Simulations in Statistical Physics

Course for MSc physics students

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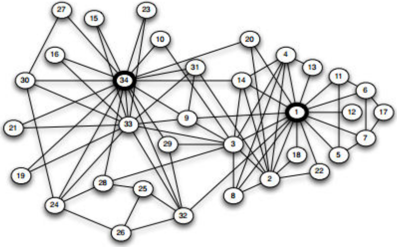
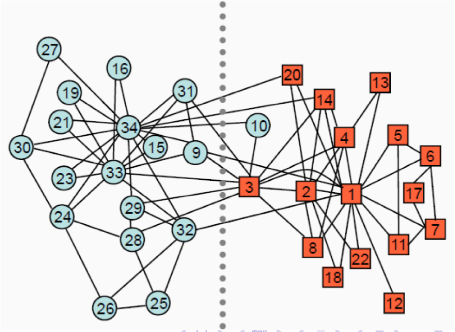
Clustering, modularity, community detection

Zachary karate club



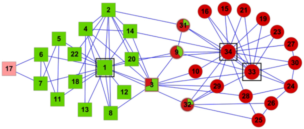


Cluster, Community definition:

- Group which is more connected to itself than to the rest
- Group of items which are more similar to each other than to the rest of the system.

Communities, Partioning:

- Strict partitioning clustering: each object belongs to exactly one cluster
- Overlapping clustering: each object may belong to more clusters
- Hierarchical clustering: objects that belong to a child cluster also belong to the parent cluster
- Outliers: which do not conform to an expected pattern



Communities, Partitioning

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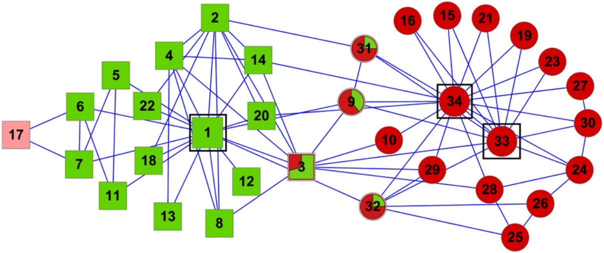


Communities, Partitioning, definitions:

- Local:
  - (Strong) Each node has more neighbors inside than outside
  - (Weak) Total degree within the community is larger than the total degree out of it.
  - Modularity by local definition (above)
  - Clique-percolation
- Global: The community structure found is optimal in a global sense
  - Modularity
  - k-means clustering
  - Agglomerative hierarchical clustering

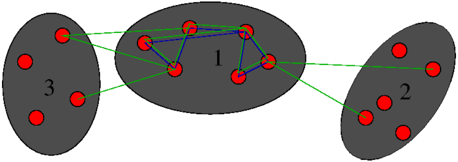
Communities, Partitioning, definitions:

- Hundreds of different algorithms, definitions
- Starting point: *adjacency matrix* A_{ij}, the strength of the link between nodes i and j
- Nodes as vectors (e.g. rows of adjacency matrix)
- Metric between nodes: $||a-b||$:
  - Euclidean distance: $||a-b||_2 = \sqrt{\sum_i (a_i - b_i)^2}$
  - Maximum distance: $||a-b||_\infty = \max_i |a_i - b_i|$
  - Cosine similarity: $||a-b||_c = \frac{a \cdot b}{||a|| \, ||b||}$
  - Hamming distance: number of different coordinates

Modularity

Global method

- e_{ii} percentage of edges in module (cluster) i
  probability edge is in module i
- a_i percentage of edges with at least 1 end in module i
  probability a random edge would fall into module i



- Modularity is

$$Q = \sum_{i=1}^{k} (e_{ii} - a_i^2)$$

- Try to maximize Q

Modularity algorithm

- Rewrite Q:
$$Q = \frac{1}{2m} \sum_{\{i,j\}} \left[A_{ij} - \frac{k_i k_j}{2m} \right]$$
where $\{i, j\}$ are pairs in the same module. $2m = \sum_i k_i$
- Only two modules
- $s_i = \pm 1$: 1 if node i is in module 1 -1 otherwise
$$Q = \frac{1}{4m} \sum_{\{i,j\}} \left[A_{ij} - \frac{k_i k_j}{2m} \right] (s_i s_j + 1)$$
- $+1$ is a constat can be omitted
- Change the vector s_i to maximize Q

