Lecture 2: Visualization Problems and Spectral Analysis

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February 12, 2018

Graphs

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Main Problem

Given a graph find a low-dimensional representation of the graph.

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As we shall see there are a several results that ultimately reduce to a spectral analysis. Today we introduce the spectral based graph representation.

We assume we are given either an adjacency matrix A or a weight matrix W. Since W is a generalization of the binary adjacency matrix, we shall use the matrix W more often. If you are given an unweighted graph, use the adjacency matrix A instead of W.

Databases of Graphs

Public Datasets

Here are several public databases:

1. Duke: https://dnac.ssri.duke.edu/datasets.php
2. Stanford: https://snap.stanford.edu/data/
3. Uni. Koblenz: http://konect.uni-koblenz.de/
4. M. Newman (U. Michigan): http://www-personal.umich.edu/ mejn/netdata/
5. A.L. Barabasi (U. Notre Dame): http://www3.nd.edu/ networks/resources.htm
6. UCI: https://networkdata.ics.uci.edu/resources.php
7. Google/YouTube: https://research.google.com/youtube8m/
8. Chemical Compounds: http://quantum-machine.org/datasets/

Visualization Problem

Consider a graph $(\mathcal{V},\mathcal{E},W)$ with n vertices and $m=|\mathcal{E}|$ edges. We want a 2-dimensional (planar) visualization of this graph.
Idea (due to Hall '70): Let $\{x(1),x(2),\cdots,x(n)\}\subset\mathbb{R}^2$ denote a collection of n points in 2D-plane. Points are chosen so to minimize the weighted sum of edge lengths:

$$J=\sum_{(k,j)\in\mathcal{E}} W_{k,j}\|x(k)-x(j)\|^2$$

This is similar to Dirichlet energy except that each vertex has a 2D vector attached to it instead of a scalar value. J can be rewritten more compactly using the $2\times n$ matrix X whose columns are the vectors $\{x(1),\cdots,x(n)\}$:

$$X=\left[\begin{array}{cccc} x(1) & x(2) & \cdots & x(n) \end{array}\right]$$

The Objective Function J

Explicit expansion of criterion J:

$$J = \sum_{(k,j)\in\mathcal{E}} W_{k,j}\|x(k)-x(j)\|^2 = \frac{1}{2}\sum_{k,j=1}^{n} W_{k,j}\|x(k)-x(j)\|^2 =$$

$$= \sum_{k,j=1}^{n} W_{k,j}\|x(k)\|^2 - \sum_{k,j=1}^{n} W_{k,j}x(k)^T x(j) =$$

$$= \sum_{k=1}^{n} D_{k,k}\left(x(k)^T x(k)\right) - \sum_{k,j} W_{k,j}\left(x(j)^T x(k)\right)$$

Remark $x(k)^T x(k) = (X^T X)_{k,k}$ and $x(j)^T x(k) = (X^T X)_{j,k}$. Next we write the sums in a more compact form using trace and matrix multiplication notations.

Traces and Commutation Relation

For a square matrix $M \in \mathbb{R}^{r\times r}$, its *trace* is defined as

$$trace(M) = \sum_{k=1}^{r} M_{k,k}$$

that is the sum of its diagonal elements.
For two matrices $A \in \mathbb{R}^{p\times q}$, $B \in \mathbb{R}^{q\times p}$:

$$trace(AB) = \sum_{k=1}^{p} (AB)_{k,k} = \sum_{k=1}^{p}\sum_{j=1}^{q} A_{k,j}B_{j,k} =$$
$$= \sum_{j=1}^{q}\sum_{k=1}^{p} B_{j,k}A_{k,j} = \sum_{j=1}^{q} (BA)_{j,j} = trace(BA).$$

This identity, $trace(AB) = trace(BA)$, allows to introduce an inner product on spaces of matrices of same size similar to the dot product betwen vectors of same size: If $U, V \in \mathbb{R}^{p\times q}$ then

$$\langle U, V\rangle = trace(U^T V) = trace(V^T U).$$

The Objective Function J - cont.

Return to J:

$$J = \sum_{k=1}^{n} D_{k,k}\left(x(k)^T x(k)\right) - \sum_{k,j} W_{k,j}\left(x(j)^T x(k)\right) =$$

$$= \sum_{k=1}^{n} D_{k,k}(X^T X)_{k,k} - \sum_{k,j} W_{k,j}(X^T X)_{j,k} = trace(DX^T X) - trace(WX^T X) =$$

$$= trace((D-W)X^T X) = trace(X \cdot \Delta \cdot X^T)$$

where the graph Laplacian $\Delta = D - W$ is defined in terms of the diagonal matrix $D = diag(W \cdot 1)$ and the weight matrix W.

