### 1.022 - Introduction to Network Models

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Lecture 7

## Graph Laplacian

- Vertex degrees often stored in the diagonal matrix $\mathbf{D}$, where $D_{i i}=d_{i}$

$$
\mathbf{D}=\left(\begin{array}{llll}
2 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 3
\end{array}\right)
$$



- The $|V| \times|V|$ symmetric matrix $\mathbf{L}:=\mathbf{D} \quad \mathbf{A}$ is called graph Laplacian

$$
L_{i j}=\left\{\begin{array}{cc}
d_{i}, & \text { if } i=j \\
1, & \text { if }(i, j) \in E \\
0, & \text { otherwise }
\end{array}, \mathbf{L}=\left(\begin{array}{cccc}
2 & 1 & 0 & 1 \\
1 & 2 & 0 & 1 \\
0 & 0 & 1 & 1 \\
1 & 1 & 1 & 3
\end{array}\right)\right.
$$

## Courant Fischer Theorem

$$
\begin{aligned}
\lambda_{1} & =\min _{x \neq 0} \frac{x^{\top} L x}{x^{\top} x} & v_{1} & =\underset{\substack{x \neq 0 \\
x \neq 0}}{\operatorname{argmin}} \frac{x^{T} L x}{x^{\top} x} \\
\lambda_{2} & =\min _{\substack{x \neq 1}} \frac{x^{\top} L x}{x^{\top} x} & v_{2} & =\underset{\substack{x \neq 0 \\
x \perp v_{1}}}{\operatorname{argmin}} \frac{x^{T} L x}{x^{\top} x}
\end{aligned}
$$

Courant Fischer Theorem: $M$ an $n \times n$ symmetric matrix with eigenvalues $\lambda_{1} \leq \ldots \leq \lambda_{n}$ and eigenvectors $v_{1}, \ldots, v_{n}$.

- $S_{k}$ : the span of $v_{1}, \ldots, v_{k}, 1 \leq k \leq n\left(S_{0}=\{0\}\right)$.
- $S_{k}^{\perp}$ :orthogonal complement of $S_{k}$.

Then,

$$
\lambda_{k}=\min _{\substack{\|x\| \neq 0 \\ x \in S_{\bar{K}}}} \frac{x^{T} M x}{x^{T} x} \quad v_{k}=\underset{\substack{\|x\| \neq 0 \\ x \in S_{k}^{\perp}}}{\operatorname{argmin}} \frac{x^{T} M x}{x^{T} x}
$$

## Community detection and spectral clustering

- Nodes in many real-world networks organize into communities Ex: families, clubs, political organizations, urban areas, ...
- Supported by the strength of weak ties theory

- Community (a.k.a. group, cluster, module) members are:
$\Rightarrow$ Well connected among themselves
$\Rightarrow$ Relatively well separated from the rest


## Graph partitioning and minimum cuts

- Community members should be well-connected among themselves
$\Rightarrow$ Loosely connected with members of other communities

- A cut $C$ is the weight of edges between blocks $V_{1}$ and $V_{2}=V \backslash V_{1}$

$$
C=\operatorname{cut}\left(V_{1}, V_{2}\right)=\sum_{i \in V_{1}, j \in V_{2}} A_{i j}
$$

- Find cut that achieves the desired sizes in $V_{1}$ and $V_{2}$ while minimizing $C$


## Graph partitioning and the Laplacian matrix

- Assign to each node $i \in V$ an identifier $s_{i} \in\{1,1\}$
$\Rightarrow$ Form the vector $\mathbf{s}=\left[s_{1}, s_{2}, \ldots, s_{|V|}\right]$
- Notice that $C(\mathbf{s})=\sum_{i j} A_{i j}$ where $s_{i}=1$ and $s_{j}=+1$
- It can be shown that $C(\mathbf{s})=\frac{1}{4} \mathbf{s}^{\top} \mathbf{L s}$, where $\mathbf{L}$ is the Laplacian matrix
$\Rightarrow$ You will show this in your homework
- We have expressed the cut (relevant graph-related quantity)
$\Rightarrow$ In terms of vectors and matrices (amenable algebraic objects)
- Find vector $\mathbf{s} \in\{1,1\}^{|V|}$ such that:

$$
\begin{aligned}
& \Rightarrow \sum_{i} s_{i}=\left|V_{2}\right| \quad\left|V_{1}\right| \text { (desired group sizes), and } \\
& \Rightarrow \text { Minimizes } C(\mathbf{s})=\frac{1}{4} \mathbf{s}^{\top} \mathbf{L s}
\end{aligned}
$$

