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 $\text{rank}(M - \lambda I) < n$ 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

$$\det(M - \lambda I) = \det(M' - \lambda I) = \prod_{i} (\lambda_i - \lambda)$$

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 $v_i^T v_j = e_i^T e_j$.

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

1. $M$ has real eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ and $n$ orthonormal eigenvectors

2. multiplicity of $\lambda_i$ as an eigenvalue = multiplicity of $\lambda_i$ as a root of the characteristic polynomial $\det(M - \lambda I) = \text{cardinality of a maximum linearly independent set of eigenvectors corresponding to } \lambda_i$

3. $\exists Q$ with $Q^T = Q^{-1}$ such that $QMQ^{-1} = \text{diag}(\lambda_1, \ldots, \lambda_n)$

4. $\det(M) = \prod_i \lambda_i$ and $\text{tr}(M) = \sum_i \lambda_i$

**Theorem 2.** Let $G$ be a graph, and $A$ its adj matrix with ordered eigenvalues $\lambda_i$, and $\Delta$ is a max degree of $G$ then

1. $\lambda_n \leq \Delta$

2. $G = G_1 \cup G_2 \implies \text{spec}(G_1) \cup \text{spec}(G_2)$

3. $G$ is bipartite $\implies$ (if $\lambda \in \text{spec}(G)$ then $-\lambda \in \text{spec}(G')$)

4. $G$ is simple cycle $\implies \text{spec}(G) = \{2 \cos \left( \frac{2\pi k}{n} \right) | k \in \{1, \ldots, n\} \}$

5. $G = K_{n_1, n_2} \implies \lambda_1 = -\sqrt{n_1 n_2}, \lambda_2 = \ldots = \lambda_{n-1} = 0,$ 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. $\sum_{i=1}^{n} \lambda_i = \text{number of loops in } G$

2. $\sum_{i=1}^{n} \lambda_i^2 = 2 \times \text{number of edges in } G$

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

Homework: Prove (any 3 out of 6 in Theorem 2) OR (any 2 out of 3 in Theorem 3)

Laplacian matrix $L = D - A$

Incidence matrix $B = (b_{i,e}) = \begin{cases} 1 & \text{i is the head of } e \\ -1 & \text{i is the tail of } e \\ 0 & \text{otherwise} \end{cases}$

For any $x \in \mathbb{C}^n$ $x^T L x = x^T B B^T x = \sum_{i,j \in E} (x_i - x_j)^2$

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 $\mathcal{L} = D^{-1/2}LD^{-1/2}$, i.e.,

$$(\mathcal{L}_{ij}) = \begin{cases} 
1 & i = j \text{ and } d(i) > 0 \\
-1/\sqrt{d(i)d(j)} & ij \in E \\
0 & \text{otherwise}
\end{cases}$$

$\lambda$ 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” $2 - \lambda(\mathcal{L}) \in \text{spectra}(\mathcal{L})$
- $\lambda_i(\mathcal{L}) = 0$, $i \in [1..k] \implies G$ has $k$ connected components

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

$$\delta - \lambda_k(A) \leq \lambda_{n+1-k}(L) \leq \Delta - \lambda_k(A)$$
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
\[
\lambda_i = \min_{X^{n-i-1}} \left( \max_{x \perp X^{n-i-1}, x \neq 0} R(x) \right) = \max_{X^i} \left( \min_{x \perp X^i, x \neq 0} R(x) \right)
\]

**Fiedler Theorem.**
\[
\lambda_2(L) = n \min_{x \in \mathbb{R}^n} \left( \frac{\sum_{ij \in E}(x_i - x_j)^2}{\sum_{ij \in \binom{V}{2}}(x_i - x_j)^2} \right)
\] same for $\lambda_n$ 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 $\lambda_1 \leq \ldots \leq \lambda_n$. Let $B \in \mathbb{R}^{(n-k) \times (n-k)}$ be a symmetric minor of $A$ with eigenvalues $\mu_1 \leq \ldots \leq \mu_{n-k}$. Then
\[
\lambda_i \leq \mu_k \leq \lambda_{i+k}.
\]
**Corollary.** Let $G$ and $H$ be two graphs with eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ and $\mu_1 \leq \ldots \leq \mu_m$ respectively. If $\mu_1 < \lambda_1$ or $\lambda_n < \mu_n$, then $H$ does not occur as an induced subgraph of $G$.

