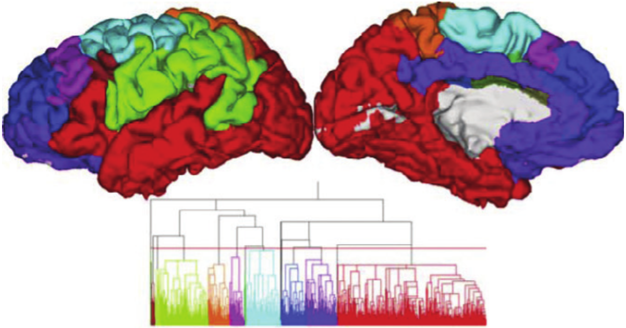
CS 4884: Modules

T. M. Murali

February 25 and 27, 2020



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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.

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Do modules exist in brain networks?
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- Focal pathology affecting a tightly interconnected brain module will be less likely to spread and affect other areas.
- Breakdown of modularity can lead to a propensity for hyper-synchronized, seizure-like dynamics.

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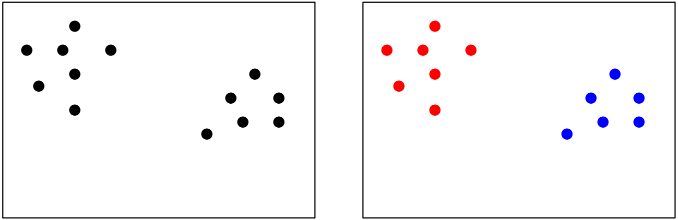
Modules and Clustering

- 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



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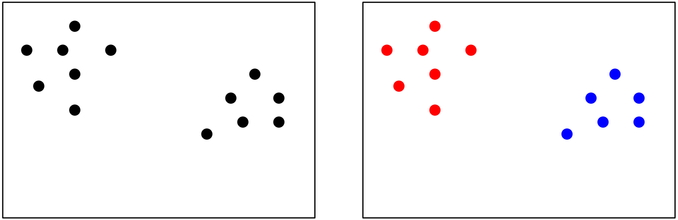

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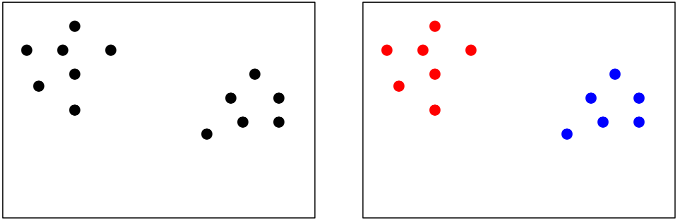

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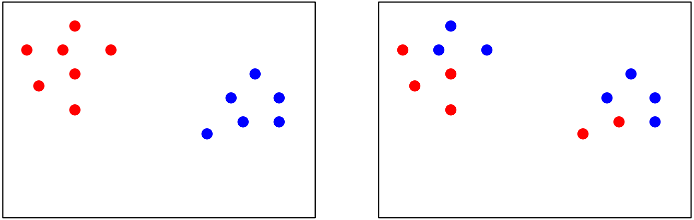

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- How do we measure how similar or close two objects are?
- How many subsets?
- How do we compare two different partitions?

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.

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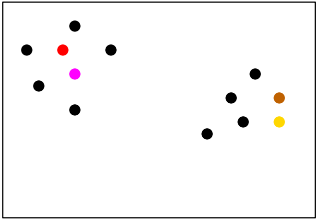
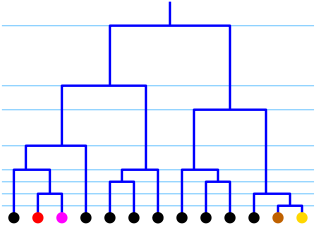
- Other distances: normalised dot product, K-L divergence, relative entropy, Pearson's correlation.
- Metrics obey triangle inequality: $d(p, q) + d(q, r) \geq d(p, r)$.
  - Euclidean, Manhattan distances are metrics.
  - Correlation, dot product are not metrics.

Hierarchical Clustering

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





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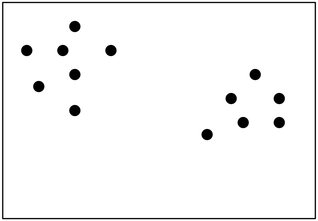

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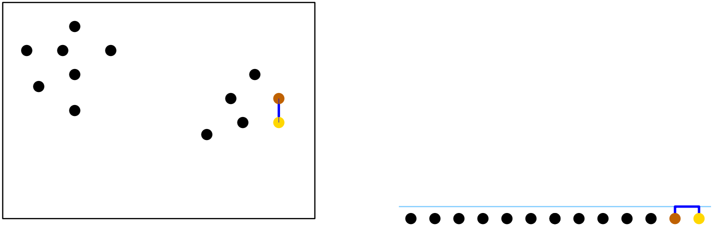

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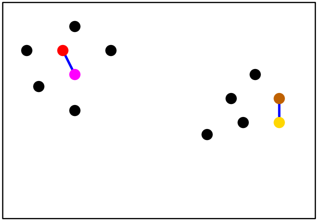

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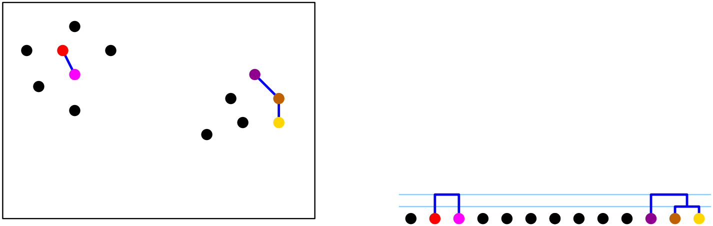

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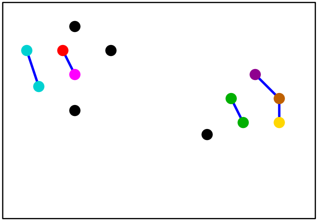