Constraints

The objective is to minimize $J = X \cdot \Delta \cdot X^T$ over the $2 \times n$ matrix X. The global minimum is reached for instance by $X = 0$. This says that all points scrum in one location (the origin). To avoid this phenomenon we introduce constraints. First, each row of X should have norm 1. However there is a non-informative solution given by the constant matrix $\frac{1}{\sqrt{n}} 1_{2\times n}$: $\Delta 1_{n\times 2} = 0$. To avoid this case we ask that each row of X to be orthogonal to the constant vector 1, i.e. $X \cdot 1 = 0$. Lastly, to make sure the first row of X does not repeat in the second row, we ask them to be linearly independent. Even stronger, we ask the rows of X to be orthogonal vectors in $\mathbb{R}^n$. A compact form of these three conditions (normalization and orthogonalities):

$$XX^T = I_2 \quad , \quad X \cdot 1 = 0$$

Optimization Problem

Putting everything together, we obtain the optimization problem

$$\min_{\substack{X \in \mathbb{R}^{2,n} \\ X1 = 0 \\ XX^T = I_2}} \quad trace(X\Delta X^T)$$

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Luckily there is an easy algorithm to solve this problem. It is based on computing eigenpairs of the graph Laplacian Δ.

Graph Visualization Spectral Algorithm

Algorithm (Graph Visualization Spectral Algorithm)

Input: An adjacency matrix A or a weight matrix W.

1. *Compute the graph Laplacian $\Delta = D - A$, or $\Delta = D - W$.*
2. *Compute the lowest three eigenpairs (e_1, λ_1), (e_2, λ_2), (e_3, λ_3), where $\Delta e_k = \lambda_k e_k$, $\|e_k\| = 1$, and $0 = \lambda_1 \leq \lambda_2 \leq \lambda_3$.*
3. *Construct the $2 \times n$ matrix X*

$$X = \begin{bmatrix} e_2^T \\ e_3^T \end{bmatrix}.$$

Output: Columns of matrix X are the n 2-dimensional vectors $\{x(1), \cdots, x(n)\}$.

Examples

See the Matlab simulations: circulant matrix case; perturbations.

Why the eigenpairs optimize the criterion?

The significant result: The Courant-Fisher criterion and Rayleight quotient.

Theorem

Assume T is a real symmetric $n \times n$ matrix. Then:

1. *All eigenvalues of T are real numbers.*
2. *There are n eigenvectors that can be normalized to form an orthonormal basis for $\mathbb{R}^n$.*
3. *The largest (principal) eigenpair (e_{max}, λ_{max}) and the smallest eigenpair (e_{min}, λ_{min}) satisfy*

$$(e_{max}), \lambda_{max}) = (arg) \max_{x \neq 0} \frac{\langle Tx, x \rangle}{\langle x, x \rangle} \quad , \quad (e_{min}, \lambda_{min}) = arg \min_{x \neq 0} \frac{\langle Tx, x \rangle}{\langle x, x \rangle}$$

Why the eigenpairs optimize the criterion? -cont

Theorem

Assume T is a real symmetric $n \times n$ matrix. Then:

4. *Assume $(e_1, ..., e_k)$ are the eigenvectors associated to the largest k eigenvalues. Then*

$$(e_{k+1}, \lambda_{k+1}) = arg \max_{x \neq 0, \langle x, e_1 \rangle = \cdots = \langle x, x_k \rangle = 0} \frac{\langle Tx, x \rangle}{\langle x, x \rangle}$$

5. *Assume $(e_{n-k+1}, ..., e_n)$ are the eigenvectors associated to the smallest k eigenvalues. Then*

$$(e_{n-k}, \lambda_{n-k}) = arg \min_{x \neq 0, \langle x, e_{n-k+1} \rangle = \cdots = \langle x, x_n \rangle = 0} \frac{\langle Tx, x \rangle}{\langle x, x \rangle}$$

Spectral Analysis
Basic Properties

Last time we learned how to construct: the Adjacency matrix A, the Degree matrix D, the (unnormalized symmetric) graph Laplacian matrix $\Delta = D - A$, the normalized Laplacian matrix $\tilde{\Delta} = D^{\dagger/2}\Delta D^{\dagger/2}$, and the normalized asymmetric Laplacian matrix $L = D^{\dagger}\Delta$.

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We denote: n the number of vertices (also known as the *size* of the graph), m the number of edges, $d(v)$ the degree of vertex v, $d(i,j)$ the distance between vertex i and vertex j (length of the shortest path connecting i to j), and by *Diam* the diameter of the graph (the largest distance between two vertices = "longest shortest path").

Spectral Analysis
Basic Properties

In this section we summarize spectral properties of the Laplacian matrices.

Theorem

1. $\Delta = \Delta^T \geq 0$, $\tilde{\Delta} = \tilde{\Delta}^T \geq 0$ *are positive semidefinite matrices.*
2. $eigs(\tilde{\Delta}) = eigs(L) \subset [0, 2]$.
3. 0 *is always an eigenvalue of* Δ, $\tilde{\Delta}$, L *with same multiplicity. Its multiplicity is equal to the number of connected components of the graph.*
4. $\lambda_{max}(\Delta) \leq 2\max_v d(v)$, *i.e. the lagest eigenvalue of* Δ *is bounded by twice the largest degree of the graph.*

