Graph mining - lesson 2
Graph Clustering
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Issue at stake:

▶ short overview of different types of methods for vertex clustering

▶ only simple clustering (although some methods for overlapping clustering, clustering according to vertex/edge attributes, clustering of bipartite graphs... also exist)
Notations for this class

Notations

In the following, a graph $G = (V, E, W)$ with:

- $V$: set of vertices $\{x_1, \ldots, x_n\}$;
- $E$: set of (undirected) edges. $m = |E|$;
- $W$: weights on edges s.t. $W_{ij} \geq 0$, $W_{ij} = W_{ji}$ and $W_{ii} = 0$ (also called, adjacency matrix).
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If needed, attributes for the nodes will be denoted by $f_j(x_i)$ ($j$th attribute for node $i$) and attributes for the edges (other than the weights) by $g_j(x_i, x_{i'})$ ($j$th attribute for the edge $(x_i, x_{i'})$).
A short overview of vertex clustering

Purpose: Find communities or modules (i.e., groups of vertices) such that vertices inside the community are strongly connected whereas vertices between two communities are slightly connected.
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Some approaches to perform such task:
- optimizing a given criterion (e.g., modularity maximization)
- spectral clustering
- model based clustering
- ... (see [Fortunato and Barthélémy, 2007, Schaeffer, 2007, Brohée and van Helden, 2006])
Outline

Modularity optimization

Spectral clustering

Model based clustering
Clustering based on criterion optimization

- “Cut” criteria: Given a number of clusters, $K$, find the partition of $V$, $C_1, \ldots, C_K$ such that it solves the mincut problem, i.e., it minimizes

$$\text{cut}(C_1, \ldots, C_K) = \frac{1}{2} \sum_{k=1}^{K} \sum_{x_i \in C_k, x_j \notin C_k} W_{ij}$$
Clustering based on criterion optimization

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**Problem:** The mincut problem often only separates individual vertices from the rest of the graph.

- **“Modularity” criterion** [Newman and Girvan, 2004]: Given a number of clusters, $K$, find the partition of $V$, $C_1, \ldots, C_K$ which maximizes

$$Q(C_1, \ldots, C_K) = \frac{1}{2m} \sum_{k=1}^{K} \sum_{x_i, x_j \in C_k} (W_{ij} - P_{ij})$$

with $P_{ij}$: weight of a "null model" (graph with the same degree distribution but no preferential attachment):

$$P_{ij} = \frac{d_i d_j}{2m}$$

where $d_i = \frac{1}{2} \sum_{j} W_{ij}$. 
Clustering based on criterion optimization

- “Cut” criteria: Given a number of clusters, $K$, find the partition of $V, C_1, \ldots, C_K$ such that it solves the “RatioCut” problem, i.e., it minimizes

$$\text{RatioCut}(C_1, \ldots, C_K) = \frac{1}{2} \sum_{k=1}^{K} \sum_{x_i \in C_k, x_j \notin C_k} \frac{W_{ij}}{|C_k|}$$

(forces larger communities than the mincut problem).

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Clustering based on criterion optimization

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$$\text{NCut}(C_1, \ldots, C_K) = \frac{1}{2} \sum_{k=1}^{K} \sum_{x_i \in C_k, x_j \notin C_k} \frac{W_{ij}}{\text{Vol}(C_k)}$$

in which $\text{Vol}(C_k) = \sum_{x_i, x_j \in C_k} W_{ij}$ (also forces larger communities than the mincut problem).

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with $P_{ij}$: weight of a “null model” (graph with the same degree distribution but no preferential attachment): $P_{ij} = \frac{d_id_j}{2m}$ with $d_i = \frac{1}{2} \sum_{j \neq i} W_{ij}$. 
Interpretation of the modularity

A good clustering should maximize the modularity:

- \( Q \uparrow \) when \((x_i, x_j)\) are in the same cluster and \( W_{ij} \gg P_{ij} \)
- \( Q \downarrow \) when \((x_i, x_j)\) are in two different clusters and \( W_{ij} \gg P_{ij} \)

\((m = 20)\)

\[ d_i = 15 \quad P_{ij} = 7.5 \quad d_j = 20 \]

\[ W_{ij} = 5 \Rightarrow W_{ij} - P_{ij} = -2.5 \]

\(i\) and \(j\) in the same cluster decreases the modularity
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$(m = 20)$

$\begin{align*}
    d_i &= 1 \\
P_{ij} &= 0.05 \\
    W_{ij} &= 5 \\
    W_{ij} - P_{ij} &= 4.95 \\
    d_j &= 2
\end{align*}$

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- Modularity
  - helps separate hubs ($\neq$ spectral clustering or min cut criterion);

- is not an increasing function of the number of clusters: useful to choose the relevant number of clusters (with a grid search: several values are tested, the clustering with the highest modularity is kept)
Advantages and drawbacks

- mincut is not adapted to vertex clustering in practice (clusters with isolated vertices)
- the other three methods are NP hard to solve...

