CS 598: Spectral Graph Theory: Lecture 2

The Laplacian

Today

- More on evectors and evalues
- The Laplacian, revisited
- Properties of Laplacian spectra, PSD matrices.
- Spectra of common graphs.
- Start bounding Laplacian evalues

A Remark on Notation

- For convenience, we will often use the bra-ket notation for vecotrs:
- We denote vector $v = \begin{pmatrix} v_1 \\ \cdots \\ v_n \end{pmatrix}$ with a "bra": $|v\rangle$
- We denote the transpose vector $v^T = (v_1 \quad \cdots \quad v_n)$ with a "ket": $\langle v|$
- We denote the inner product $v^T u$ between two vectors v and u with a "braket": $\langle v|u\rangle = \langle v, u\rangle$

Evectors and Evalues

- Vector v is evector of matrix A with evalue μ if $Av=\mu v$.
- We are interested (almost always) in symmetric matrices, for which the following special properties hold:

  - If v1,v2 are evectors of A with evalues μ1, μ2 and μ1≠ μ2, then v1 is orthogonal to v2.

    Proof: $\mu_1 v_1^T v_2 = v_1^T A v_2 = v_1^T \mu_2 v_2 = \mu_2 v_1^T v_2$. Assuming μ1≠ μ2 it implies $v_1^T v_2 = 0$.

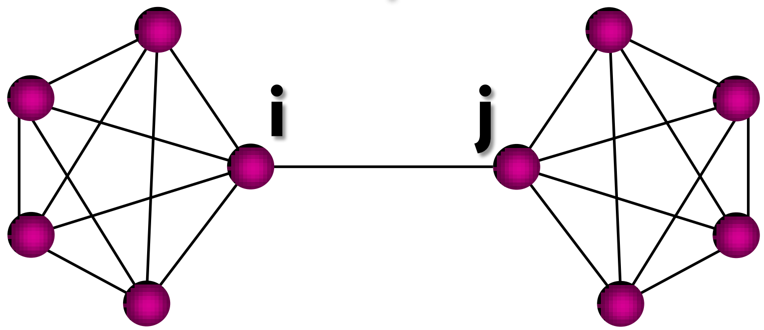
  - If v1,v2 are evectors of A with the same evalue μ, then v1+v2 is as well. The multiplicity of evalue μ is the dimension of the space of evectors with evalue μ.

  - Every n-by-n symmetric matrix has n evalues $\{\mu_1 \leq \cdots \leq \mu_n\}$ counting multiplicities, and and orthonormal basis of corresponding evectors $\{v_1, \dots, v_n\}$, so that $Av_i = \mu_i v_i$

  - If we let V be the matrix whose i-th column is v_i, and M the diagonal matrix whose i-th diagonal is μ_i, we can compactly write AV=VM. Multiplying by V^T on the right, we obtain the eigendecomposition of A:

    $$A = AV\ V^T = VM\ V^T = \sum_i \mu_i v_i v_i^T$$

The Laplacian: Definition Refresher



G = {V,E}

$$L_G = \begin{array}{c|cccccc} & & & & & j & \\ \hline & d_1 & & & & & \\ & & d_2 & & & & \\ & & & d_3 & & & \\ i & & & & d_i & -1 & \\ & & & & & \cdots & \\ & & & & & & d_n \end{array}$$

$$L_G(i,j) = \begin{cases} d_i & if \;\; i = j \\ -1 & if \;\; (i,j)\; edge \\ 0 & otherwise \end{cases}$$

Where d_i is the degree of i-th vertex.
For convenience, we have unweighted graphs

- D_G = Diagonal matrix of degrees
- A_G = Adjacency matrix of the graph
- $L_G = D_G - A_G$

The Laplacian: Properties Refresher

- The constant vector **1** is an eigenvector with eigenvalue zero.

$$L_G \vec{1} = 0$$

- Has n eigenvalues (spectrum) $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$
- Second eigenvalue is called "algebraic connectivity".
  G is connected if and only if $\lambda_2 > 0$
- We will see the further away from zero,
  the more connected G is.

