### On sums of graph eigenvalues

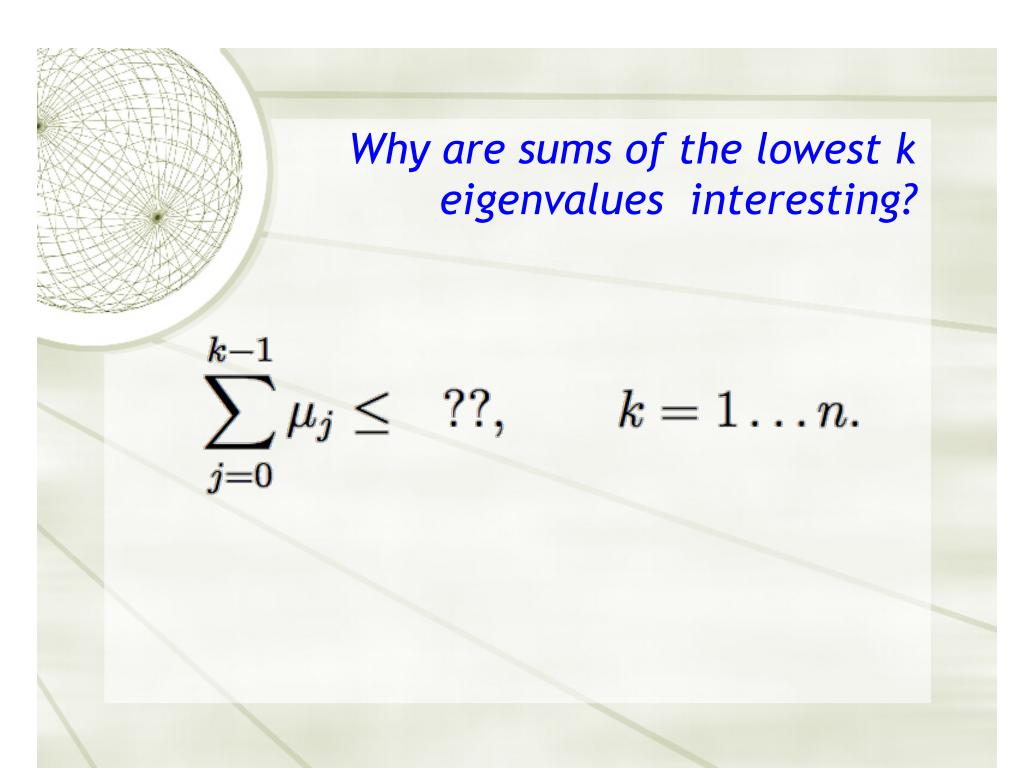
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Why are sums of the lowest k eigenvalues interesting?

Physically: This is the lowest energy (up to physical constants) of a Fermionic system of k( $2\sigma$ +1) particles with spin  $\sigma$ .

Why are sums of the lowest k eigenvalues interesting?

Information about sums of eigenvalues for arbitrary k is equivalent to information about the partition function.

$$egin{aligned} R_1(z) &:= \sum_j \, (z-\lambda_j)_+ = z \mathcal{N}(z) - \sum_j^{\mathcal{N}(z)} \lambda_j \ \mathcal{L}[R_1(z)] &= \sum_j \, \int_{\lambda_j}^{\infty} (z-\lambda_j) e^{-zt} = \cdots = rac{1}{t^2} \sum_j e^{-t\lambda_j} \end{aligned}$$

### Embeddings of graphs in regular lattices

Suppose I am given the adjacency matrix A of some enormous graph about which I don't know anything geometrical. How can I tell whether it embeds in a regular lattice of dimension v? Can I find conditions in terms of the eigenvalues of A or of the graph Laplacian?

# The same graph can embed in lattices of various dimension

### Embeddings of graphs in regular lattices

It will turn out that the sums of graph eigenvalues will offer necessary conditions for such embeddings, which, numerically, are pretty good.

### Embeddings of graphs in regular lattices

It will turn out that the sums of graph eigenvalues will offer necessary conditions for such embeddings, which, numerically, are pretty good. Our larger project is to see what information about a graph can be recognized in the statistical properties of spectra.

In some standard PDE problems, eigenvalues obey an asymptotic law of Weyl, where the dimension of the space appears in an exponent. The same will be shown for graphs embedded in regular lattices.

### **Conventions and notation**

Graphs are assumed connected, not directed, on a finite number n of vertices, no self-connections or multiple edges. The adjacency matrix is A, with entries a<sub>ij</sub>. It will be one of three operators whose spectra we consider.