Modularity algorithm

$$Q = \frac{1}{4m} \sum_{\{i,j\}} \left[A_{ij} - \frac{k_i k_j}{2m} \right] s_i s_j$$

- Try to find ± 1 vector s_i that maximizes the modularity.
- Start with two groups
- Then split one of the two groups using the same technique
- Very similar to spin glass Hamiltonian
- Generally a np-complete problem, we can use the same techniques.
- Often steepest descent is used, (greedy method): change the site that would increase the modularity the most.

Problems with modularity

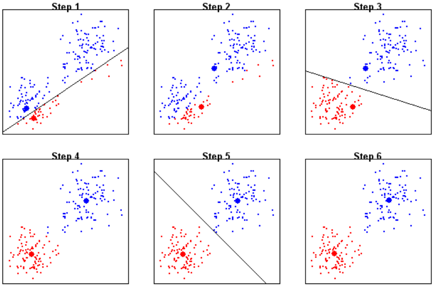
Resolution

$$Q = \frac{1}{4m} \sum_{\{i,j\}} \left[A_{ij} - \frac{k_i k_j}{2m} \right] s_i s_j$$

- On large networks normalization factor m can be very large
- (It relies on random network model)
- The expected edge between modules decreases and drops below 1
- A single link is a strong connection.
- Small modules will not be found

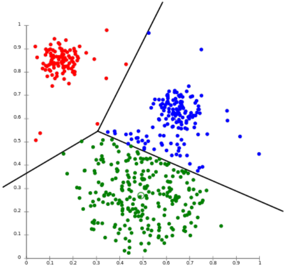
k-means clustering

- Cut the system into exactly k parts
- Let μ_i be the mean of each cluster (using a metric)
- The cluster i is the set of points which are closer to μ_i than to any other μ_j
- The result is a partitioning of the data space into Voronoi cells



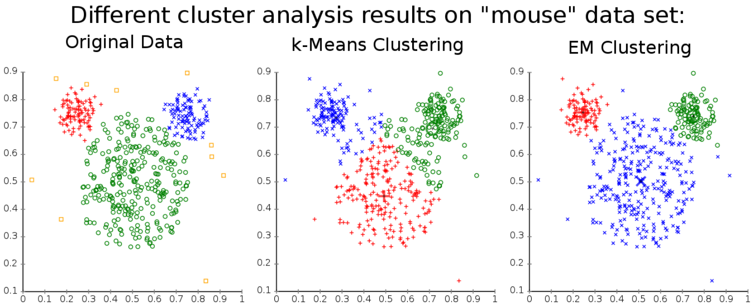
k-means clustering, standard algorithm:

- Define a norm between nodes
- Give initial positions of the means m_i
- Assignment step: Assign each node to cluster whoose mean m_i is the closest to node.
- Update step: Calculate the new means of the clusters
- Go to Assignment step.

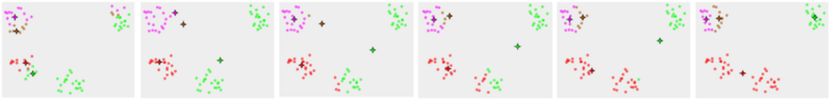


k-means clustering, problems:

- k has to fixed beforhand
- Fevorizes equal sized clusters:



- Very sensitive on initial conditions:



- No guarantee that it converges

Hierarchical clustering

1. Define a norm between nodes $d(a, b)$
2. At the beginning each node is a separate cluster
3. Merge the two closest cluster into one
4. Repeat 3.

