Spectral Methods (aka Algebraic Graph Theory, see Chapter 14 in [BE] "Network analysis")

Three main objects of interest:

- adjacency matrix,
- Laplacian, and
- normalized Laplacian

What their spectrums (all eigenvalues, including algebraic multiplicity) can tell about network statistics, existence of subgraphs, classification, etc.?

Let $M \in \mathbb{C}^{n \times n}$. A non-zero vector $x \in \mathbb{C}^n$ is an eigenvector of M with corresponding eigenvalue $\lambda \in \mathbb{C}$ if

$$Mx = \lambda x$$

The solution exists iff $\operatorname{rank}(M\lambda I) < n$ iff $\det(M\lambda I) = 0$, i.e., the eigenvalues are roots of $\det(M\lambda I) = 0$.

Spectral Methods

- If Q is non-singular then M and $Q^{-1}MQ$ have the same eigenvalues.
- If $M \in \mathbb{R}^{n \times n}$ and $M = M^T$ then \exists non-singular Q s.t. $Q^{-1} = Q^T$ and $M' = Q^{-1}MQ$ is diagonal. Eigenvectors of M' are e_i and

$$\det(M\lambda I) = \det(M'\lambda I) = \prod_i (\lambda_i - \lambda)$$
 diagonal entry of *M*'

• One can infer $tr(M) = \sum_{i=1}^{n} \lambda_i$ (check at home).

• If
$$v_i = Qe_i$$
 then $Mv_i = \lambda_i v_i$ and $v_i^T v_j = e_i^T e_j$.

orthonormal eigenvectors of M

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Theorem 1. Let $M \in \mathbb{R}^{n \times n}$ and $M = M^T$, then

eigen-M h. Ar indsriear eigenvalues $\lambda_1 \leq \dots \leq \lambda_n$ and he or monorhrinar evectors

 λ_i as a root 2. multiplicity of λ_i as an eigenvalue = multiplicity of λ_i nality of a of the characteristic polynomial det $(M\lambda I)$ = cardi tors correspond- maximum linearly independent set of eigenvec ing to λ_j .

diag
$$(\lambda_1, ..., \lambda_n)$$
 3. $\exists Q \text{ with } Q^T = Q^1 \text{ such that } QMQ^{-1} =$
4. $\det(M) = \prod_i \lambda_i \text{ and } tr(M) = \sum_i \lambda_i$

Theorem 2. Let G be a graph, and A its adj matrix with ordered eigenvalues λ_i , and Δ is a max degree of G then

1.
$$\lambda_n \leq \Delta$$

2. $G = G_1 \cup G_2 \Longrightarrow spec(G) = spec(G_1) \cup spec(G_2)$
3. G is bipartite \Longrightarrow (if $\lambda \in spec(G)$ then $-\lambda \in spec(G)$)
4. G is simple cycle \Longrightarrow $spec(G) = \{2\cos(\frac{2\pi k}{n}) | k \in \{1, ..., n\}\}$
5. $G = K_{n_1, n_2} \implies \lambda_1 = \sqrt{n_1 n_2}, \lambda_2 = ... = \lambda_{n_1} = 0$, and $\lambda_n = \sqrt{n_1 n_2}$

6.
$$G = K_{n_1} \implies \lambda_1 = \ldots = \lambda_{n_1}, \lambda_n = n - 1$$

Theorem 3.

- 1. $\sum_{i=1}^{n} \lambda_i$ = number of loops in G
- 2. $\sum_{i=1}^{n} \lambda_i^2 = 2 \times$ number of edges in G
- 3. $\sum_{i=1}^{n} \lambda_i^3 = 6 \times$ number of triangles in G

Homework "Spectral Methods": Prove any 2 out of 3 in Theorem 3 (submit by 9/29/2016)

Laplacian matrix L = D - AIncidence matrix $B = (b_{i,e}) = \begin{cases} 1 & i \text{ is the head of } e \\ -1 & i \text{ is the tail of } e \\ 0 & \text{otherwise} \end{cases}$ For any $x \in \mathbb{C}^n \ x^T L x = x^T B B^T x = \sum_{ij \in E} (x_i - x_j)^2$ A graph G consists of k connected components if and only if $\lambda_1(L) = \dots = \lambda_k(L) = 0$ and $\lambda_{k+1}(L) > 0$.