### **Conventions and notation**

The graph Laplacian is a matrix that compares values of a function at a vertex with the average of its values at the neighbors.

H :=  $-\Delta$  := Deg – A, where Deg := diag(d<sub>v</sub>), d<sub>v</sub> := # neighbors of v. Its weak form is:

$$\rightarrow \frac{1}{2} \sum_{u} \sum_{v \sim u} |f_u - f_v|^2$$

### **Conventions and notation**

Graph are assumed connected, not directed, on a finite number n of vertices, no self-connections or multiple edges. The adjacency matrix is A, with entries a<sub>ii</sub>.

### Variational bounds on graph spectra

### Variational bounds on sums The classical min-max inequality: With a suitable orthonormal set,

$$\sum_{\ell=0}^{k-1} \mu_{\ell} \leq \sum_{\ell=0}^{k-1} \left\langle M\phi^{(\ell)}, \phi^{(\ell)} \right\rangle,$$

$$\sum_{\ell=k}^{n-1} \mu_{\ell} \ge \sum_{\ell=k}^{n-1} \left\langle M\phi^{(\ell)}, \phi^{(\ell)} \right\rangle,$$

### A new method: an averaged variational inequality for sums

A new variational inequality for sums

Historical remark. This was suggested by Pawel Kröger's proof of a Weyl-sharp upper bound for the Neumann eiganvalues of the Laplacian on a domain. (1990's)

# A new method: an averaged variational inequality for sums

**Theorem 3.1** Consider a self-adjoint operator M on a Hilbert space  $\mathcal{H}$ , with ordered, entirely discrete spectrum  $-\infty < \mu_0 \leq \mu_1 \leq \ldots$  and corresponding normalized eigenvectors  $\{\psi^{(\ell)}\}$ . Let  $f_z$  be a family of vectors in  $\mathcal{Q}(M)$  indexed by a variable z ranging over a measure space  $(\mathfrak{M}, \Sigma, \sigma)$ . Suppose that  $\mathfrak{M}_0$  is a subset of  $\mathfrak{M}$ . Then for any eigenvalue  $\mu_k$  of M,

$$\begin{aligned}
\mu_k \left( \int_{\mathfrak{M}_0} \langle f_z, f_z \rangle \, d\sigma - \sum_{j=0}^{k-1} \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma \right) \\
\leq \\
\int_{\mathfrak{M}_0} \langle Hf_z, f_z \rangle \, d\sigma - \sum_{i=0}^{k-1} \mu_j \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma,
\end{aligned} \tag{3.2}$$

provided that the integrals converge.

# How to use the averaged variational bound to get sharp results for graphs? (A deep question)

$$\begin{split} & \mu_k \left( \int_{\mathfrak{M}_0} \langle f_z, f_z \rangle \, d\sigma - \sum_{j=0}^{k-1} \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma \right) \\ & \leq \\ & \int_{\mathfrak{M}_0} \langle Hf_z, f_z \rangle \, d\sigma - \sum_{j=0}^{k-1} \mu_j \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma, \end{split}$$

(3.2)

# How to use the averaged variational bound to get sharp results for graphs? (A deep question)

$$\int_{\mathfrak{M}_{0}} \langle Hf_{z}, f_{z} \rangle d\sigma - \sum_{j=0}^{k-1} \mu_{j} \int_{\mathfrak{M}} |\langle f_{z}, \psi^{(j)} \rangle|^{2} d\sigma,$$

 $d\sigma$ 

(3.2)

How to use the averaged variational bound to get sharp results for graphs? (A deep question)

$$\sum_{j=0}^{\kappa-1} \mu_j \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma \leq \int_{\mathfrak{M}_0} \langle M f_z, f_z \rangle d\sigma.$$

provided that the subset  $\mathfrak{M}_0$  is large enough.

Orthogonalization has been replaced by averaging!

 $\sum_{j=0}^{k-1} \mu_j \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma \leq \int_{\mathfrak{M}_0} \langle M f_z, f_z \rangle d\sigma.$ 

Given an abstract graph, when can it be embedded as a subgraph of a regular lattice? What is the minimal dimension of the enveloping lattice?

I'll describe the case when G is isomorphic to a subgraph of a rectangular lattice with no diagonal connections.

