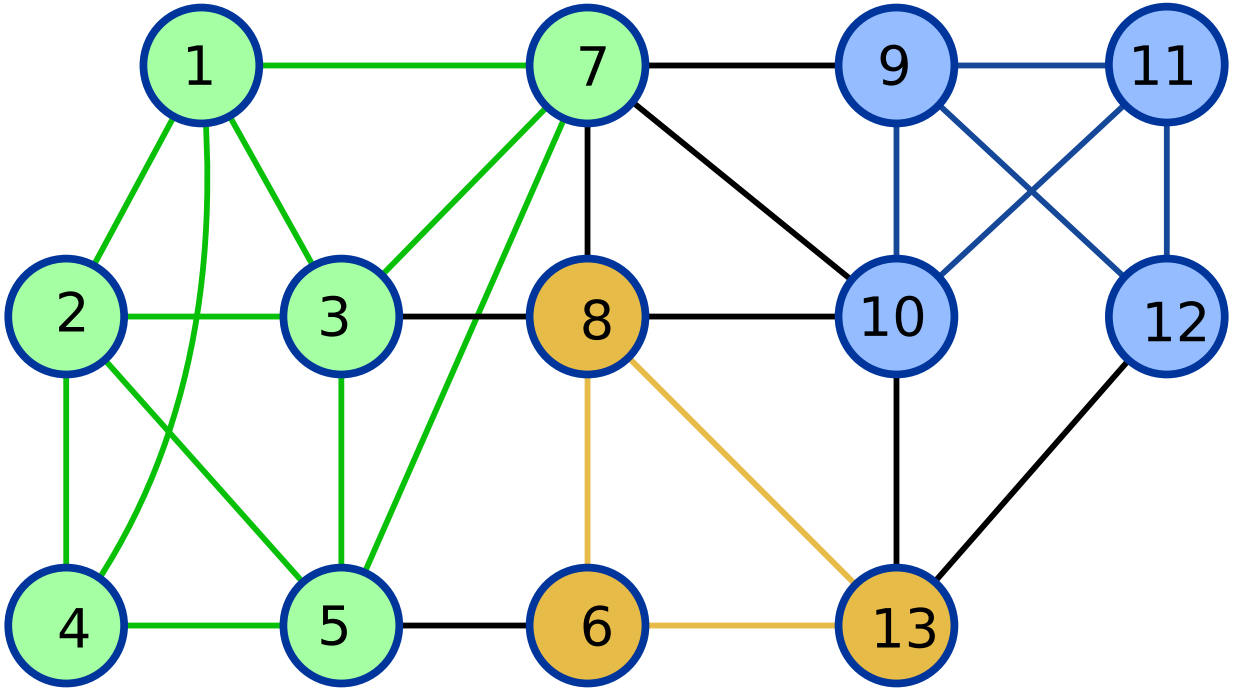
$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} a(u,v)\delta(c(u),c(v))$$

- Should we maximise or minimise $q(\mathcal{C})$? Maximise it.
- What is the value of $q(\mathcal{C})$ if we place all nodes in G in a single cluster? 1!

Two Criteria for High Quality Partitions

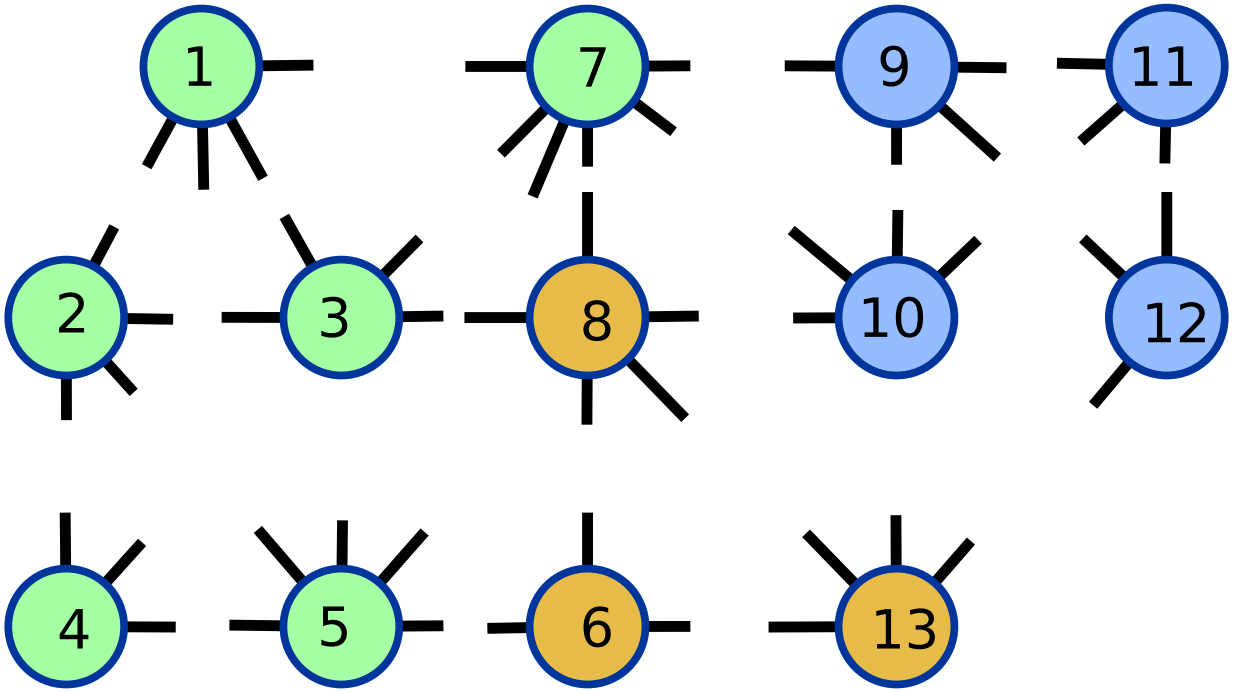
1. Nodes are in highly cohesive modules, i.e., nodes within the same module will be strongly connected with each other.
2. The amount of intramodule connectivity in a good partition will be greater than expected by chance, as defined by a network in which edges are placed between nodes at random.
3. Proposed by Newman and Girvan, 2004.

