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 spectrum (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 $\mathrm{rank}(M-\lambda I) < n$ iff $\det(M-\lambda I) = 0$, i.e., the eigenvalues are roots of $\det(M-\lambda I) = 0$.

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 $M' = Q^{-1}MQ$ has diagonal form. Eigenvectors of M' are e_i and

diagonal entry of *M'*

$$\det(M-\lambda I) = \det(M'-\lambda I) = \prod_i (\lambda_i - \lambda)$$

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*

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

1. M has real eigenvalues $\lambda_1 \leq ... \leq \lambda_n$ and n orthonormal eigenvectors
2. multiplicity of λ_i as an eigenvalue = multiplicity of λ_i as a root of the characteristic polynomial $\det(M - \lambda I)$ = cardinality of a maximum linearly independent set of eigenvectors corresponding to λ_i
3. $\exists\, Q$ with $Q^T = Q^{-1}$ such that $QMQ^{-1} = \mathrm{diag}(\lambda_1, ..., \lambda_n)$
4. $\det(M) = \prod_i \lambda_i$ 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. $G = G_1 \cup G_2 \implies spec(G) = spec(G_1) \cup spec(G_2)$
3. G is bipartite $\implies$ (if $\lambda \in spec(G)$ then $-\lambda \in spec(G)$)
4. G is simple cycle $\implies\ spec(G) = \{2\cos(\frac{2\pi k}{n}) | k \in \{1, ..., n\}\}$
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. $G = K_{n_1} \implies \lambda_1 = ... = \lambda_{n-1}, \lambda_n = n - 1$

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: Prove any 2 out of 3 in Theorem 3 (submit by 3/6/2014)

Laplacian matrix $L = D - A$

Incidence 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 $\lambda_1(L) = \ldots = \lambda_k(L) = 0$ and $\lambda_{k+1}(L) > 0$.

Trees and Laplacian: for every $i \in \{1, \ldots, n\}$ 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 $\frac{1}{n} \prod_{i \geq 2} \lambda_i(L)$.

Normalized Laplacian $\mathcal{L} = D^{-1/2} L D^{-1/2}$, 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* on nodes

λ is an eigenvalue of $\mathcal{L}$, 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 $\lambda_n(\mathcal{L}) \leq 2$
- 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: $\forall k$ $\lambda_k(A)$ kth smallest eigenvalue of A and $\lambda_{n-k+1}(L)$ kth 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 $\lambda_0 \leq ... \leq \lambda_{n-1}$. Let X^k be a k-dim subspace of $\mathbb{R}^n$ and $x \perp X^k$. Then

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

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

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

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	spectrum(A)	spectrum(L)	spectrum($\mathcal{L}$)
simple path $G = P_n$	$2\cos\left(\frac{\pi k}{n+1}\right)$, $k \in \{1, \ldots, n\}$	$2 - 2\cos\left(\frac{\pi(k-1)}{n}\right)$, $k \in \{1, \ldots, n\}$	$1 - \cos\left(\frac{\pi(k-1)}{n-1}\right)$, $k \in \{1, \ldots, n\}$
simple cycle $G = C_n$	$2\cos\left(\frac{2\pi k}{n}\right)$, $k \in \{1, \ldots, n\}$	$2 - 2\cos\left(\frac{2\pi k}{n}\right)$, $k \in \{1, \ldots, n\}$	$1 - \cos\left(\frac{2\pi k}{n}\right)$, $k \in \{1, \ldots, n\}$
star $G = K_{1,n}$	$-\sqrt{n}, \sqrt{n}$, 0 ($n-2$ times)	$0, n$, 1 ($n-2$ times)	$0, 2$, 1 ($n-2$ times)
$G = K_{n_1,n_2}$	$-\sqrt{n_1 n_2}, \sqrt{n_1 n_2}$, 0($n-2$ times)	$0, n_1$ ($n_2 - 1$ times) n_2 ($n_1 - 1$ times), n	$0, 2$ 1 ($n-2$ times)
$G = K_n$	$1, -1$ ($n-1$ times)	$0, n$ ($n-1$ times)	$0, \frac{n}{n-1}$ ($n-1$ times)