Trees and Laplacian: for every $i \in \{1, ..., n\}$ the number of spanning trees in G is equal to $|\det(L_i)|$, where L_i is obtained from the Laplacian L by deleting row i and column i. Moreover, the number of spanning trees is equal to $\frac{1}{n} \prod_{i>2} \lambda_i(L)$.

Normalized Laplacian
$$\mathcal{L} = D^{-1/2}LD^{-1/2}$$
, i.e.,
 $(\mathcal{L}_{ij}) = \begin{cases} 1 & i = j \text{ and } d(i) > 0 \\ -1/\sqrt{d(i)d(j)} & ij \in E \\ 0 & \text{otherwise} \end{cases}$ There exists some nonzero function
 $w \text{ on nodes} \end{cases}$
 $\lambda \text{ is an eigenvalue of } \mathcal{L}, \text{ i.e., } \lambda w(i) = \frac{1}{\sqrt{d(i)}} \sum_{j \in N(i)} \left(\frac{w(i)}{\sqrt{d(i)}} - \frac{w(j)}{\sqrt{d(j)}} \right)$

•
$$\lambda_1(\mathcal{L}) = 0$$
 and $\lambda_n(\mathcal{L}) \le 2$

- G is bipartite iff for every $\lambda(\mathcal{L})$ its "complement" $2 \lambda(\mathcal{L}) \in spectra(\mathcal{L})$
- $\lambda_i(\mathcal{L}) = 0, \ i \in [1..k] \implies G$ has k connected components

For d-regular graphs, the three spectra are equivalent

• $spectra(A) = \{\lambda_1, ..., \lambda_n\}$

•
$$spectra(L) = \{d - \lambda_n, ..., d - \lambda_1\}$$

•
$$spectra(\mathcal{L}) = \{1 - \lambda_n/d, ..., 1 - \lambda_1/d\}$$

Theorem: $\forall k \ \lambda_k(A) \ k$ th smallest eigenvalue of A and $\lambda_{n-k+1}(L) \ k$ th largest eigenvalue of L

$$\delta-\lambda_k(A)\leq \lambda_{n+1-k}(L)\leq \Delta-\lambda_k(A)$$
 min degree max degree

For a nonzero $x \in \mathbb{R}^n$ and $M \in \mathbb{R}^{n \times n}$ the Raleigh quotient is defined

$$R(x) = \frac{x^T M x}{x^T x}$$

Courant-Fischer Theorem. Let $M \in \mathbb{R}^{n \times n}$ be symmetric with eigenvalues $\lambda_0 \leq \ldots \leq \lambda_{n-1}$. Let X^k be a k-dim subspace of \mathbb{R}^n and $x \perp X^k$. Then

$$\lambda_{i} = \min_{X^{n-i-1}} (\max_{x \perp X^{n-i-1}, x \neq 0} R(x)) = \max_{X^{i}} (\min_{x \perp X^{i}, x \neq 0} R(x))$$

Fiedler Theorem.

$$\lambda_2(L) = n \min_{x \in \mathbb{R}^n} \left(\frac{\sum_{ij \in E} (x_i - x_j)^2}{\sum_{ij \in \binom{V}{2}} (x_i - x_j)^2} \right) \text{ same for } \lambda_n \text{ and } \max$$

A symmetric minor of A is a submatrix B obtained by deleting some rows and the corresponding columns.

Theorem (Interlacing eigenvalues). Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix with eigenvalues $\lambda_1 \leq ... \leq \lambda_n$. Let $B \in \mathbb{R}^{(n-k) \times (n-k)}$ be a symmetric minor of A with eigenvalues $\mu_1 \leq ... \leq \mu_{n-k}$. Then

$$\lambda_i \le \mu_i \le \lambda_{i+k}.$$

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Corollary. Let G and H be two graphs with eigenvalues $\lambda_1 \leq ... \leq \lambda_n$ and $\mu_1 \leq ... \leq \mu_m$ respectively. If $\mu_1 < \lambda_1$ or $\lambda_n < \mu_n$, then H does not occur as an induced subgraph of G.