Redefining the Laplacian

- Let Le be the Laplacian of the graph on n vertices consisting of just one edge e=(u,v).

$$L_e(i,j) = \begin{cases} 1 & if\ \ i = j, i \in u,v \\ -1 & if\ \ i = u,\ j = v,\ or\ vice\ versa \\ 0 & otherwise \end{cases}$$

$$L_e = \begin{array}{cc} & \begin{array}{cc} \mathbf{u} & \mathbf{v} \end{array} \\ \begin{array}{c} \mathbf{u} \\ \mathbf{v} \end{array} & \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \end{array} \otimes [zeros]$$

- For a graph G with edge set E we now define

$$L_G = \sum_{e \in E} L_e$$

- Many elementary properties of the Laplacian now follow from this definition as we will see next (prove facts for one edge and then add).

Laplacian of an edge, contd.

$$L_e = \begin{array}{c c} & \begin{array}{cc} u & v \end{array} \\ \begin{array}{c} u \\ v \end{array} & \begin{array}{|c|c|} \hline 1 & -1 \\ \hline -1 & 1 \\ \hline \end{array} \end{array} \otimes [zeros]$$

eigenvalue

eigenvector

$$\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} (1 \quad -1) = 2 \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} (1/\sqrt{2} \quad -1/\sqrt{2})$$

- Since evalues are zero and 2, we see that L_e is P.S.D. Moreover,

$$x^T L_e x = (x_1 x_2) \begin{pmatrix} 1 \\ -1 \end{pmatrix} (1 \quad -1) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = (x_1 - x_2)^2$$

Review of Positive Semidefiniteness

- **Definition:** A symmetric matrix M is positive semidefinite (PSD) if:

$$x^T M x \geq 0 \ \forall x \in R^n$$

Positive definite (PD) if inequality is strict for all x≠0.

- PSD iff all evalues are non-negative (exercise.)

- PSD iff M can be written as $M = A^T A$, where A can be n-by-k (not necessarily symmetric) and is not unique.

  Proof: see blackboard

Review of Positive Semidefiniteness

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Proof

($\Rightarrow$) If M is positive semidefinite, recall that M can be diagonalized as

$$M = Q^T \Lambda Q,$$

thus

$$M = Q^T \Lambda^{1/2} \Lambda^{1/2} Q = \left(\Lambda^{1/2} Q\right)^T \left(\Lambda^{1/2} Q\right),$$

where $\Lambda^{1/2}$ has $\sqrt{\lambda_i}$ on the diagonal.

($\Leftarrow$) If $M = A^T A$, then

$$x^T M x = x^T A^T A x = (Ax)^T (Ax)$$

Letting $y = (Ax) \in \mathbb{R}^k$, we see that:

$$x^T M x = y^T y = ||y||^2 \geq 0. \quad \blacksquare$$

More Properties of Laplacian

From the definition using edge sums, we get:

- **(PSD-ness)** The Laplacian of any graph is PSD.

$$x^T L_G x = x^T (\sum_{e \in E} L_e) x = \sum_{e \in E} x^T L_e x = \sum_{(i,j) \in E} (x_i - x_j)^2$$

- **(Connectivity)** G is connected iff **λ2** positive or alternatively, the null space is 1-d and spanned by the vector **1.**

Proof Let $x \in \text{null}(L)$, i.e. $L_G x = 0$. This implies

$$x^T L_G x = \sum_{(i,j) \in E} (x_i - x_j)^2 = 0.$$

Thus, $x_i = x_j$ for every $(i,j) \in E$. As G is connected, this means that all x_i are equal. Thus every member of the null space is a multiple of 1. ∎

- **Corollary:** The multiplicity of zero as an eigenvalue equals the number of connected components of the graph.

More Properties of Laplacian

- **(Edge union)** If G and H are two graphs on the same vertex set, with disjoint edge set then

$$L_{G \cup H} = L_G + L_H \ \text{(additivity)}$$

- If a vertex is isolated, the corresponding row and column of Laplacian are zero
- **(Disjoint union)** Together these imply that for the disjoint union of graphs G and H

$$L_{G \coprod H} = L_G \oplus L_H = \begin{pmatrix} L_G & 0 \\ 0 & L_H \end{pmatrix}$$

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- **(Disjoint union spectrum)** If L_G has evectors $v_1,\ldots, v_n$ with evalues $\lambda_1,\ldots, \lambda_n$ and L_H has evectors $w_1,\ldots, w_n$ with evalues $\mu_1,\ldots, \mu_n$ then $L_G \coprod L_H$ has evectors $v_1 \oplus 0, \ldots, v_n \oplus 0, 0 \oplus w_1, \ldots, 0 \oplus w_n$ with evalues $\lambda_1, \ldots, \lambda_n, \mu_1, \ldots, \mu_n$.