Spectral Analysis
Basic Properties

Theorem

Let $0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 2$ *be the eigenvalues of* $\tilde{\Delta}$ *(or* L*), that is* $eigs(\tilde{\Delta}) = \{\lambda_0, \lambda_1, \cdots, \lambda_{n-1}\} = eigs(L)$*. Then:*

1. $\sum_{i=0}^{n-1} \lambda_i \leq n$.
2. $\sum_{i=0}^{n-1} \lambda_i = n - \#\text{isolated vertices}$.
3. $\lambda_1 \leq \frac{n}{n-1}$.
4. $\lambda_1 = \frac{n}{n-1}$ *if and only if the graph is complete (i.e. any two vertices are connected by an edge).*
5. *If the graph is not complete then* $\lambda_1 \leq 1$.
6. *If the graph is connected then* $\lambda_1 > 0$*. If* $\lambda_i = 0$ *and* $\lambda_{i+1} \neq 0$ *then the graph has exactly* $i+1$ *connected components.*
7. *If the graph is connected (no isolated vertices) then* $\lambda_{n-1} \geq \frac{n}{n-1}$.

Spectral Analysis

Smallest nonnegative eigenvalue

Theorem

Assume the graph is connected. Thus $\lambda_1 > 0$. *Denote by D its diameter and by* $d_{max}, \bar{d}, d_H$ *the maximum, average, and harmonic avergae of the degrees* $(d_1, \cdots, d_n)$*:*

$$d_{max} = \max_j d_j \quad , \quad \bar{d} = \frac{1}{n}\sum_{j=1}^{n} d_j \quad , \quad \frac{1}{d_H} = \frac{1}{n}\sum_{j=1}^{n}\frac{1}{d_j}.$$

Then

1. $\lambda_1 \geq \frac{1}{nD}$.
2. *Let* $\mu = \max_{1 \leq j \leq n-1} |1 - \lambda_j|$. *Then*

$$1 + (n-1)\mu^2 \geq \frac{n}{d_H}(1 - (1+\mu)(\frac{\bar{d}}{d_H} - 1)).$$

Spectral Analysis
Smallest nonnegative eigenvalue

Theorem

[continued]

3. *Assume $D \geq 4$. Then*

$$\lambda_1 \leq 1 - 2\frac{\sqrt{d_{max} - 1}}{d_{max}}(1 - \frac{2}{D}) + \frac{2}{D}.$$

Spectral Analysis

Comments on the proof

"Ingredients" and key relations:

1. Let $f = (f_1, f_2, \cdots, f_n) \in \mathbb{R}^n$ be a n-vector. Then:

$$\langle \Delta f, f \rangle = \sum_{x \sim y} (f_x - f_y)^2$$

where $x \sim y$ if there is an edge between vertex x and vertex y (i.e. $A_{x,y} = 1$).
This proves positivity of all operators.

2. Last time we showed $eigs(\tilde{\Delta}) = eigs(L)$ because $\tilde{\Delta}$ and L are similar matrices.

3. 0 is an eigenvalue for Δ with eigenvector $1 = (1, 1, \cdots, 1)$. If multiple connected components, define such a 1 vector for each component (and 0 on rest).

4. $\lambda_{max}(\tilde{\Delta}) = 1 - \lambda_{min}(D^{-1/2}AD^{-1/2}) \leq 1 + |\lambda_{min}(D^{-1/2}AD^{-1/2})|$.

Spectral Analysis
Comments on the proof - 2

$$\lambda_{max}(D^{-1/2}AD^{-1/2}) = \max_{\|f\|=1} \langle D^{-1/2}AD^{-1/2}f, f\rangle = \max_{\|f\|=1} \sum_{i,j} A_{i,j}\frac{f_i}{\sqrt{d_i}}\frac{f_j}{\sqrt{d_j}}$$

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$$|\lambda_{min,max}(D^{-1/2}AD^{-1/2})| \leq \max_{\|f\|=1} \left|\langle D^{-1/2}AD^{-1/2}f, f\rangle\right| = \max_{\|f\|=1} \left|\sum_{i,j} A_{i,j}\frac{f_i}{\sqrt{d_i}}\frac{f_j}{\sqrt{d_j}}\right|$$

Next use Cauchy-Schwartz to get

$$\left|\sum_{i,j} A_{i,j}\frac{f_i}{\sqrt{d_i}}\frac{f_j}{\sqrt{d_j}}\right| \leq \sum_i \frac{f_i^2}{d_i}\sum_j A_{i,j} = \sum_i f_i^2 = \|f\|^2 = 1.$$

Thus $\lambda_{max}(\tilde{\Delta}) \leq 2$. Similarly $\lambda_{max}(\Delta) \leq 2(\max_i d_i)$.

Spectral Analysis
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Spectral Analysis
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Spectral Analysis
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Spectral Analysis

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Consequence: The normalized Laplacian has the following eigenvalues:

1. For cycle graph on n vertices: $\lambda_k = 1 - cos\frac{2\pi k}{n}$, $0 \leq k \leq n-1$.
2. For the complete graph on n vertices:

$$\lambda_0 = 0\ ,\ \ \lambda_1 = \cdots = \lambda_{n-1} = \frac{n}{n-1}.$$

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