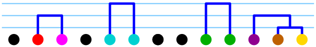

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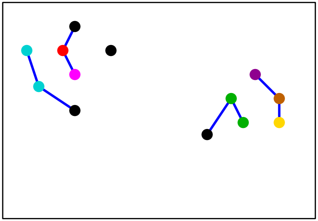

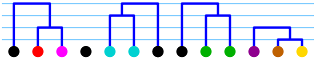

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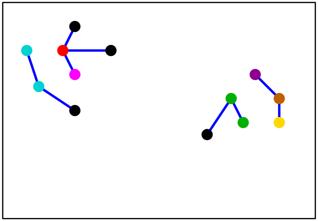

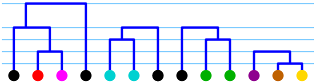

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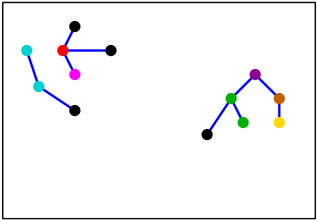

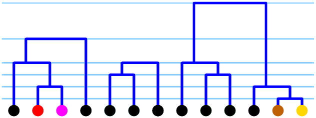

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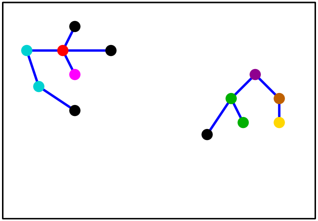

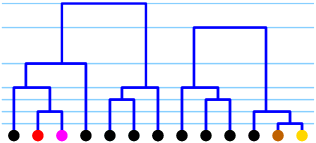

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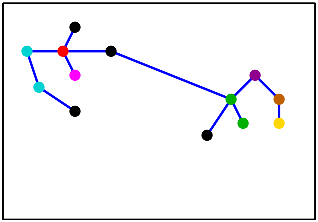
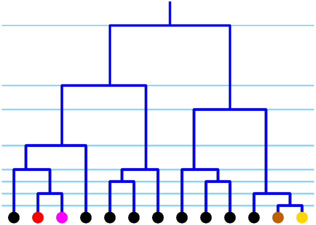
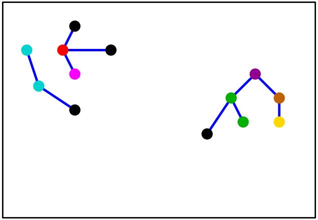
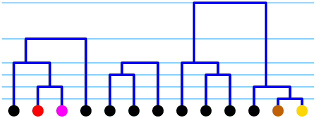




Measuring Distance between Clusters





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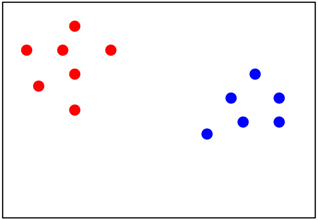

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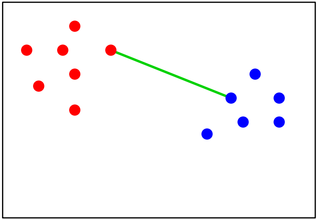

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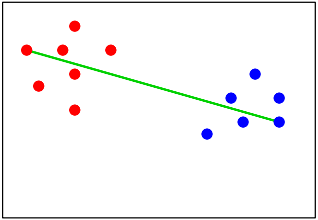

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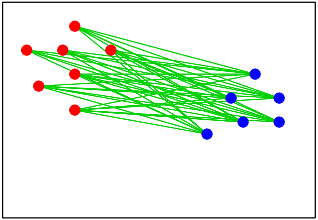

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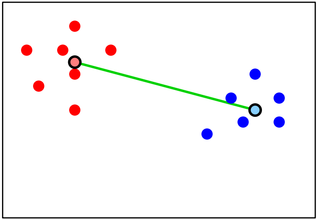

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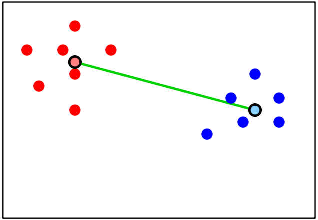

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- $d_{centroid}(C_i, C_j) = d(\mu_i, \mu_j)$, where μ_i is the centroid of C_i.
- Methods are called minimum linkage, maximum linkage, mean linkage, and centroid linkage clustering, respectively.

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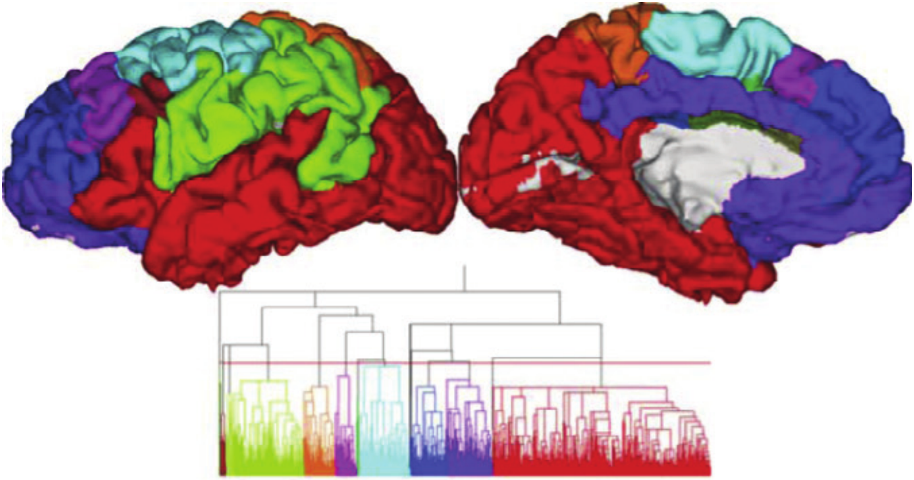
- Assume computing distance between two objects takes $O(1)$ time.
- Store all $O(n^2)$ inter-object distances.
- At each iteration, compute distance between every pair of clusters: takes $O(n^2)$ time in total.
- There are n iterations, so overall running time is $O(nn^2) = O(n^3)$.