[Fortunato and Barthélémy, 2007] showed that modularity has a resolution issue. [Bickel and Chen, 2009] gave conditions for consistency of the clusters obtained by modularity optimization in Stochastic Block Models (SBM).

Remark: Relaxation of RatioCut problem and NCut problem gives spectral clustering. Modularity optimization is often solved by approximation methods.
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A short description of approximation methods for modularity optimization

- simple greedy algorithms ([Newman, 2004] and [Clauset et al., 2004] for a fast version): hierarchical clustering which merges pairs of vertices with the highest contribution to modularity

- multi-level greedy algorithms ([Blondel et al., 2008], also known as “Louvain algorithm” and [Noack and Rotta, 2009] for an improved version): hierarchical approach in which vertices are sometimes re-assigned to a different community in a greedy way

- simulated annealing ([Reichardt and Bornholdt, 2006] uses a spin-glass model which, in some cases, is equivalent to modularity maximization)

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Computational time needed by the different solution to find a clustering for NVV network:

<table>
<thead>
<tr>
<th>Method</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>hierarchical</td>
<td>0.003</td>
</tr>
<tr>
<td>multilevel</td>
<td>0.002</td>
</tr>
<tr>
<td>annealing</td>
<td>1.266</td>
</tr>
</tbody>
</table>
Computational time (greedy approaches)

Difference (computational time) between the first two approaches (100 evaluations):

## Coordinate system already present. Adding new coordinate system, which will replace the existing one.
Accuracy of the clustering

- Hierarchical: 0.567, 7
- Multilevel: 0.567, 7
- Simulated annealing: 0.5628, 10
Outline

Modularity optimization

Spectral clustering

Model based clustering
Relation between RatioCut and Laplacian

[von Luxburg, 2007] shows that minimizing

$$\text{RatioCut}(C_1, C_2) = \frac{1}{2} \sum_{k=1}^{2} \sum_{x_i \in C_k, x_j \notin C_k} \frac{W_{ij}}{|C_k|}$$

is equivalent to the following constrained problem:

$$\min_{C_1, C_2} \mathbf{v}^T L \mathbf{v} \text{ st } \mathbf{v} \perp \mathbf{1}_n \text{ and } \|\mathbf{v}\| = \sqrt{n}$$

for $\mathbf{v}$ the vector of $\mathbb{R}^n$ obtained from the partition by:

$$v_i = \begin{cases} \sqrt{\frac{|C_2|}{|C_1|}} & \text{if } v_i \in C_1 \\ -\sqrt{\frac{|C_1|}{|C_2|}} & \text{otherwise.} \end{cases}$$

and $L$ is the Laplacian of the graph, $n \times n$-matrix with entries:

$$L_{ij} = \begin{cases} -W_{ij} & \text{if } i \neq j \\ d_i = \sum_{j \neq i} W_{ij} & \text{otherwise.} \end{cases}$$
... and more remarks

- this is a discrete (since $v$ can only have two values) and NP-hard problem;
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- the same relation holds between NCut problem and normalized Laplacian \( D^{-1/2}LD^{-1/2} \) is which
  \( D = \text{Diag}(d_1, \ldots, d_n) \);
... and more remarks

- this is a **discrete** (since $v$ can only have two values) and **NP-hard** problem;

- the same relation holds between **NCut problem** and normalized Laplacian $D^{-1/2}LD^{-1/2}$ is which $D = \text{Diag}(d_1, \ldots, d_n)$;

- a generalization of these results exist for $K > 2$. 
Some properties of the Laplacian

Relations with the graph structure:

The Laplacian matrix of the graph has a null space spanned by the vectors

\[
\begin{pmatrix}
1 \\
1 \\
1 \\
0 \\
0
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
0 \\
0 \\
0 \\
1 \\
1
\end{pmatrix}.
\]

Random walk point of view: If we consider a random walk on the graph with probability to jump from one node to the other equal to \( W_{ij} \), then the average time to go from one node to another (commute time) is given by \( L + [\text{Fouss et al., 2007}] \).
Some properties of the Laplacian

Relations with the graph structure: the vector $1_n$ spans the null space for connected graphs.
Random walk point of view: If we consider a random walk on the graph with probability to jump from one node to the other equal to $\frac{w_{ij}}{d_i}$ then NCut($A_1, A_2$) is interpreted as the probability to go from $C_1$ to $C_2$ or from $C_2$ to $C_1$.
Some properties of the Laplacian

Relations with the graph structure:

Random walk point of view: If we consider a random walk on the graph with probability to jump from one node to the other equal to $\frac{W_{ij}}{d_i}$, then the average time to go from one node to another (commute time) is given by $L^+$ \cite{Fouss et al., 2007}. 
Spectral clustering: relaxing the constrains

$K$ has to be given. Solving $\min_{C_1, C_2} \text{Tr}(U^T L U)$ for a $K \times n$ matrix $U$ st $U^T U = 1$:

1. Compute the first $K$ eigenvectors of $L$, $u^1, \ldots, u^K$ and write $U = (u^1, \ldots, u^K)$ (a $n \times K$ matrix).
Spectral clustering: relaxing the constrains

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1. Compute the first \( K \) eigenvectors of \( L \), \( u^1, \ldots, u^K \) and write \( U = (u^1, \ldots, u^K) \) (a \( n \times K \) matrix).