Norm between clusters $||A - B||$

- Maximum or complete linkage clustering:

$$\max\{d(a, b) : a \in A, b \in B\}$$

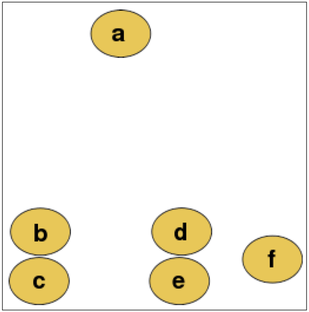
- Minimum or single-linkage clustering:

$$\min\{d(a, b) : a \in A, b \in B\}$$

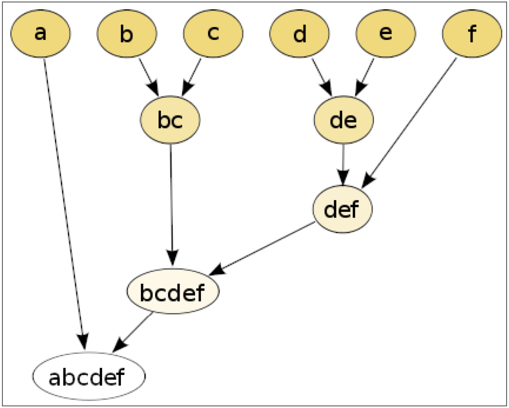
- Mean or average linkage clustering:

$$\frac{1}{||A|| \, ||B||} \sum_{a \in A} \sum_{b \in B} d(a, b)$$

Hierarchical clustering

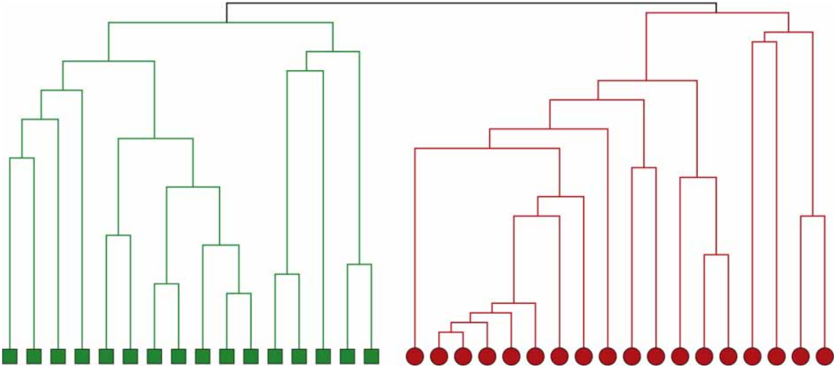


Original



Dendogram

Dendograph of the Zachary karate club



Example: Temperatures in capitals

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Tallinn	-3	-5	-1	3	10	13	16	15	10	6	1	-2
Beijing	-3	0	6	13	20	24	26	25	20	13	5	-1
Berlin	0	-1	4	7	12	16	18	17	14	9	4	1
Buenos Aires	23	22	20	16	13	10	10	11	13	16	18	22
Cairo	13	15	17	21	25	27	28	27	26	23	19	15
Canberra	20	20	17	13	9	6	5	7	9	12	15	18
Cape Town	21	21	20	17	15	13	12	13	14	16	18	20
Helsinki	-5	-6	-2	3	10	13	16	15	10	5	0	-3
London	3	3	6	7	11	14	16	16	13	10	6	5
Moscow	-8	-7	-2	5	12	15	17	15	10	3	-2	-6
Ottawa	-10	-8	-2	6	13	18	21	20	14	7	1	-7
Paris	3	4	7	10	13	16	19	19	16	11	6	5
Riga	-3	-3	1	5	11	15	17	16	12	7	2	-1
Rome	8	8	11	12	17	20	23	23	21	17	12	9
Singapore	27	27	28	28	28	28	28	28	27	27	27	26
Stockholm	-2	-3	0	3	10	14	17	16	11	6	1	-2
Washington D.C.	2	3	7	13	18	23	26	25	21	15	9	3