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 Including enough diagonal connections to embed an arbitrary graph will add at most a factor of 2, cf. GT grad student Shane Scott. (We are seeking the optimal constant.) **Corollary 6** Suppose that G is a finite subgraph of  $\mathfrak{Q}^{\nu}$ . Then for  $k \geq 2$  the eigenvalues of the graph Laplacian  $H_G$  satisfy

$$\sum_{j=1}^{k-1} \lambda_j \le 2\mathcal{E}\left(1 - \frac{\sin((k/n)^{1/\nu}\pi)}{(k/n)^{1/\nu}\pi}\right) \frac{k}{n},\tag{2.17}$$

where  $\mathcal{E}$  denotes the number of edges of G.

**Remark 2.2** In particular, it is true independently of dimension that

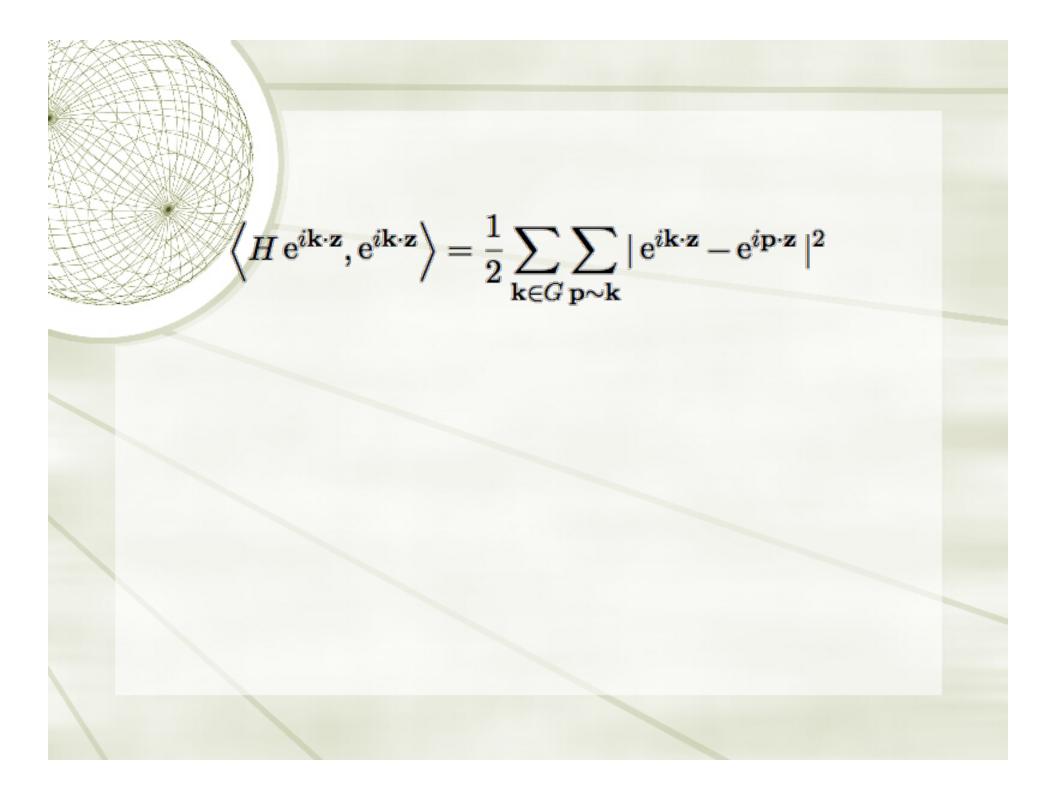
$$\sum_{j=1}^{k-1} \lambda_j \le \frac{2\mathcal{E}k}{n},$$

which becomes a standard equality when k = n. In the complementary situation where  $k \ll n$  the upper bound is

$$\sim \frac{\pi^2 \mathcal{E}}{3} \left(\frac{k}{n}\right)^{1+\frac{2}{\nu}},$$

which has the form of the Weyl law for Laplacians on domains  $\Omega \subset \mathbb{R}^{\nu}$ .