Configuration Model



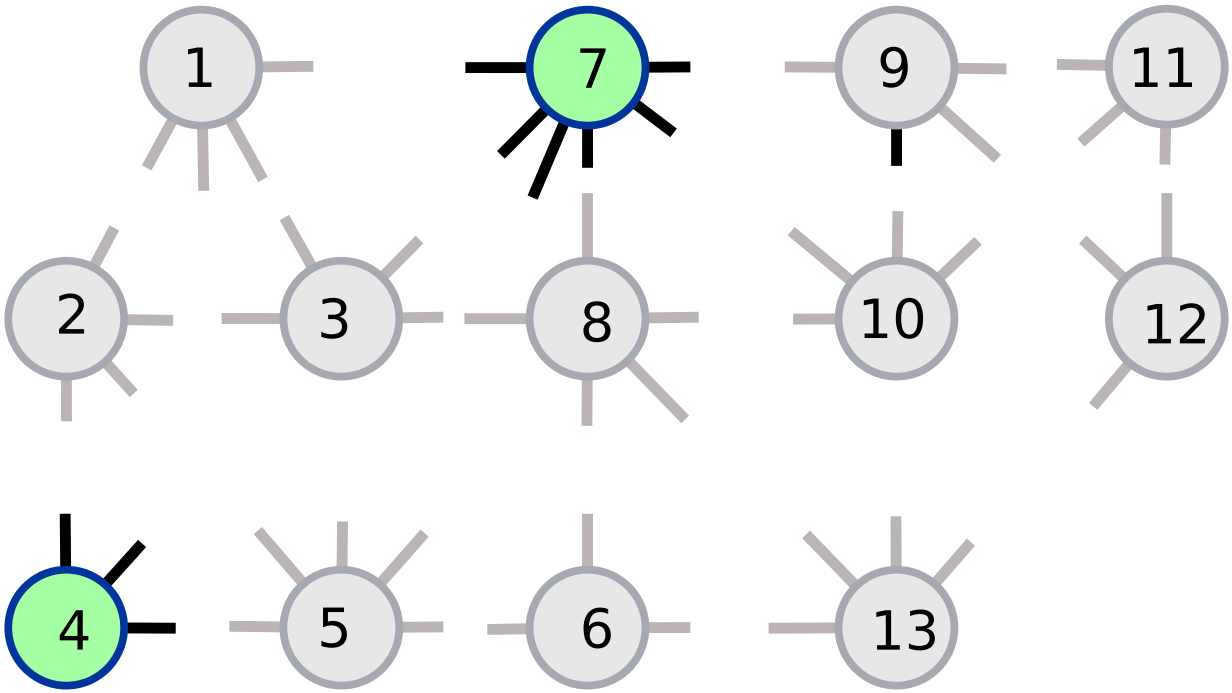
- Method to generate random graphs like Erdös-Renyi and Watts-Strogatz models.
- Ensure that the random graphs have the same degree sequence as G, but allow self loops and multi-edges.

Configuration Model



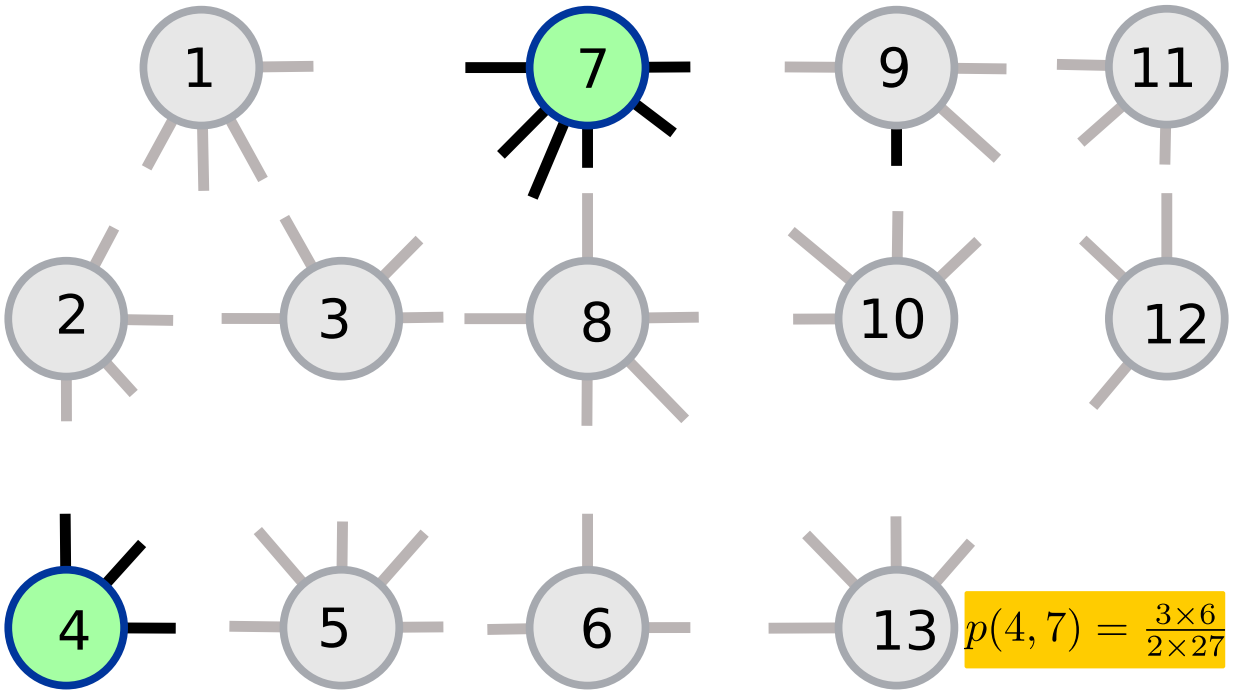
- Cut each edge in G in half.
- Each node u has $d(u)$ stubs; total number of stubs is $2m$.
- For each stub select another stub uniformly at random and connect them by an edge.