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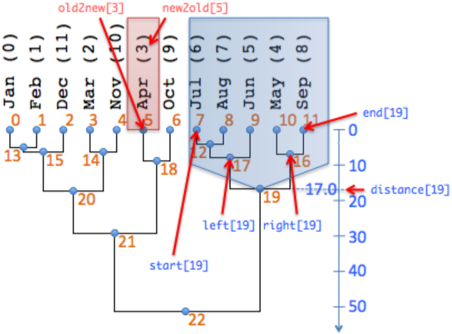
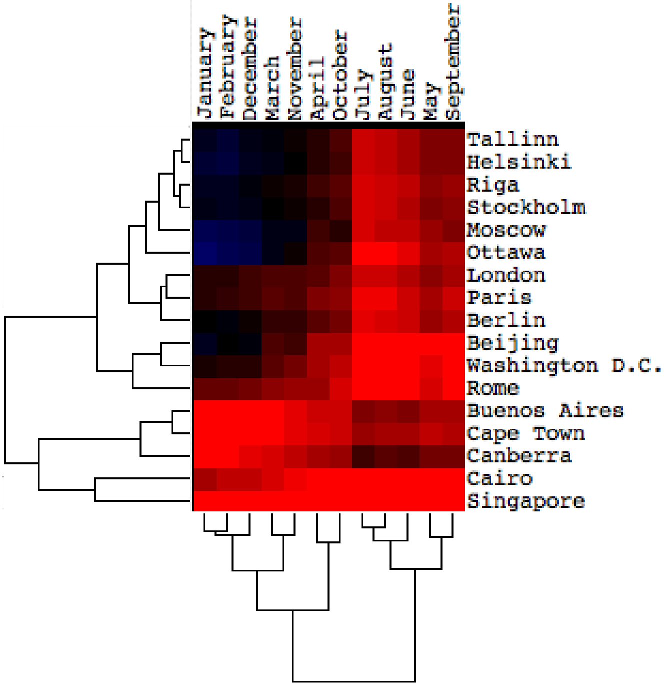


Euclidean distance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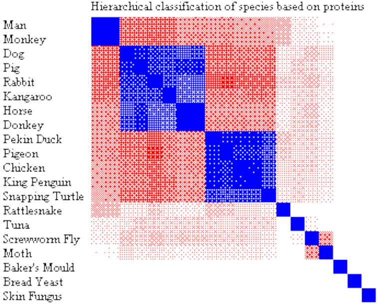
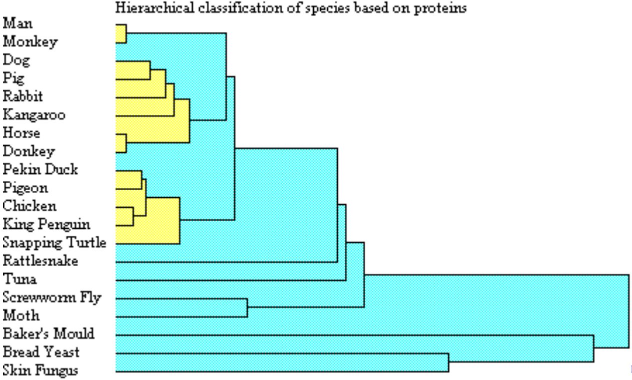

Hierarchical classification of species based on proteins
Man
Monkey
Dog
Pig
Rabbit
Kangaroo
Horse
Donkey
Pekin Duck
Pigeon
Chicken
King Penguin
Snapping Turtle
Rattlesnake
Tuna
Screwworm Fly
Moth
Baker's Mould
Bread Yeast
Skin Fungus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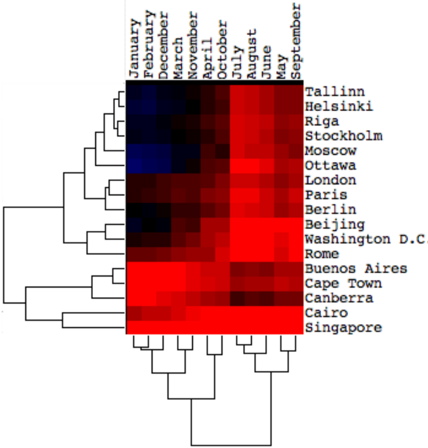
Hierarchical clustering: problems