$$\begin{split} M &= [-\pi,\pi]^{\nu} \qquad f_{\mathbf{x}} = \exp(i\mathbf{k}\cdot\mathbf{x}) \\ M_0 &:= [-a\pi,a\pi]^{\nu} \qquad f_{\mathbf{x}} = \exp(i\mathbf{k}\cdot\mathbf{x}) \\ \hat{\phi}(\mathbf{x}) &:= \sum_{\mathbf{k}\in G} e^{-i\mathbf{k}\cdot\mathbf{x}} \phi_{\mathbf{k}}, \qquad \phi_{\mathbf{k}} = \frac{1}{(2\pi)^{\nu}} \int_{[-\pi,\pi]^{\nu}} e^{i\mathbf{k}\cdot\mathbf{x}} \hat{\phi}(\mathbf{x}) \end{split}$$



$$\left\langle H \, \mathrm{e}^{i \mathbf{k} \cdot \mathbf{z}}, \mathrm{e}^{i \mathbf{k} \cdot \mathbf{z}} 
ight
angle = rac{1}{2} \sum_{\mathbf{k} \in G} \sum_{\mathbf{p} \sim \mathbf{k}} | \, \mathrm{e}^{i \mathbf{k} \cdot \mathbf{z}} - \mathrm{e}^{i \mathbf{p} \cdot \mathbf{z}} |^2$$

 $|e^{i\mathbf{k}\cdot\mathbf{z}} - e^{i\mathbf{p}\cdot\mathbf{z}}|^2$  simplifies to  $|e^{\pm iz_q} - 1|^2 = 4\sin^2\left(\frac{z_q}{2}\right)$ 

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 $A_0 = 2(a\pi - \sin(a\pi))(2a\pi)^{\nu - 1} \sum_{\mathbf{k} \in G} d_{\mathbf{k}} = (2a\pi)^{\nu} 2\left(1 - \frac{\sin(a\pi)}{a\pi}\right) \mathcal{E}_{\mathbf{k}}$ 

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$$A_0 = 2(a\pi - \sin(a\pi))(2a\pi)^{\nu-1} \sum_{\mathbf{k}\in G} d_{\mathbf{k}} = (2a\pi)^{\nu} 2\left(1 - \frac{\sin(a\pi)}{a\pi}\right) \mathcal{E}$$

 $\int_{[-\pi,\pi]^{\nu}} |\langle e^{i\mathbf{k}\mathbf{x}}, \phi_j \rangle|^2 = (2\pi)^{\nu} ||\phi_j||^2 = (2\pi)^{\nu}$ 

#### Meanwhile, on the left,

$$n(2a\pi)^{\nu} - k(2\pi)^{\nu} \ge 0,$$

so  $a^{\nu} \rightarrow k/n$ 

#### Giving

$$\sum_{j=1}^{k-1} \lambda_j \le 2\mathcal{E}\left(1 - \frac{\sin((k/n)^{1/\nu}\pi)}{(k/n)^{1/\nu}\pi}\right) \frac{k}{n}$$

# There are many variants of these inequalities

# Variants

$$\sum_{j=0}^{\infty} \lambda_j^2 \leq \kappa \left(1 - \operatorname{sinc}(\pi \kappa^{1/\nu})\right)^2 \operatorname{Tr}(H^2)$$

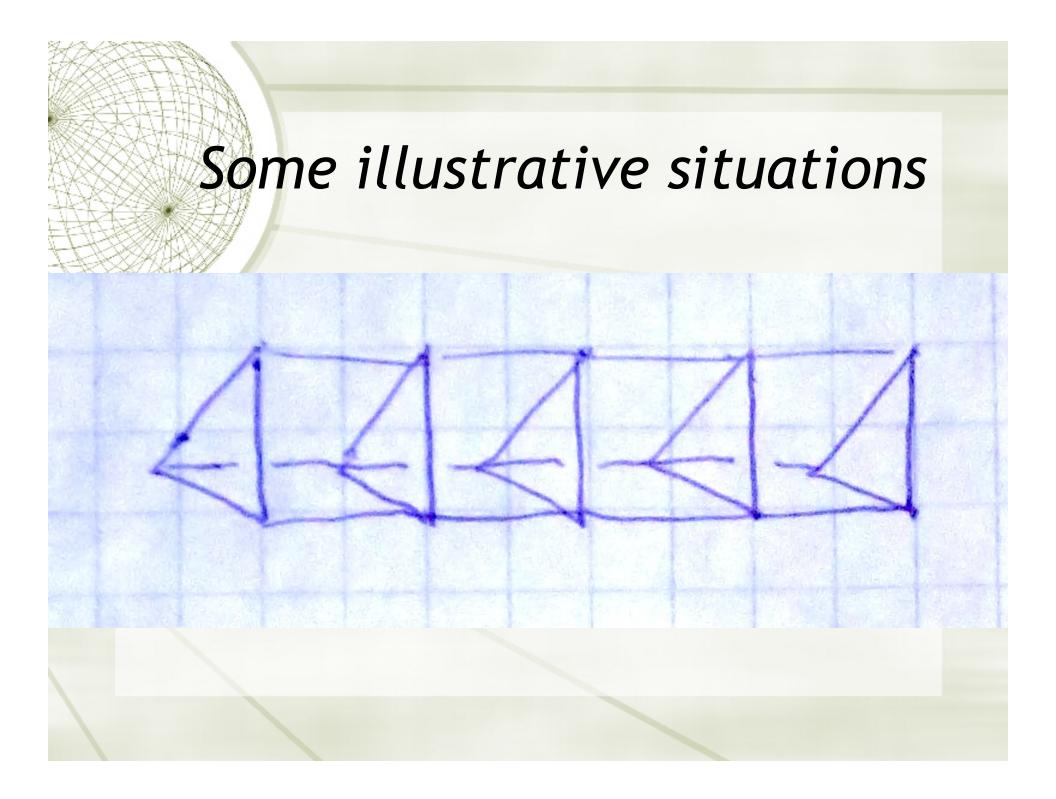
$$+ 2\kappa \operatorname{sinc}(\pi \kappa^{1/\nu}) (1 - \operatorname{sinc}(\pi \kappa^{1/\nu})) \sum_{\mathbf{x} \in G} d_{\mathbf{x}}$$
$$- 2\kappa \operatorname{sinc}(\pi \kappa^{1/\nu}) (1 - \cos(\pi \kappa^{1/\nu})) \sum_{\mathbf{x} \in G} d_{\mathbf{x}}^{\parallel}.$$