2. For \( i = 1, \ldots, n \), denote \( u_i \in \mathbb{R}^K \) the \( i \)-th row of \( U \). Cluster the points \( (u_i)_{i=1,\ldots,n} \) using a clustering algorithm (e.g., k-means).
Spectral clustering in practice

For NVV network, computation time is equal to 0.039 (between the greedy approaches for modularity optimization and simulated annealing for modularity optimization).
Modularity is smaller (as expected) and clusters tend to be more unbalanced. An empirical comparison between the performance of spectral clustering and modularity optimization is provided in [Bickel and Chen, 2009]. [Lei and Rinaldo, 2015] gives conditions for the consistency of spectral clustering in stochastic block models.
Outline

Modularity optimization

Spectral clustering

Model based clustering
A mixture model for networks

[Snijders and Nowicki, 1997]: The observed network $G$ is supposed to be the realization of some random graph model in which vertices are organized in groups.

**description of the model**

- vertices $x_i$ belong to an unknown class in $\{C_1, ..., C_K\}$ ($K$ is given) $\Rightarrow$ latent (unobserved) variables

$$Z_i \sim \mathcal{M}(1, \alpha = (\alpha_1, \ldots, \alpha_K))$$

in which $\alpha_k$ is the probability that $x_i$ belongs to $C_k$
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- given the class membership, the probabilities to have an edge between $x_i$ and $x_j$ are all independent and obtained by:

$$W_{ij} = 1|Z_{ik}Z_{jk'} = 1 \sim \mathcal{L}(., \pi_{kk'})$$

distributition $\mathcal{L}$

for a given distribution $\mathcal{L}$
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- given the class membership, the probabilities to have an edge between $x_i$ and $x_j$ are all independent and obtained by:

typically, the Bernoulli distribution with probability $\pi_{kk'}$ with

$$\pi_{kk'} = \begin{cases} 
  p_1 & \text{if } k = k' \\
  p_0 & \text{if } k \neq k'
\end{cases} \text{ for } p_1 > p_0.$$
Basic principle for using SBM

1. assignments of vertices to groups;
2. parameter estimation \((\alpha_k)_k\) and \((\pi_{kk'})_{k,k'}\);
3. estimation of the number of groups.
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1. assignments of vertices to groups;
2. parameter estimation \(((\alpha_k)_k \text{ and } (\pi_{k,k'})_{k,k'})\);
3. estimation of the number of groups.

Estimation is made by Bayesian or frequentist approaches and Variational EM (see e.g., [Daudin et al., 2008] for the more computationally efficient frequentist approach). Number of nodes can be chosen using ICL [Biernacki et al., 2000].
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All this is implemented in the package **blockmodels** [Léger, 2016].
SBM in practice

For NVV network, the computational time of SBM clustering is 2.104. The number of clusters found by the method is 6.
Accuracy of the clustering

SBM clustering – 0.4037 – 6

multilevel – 0.567 – 7

Modularity is smaller (as expected) but groups can be interpreted by being sets of vertices with similar connecting patterns.
Comparing clustering

Various metrics ((di)similarities) exist to compare clustering, among which:

- **Rand Index** [Rand, 1971]

  \[
  \text{number of agreements between the two clusterings} \quad \frac{n(n - 1)}{2}
  \]

- **Normalized Mutual Information** [Danon et al., 2005]

  \[
  \sum_{k=1}^{K_1} \sum_{k'=1}^{K_2} \frac{n_{k k'}}{n} \log \left( \frac{n_{k k'} n}{n_k^1 n_k^2} \right)
  \]

  in which \( K_j \) is the number of clusters in clustering \( j \), \( n_k^j \) is the number of vertices classified into cluster \( k \) for clustering \( j \) and \( n_{k k'} \) is the number of vertices classified into cluster \( k \) for clustering 1 and cluster \( k' \) for clustering 2. The similarity is normalized so that it is between 0 and 1 (1 is for a perfect match).
How do clusterings relate?

Method:

1. compute a dissimilarity based on Rand index or NMI (1 – value)

2. perform clustering (of the results of vertex clustering) using hierarchical clustering \texttt{hclust}
How do clusterings relate?

Rand index

NMI

sbm
spectral
annealing
hierarchical
multilevel

Height

sbm
spectral
annealing
hierarchical
multilevel

Rand index

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Height
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Assessing a mixture model for clustering with the integrated completed likelihood.

Fast unfolding of communities in large networks.

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Comparing community structure identification.

A mixture model for random graphs.

Resolution limit in community detection.
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Random-walk computation of similarities between nodes of a graph, with application to collaborative recommendation.

Blockmodels: a R-package for estimating in LBM and SBM, with many pdf, with or without covariates.

Consistency of spectral clustering in stochastic block models.

Fast algorithm for detecting community structure in networks.

Finding and evaluating community structure in networks.

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Objective criteria for the evaluation of clustering methods.

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A tutorial on spectral clustering.