- Advantages
  - Simple
  - Fast
  - Number of clusters can be controlled
  - Hierarchical relationship
- Disadvantages
  - No a priori cutting level
  - Meaning of clusters unclear
  - Important links may be missed
  - Different result if one item omitted



LFK method

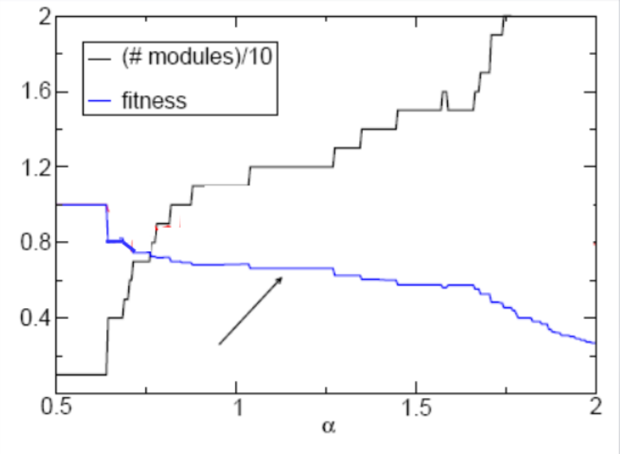
- Try to use definition: more links in than out in cluster

$$f_G = \frac{k_{in}^G}{(k_{in}^G + k_{out}^G)^\alpha}$$

- Try tomaximize fitness:
  - Add node if it increases fitness
  - Check all others whether they decrease it
- Algorithm:
  1. Loop for all neighboring nodes of G not included in G
  2. The neighbor with the largest fitness is added to G, yielding a larger subgraph G'
  3. The fitness of each node of G' is recalculated
  4. if a node turns out to have negative fitness, it is removed from G', yielding a new subgraph G''
  5. if 4 occurs go to 3 than repeat from 1 with G''

LFK method

- α resolution factor



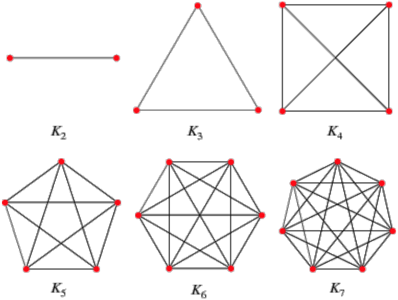
- Long plateaus indicate stable structure, (as e.g. hierarchical)

LFK method: problems

- Advantages
  - Resolution can be controlled
  - Close to most trivial definition
  - Can be extended to overlapping clusters
- Disadvantages
  - Code runs for ages
  - Heuristic cutting

Clique percolation

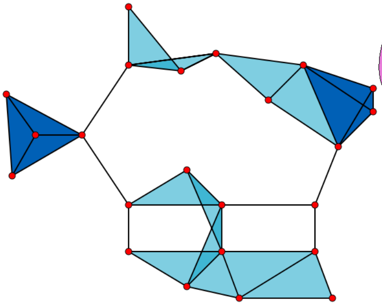
- Motication: clusters are formed with at least triangles
- Can be generalized to any k-clique

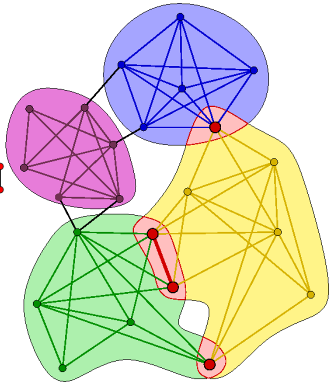


- $k = 2$ normal percolation

Clique percolation

- It will definitely lead to overlapping communities, but overlap is limited to $k-1$ nodes
- k-clusters are included in $k-1$ clusters





Clique percolation

- Algorithm
  - Similar to normal percolation on networks but with multiple loops
- Advantages
  - Different level of clusters
  - Clusters are generally relevant
  - No heuristics
- Disadvantages
  - Running time cannot be guessed (finding the maximal clique is an np-complete problem)
  - Code may run for ages