graph class	$\operatorname{spectrum}(A)$	$\operatorname{spectrum}(L)$	$\operatorname{spectrum}(\mathcal{L})$
simple path $G = P_n$	$2\cos\left(\frac{\pi k}{n+1}\right),\ k \in \{1,\ldots,n\}$	$2 - 2\cos\left(\frac{\pi(k-1)}{n}\right),\$ $k \in \{1, \dots, n\}$	$1 - \cos\left(\frac{\pi(k-1)}{n-1}\right),$ $k \in \{1, \dots, n\}$
simple cycle $G = C_n$	$2\cos\left(\frac{2\pi k}{n}\right),\ k \in \{1,\ldots,n\}$	$2 - 2\cos\left(\frac{2\pi k}{n}\right),\ k \in \{1, \dots, n\}$	$ \begin{array}{l} 1 - \cos\left(\frac{2\pi k}{n}\right), \\ k \in \{1, \dots, n\} \end{array} $
$\overset{\text{star}}{G = K_{1,n}}$	$ \begin{array}{c} -\sqrt{n}, \sqrt{n}, \\ 0 \ (n-2 \text{ times}) \end{array} $	$\begin{array}{c} 0, n, \\ 1 \ (n-2 \text{ times}) \end{array}$	0, 2, 1 (n-2 times)
$G = K_{n_1, n_2}$	$\begin{array}{c} -\sqrt{n_1 n_2}, \sqrt{n_1 n_2}, \\ 0(n-2 \text{ times}) \end{array}$	$0, n_1 \ (n_2 - 1 \text{ times}) \\ n_2 \ (n_1 - 1 \text{ times}), n$	0, 2 1 (<i>n</i> - 2 times)
$G = K_n$	$1, -1 \ (n-1 \text{ times})$	0, n (n-1 times)	$0, \frac{n}{n-1} \ (n-1 \text{ times})$

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Computing Part of the Spectrum, Lanczos Algorithm

1. Initialization: Choose the number of steps k, the desired number of eigenvalues r and an initial vector x_1 ; let $\beta_0 := x_1^{\top} x_1$, $x_1 := x_1/\beta_0$

2. Lanczos steps: for i = 1 to k do $\begin{vmatrix}
(i) \ y := M x_i \\
(ii) \ \alpha_i := x_i^\top y \\
(iii) \ x_{i+1} := y - \alpha_i x_i - \beta_{i-1} x_{i-1} \\
(iv) \ \beta_i := x_{i+1}^\top x_{i+1} \\
(v) \ x_{i+1} := x_{i+1} / \beta_i;
\end{cases}$ Set $X_i := \operatorname{Mat}(x_1, \dots, x_i)$

3. Eigenvalue computation: Compute the eigenvalues of $T := X_i^\top M X_i$.

4. Convergence test and restart: If the first r columns of T satisfy the convergence criteria then accept the corresponding eigenvalues and stop. Otherwise restart with a suitable new x_1 .

Grafting

Q: How to modify G by adding to it eigenvalues of H? What if we want to add λ to G?



Eigenvalues and Global Properties

•
$$\frac{1}{n} \sum_{i \in V} d(i) \le \lambda_n(A)$$

•
$$\left\lceil \frac{4}{n\lambda_2(L)} \right\rceil \le \operatorname{diam}(G) \le 2 \left\lfloor \frac{\cosh^{-1}(n-1)}{\cosh^{-1}\left(\frac{\lambda_n(L)+\lambda_2(L)}{\lambda_n(L)-\lambda_2(L)}\right)} \right\rfloor + 1$$

•
$$\frac{1}{n-1} \left(\frac{2}{\lambda_2(L)} + \frac{n-2}{2} \right) \le \bar{\rho}(G) \le \frac{n}{n-1} \left\lceil \frac{\Delta + \lambda_2(L)}{4\lambda_2(L)} \ln(n-1) \right\rceil$$

mean distance in *G*

• Isopermetric number $i(G) = \min\{\frac{|cut(X,Y)|}{\min\{|X|,|Y|\}}; X \subset V, X \neq \emptyset, Y = V \setminus X\}$

$$i(G) \ge \min\left\{1, \frac{\lambda_2(L)\lambda_n(L)}{2(\lambda_n(L) + \lambda_2(L) - 2)}\right\} \qquad i(G) \le \sqrt{\lambda_2(L)(2\Delta - \lambda_2(L))}$$

• Expansion $c_V := \min\left\{\frac{|N(S) \setminus S|}{|S|}; S \subseteq V, |S| \le \frac{n}{2}\right\} \qquad \frac{\lambda_2(L)}{\frac{\Delta}{2} + \lambda_2(L)} \le c_V = \mathcal{O}(\sqrt{\lambda_2(L)})$

... chromatic number, minimum independent set, ...

