Learning from Networks

Graph Clustering

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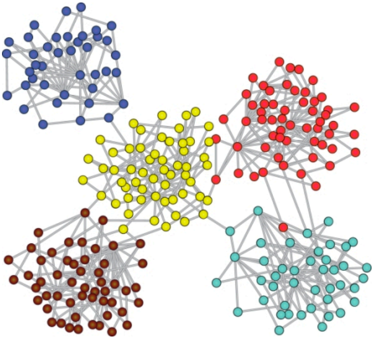
Graph Clustering: Definition

Given: graph $G = (V, E)$

Goal: partition V into clusters so that *similar vertices* are in the same cluster and *different vertices* are in different clusters.

Graph Clustering: Definition (continue)

Intuition: the similarity between vertices are represented by the edges



Given: *connected* graph $G = (V, E)$
Goal: partition V so that there are many edges *within* each cluster and few edges *between* clusters.

Many different formalizations based on this intuition.

Note: sometimes clusters in a graph are called *communities*

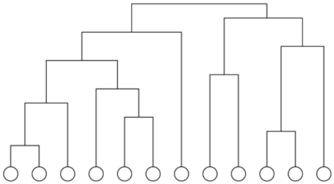
Graph Clustering: Approaches

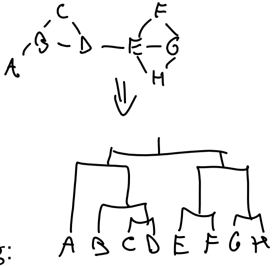
We will see different types of approaches for clustering:

- hierarchical clustering
- cost-based clustering
- (spectral clustering)

Hierarchical Clustering

The output is a **dendrogram**, representing the clustering structure of the whole graph G.





Two general approaches to hierarchical clustering:

- *agglomerative approach*: start with each node in a cluster, iteratively join clusters $\Rightarrow$ Ravasz algorithm
- *divisive approach*: start with all nodes in a cluster, iteratively split clusters $\Rightarrow$ Girvan-Newman algorithm

Ravasz Algorithm

Algorithm `AgglomerativeClustering(`G`)`
Input: connected graph $G = (V, E)$
Output: dendrogram whose leaves are the elements of V

```
assign each node u to its own cluster C_u;
for all pairs u, v ∈ V, u ≠ v: compute their similarity sim(u, v)
repeat until all nodes are in a single cluster:
    find the pair of clusters C_1, C_2 with highest similarity
    sim(C_1, C_2) (ties broken arbitrarily)
    merge clusters C_1, C_2 in a single cluster C'
    compute similarity between C' and all other clusters
return the corresponding dendrogram
```

$\Theta(n)$

$\leq n$ calcoli di $sim(C_1, C_2)$

Different variants depending on the definition of $sim(u, v)$ and the definition of $sim(C_1, C_2)$.

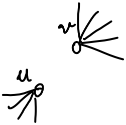
Complexity? In general: $\Theta\left(|V|^2\right)$ computations of $sim(u, v)$ and of $sim(C_1, C_2)$

Ravasz Algorithm (continue)

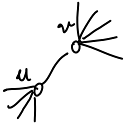
Common choice for $sim(u, v)$:

$$\boxed{sim(u,v) = \frac{|\mathcal{N}(u) \cap \mathcal{N}(v)| + A_{uv}}{\min\{deg(u), deg(v)\} + 1 - A_{uv}}}$$

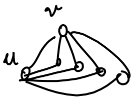
where $\boxed{A}$ is the adjacency matrix of G

a) 

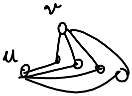
$\Rightarrow sim(u,v) = 0$

b) 

$\Rightarrow sim(u,v) = \dfrac{1}{\min\{deg(u), deg(v)\}}$

c) 

$(deg(u) = deg(v)) \Rightarrow sim(u,v) = \dfrac{deg(u)}{deg(u)} = 1$

d) 

$(deg(u) = deg(v)) \Rightarrow sim(u,v) = \dfrac{deg(u)}{deg(u)+1}$

Ravasz Algorithm (continue)

Common choices for $sim(C_1, C_2)$ define different types of *linkage clustering*:

- *single linkage clustering*: $\boxed{sim(C_1, C_2) = \min_{u \in C_1, v \in C_2} sim(u, v)}$
- *average linkage clustering*:
$$\boxed{sim(C_1, C_2) = \frac{1}{|C_1| \cdot |C_2|} \sum_{u \in C_1, v \in C_2} sim(u, v)}$$
- *complete linkage clustering*: $\boxed{sim(C_1, C_2) = \max_{u \in C_1, v \in C_2} sim(u, v)}$

Example

Girvan-Newman Algorithm

Based on the idea of iteratively removing the most *central* edge in the graph $G = (V, E)$.

Various definitions of *centrality* for edges, but the most common one is *link betweenness*.

Link betweenness

Let $\boxed{\sigma_{s,t}}$ be the number of shortest paths from node s to node t.
Let $\boxed{\sigma_{s,t}(e)}$ be the number of shortest paths from node s to node t that pass through *edge* e.