### Variants

For any positive nonincreasing convex function, like  $x \rightarrow exp(-t x)$ ,

$$\sum_{j=0}^{k-1} \Psi(\mu_j) \ge \sum_{j=0}^{k-1} \Psi\left(\left(1+\frac{2}{\nu}\right) \frac{\pi^2 m j^{2/\nu}}{3n^{1+2/\nu}}\right).$$

# Some illustrative situations



Another way to apply the averaged variational principle to graphs is to let M be the set of pairs of vertices. The reason is that the complete graph has a superbasis of nontrivial eigenfunctions consisting of functions equal to 1 on one vertex, -1 on a second, and 0 everywhere else. Let these functions be  $h_z$ , where z is a vertex pair.

Two facts are easily seen:

2.

1. For vectors of mean 0 (orthogonal to  $\phi_0 = 1$ ),

$$\sum_{\text{IL pairs}} |\langle h_{uv}, f \rangle|^2 = 2 ||f||^2 (n-1).$$

$$\langle Hh_{uv},h_{uv}
angle = d_u+d_v+2a_{uv}$$

From the averaged variational principle,

$$\sum_{j \leq L} \lambda_j \leq rac{1}{2n} \min_{ ext{choices of nL pairs}} \sum_{uv} (d_u + d_v + 2a_{uv})$$

#### Variants

For the normalized graph Laplacian,

$$\sum_{j=1}^{k-1} c_j \leq \frac{1}{4m} \sum_{\mathfrak{M}_0} (d_u + d_v + 2a_{uv}),$$

#### Variants

**Corollary 9** Let G be a finite connected graph on n vertices. Then for  $1 \leq k < n-1$ , the eigenvalues  $\alpha_0 \geq \alpha_1 \geq \cdots \geq \alpha_{n-1}$  of the adjacency matrix  $A_G$  satisfy the elementary inequalities

$$\sum_{j=0}^{n-k-1} \alpha_j \ge \min\left(k, \left\lfloor \frac{2m}{n} \right\rfloor\right),$$

$$\sum_{j=n-k}^{n-1} \alpha_j \le -\min\left(k, \left\lfloor \frac{2m}{n} \right\rfloor\right).$$
(3.25)

Now let  $\{\alpha_{\ell_j}\}, \ell = 0, ..., n-1$  denote the eigenvalues  $\alpha_j$  reordered by magnitude, so that  $|\alpha_{\ell_0}| \leq |\alpha_{\ell_1}| \leq ...$  Then for any set  $\mathfrak{M}_0$  of nk ordered pairs of vertices,

$$\sum_{j=0}^{n-1} \alpha_{\ell_j}^2 \le \frac{1}{2n} \sum_{(u,v) \in \mathfrak{M}_0} (d_u + d_v - 2(A^2)_{uv}).$$
(3.26)

## Standard variational bounds on graph spectra

Inequalities that arise from min-max and good choices of trial functions.