Hierarchical Clustering Result



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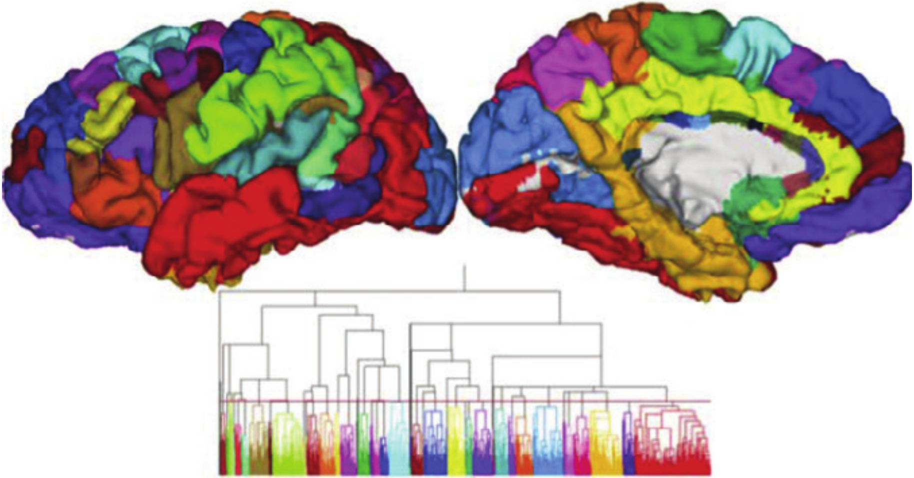

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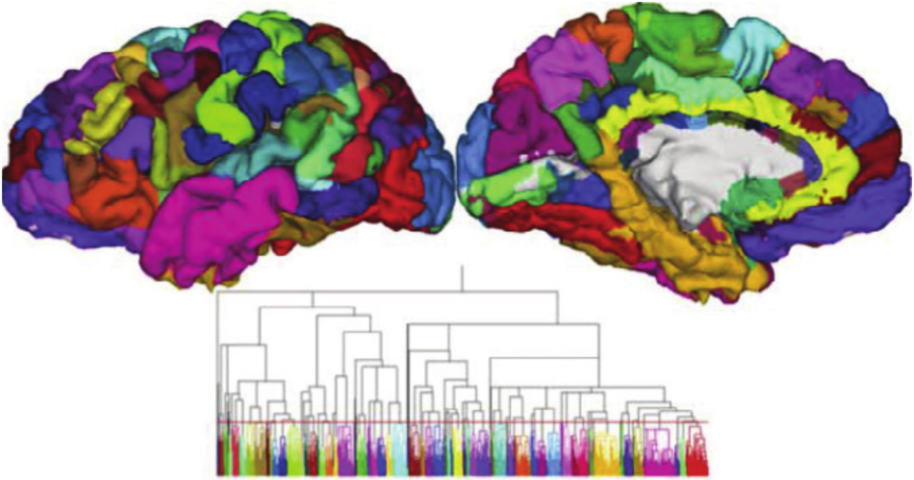

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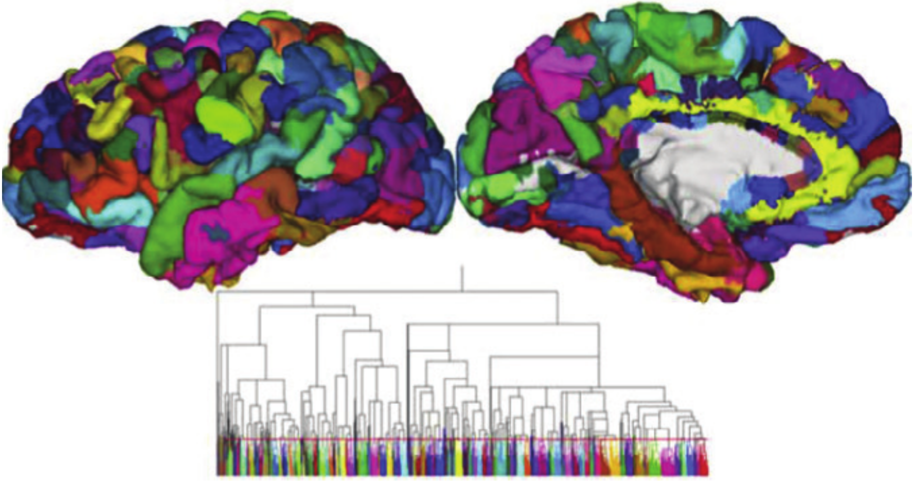

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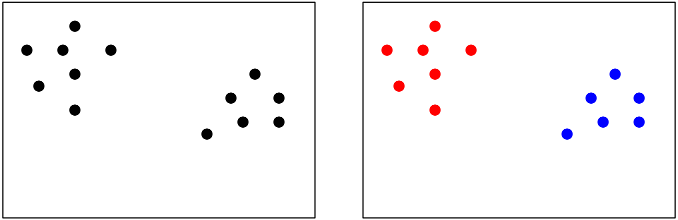

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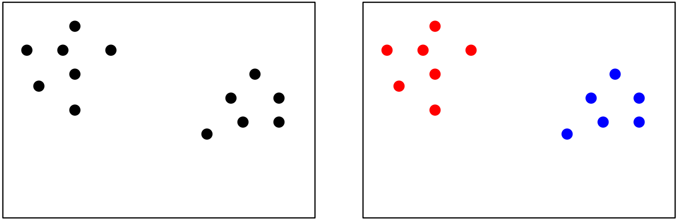

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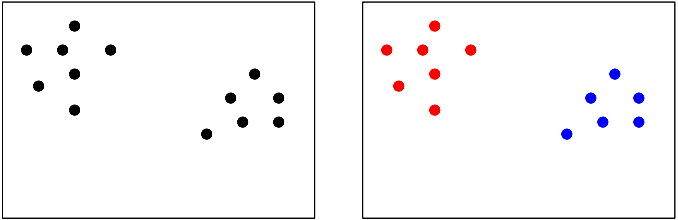

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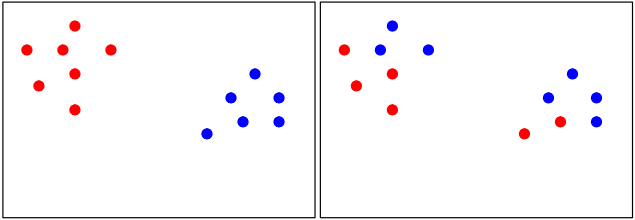
- How many subsets? Not specified in hierarchical clustering.