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**

- *(i)* $y := Mx_i$
- *(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)* $x_{i+1} := x_{i+1}/\beta_i$;

Set $X_i :=\mathrm{Mat}(x_1, \ldots, x_i)$

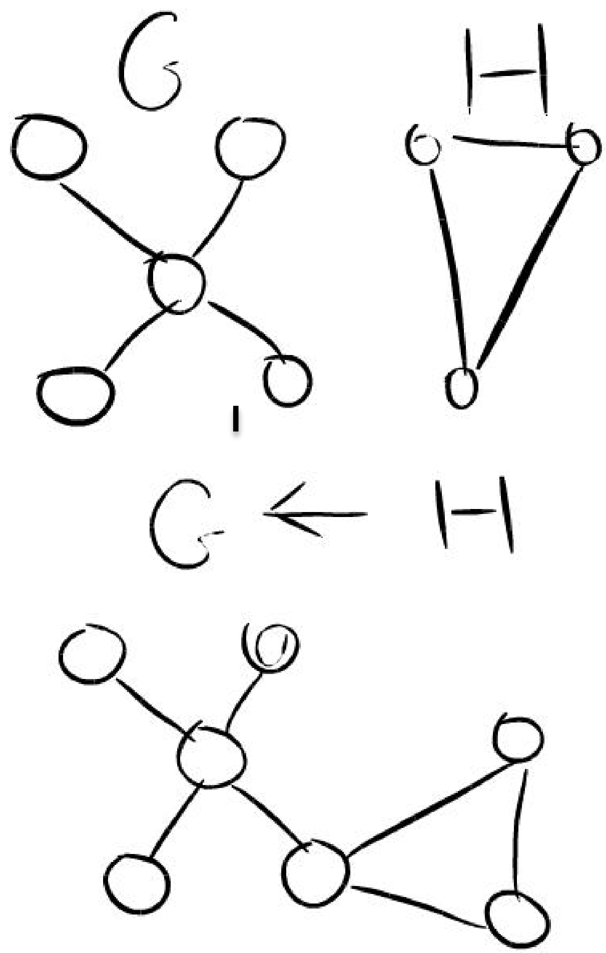
3. Eigenvalue computation: Compute the eigenvalues of $T := X_i^\top M X_i$.

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

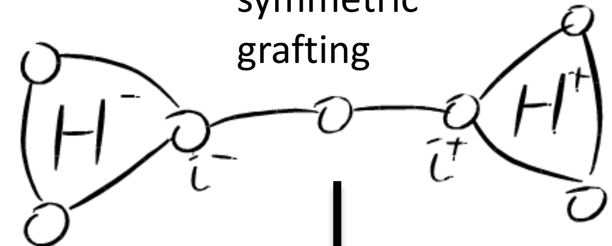
Q: How to modify G by adding to it eigenvalues of H? What if we want to add λ to G?

(λ, x) is eigenpair of H, $\exists\, i \in V_H\ x_i = 0$

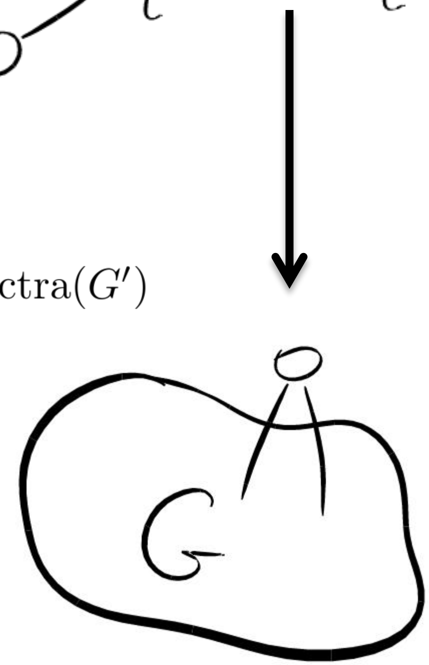


(λ, x) is eigenpair of H

new node for
symmetric
grafting



$\lambda \in \mathrm{spectra}(G')$



Eigenvalues and Global Properties

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

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

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

mean distance in *G*

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

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

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

… chromatic number, minimum independent set, …