Configuration Model



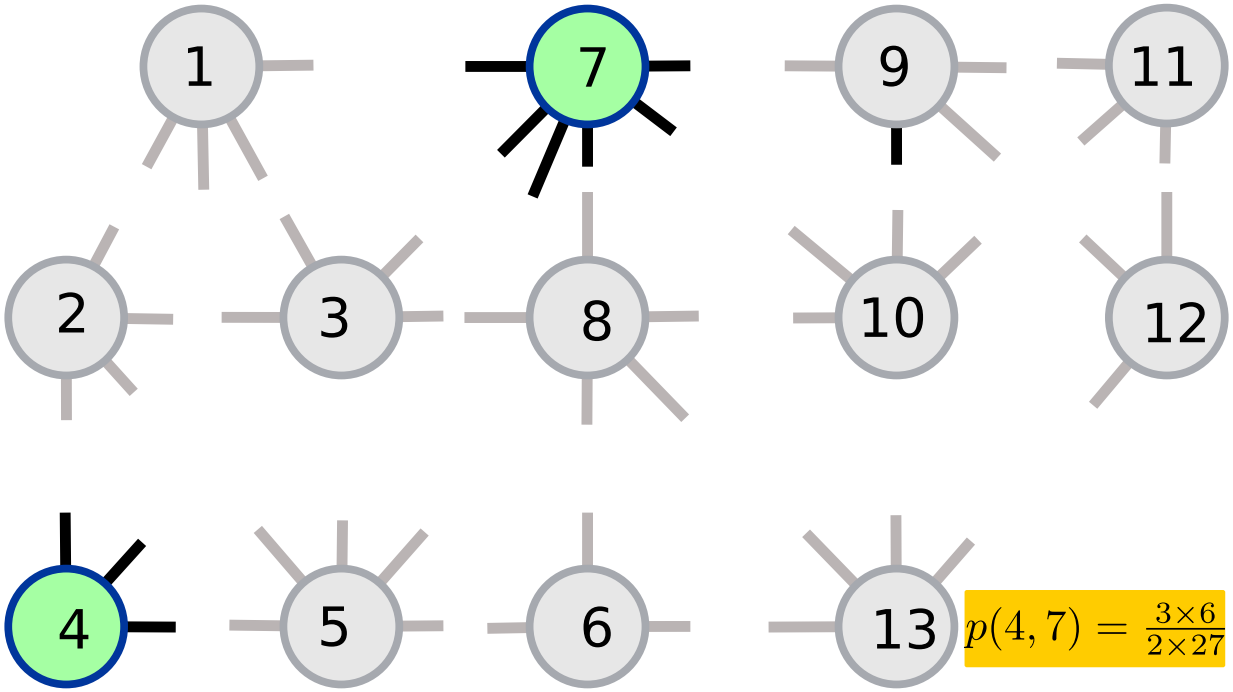
- What is the probability of an edge between nodes u and v?

Configuration Model



- What is the probability of an edge between nodes u and v? $\frac{d(u)d(v)}{2m}$.

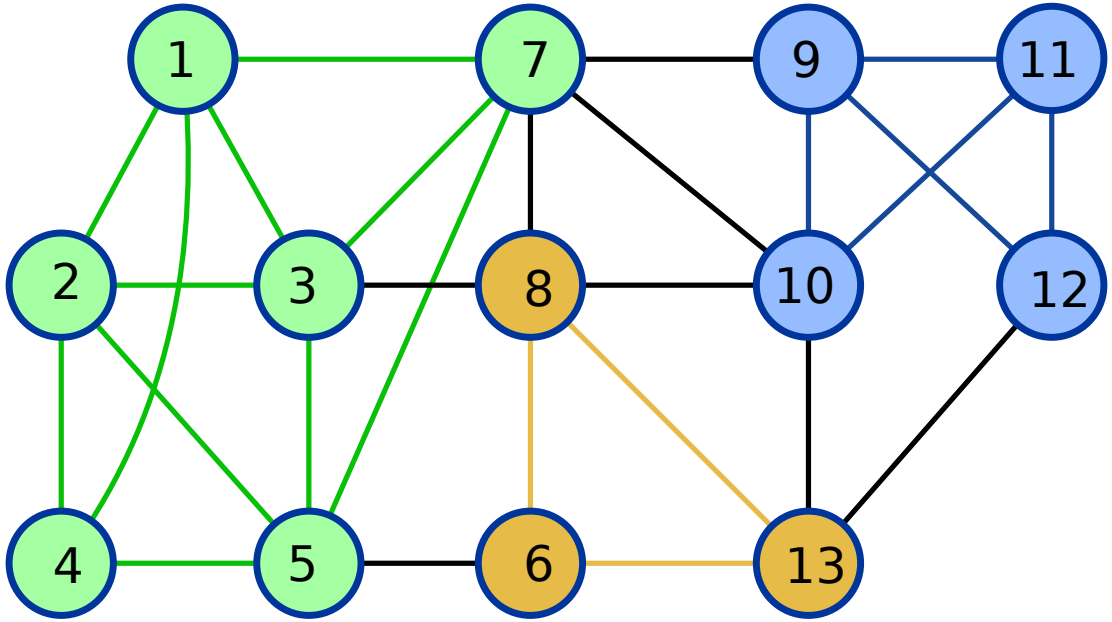
Configuration Model



- What is the probability of an edge between nodes u and v? $\frac{d(u)d(v)}{2m}$.
- Therefore modularity of the partition of a random graph in the configuration model into the same modules $\mathcal{C} = C_1, C_2, \ldots C_k$