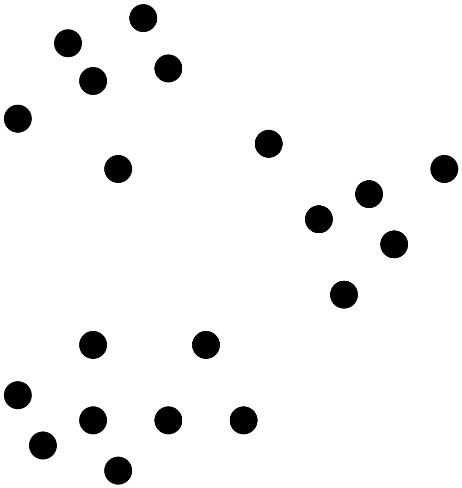
Definition of Clustering



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



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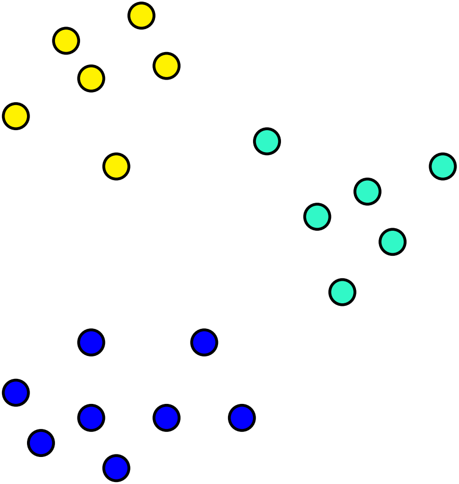

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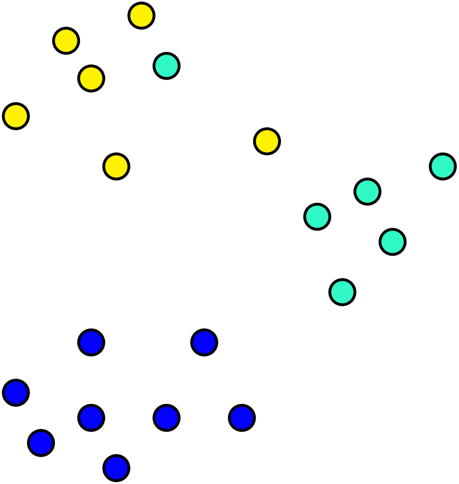

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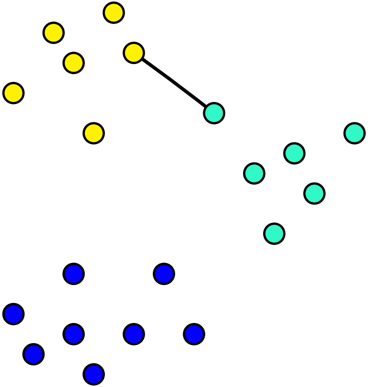

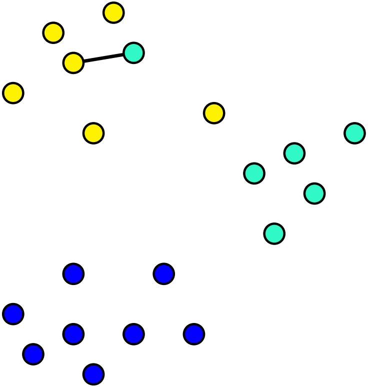

Formalising the Clustering Problem

- 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 $d(p_i, p_j) = d(p_j, p_i)$

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

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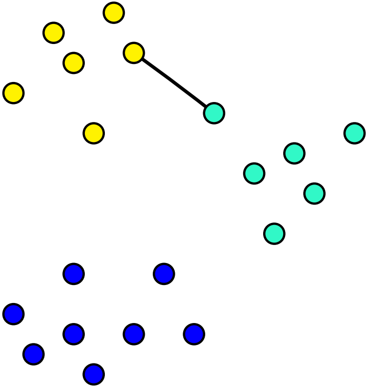
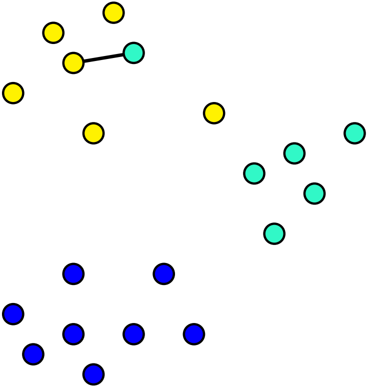
Clustering of Maximum Spacing

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

Example of Clustering of Maximum Spacing

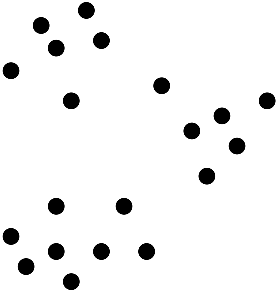


Spacing is large



Spacing is small

Algorithm for Clustering of Maximum Spacing



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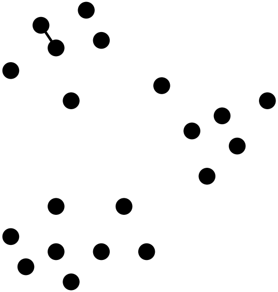

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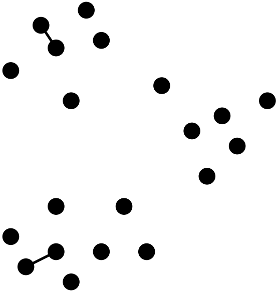

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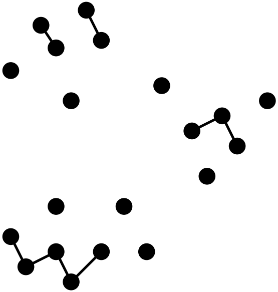