For example, Fiedler showed in 1973 that for the graph Laplacian  $(0 = \lambda_0 < \lambda_1 \le ... \le \lambda_{n-1} \le n)$  $\lambda_1 \le \frac{n}{n-1} \min_k d_k, \quad \frac{n}{n-1} \max_k d_k \le \lambda_{n-1}$ 

## Standard min-max bounds on sums With a suitable orthonormal set,

$$\sum_{\ell=0}^{k-1} \mu_{\ell} \leq \sum_{\ell=0}^{k-1} \left\langle M\phi^{(\ell)}, \phi^{(\ell)} \right\rangle,$$

 $\sum_{\ell=k}^{n-1} \mu_\ell \geq \sum_{\ell=k}^{n-1} \Big\langle M \phi^{(\ell)}, \phi^{(\ell)} \Big\rangle,$ 

#### Variational bounds on sums

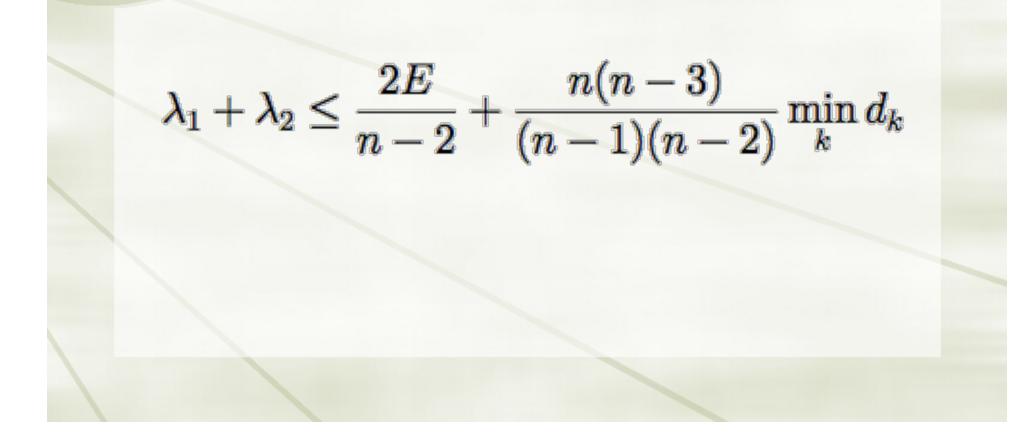
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#### Variational bounds on sums

A good way to generate an o.n. set is with eigenvectors of a reference operator. Here is a new choice of that reference operator

$$T_p := \begin{pmatrix} p & 0 & \dots & 0 & -1 & -1 & \dots & -1 \\ 0 & p & \dots & 0 & -1 & -1 & \dots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & p & -1 & -1 & \dots & -1 \\ -1 & -1 & \dots & -1 & n & -1 & \dots & -1 \\ -1 & -1 & \dots & -1 & n & -1 & \dots & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -1 & -1 & \dots & -1 & -1 & \dots & n & -1 \end{pmatrix}$$

Variational bounds on sums Alternative for  $\lambda_1 + \lambda_2$ :



### Variational bounds on graph spectra $\sum_{\ell=1}^{L} \lambda_{\ell} \leq \frac{(n-L+1)\sum_{k=n-L+1}^{n} d_{k} - 1}{n-L}$

(where the degrees are in decreasing order)

 $\sum_{\ell}^{L} \lambda_{\ell} \leq \frac{L \sum_{k}^{L+1} d_{k} - 1}{L+1}$  optimal for the complete and star graphs