$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} \frac{d(u)d(v)}{2m} \delta(c(u), c(v))$$

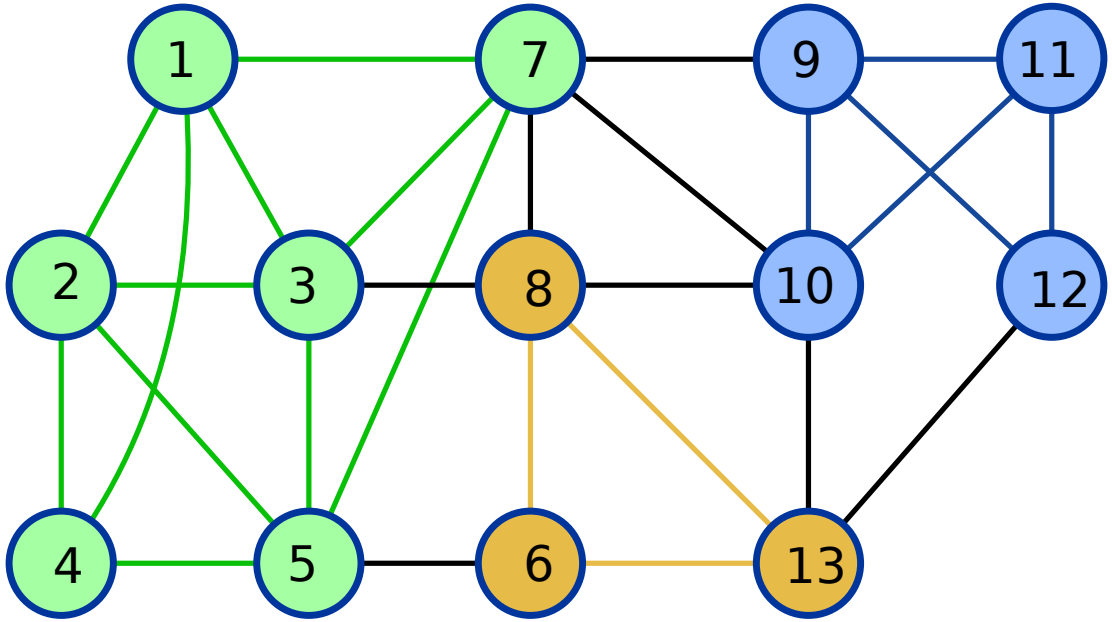
Final Definition of Modularity



$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} \left(a(u,v) - \frac{d(u)d(v))}{2m} \right) \delta(C(u), C(v))$$

- What is the range of $q(\mathcal{C})$?

Final Definition of Modularity



$$q(\mathcal{C}) = \frac{1}{2m} \sum_{u,v \in V} \left(a(u,v) - \frac{d(u)d(v))}{2m} \right) \delta(C(u), C(v))$$

- What is the range of $q(\mathcal{C})$? Between -1 and 1.
  - $q(\mathcal{C}) > 0$: $\mathcal{C}$ has higher intramodule connectivity than expected by chance from configuration model.
  - $q(\mathcal{C}) = 0$: $\mathcal{C}$ has same intramodule connectivity as expected in a random graph.
  - $q(\mathcal{C}) < 0$: $\mathcal{C}$ has no modular structure.

Using Modularity

- Now that we have defined a nice measure for the quality of a partition, how do we use it?
- Definition of q does not specify the number of clusters.

Using Modularity

- Now that we have defined a nice measure for the quality of a partition, how do we use it?
- Definition of q does not specify the number of clusters.
- Hierarchical clustering: Compute modularity after every merge and output the clustering with the largest value.
- Any other clustering algorithm: compute the modularity of the result.

Using Modularity

- Now that we have defined a nice measure for the quality of a partition, how do we use it?
- Definition of q does not specify the number of clusters.
- Hierarchical clustering: Compute modularity after every merge and output the clustering with the largest value.
- Any other clustering algorithm: compute the modularity of the result.
- Develop a new algorithm to maximise modularity.
  - Maximising modularity is NP-hard.
  - We must rely on heuristics to make the modularity as large as possible.

Greedy Algorithm

- Proposed by Newman, 2004.

1. Start with every node in its own module.
2. While there are at least two modules
   1. Compute the pair of modules whose merger will result in the largest increase or smallest decrease in q.
   2. Merge this pair of modules into one.
3. Return the clustering with the largest value of q.

Greedy Algorithm

- Proposed by Newman, 2004.

1. Start with every node in its own module.
2. While there are at least two modules
   1. Compute the pair of modules whose merger will result in the largest increase or smallest decrease in q.
   2. Merge this pair of modules into one.
3. Return the clustering with the largest value of q.

- Hierarchical clustering algorithm built directly around maximisation of q.
- Allows q to decrease to preserve the principle of hierarchical clustering.
- Why is the algorithm "greedy"?

Greedy Algorithm

- Proposed by Newman, 2004.

1. Start with every node in its own module.
2. While there are at least two modules
   1. Compute the pair of modules whose merger will result in the largest increase or smallest decrease in q.
   2. Merge this pair of modules into one.
3. Return the clustering with the largest value of q.

- Hierarchical clustering algorithm built directly around maximisation of q.
- Allows q to decrease to preserve the principle of hierarchical clustering.
- Why is the algorithm "greedy"? Merging of two modules cannot be undone.

Louvain Algorithm

- Proposed by Blondel *et al.*, 2008.

1. Start with every node in its own module.
2. For every node $u \in V$ and every neighbour v of u, evaluate the change in q when we remove u from its module and add it to v's module.
3. Move u to that neighbour's module for which increase in q is largest.
4. Repeat the previous two steps until q does not increase.

Louvain Algorithm

- Proposed by Blondel *et al.*, 2008.