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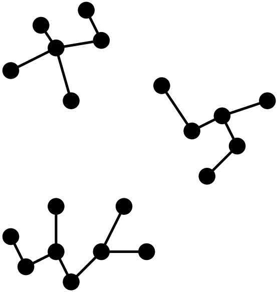

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- Let $\mathcal{C}$ be a set of n clusters, with each object in U in its own cluster.
- Process pairs of objects in increasing order of distance.
  - Let (p, q) be the next pair with $p \in C_p$ and $q \in C_q$.
  - If $C_p \neq C_q$, add new cluster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

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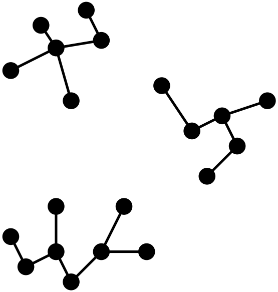

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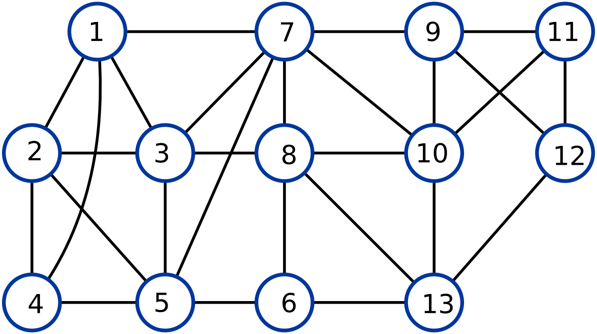
- Stop when there are k clusters in $\mathcal{C}$.
- Same as Kruskal's algorithm but do not add last $k - 1$ edges in MST.

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 $\mathcal{C} = C_1, C_2, \ldots C_k$.
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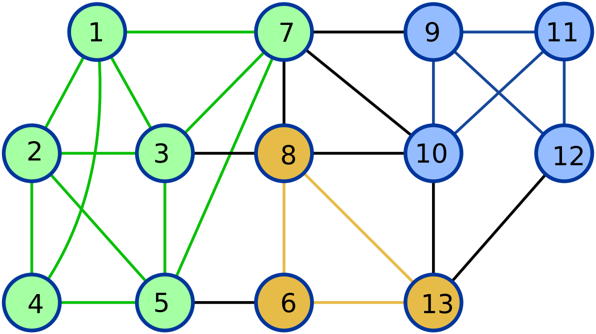

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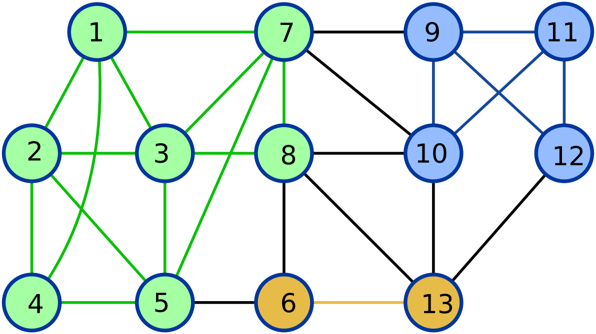

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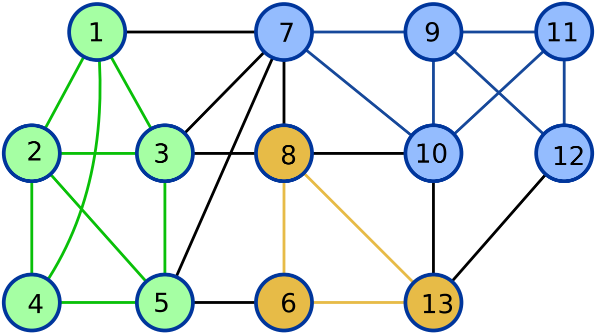

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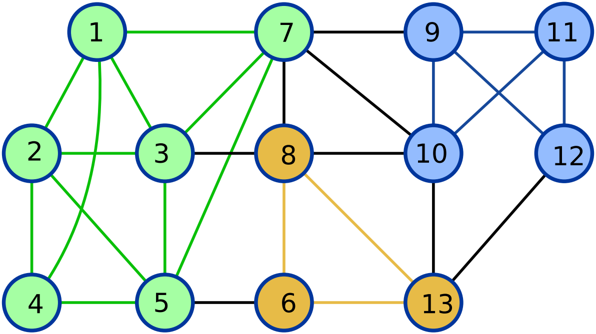

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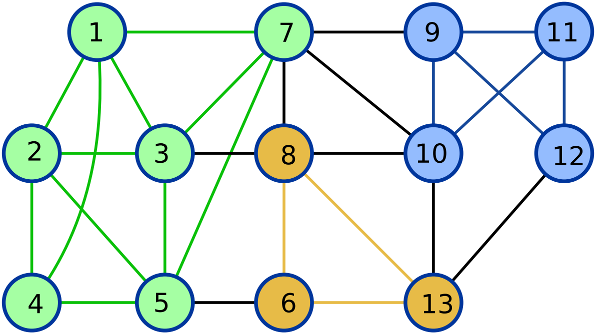

- How do we count the number of edges within modules?
- For every node $u \in V$, define $c(u)$ as the index of u's module.