# Variational bounds on graph spectra Generalization of Fiedler:

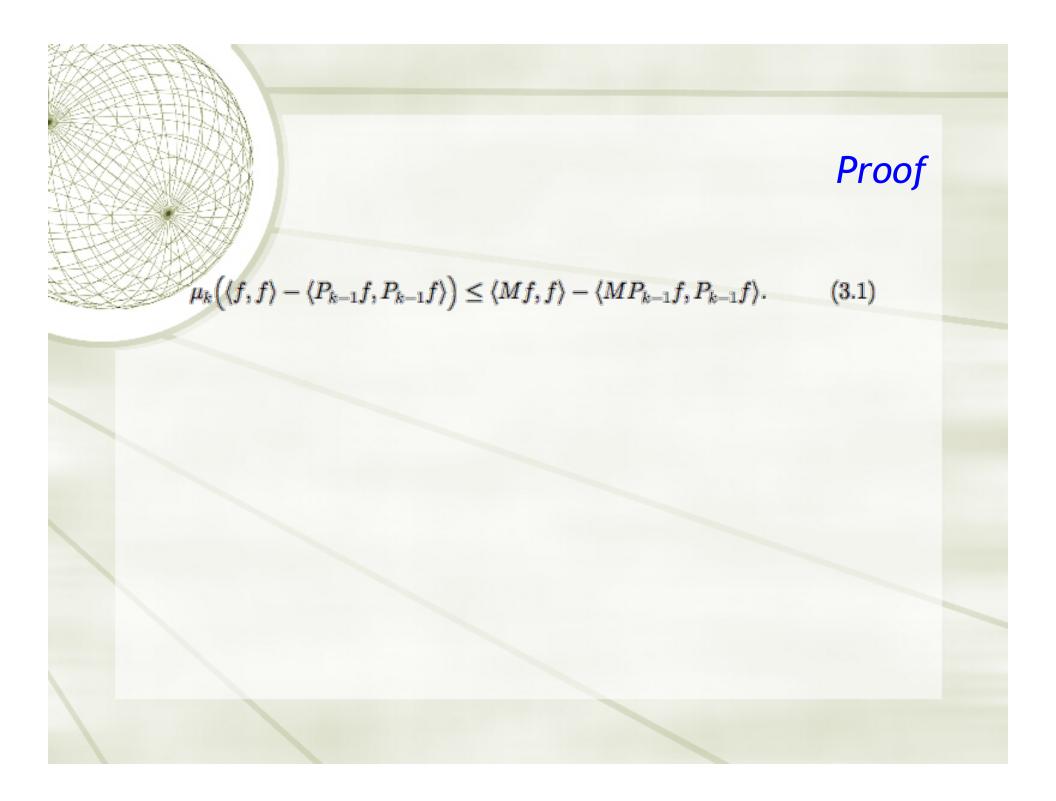
$$\begin{aligned} & \text{For any } L = 1, \dots, n-1 \text{ we get} \\ & \sum_{i=1}^{L} \lambda_i \leq \frac{L}{L+1} \sum_{i=1}^{L+1} d_i + \frac{1}{L+1} \sum_{\substack{\alpha=1 \ \beta=1 \\ \beta \neq \alpha}}^{L+1} A_{\alpha\beta} \leq \sum_{i=N-L+1}^{N} \lambda_i \\ & \sum_{i=1}^{L} \lambda_i \leq \frac{n-L+1}{n-L} \sum_{i=n-L+1}^{n} d_i + \frac{1}{n-L} \sum_{\substack{\alpha=n-L+1 \ \beta=n-L+1 \\ \beta \neq \alpha}}^{n} \sum_{\substack{\alpha=n-L+1 \\ \beta \neq \alpha}}^{n} A_{\alpha\beta} \leq \sum_{i=N-L+1}^{N} \lambda_i. \end{aligned}$$

#### **Proof of the averaged variational inequality for sums**

**Theorem 3.1** Consider a self-adjoint operator M on a Hilbert space  $\mathcal{H}$ , with ordered, entirely discrete spectrum  $-\infty < \mu_0 \leq \mu_1 \leq \ldots$  and corresponding normalized eigenvectors  $\{\psi^{(\ell)}\}$ . Let  $f_z$  be a family of vectors in  $\mathcal{Q}(M)$  indexed by a variable z ranging over a measure space  $(\mathfrak{M}, \Sigma, \sigma)$ . Suppose that  $\mathfrak{M}_0$  is a subset of  $\mathfrak{M}$ . Then for any eigenvalue  $\mu_k$  of M,

$$\begin{aligned}
\mu_k \left( \int_{\mathfrak{M}_0} \langle f_z, f_z \rangle \, d\sigma - \sum_{j=0}^{k-1} \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma \right) \\
\leq \\
\int_{\mathfrak{M}_0} \langle Hf_z, f_z \rangle \, d\sigma - \sum_{j=0}^{k-1} \mu_j \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma,
\end{aligned} \tag{3.2}$$

provided that the integrals converge.





$$\mu_k \Big( \langle f, f \rangle - \langle P_{k-1}f, P_{k-1}f \rangle \Big) \le \langle Mf, f \rangle - \langle MP_{k-1}f, P_{k-1}f \rangle. \tag{3.1}$$