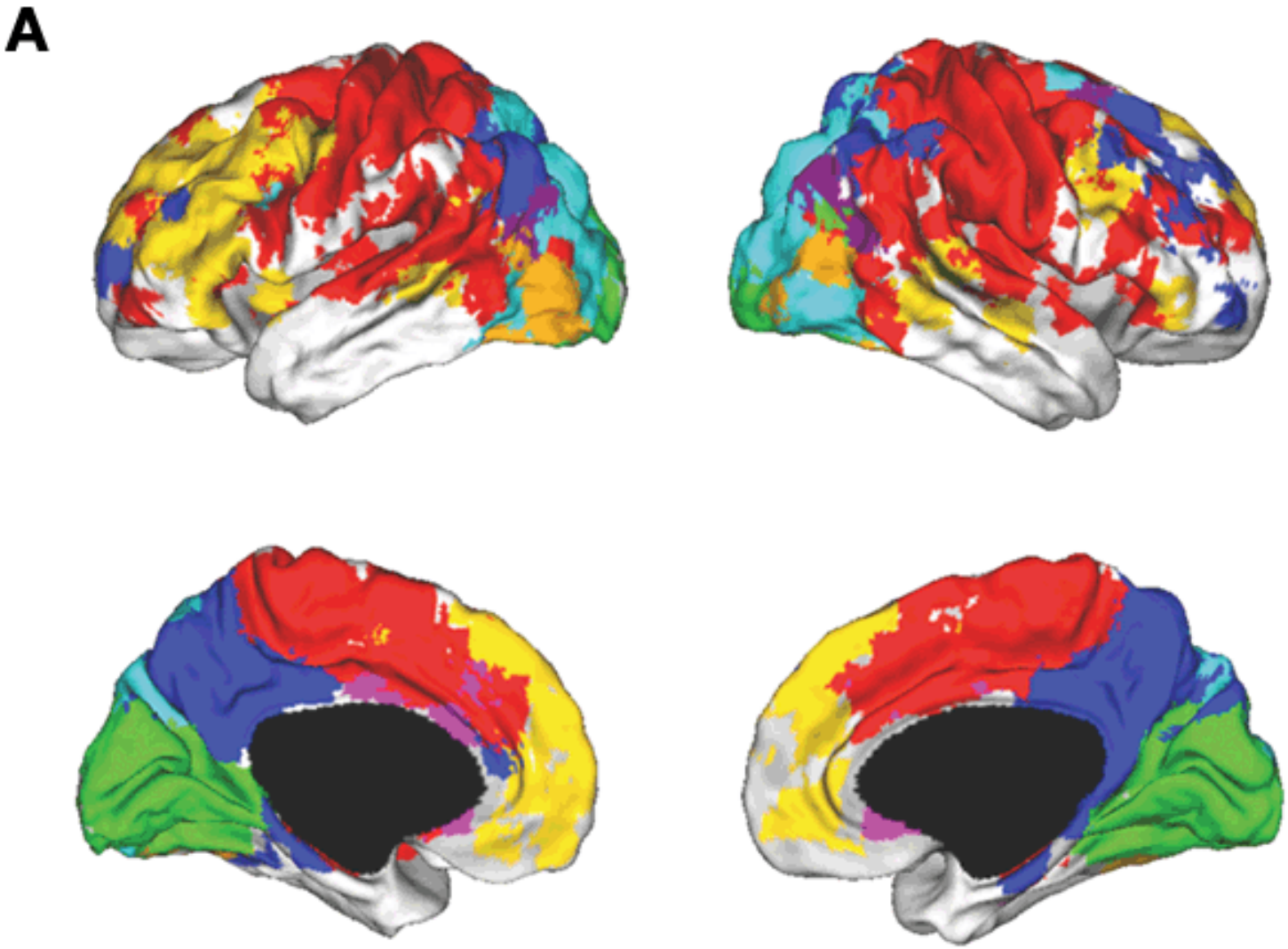
1. Start with every node in its own module.
2. For every node $u \in V$ and every neighbour v of u, evaluate the change in q when we remove u from its module and add it to v's module.
3. Move u to that neighbour's module for which increase in q is largest.
4. Repeat the previous two steps until q does not increase.
5. Construct a new graph where every module is a node and a weighted edge represents (multiple) connections between two modules.
6. Repeat steps 2–5 until no further gains in q are possible.

Louvain Algorithm

- Proposed by Blondel *et al.*, 2008.