The Incidence Matrix: Factoring the Laplacian

- We can factor L as $L = V^T V$ using evectors but also exists nicer factorization
- Define the incidence matrix B to be the m-by-n matrix

$$B(e,v) = \begin{cases} 1, if\ e = (v,w) and\ v < w \\ -1, if\ e = (v,w) and\ w < v \\ 0, otherwise \end{cases}$$

- Example of incidence matrix

$$B = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix} \qquad L = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

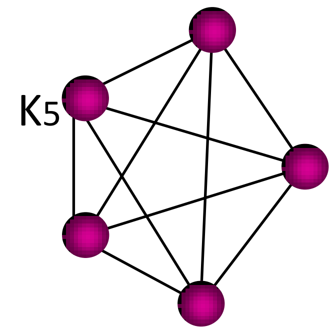
- Claim: $L = B^T B$ (exercise)
- Gives another proof that L is PSD.

Spectra of Some Common Graphs

- The complete graph K_n on n vertices with edge set $\{(u, v): u \neq v\}$
- The path graph P_n on n vertices with edge set $\{(u, u+1): 0 \leq u < n\}$
- The ring graph R_n on n vertices with edge set $\{(u, u+1): 0 \leq u < n\} \cup (0, n-1)$
- The grid graph G_{nxm} on nxm vertices with edges from node (u_1, u_2) to nodes that differ by one in just one coordinate
- Product graphs in general

The Complete Graph

- Kn: $\{(u, v) : u \neq v\}$

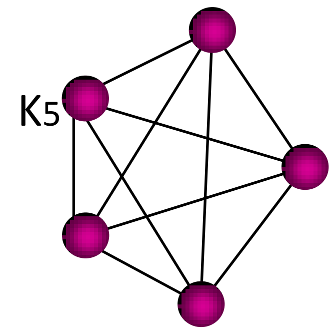


- The Laplacian of Kn has eigenvalue zero with multiplicity 1 (since it is connected) and n with multiplicity n-1.

- Proof: see blackboard

The Complete Graph

- $K_n: \{(u, v): u \neq v\}$



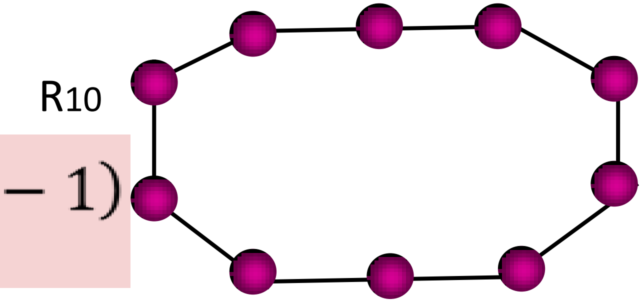
- The Laplacian of Kn has eigenvalue zero with multiplicity 1 (since it is connected) and n with multiplicity n-1.

Proof. Let L be the Laplacian of K_n. Let x be any vector orthogonal to the all 1s vector. Consider the first coordinate of Lx. It will be $n-1$ times x_1, minus

$$\sum_{u>1} x_u = -x_1,$$

as x is orthogonal to 1. Thus, x is an eigenvector of eigenvalue n. $\square$

The Ring Graph



- Rn: $\{(u, u+1) : 0 \le u < n\} \cup (0, n-1)$

- The Laplacian of Rn has eigenvectors

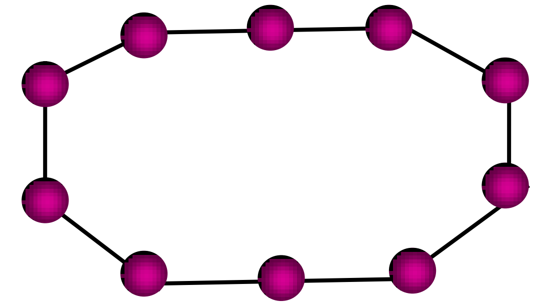
$$x_k(u) = \sin(\frac{2\pi k u}{n}) \text{ and}$$
$$y_k(u) = \cos(\frac{2\pi k u}{n})$$

for k≤n/2. Both have eigenvalue $2 - 2\cos(\frac{2\pi k}{n})$. Note x_0 should be ignored and y_0 is the all ones vector. If n is even, then $x_{n/2}$ should be ignored.