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

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

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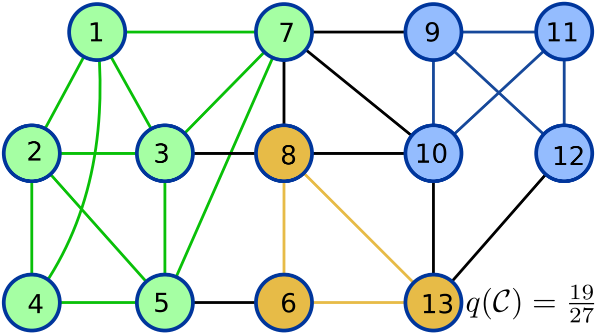

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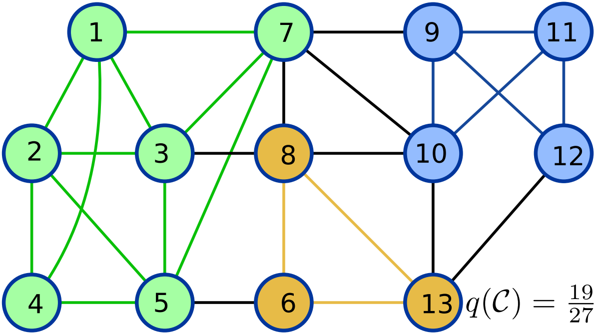

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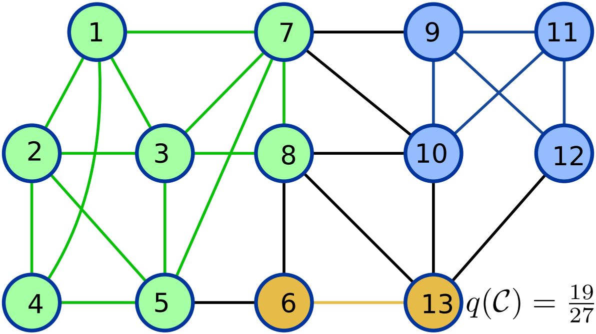

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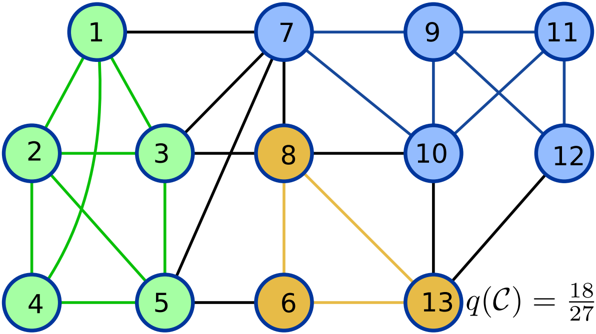

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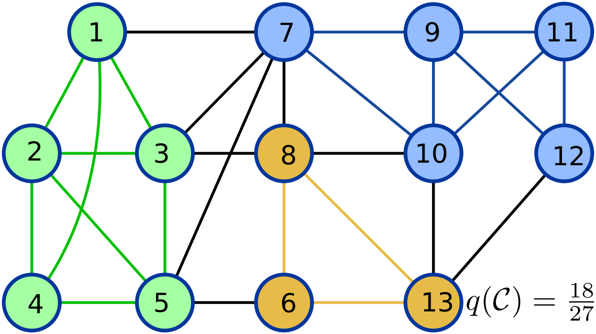

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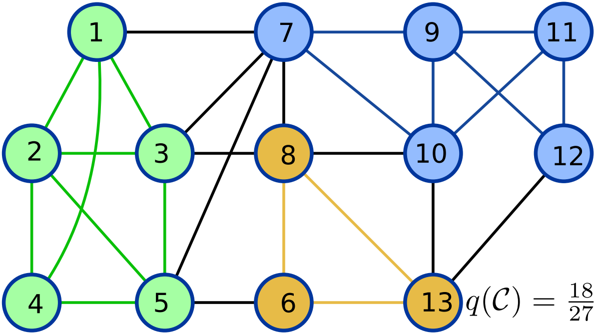

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- Should we maximise or minimise $q(\mathcal{C})$? Maximise it.
- What is the maximum value we can get for $q(\mathcal{C})$?

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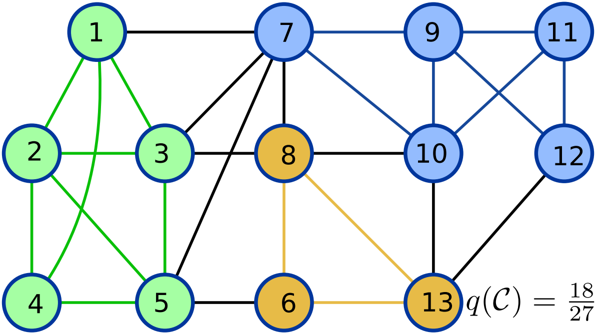

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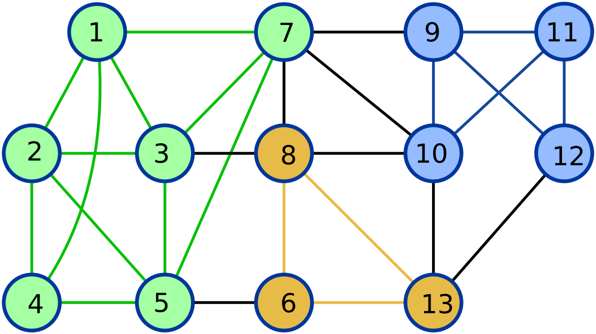
- Should we maximise or minimise $q(\mathcal{C})$? Maximise it.
- What is the maximum value we can get for $q(\mathcal{C})$? If we place all nodes in G in a single cluster, $q(\mathcal{C}) = 1$!

Two Criteria for High Quality Partitions

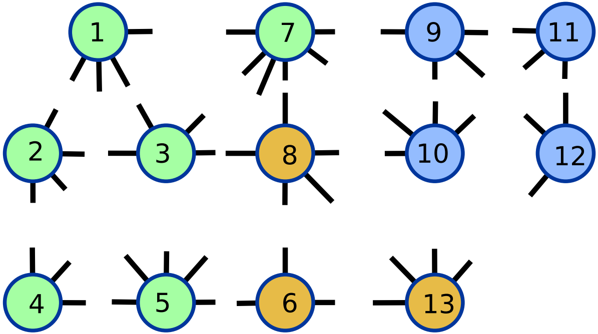
1. Nodes are in highly cohesive modules, i.e., nodes within the same module will be strongly connected with each other.
2. The amount of intramodule connectivity in a good partition will be greater than expected by chance, as defined by a network in which edges are placed between nodes at random.
3.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

Configuration Model



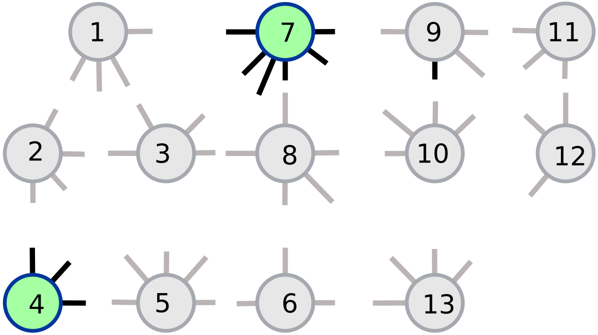
- Method to generate random graphs like Erdös-Renyi and Watts-Strogatz models.
- Ensure that the random graphs have the same degree sequence as G, but allow self loops and multi-edges.