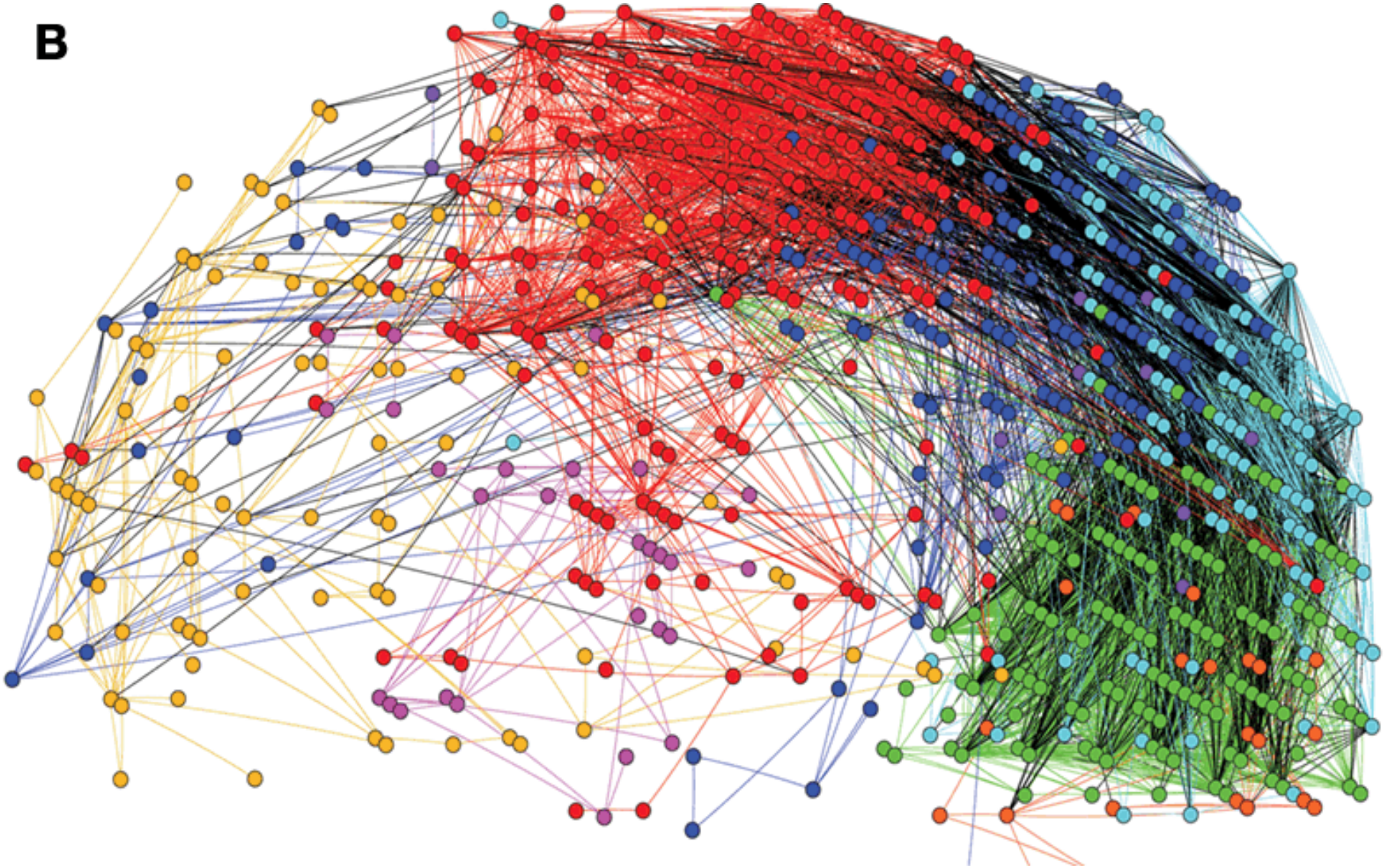
1. Start with every node in its own module.
2. For every node $u \in V$ and every neighbour v of u, evaluate the change in q when we remove u from its module and add it to v's module.
3. Move u to that neighbour's module for which increase in q is largest.
4. Repeat the previous two steps until q does not increase.
5. Construct a new graph where every module is a node and a weighted edge represents (multiple) connections between two modules.
6. Repeat steps 2–5 until no further gains in q are possible.

- Efficient calculation of change in q upon swapping makes this algorithm very fast.



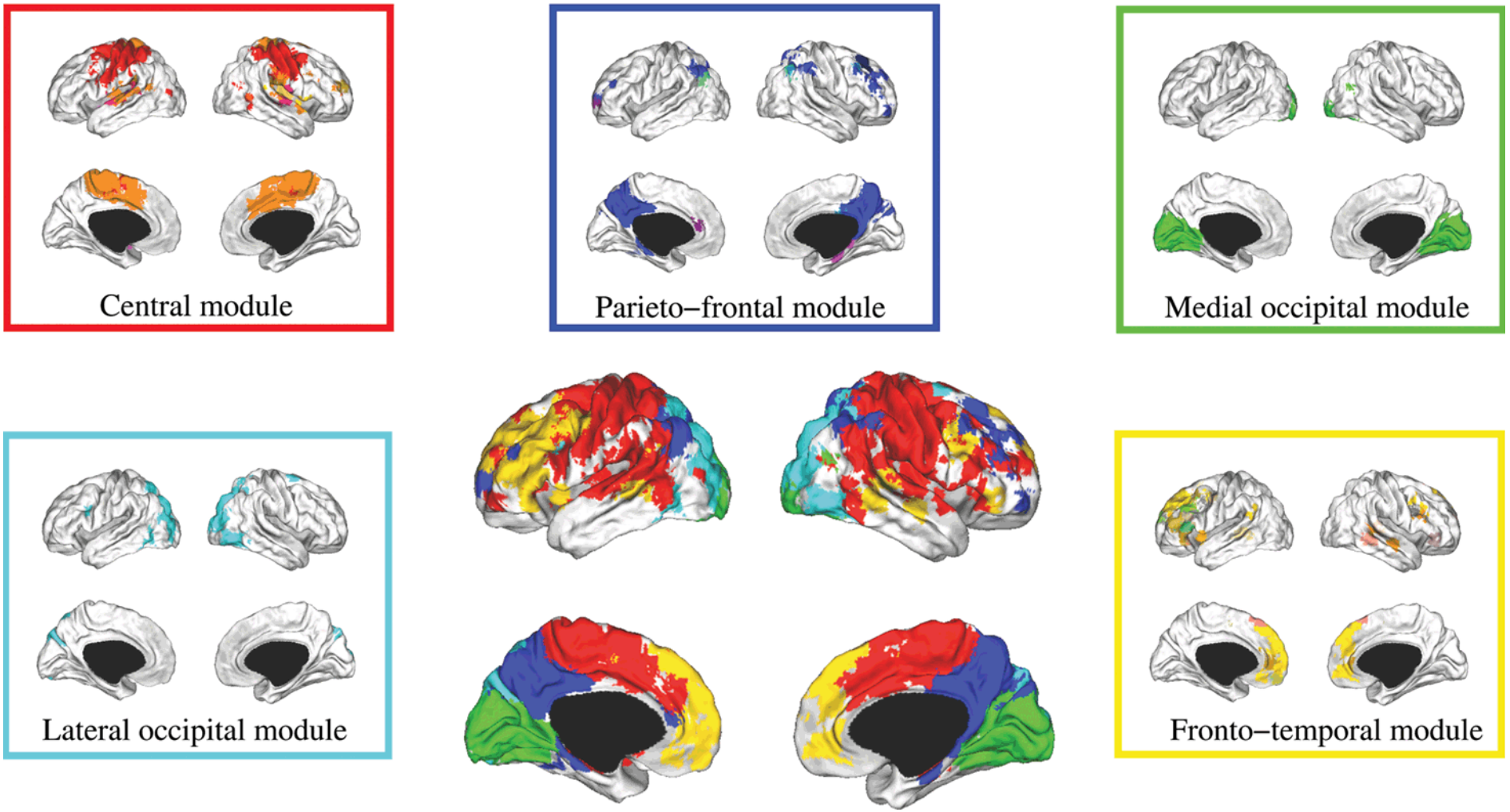
Human resting-state fMRI networks, 1800 nodes, 4mm^3 voxels, had three hierarchical levels: eight modules at the highest level, each with > 10 nodes, 57 modules at the lowest level of the hierarchy.