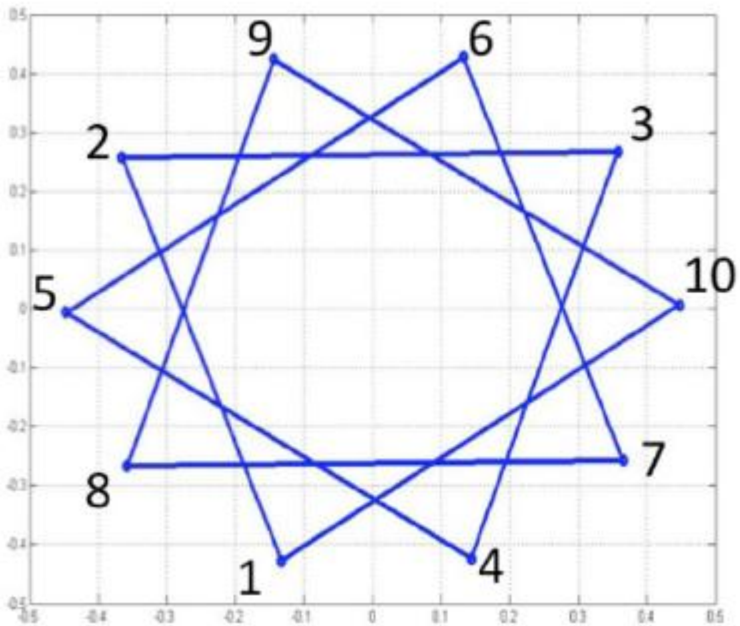
Proof: By plotting the graph on the circle using these vectors as coordinates.

The Ring Graph

R10



Spectral embedding for k=3



Let $z(u)$ be the point $(x\_k(u), y\_k(u))$ on the plane.

Consider the vector $z(u-1) - 2\,z(u) + z(u+1)$. By the reflection symmetry of the picture, it is parallel to $z(u)$

Let $z(u-1) - 2\,z(u) + z(u+1) = \lambda z(u)$. By rotational symmetry, the constant λ is independent of u.

To compute λ consider the vertex $u=1$.

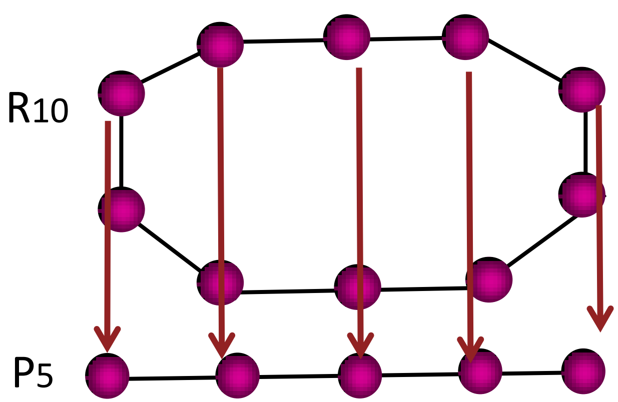
Verify details as excercise

The Path Graph

- Pn:$\{(u, u+1) : 0 \le u < n\}$

- The Laplacian of P_n has the same eigenvalues as R_{2n} and eigenvectors $z_k(u) = \sin\left(\frac{\pi k u}{n} + \frac{\pi}{2n}\right)$, for k<n.

Proof: Treat P_n as a quotient of R_{2n}. Use projection



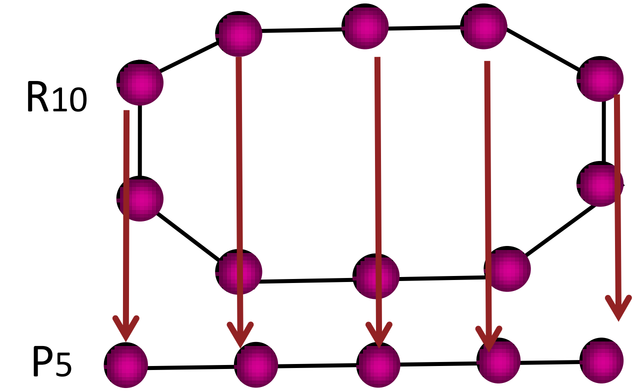
$$f : R_{2n} \to P_n$$

$$f(u) = \begin{cases} u, if\ u < n \\ 2n - 1 - u, if\ u \ge n \end{cases}$$

The Path Graph

Proof: Treat P_n as a quotient of R_{2n}.