Bisection



Algorithm for finding sparse cuts: compute Fiedler vector, sort the vertices according to its values , and find the best cut .

Partitioning problem, Walshaw's partitioning archive, DIMACS competition [BMSSS] "Recent advances in graph partitioning", 2013

p-discrepancy

We define $p - discrepancy \sigma_p(G, \psi)$ of labeling ψ as

$$\sigma_p(G,\psi) = \left(\sum_{ij\in E} w_{ij}|\psi(i) - \psi(j)|^p\right)^{1/p} \text{ and } \sigma_\infty(G,\psi) = \max_{ij\in E} w_{ij}|\psi(i) - \psi(j)|$$

Finding minimum p - discrepancy (such as minimum linear arrangement, 2sum, bandwidth) is NP-hard. Basic facts:

$$\lambda_2 \frac{n(n^2 - 1)}{12} \le \sigma_2(G, \psi)^2 \le \lambda_n \frac{n(n^2 - 1)}{12}$$
$$\lambda_2 \frac{(n^2 - 1)}{6} \le \sigma_1(G, \psi) \le \lambda_n \frac{(n^2 - 1)}{6}$$

Homework: Juvan, Mohar "Optimal linear labelings and eigenvalues of graphs" (submit by 9/24)



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Random Walks

Let $p_i(t)$ be the probability that the walk is at *i* at time *t*

$$p_i(t) = \sum_j \frac{A_{ij}}{d(j)} p_j(t-1) \text{ or } p(t) = AD^{-1}p(t-1)$$

Another useful form of this relation is

$$D^{-1/2}p(t) = \left(D^{-1/2}AD^{-1/2}\right)\left(D^{-1/2}p(t-1)\right)$$

As $t \to \infty$ the probability distribution is represented by $p = AD^{-1}p$ or

$$(I - AD^{-1})p = (D - A)D^{-1}p = LD^{-1}p = 0,$$

i.e., $D^{-1}p$ is an eigenvector of L with eval 0. **Example**: G is connected \Rightarrow there is only one eval $0 \Rightarrow D^{-1}p = \alpha 1$, i.e.,

$$p_i = d(i) / \sum_j d(j) = \frac{d(i)}{2m}$$

Intuition: high degree nodes are more likely to be visited.

First Passage Time

Q: what is the mean first passage time the random walk started at *i* reaches *j*? **Absorbing random walk** = random walk with one or more nodes we can move to but not leave We consider an absorbing random walk with **single absorbing vertex** *v*. Probability that rw has fpt exactly *t* is $p_v(t) - p_v(t-1)$, i.e., the mean is

$$\tau = \sum_{t=0}^{\infty} t(p_v(t) - p_v(t-1)).$$

For any
$$i \neq v \ p_i(t) = \sum_j \frac{A_{ij}}{d(j)} p_j(t-1) = \sum_{j \neq v} \frac{A_{ij}}{d(j)} p_j(t-1)$$
, i.e.,

 $p'(t) = A'D'^{-1}p'(t-1) = (A'D'^{-1})^t p'(0) \quad (' \text{ means } v \text{ is removed})$ Since $\sum_i p_i(t) = 1$ at all times

$$p_v(t) = 1 - \sum_{i \neq v} p_i(t) = 1 - 1^T p'(t)$$
 and

 $\tau = \sum_{t=0}^{\infty} t \mathbf{1}^T (p'_v(t-1) - p'_v(t-1)) = \mathbf{1}^T \left(I - A'D'^{-1} \right)^{-1} p'(0) = \dots = \mathbf{1}^T D'L'^{-1} p'(0)$