Meunier *et al.*, 2009



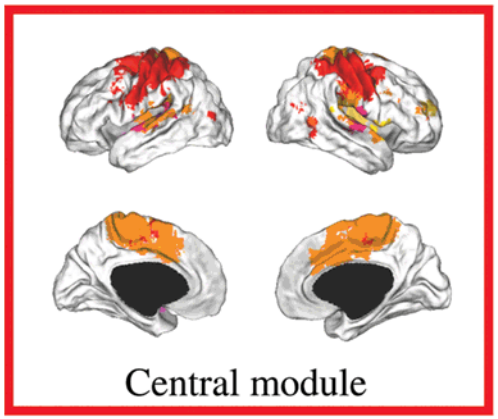
Visualisation of modules. View of brain is from the left side with the frontal cortex on the left and the occipital cortex on the right.

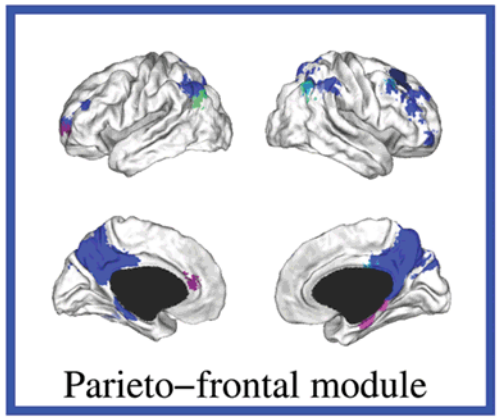
Meunier *et al.*, 2009

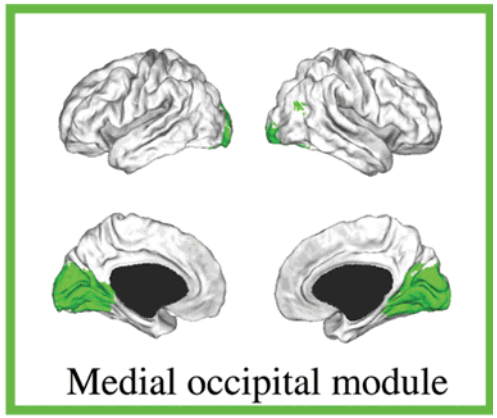


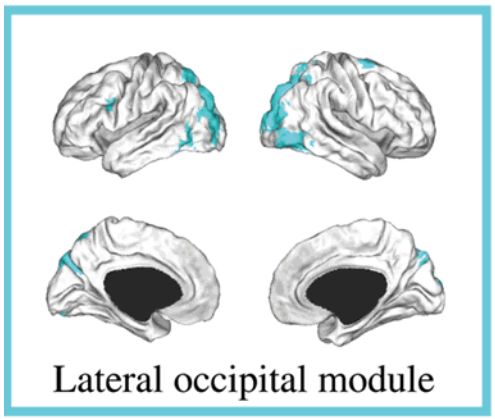
Decomposition of the five largest modules (in the centre): medial occipital module has no major sub-modules whereas the fronto-temporal modules has many sub-modules.