Use projection $f: R_{2n} \to P_n$



$$f(u) = \begin{cases} u, if\ u < n \\ 2n - 1 - u, if\ u \geq n \end{cases}$$

- Let z be an eigenvector of the ring, with z(u)=z(2n-1-u) for all u.
- Take the first n components of z and call this vector v.
- To see that v is an eigenvector of P_n, verify that it satisfies for some λ:

  2v(u)-v(u-1)-v(u+1)= λv(u), for 0<u<n-1

  v(0)-v(1)= λv(1)

  v(n-1)-v(n-2)= λv(n-1)

- Take z as claimed, i.e. $z_k(u) = \sin\left(\frac{\pi k u}{n} + \frac{\pi}{2n}\right)$, which is in the span of x_k and y_k.

- (verify details as exercise)

Graph Products

- (Definition): Let G(V,E) and H(W,F). The graph product GxH is a graph with vertex set VxW and edge set $((v_1,w),(v_2,w))$ for $(v_1,v_2)\in E$

  $((v,w_1),(v,w_2))$ for $(w_1,w_2)\in F$
- If G has evals $\lambda_1,\ldots,\lambda_n$, evecs $x_1,\ldots,x_n$

  H has evals $\mu_1,\ldots,\mu_m$, evecs $y_1,\ldots,y_m$

Then GxH has for all i,j in range, an evector

$z_{ij}(v,w)=x_i(v)y_j(w)$ of evalue $\lambda_i + \mu_j$

- Proof: see blackboard

Graph Products

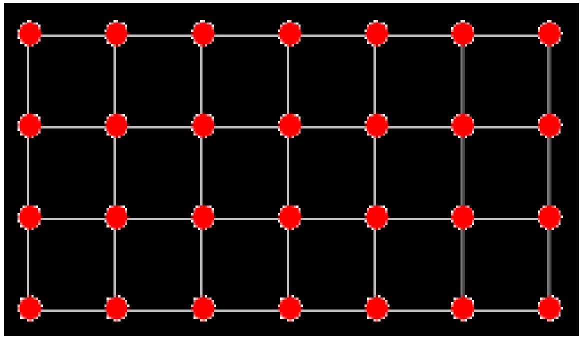
Proof. To see that this eigenvector has the propper eigenvalue, let L denote the Laplacian of $G \times H$, d_v the degree of node v in G, and e_w the degree of node w in H. We can then verify that

$$
\begin{aligned}
(Lz)(v,w) &= (d_v + e_w)(x_i(v)y_j(w)) - \sum_{(v,v_2)\in E} (x_i(v_2)y_j(w)) - \sum_{(w,w_2)\in F} (x_i(v)y_j(w_2)) \\
&= (d_v)(x_i(v)y_j(w)) - \sum_{(v,v_2)\in E} (x_i(v_2)y_j(w)) + (e_w)(x_i(v)y_j(w)) - \sum_{(w,w_2)\in F} (x_i(v)y_j(w_2)) \\
&= y_j(w)\left(d_v x_i(v) - \sum_{(v,v_2)\in E} (x_i(v_2))\right) + x_i(v)\left(e_w y_j(w) - \sum_{(w,w_2)\in F} (x_i(v)y_j)\right) \\
&= y_j(w)\lambda_i x_i)(v) + x_i(v)\mu_j y_j(w) \\
&= (\lambda_i + \mu_j)(x_i(v)y_j(w)).
\end{aligned}
$$

□

Graph Products: Grid Graph

$$G_{n\times m} = P_n \times P_m$$



- Immediately get spectra from path.

Start Bounding Laplacian Eigenvalues

Sum of Eigenvalues, Extremal Eigenvalues

- $\sum_i \lambda_i = \sum_i d_i \leq d_{max} n$ where d_i is the degree of vertex i.

  Proof: take the trace of L
- $\lambda_2 \leq \frac{\sum_i d_i}{n-1}$ and $\lambda_n \geq \frac{\sum_i d_i}{n-1}$

  Proof: previous inequality + $\lambda_1 = 0$.