Definition

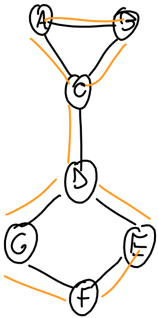
Given a connected graph $\boxed{G = (V, E)}$ and an edge $\boxed{e \in E}$ the link betweenness $\boxed{b(e, G)}$ of e in G:

$$\boxed{b(e, G) = \sum_{s,t \in V : s \neq t} \frac{\sigma_{s,t}(e)}{\sigma_{s,t}}}$$

Complexity of computing $b(e, G)$ for all edges $e \in E$?
$\boxed{\Theta\left(|V| \cdot |E|\right)}$

Example

G:



e	$b(e, G)$
A, B	1
A, C	
B, C	
C, D	12 ⇒ (nodo in triangolo) → (nodo in diamante)
D, E	
E, F	3.5

Girvan-Newman Algorithm (continue)

Algorithm `GNClustering(`G`)`
Input: connected graph $G = (V, E)$
Output: dendrogram whose leaves are the elements of V

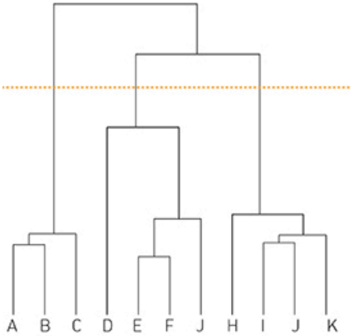
- assign all nodes u to a single cluster C;
- repeat until all nodes are in different clusters: m iterazioni
  - $O(mn)$ for each cluster C:
    - for each edge $e \in C$: compute $b(e, C)$
  - let $e_{\max}$ the edge of maximum betweenness, and let $C(e)$ its cluster;
  - remove e from $C(e)$;
- report the corresponding dendrogram

Complexity? In general: $\boxed{\Theta\left(|E|^2|V|\right)}$.

$|E| = m$, $|V| = n$

Hierarchical Clustering: Getting a Clustering

The output of hierarchical clustering is a dendrogram, not a clustering. How do we obtain a clustering?

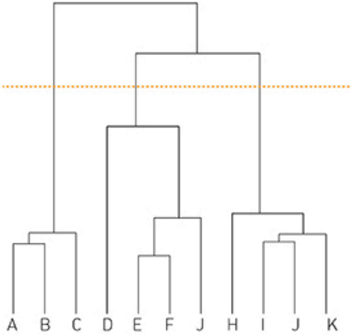


By cutting the dendrogram at a given level.

How do we select where to cut?

Hierarchical Clustering: Getting a Clustering (continue)

How do we select where to cut?



- if we know the number k of clusters we want: pick a level resulting in k clusters
- if we do not know k: define a score for clusterings, and pick the clustering from the dendrogram of maximum score

Cost-based Clustering

Common approach in clustering (not only for graphs):

- define a cost function over possible partitions of the objects
- find the partition (=clustering) of minimal cost

Modularity

Idea:a cluster should contain more edges than expected in a random graph.

Definition

Given a graph $\boxed{G = (V, E)}$ with $|V| = n$, $|E| = m$ the $\boxed{\text{modularity}}$ $\boxed{M(S)}$ of a subset $\boxed{S \subseteq V}$ of the vertices of G is

$$\boxed{M(S) = \frac{1}{2m} \sum_{u,v \in S} \left(A_{uv} - \frac{deg(u)deg(v)}{2m} \right)}$$

Intuition: measures the difference between the number of edges within each cluster with the *expected* number of edges under the Chung-Lu model for random graphs.

Modularity (continue)

The modularity of a clustering of G is the sum of the modularity of each cluster.

Definition

Given a clustering $\boxed{\mathcal{C} = C_1, C_2, \ldots}$ of graph $G = (V, E)$ with $|V| = n$, $|E| = m$, the modularity $M(\mathcal{C})$ of $\mathcal{C}$ is:

$$\boxed{\begin{aligned} M(\mathcal{C}) &= \sum_{C \in \mathcal{C}} M(C) \\ &= \frac{1}{2m} \sum_{C \in \mathcal{C}} \sum_{u,v \in C} \left(A_{uv} - \frac{deg(u)deg(v)}{2m} \right) \end{aligned}}$$

Modularity (continue)

Proposition

Given a clustering $\boxed{\mathcal{C} = C_1, C_2, \dots}$ of graph $\boxed{G = (V, E)}$ with $\boxed{|V| = n,\ |E| = m,}$ the modularity $M(\mathcal{C})$ of $\mathcal{C}$ is equal to

$$\boxed{M(\mathcal{C}) = \sum_{C \in \mathcal{C}} \left(\frac{|E(C)|}{m} - \left(\frac{\sum_{u \in C} deg(u)}{2m} \right)^2 \right)}$$

where $E(C)$ are the edges between nodes in cluster C:
$\boxed{E(C) = \{(u, v) \in E : u \in C, v \in C\}}$

ci serve solo sapere $|E(C)|$ e iterare su nodi (non coppie di nodi)