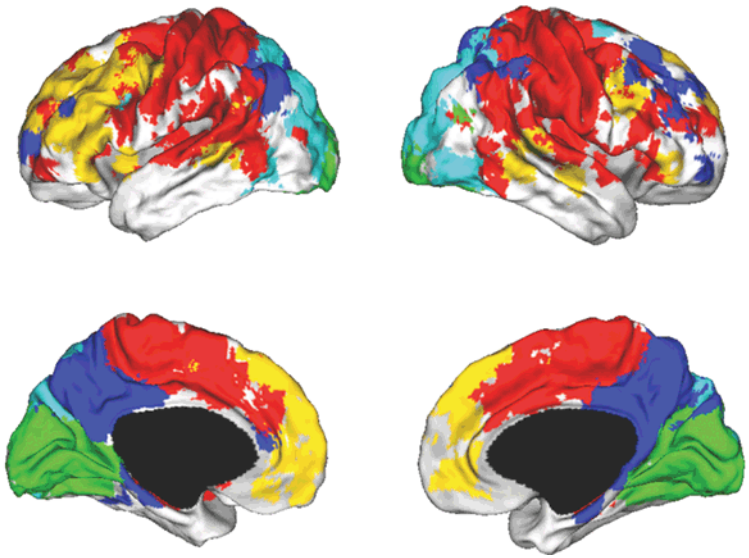
Meunier *et al.*, 2009

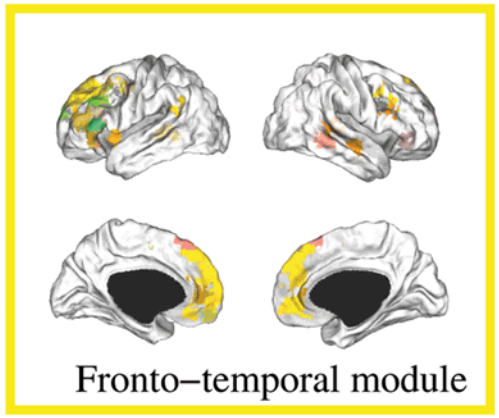






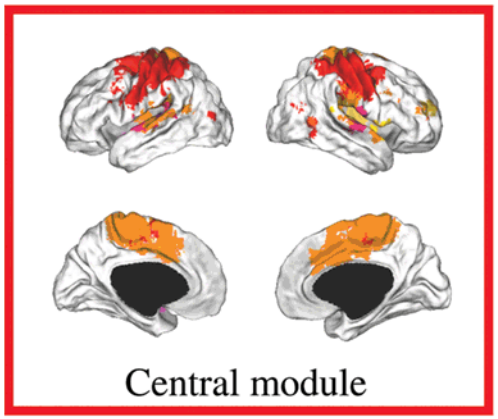


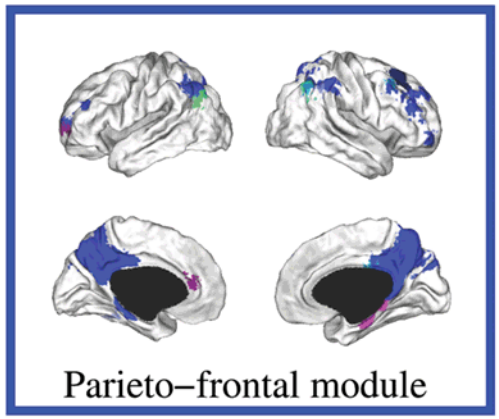


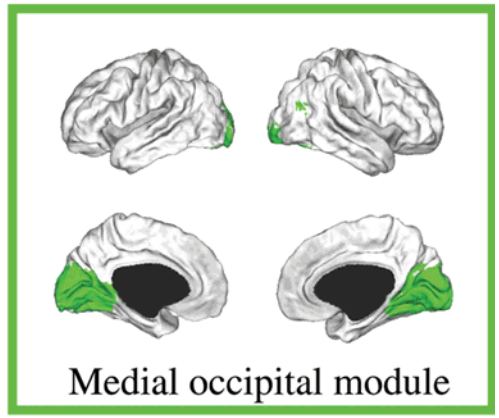


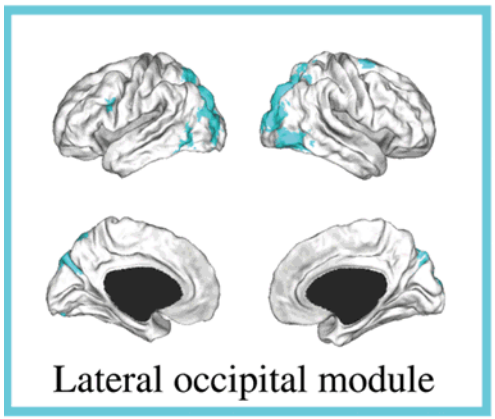
Medial occipital module (primary visual): This module comprised medial occipital cortex and occipital pole, including primary visual areas.

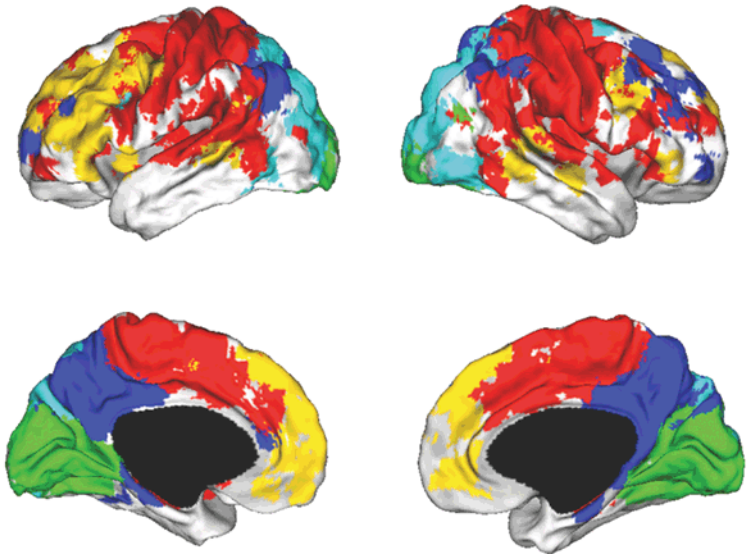
Meunier *et al.*, 2009

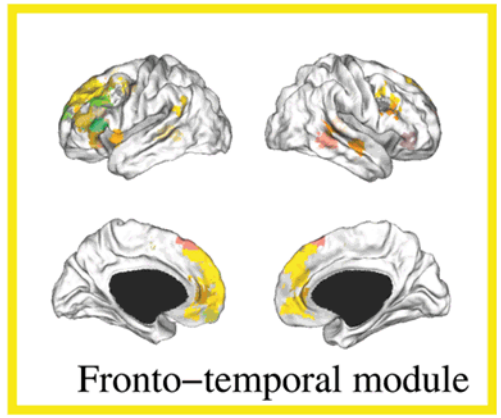












Fronto-temporal module (symbolic): less symmetrically organized than most of the other high level modules and contained larger number of sub-modules at lower levels.

Meunier *et al.*, 2009

Limitations of Modularity

- Modularity generally increases as number of nodes and modules in a graph increase.
- Many very similar partitions have similar values of q.
- Modularity has a resolution limit: small modules may be combined simply to increase q. (Read Box 9.2 in the textbook.)
- Random graph model is quite simple: assumes every node has an equal probability of connecting to every other node.

Limitations of Modularity

- Modularity generally increases as number of nodes and modules in a graph increase.
- Many very similar partitions have similar values of q.
- Modularity has a resolution limit: small modules may be combined simply to increase q. (Read Box 9.2 in the textbook.)
- Random graph model is quite simple: assumes every node has an equal probability of connecting to every other node.
- Many alternatives proposed to address these limitations.