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



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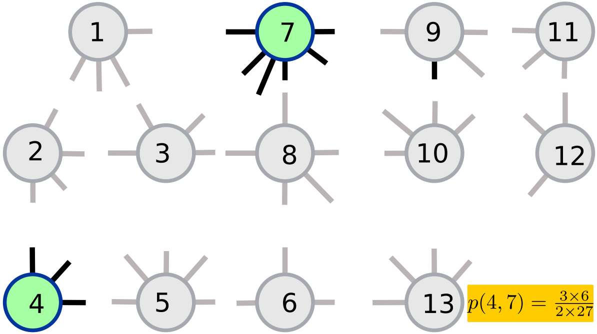

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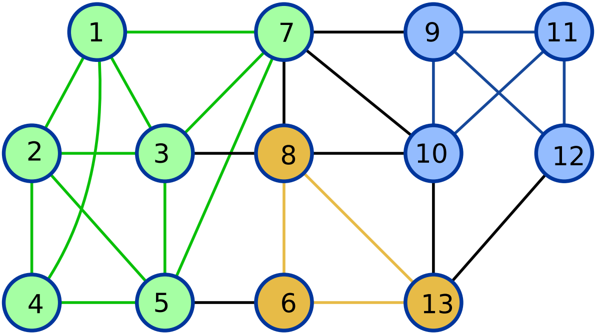
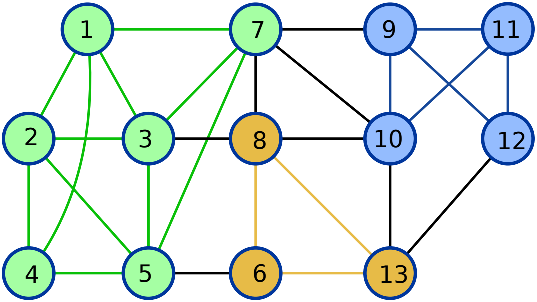


- What is the probability of an edge between nodes u and v? $\frac{d(u)d(v)}{2m}$.
- Therefore modularity of the partition of a random graph in the configuration model into the same modules $\mathcal{C} = C_1, C_2, \ldots C_k$

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

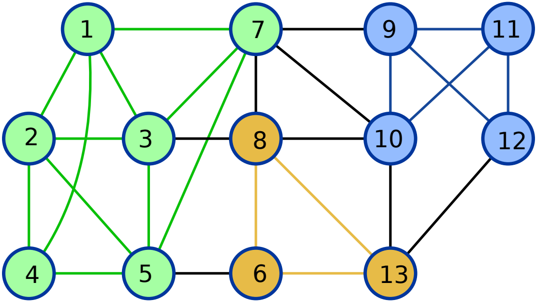
Final Definition of Modularity



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

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

Final Definition of Modularity



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- 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?
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- 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.

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- 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

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Gemma (Jemme Reinerszoon) Frisius

Biography

Magister Philosophiae, Medicinae Doctor Université Catholique de Louvain 1529, 1536

Dissertation:

Advisor: Petrus (Pieter de Corte) Curtius

Students:
Click here to see the students listed in chronological order.

Name	School	Year	Descendants
John Dee	University of Cambridge and Université Catholique de Louvain	1546	1
Gerardus Mercator	Université Catholique de Louvain	1532	2
Johannes Stadius	Université Catholique de Louvain		2
Andreas Vesalius	Università degli Studi di Padova and Université Catholique de Louvain	1537	105089

According to our current on-line database, Gemma Frisius has 4 students and 105096 descendants.
We welcome any additional information.

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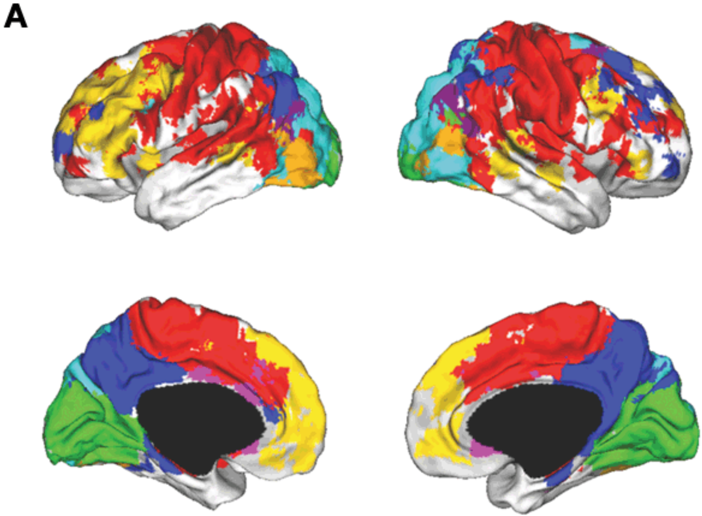
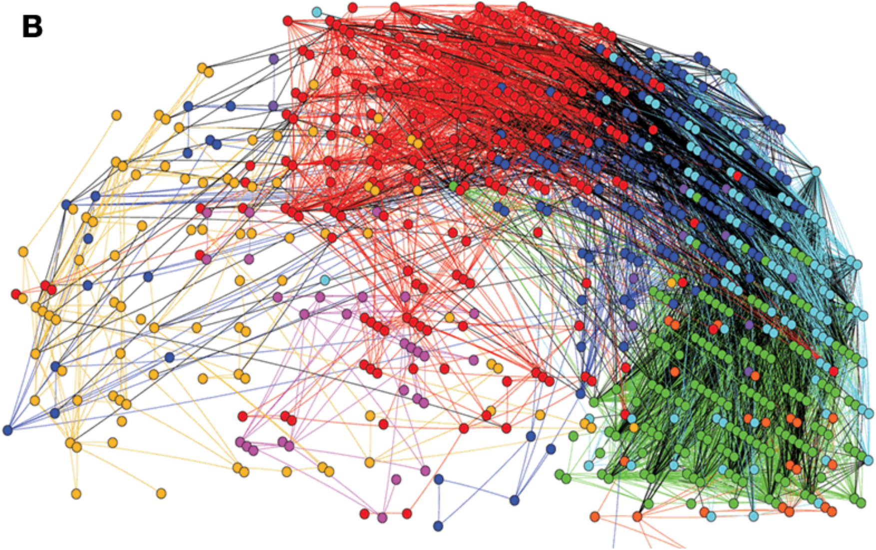
- Efficient calculation of change in q upon swapping makes this algorithm very fast.