- Courant-Fisher formula (for extreme evalues): For any nxn symmetric matrix A (eigenvalues in increasing order),

$$\lambda_1 = \min_{\|x\|=1} x^T A x = \min_{x \neq 0} \frac{x^T A x}{x^T x} \qquad \lambda_2 = \min_{\|x\|=1, x \perp v_1} x^T A x = \min_{x \perp v_1, x \neq 0} \frac{x^T A x}{x^T x}$$

$$\lambda_{\max} = \max_{\|x\|=1} x^T A x = \max_{x \neq 0} \frac{x^T A x}{x^T x}$$

Courant-Fischer.

- Courant-Fischer Formula: For any nxn symmetric matrix A,

$$\lambda_k = \min_{S\, of\, \dim k} \max_{x \in S} \frac{x^T A x}{x^T x}$$

$$\lambda_k = \max_{S\, of\, \dim n-k-1} \min_{x \in S} \frac{x^T A x}{x^T x}$$

- Proof: see blackboard

- Courant-Fischer Formula: $$\lambda_k = \max_{S\, of\, \dim n-k-1} \min_{x \in S} \frac{x^T A x}{x^T x}$$

Proof Let $A = Q^T \Lambda Q$ be the eigendecomposition of A. We observe that $x^T A x = x^T Q^T \Lambda Q x = (Qx)^T \Lambda (Qx)$, and since Q is orthogonal, $\|Qx\| = \|x\|$. Thus it suffices to consider the case when $A = \Lambda$ is a diagonal matrix with the eigenvalues $\lambda_1, \ldots, \lambda_n$ in the diagonal. Then we can write

$$x^T A x = \begin{pmatrix} x_1 & \cdots & x_n \end{pmatrix} \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \sum_{i=1}^{n} \lambda_i x_i^2.$$

We note that when A is diagonal, the eigenvectors of A are $v_k = e_k$, the standard basis vector in $\mathbb{R}^n$, i.e. $(e_k)_i = 1$ if $i = k$, and $(e_k)_i = 0$ otherwise. Then the condition $x \in S_{k-1}^{\perp}$ implies $x \perp e_i$ for $i = 1, \ldots, k-1$, so $x_i = \langle x, e_i \rangle = 0$. Therefore, for $x \in S_{k-1}^{\perp}$ with $\|x\| = 1$, we have

$$x^T A x = \sum_{i=1}^{n} \lambda_i x_i^2 = \sum_{i=k}^{n} \lambda_i x_i^2 \geq \lambda_k \sum_{i=k}^{n} x_i^2 = \lambda_k \|x\|^2 = \lambda_k.$$

- Courant-Fischer Formula: $$\lambda_k = \max_{S\, of\, \dim n-k-1} \min_{x \in S} \frac{x^T Ax}{x^T x}$$

On the other hand, plugging in $x = e_k \in S_{k-1}^{\perp}$ yields $x^T Ax = (e_k)^T Ae_k = \lambda_k$. This shows that

$$\lambda_k = \min_{\substack{\|x\|=1 \\ x \in S_{k-1}^{\perp}}} x^T Ax.$$

Similarly, for $\|x\| = 1$,

$$x^T Ax = \sum_{i=1}^{n} \lambda_i x_i^2 \leq \lambda_{\max} \sum_{i=1}^{n} x_i^2 = \lambda_{\max} \|x\|^2 = \lambda_{\max}.$$

On the other hand, taking $x = e_n$ yields $x^T Ax = (e_n)^T Ae_n = \lambda_{\max}$. Hence we conclude that

$$\lambda_{\max} = \max_{\|x\|=1} x^T Ax.$$

Courant-Fischer.

- Courant-Fischer Formula: For any nxn symmetric matrix A,

$$\lambda_k = \min_{S\, of\, \dim k} \max_{x \in S} \frac{x^T A x}{x^T x}$$

$$\lambda_k = \max_{S\, of\, \dim n-k-1} \min_{x \in S} \frac{x^T A x}{x^T x}$$

- Proof: see blackboard

- Definition (Rayleigh Quotient): The ratio $\frac{x^T A x}{x^T x}$ is called the *Rayleigh Quotient* of x with respect to A.
- Next lecture we will use it to bound evalues of Laplacians.