## Spectral graph partitioning

- Finding such optimal s is still challenging
$\Rightarrow$ Due to the integer restriction $\mathbf{s} \in\{1,1\}^{|V|}$
- Relax this requirement into $\sum_{i} s_{i}^{2}=|V|$
$\Rightarrow$ Note that $\mathbf{s} \in\{1,1\}^{|V|}$ implies $\sum_{i} s_{i}^{2}=|V|$ but not vice versa
- New relaxed problem: Find $\mathbf{s}$ that minimizes $C(\mathbf{s})=\frac{1}{4} \mathbf{s}^{\top} \mathbf{L s}$
$\Rightarrow$ Subject to $\sum_{i} s_{i}=\left|V_{2}\right| \quad\left|V_{1}\right|$ and $\sum_{i} s_{i}^{2}=|V|$
- The optimal $\mathbf{s}^{*}$ is given by

$$
\mathbf{s}^{*}=\mathbf{v}_{2}+\frac{\left|V_{2}\right| \quad\left|V_{1}\right|}{|V|} \mathbf{1}
$$

$\Rightarrow$ where $\mathbf{v}_{2}$ is the eigenvector of $\mathbf{L}$ with the second smallest eigenvalue

## Recovering the partitions

- How do we go back to two groups from the (non-integer) s*?
$\Rightarrow$ Find $\mathbf{s} \in\{1,+1\}^{|V|}$ that is most aligned with $\mathbf{s}^{*}$
- Algorithm: Spectral graph partitioning
$\Rightarrow 1)$ Compute Laplacian matrix $\mathbf{L}$ of graph of interest
$\Rightarrow 2$ ) Find $\mathbf{v}_{2}$, the eigenvector of $\mathbf{L}$ with the second smallest eigenvalue
$\Rightarrow 3$ ) Order the entries of $\mathbf{v}_{2}$ in decreasing order
$\Rightarrow 4)$ Assign $s_{i}=1$ to the $\left|V_{1}\right|$ top-sorted entries and rest $s_{i}=+1$
- Minor subtlety $\Rightarrow$ Both $\mathbf{v}_{2}$ and $\mathbf{v}_{2}$ are eigenvectors
$\Rightarrow$ Repeat the above procedure for $\mathbf{v}_{2}$
$\Rightarrow$ Choose partition (from those two) that minimizes the cut


## Community detection problem

- What if we do not know a priori the sizes of the sought communities?
$\Rightarrow$ We cannot implement the above procedure
$\Rightarrow$ More importantly, the cut might not be the right criterion

- Consider the ratio cut $R$ instead

$$
R\left(V_{1}, V_{2}\right)=\frac{C\left(V_{1}, V_{2}\right)}{\left|V_{1}\right|}+\frac{C\left(V_{1}, V_{2}\right)}{\left|V_{2}\right|}
$$

$\Rightarrow$ Small groups are penalized $\Rightarrow$ Balanced partition

## Spectral community detection

- The ratio cut criterion can be relaxed in a similar way
- Main difference $\Rightarrow$ Unknown group sizes
- Algorithm: Spectral community detection
$\Rightarrow 1)$ Compute Laplacian matrix $\mathbf{L}$ of graph of interest
$\Rightarrow 2)$ Find $\mathbf{v}_{2}$, the eigenvector of $\mathbf{L}$ with the second smallest eigenvalue
$\Rightarrow 3)$ Assign $s_{i}=1$ if $\left[\mathbf{v}_{2}\right]_{i}<0$ and $s_{i}=+1$ otherwise
- What if we want to detect more than two groups?
- Opt. 1: Apply the above process iteratively


## Clustering via other low-dimensional representations ||||l|

- Votes by $n=100$ senators in the 2004-2006 US Senate about $m=542$ bills

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- Republicans tend to vote similar to other republicans [El Ghaoui 17]
$\Rightarrow$ Same occurs with democrats
$\Rightarrow$ How can we capture this? $\Rightarrow$ Notion of covariance


## Principal Component Analysis (PCA)

- One can interpret the covariance matrix as a weighted graph
$\Rightarrow$ Large positive values indicate similar voting patterns between senators
- PCA projects senators onto the top eigenvectors of the covariance matrix
$\Rightarrow$ These are the direction of maximum variance

- The parties can be recovered almost perfectly from the 2D representation


## Example of more than two groups

- Genes mirror geography within Europe, Novembre et al., Nature (2008)
- Two-dimensional embedding of 'gene similarity' matrix
$\Rightarrow$ Consistent with origins of individuals in European map


Novembre, John, Toby Johnson, Katarzyna Bryc, et al. "Genes mirror geography within Europe." Nature 456 (2008): 98-101. © Springer Nature. All rights reserved. This content is excluded from our Creative Commons license. For more information, see

## Using centrality for community detection

- Communities as connected components when deleting bridges

- How can we automatically detect bridges?
- Can we use the notion of (betweenness) centrality but for edges?
$\Rightarrow$ For the interested, see Chapter 3.6 of our main text

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