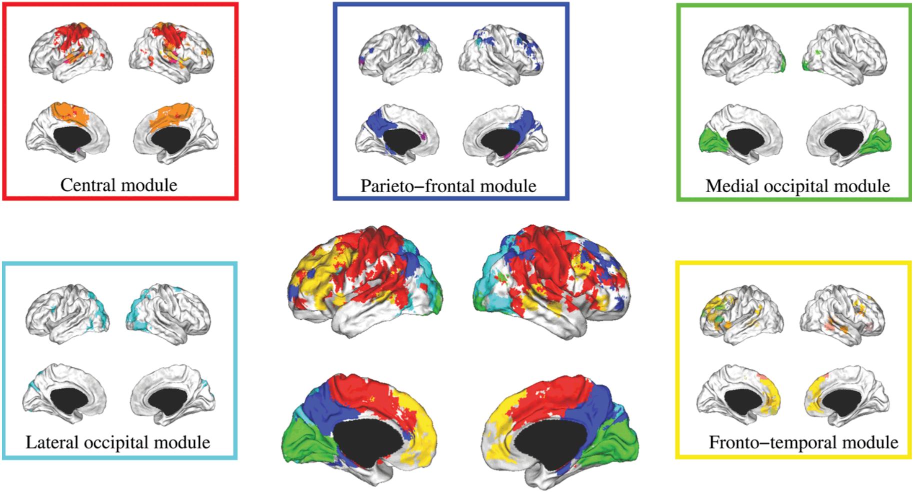
Human resting-state fMRI networks, 1800 nodes, 4mm^3 voxels, had three hierarchical levels: eight modules at the highest level, each with > 10 nodes, 57 modules at the lowest level of the hierarchy.

Meunier *et al.*, 2009



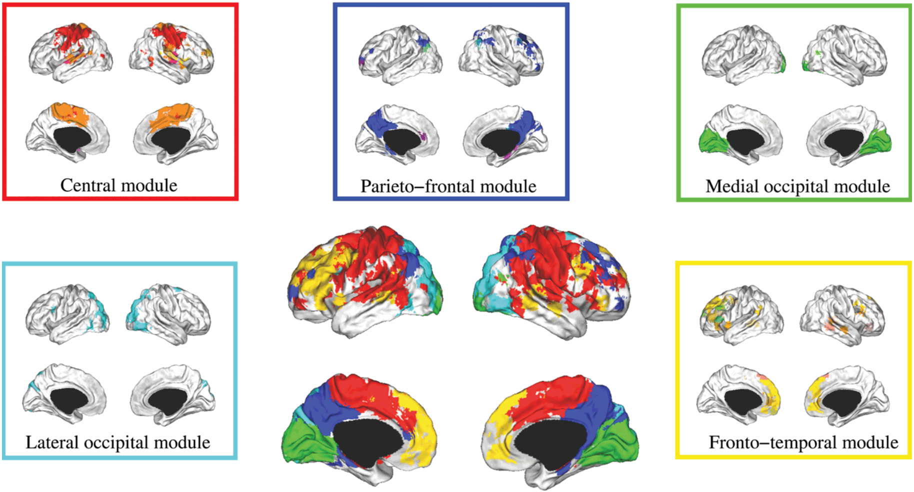
Visualisation of modules. View of brain is from the left side with the frontal cortex on the left and the occipital cortex on the right.

Meunier *et al.*, 2009



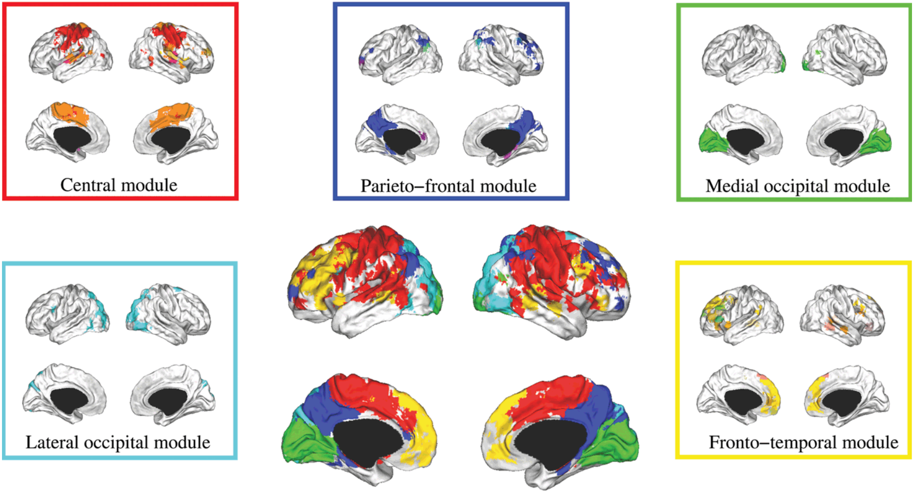
Decomposition of the five largest modules (in the centre): medial occipital module has no major sub-modules whereas the fronto-temporal modules has many sub-modules.

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.

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- 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.