By integrating (3.1),

$$\mu_{k} \int_{\mathfrak{M}_{0}} \left( \langle f_{z}, f_{z} \rangle - \langle P_{k-1}f, P_{k-1}f_{z} \rangle \right) d\sigma$$

$$\leq \int_{\mathfrak{M}_{0}} \langle Mf_{z}, f_{z} \rangle \, d\sigma - \int_{\mathfrak{M}_{0}} \langle MP_{k-1}f_{z}, P_{k-1}f_{z} \rangle \, d\sigma,$$
(3.3)



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(3.3)

$$\begin{split} \mu_k \int_{\mathfrak{M}_0} \left( \langle f_z, f_z \rangle - \sum_{j=0}^{k-1} |\langle f_z, \psi^{(j)} \rangle|^2 \right) d\sigma \qquad (3.4) \\ &\leq \int_{\mathfrak{M}_0} \langle M f_z, f_z \rangle \, d\sigma - \int_{\mathfrak{M}_0} \sum_{j=0}^{k-1} \mu_j |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma. \end{split}$$

Since  $\mu_k$  is larger than or equal to any weighted average of  $\mu_1 \dots \mu_{k-1}$ , we add to (3.4) the inequality

$$-\mu_k \int_{\mathfrak{M}\setminus\mathfrak{M}_0} \left( \sum_{j=0}^{k-1} |\langle f_z, \psi^{(j)} \rangle|^2 \right) d\sigma \leq -\int_{\mathfrak{M}\setminus\mathfrak{M}_0} \sum_{j=0}^{k-1} \mu_j |\langle f_z, \psi^{(j)} \rangle|^2 d\sigma, \quad (3.5)$$

and obtain the claim.

or

How to use the averaged variational bound to get sharp results for graphs?

$$\begin{aligned}
\mu_k \left( \int_{\mathfrak{M}_0} \langle f_z, f_z \rangle \, d\sigma - \sum_{j=0}^{k-1} \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma \right) \\
\leq \\
\int_{\mathfrak{M}_0} \langle Hf_z, f_z \rangle \, d\sigma - \sum_{i=0}^{k-1} \mu_j \int_{\mathfrak{M}} |\langle f_z, \psi^{(j)} \rangle|^2 \, d\sigma,
\end{aligned} \tag{3.2}$$



Extensions to other functions of eigenvalues

**Lemma 3.1 (Karamata-Ostrowski)** Let two nondecreasing ordered sequences of real numbers  $\{\mu_j\}$  and  $\{m_j\}$ , j = 0, ..., n - 1, satisfy

$$\sum_{j=0}^{k-1} \mu_j \le \sum_{j=0}^{k-1} m_j \tag{3.7}$$

for each k. Then for any differentiable convex function  $\Psi(x)$ ,

$$\sum_{j=0}^{k-1} \Psi(\mu_j) \geq \sum_{j=0}^{k-1} \Psi(m_j) + \Psi'(m_{k-1}) \cdot \sum_{j=0}^{k-1} (\mu_j - m_j)$$

In particular, assuming either that  $\Psi$  is nonincreasing or that  $\sum_{j=0}^{k-1} \mu_j = \sum_{j=0}^{k-1} m_j$ ,

$$\sum_{j=0}^{k-1} \Psi(\mu_j) \ge \sum_{j=0}^{k-1} \Psi(m_j)$$

#### Abstract

We use two variational techniques to prove upper bounds for sum of the lowest several eigenvalues of matrices associated with finite, simple, combinatorial graphs. These include estimates for the adjacency matrix of a graph and for both the standard combinatorial Laplacian and the renormalized Laplacian. We also provide upper bounds for sums of squares of eigenvalues of these three matrices.

 Using a traditional variational method, we generalize an inequality of Fiedler for the extreme eigenvalues of the graph Laplacian, producing a sharp bound on the sums of the smallest (or largest) k such eigenvalues, k < n.</li>

#### Abstract

- We also introduce a new variational principle for sums of eigenvalues, in which orthogonalization plays no role, but is replaced by an averaging. We use this principle to obtain further sharp bounds resembling the classic Weyl law for continuous Laplacians, i.e., which connect the distribution of the eigenvalues to the dimension. In this case the dimension is that of a regular lattice in which the graph can be embedded as a subgraph.
- This and related estimates for provide a family of necessary conditions for the embeddability of the graph in a regular lattice of dimension v.
- This is joint work with J. Stubbe of EPFL. Most of these results will appear in Linear Alg. Appl..and are available in arXiv: 1308.5340