Proof

Dim: $M(\mathcal{C}) = \frac{1}{2m} \sum_{c \in \mathcal{C}} \sum_{u,v \in C} \left(A_{uv} - \frac{deg(u)\,deg(v)}{2m} \right) =$

$\frac{1}{2m} \sum_{c \in \mathcal{C}} \sum_{u,v \in C} A_{u,v} = \frac{1}{2m} \sum_{c \in \mathcal{C}} 2|E(C)| = \frac{1}{m} \sum_{c \in \mathcal{C}} |E(C)|$

$\frac{1}{2m} \sum_{c \in \mathcal{C}} \sum_{u,v \in C} \frac{deg(u)\,deg(v)}{2m} = \frac{1}{(2m)^2} \sum_{c \in \mathcal{C}} \sum_{u,v \in C} deg(u)\,deg(v) =$

$= \frac{1}{(2m)^2} \sum_{c \in \mathcal{C}} \left(\sum_{u \in C} deg(u) \left(\sum_{v \in C} deg(v) \right) \right) =$

$= \frac{1}{(2m)^2} \sum_{c \in \mathcal{C}} \left(\left(\sum_{u \in C} deg(u) \right) \left(\sum_{v \in C} deg(v) \right) \right) = \frac{1}{(2m)^2} \sum_{c \in \mathcal{C}} \left(\sum_{u \in C} deg(u) \right)^2 =$

$= \sum_{c \in \mathcal{C}} \left(\frac{\sum_{u \in C} deg(u)}{2m} \right)^2$

$=$ QED ■

Example

Modularity-Based Clustering

Input: graph $\boxed{G = (V, E)}$
Goal: find the clustering $\boxed{\mathcal{C} = C_1, C_2, \ldots}$ that maximizes the modularity

$$\boxed{M(\mathcal{C}) = \sum_{C \in \mathcal{C}} \left(\frac{|E(C)|}{m} - \left(\frac{\sum_{u \in C} deg(u)}{2m} \right)^2 \right)}$$

Equivalent formulation: since the cost of clustering $\mathcal{C}$ is $-M(\mathcal{C})$, the following formulation is equivalent:

Input: graph $G = (V, E)$
Goal: find the clustering $\mathcal{C} = C_1, C_2, \ldots$ of minimum cost $\boxed{-M(\mathcal{C})}$.

Modularity-Based Clustering: Complexity

Informal: finding a clustering of maximum modularity is hard!

Problem (Modularity Clustering Problem)

Given a graph G *and a value* K*, is there a clustering* $\mathcal{C}$ *of* G *such that* $M(\mathcal{C}) \geq K$*?*

Proposition

The Modularity Clustering Problem is NP-complete.

So? (Greedy) agglomerative algorithm

Modularity-Based Clustering: Greedy Agglomerative Approach

Algorithm `GreedyModularityClustering(`G`)`

Input: connected graph $G = (V, E)$

Output: clustering of the elements of V

1 $\mathcal{C}_1 \leftarrow$ clustering where each node u is assigned to its own cluster C_u; $i \leftarrow 1$;

2 repeat until all nodes are in a single cluster:

   3 for each pair of clusters C_1, C_2 such that there exists one edge between C_1 and C_2: compute $\delta(\mathcal{C}_i, C_1, C_2) = M(\mathcal{C}_i - C_1 - C_2 + (C_1 \cup C_2)) - M(\mathcal{C}_i)$;

   4 find C', C'' that maximize $\delta(\mathcal{C}_i, C', C'')$

   5 $\mathcal{C}_{i+1} \leftarrow \mathcal{C}_i - C' - C'' + (C' \cup C'')$; $i \leftarrow i + 1$;

6 return the clustering $\mathcal{C}^*$, across iterations, of maximum modularity: $\mathcal{C}^* = \arg\max_{\mathcal{C}_i, i=1,2,\ldots} M(\mathcal{C}_i)$

Complexity? In general: $O\left(|E| \cdot |V|\right)$ computations of $\delta(\mathcal{C}_i, C_1, C_2)$

Modularity-Based Clustering: Efficient Computation

Proposition

Let $E(C_1, C_2)$ be the edges between cluster C_1 and cluster C_2: $E(C_1, C_2) = \{(u, v) \in E : u \in C_1, v \in C_2\}$. Then

$$\delta(\mathcal{C}_i, C_1, C_2) = \frac{|E(C_1, C_2)|}{m} - \frac{\left(\sum_{u \in C_1} deg(u)\right)\left(\sum_{v \in C_2} deg(v)\right)}{2m^2}$$

Modularity-Based Clustering: Efficient Computation (continue)

Proposition

In every iteration of the repeat-until loop, the values $|E(C_1, C_2)|$ for all $C_1, C_2 \in \mathcal{C}$ and $\sum_{u \in C} deg(u)$ for all $C \in \mathcal{C}$ can be efficiently updated in total time $O(|E|)$.

Example