<table>
<thead>
<tr>
<th>graph class</th>
<th>spectrum($A$)</th>
<th>spectrum($L$)</th>
<th>spectrum($\mathcal{L}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>simple path $G = P_n$</td>
<td>$2 \cos \left( \frac{\pi k}{n+1} \right)$, $k \in {1, \ldots, n}$</td>
<td>$2 - 2 \cos \left( \frac{\pi (k-1)}{n} \right)$, $k \in {1, \ldots, n}$</td>
<td>$1 - \cos \left( \frac{\pi (k-1)}{n-1} \right)$, $k \in {1, \ldots, n}$</td>
</tr>
<tr>
<td>simple cycle $G = C_n$</td>
<td>$2 \cos \left( \frac{2\pi k}{n} \right)$, $k \in {1, \ldots, n}$</td>
<td>$2 - 2 \cos \left( \frac{2\pi k}{n} \right)$, $k \in {1, \ldots, n}$</td>
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</tr>
<tr>
<td>star $G = K_{1,n}$</td>
<td>$-\sqrt{n}$, $\sqrt{n}$, $0$ ($n-2$ times)</td>
<td>$0, n$, $1$ ($n-2$ times)</td>
<td>$0, 2$, $1$ ($n-2$ times)</td>
</tr>
<tr>
<td>$G = K_{n_1,n_2}$</td>
<td>$-\sqrt{n_1n_2}$, $\sqrt{n_1n_2}$, $0$ ($n-2$ times)</td>
<td>$0, n_1$ ($n_2 - 1$ times), $n_2$ ($n_1 - 1$ times), $n$</td>
<td>$0, 2$, $1$ ($n-2$ times)</td>
</tr>
<tr>
<td>$G = K_n$</td>
<td>$1, -1$ ($n - 1$ times)</td>
<td>$0, n$ ($n - 1$ times)</td>
<td>$0, \frac{n}{n-1}$ ($n - 1$ times)</td>
</tr>
</tbody>
</table>
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 $\beta_0 := x_1^T x_1$, $x_1 := x_1 / \beta_0$

2. **Lanczos steps:**
   \[
   \text{for } i = 1 \text{ to } k \text{ do }
   \]
   \[
   \begin{align*}
   & (i) \quad y := Mx_i \\
   & (ii) \alpha_i := x_i^T y \\
   & (iii) x_{i+1} := y - \alpha_i x_i - \beta_{i-1} x_{i-1} \\
   & (iv) \beta_i := x_{i+1}^T x_{i+1} \\
   & (v) \quad x_{i+1} := x_{i+1} / \beta_i;
   \end{align*}
   \]
   Set $X_i := \text{Mat}(x_1, \ldots, x_i)$

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

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 $x_1$. 

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Introduction to Network Analysis
**Grafting**

Q: How to modify $G$ by adding to it eigenvalues of $H$?

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

$(\lambda, x)$ is eigenpair of $H$

(new node for symmetric grafting)

$\lambda \in \text{spectra}(G')$
Eigenvalues and Global Properties

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

- $\left[ \frac{4}{n\lambda_2(L)} \right] \leq \text{diam}(G') \leq 2 \left[ \frac{\cosh^{-1}(n-1)}{\cosh^{-1}\left(\frac{\lambda_n(L)+\lambda_2(L)}{\lambda_n(L)-\lambda_2(L)}\right)} \right] + 1$

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

  mean distance in $G$

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

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

  $i(G') \leq \sqrt{\lambda_2(L)(2\Delta - \lambda_2(L))}$

- Expansion $c_V := \min \left\{ \frac{|N(S) \setminus S|}{|S|}; S \subseteq V, |S| \leq \frac{n}{2} \right\}$

  $\frac{\lambda_2(L)}{\frac{4}{2} + \lambda_2(L)} \leq c_V = O(\sqrt{\lambda_2(L)})$

  ... chromatic number, minimum independent set, ...
Algorithm for finding sparse cuts: take a Fiedler vector, sort the vertices according to its values, and find the best cut.
p-discrepancy

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

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

and $\sigma_\infty(G, \psi) = \max_{i,j \in E} w_{ij} |\psi(i) - \psi(j)|$

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

Basic facts:

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

Homework for submission:

$$
\lambda_2 \frac{(n^2 - 1)}{6} \leq \sigma_1(G, \psi) \leq \lambda_n \frac{(n^2 - 1)}{6}
$$
Introduction to Network Analysis

Matlab demo
Random Walks

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

\[
p_i(t) = \sum_j \frac{A_{i,j}}{d(j)} p_j(t-1) \text{ or } p(t) = AD^{-1}p(t-1)
\]

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

\[
(I - AD^{-1})p = LD^{-1}p,
\]

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.,

\[
p_i = d(i)/\sum_j d(j)
\]

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

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

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