Randomised Algorithms

Lecture 12: Spectral Graph Clustering

Thomas Sauerwald (tms41@cam.ac.uk)

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Outline

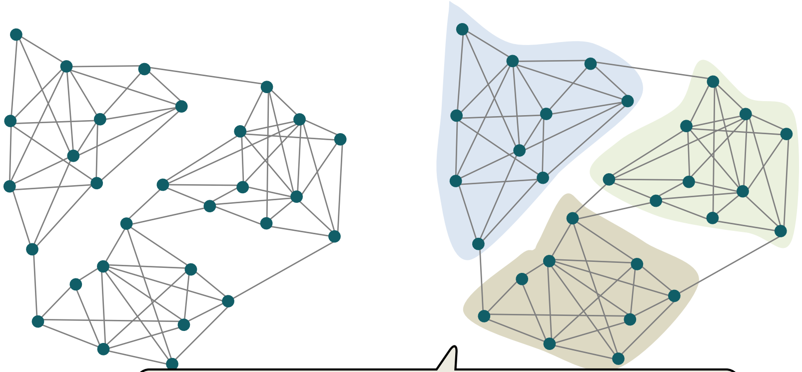
Conductance, Cheeger's Inequality and Spectral Clustering

Illustrations of Spectral Clustering and Extension to Non-Regular Graphs

Appendix: Relating Spectrum to Mixing Times (non-examinable)

Graph Clustering

*Partition the graph into **pieces (clusters)** so that vertices in the same piece have, on average, more connections among each other than with vertices in other clusters*



Let us for simplicity focus on the case of **two clusters**!

Conductance

Conductance

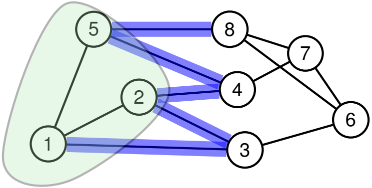
Let $G = (V, E)$ be a d-regular and undirected graph and $\emptyset \neq S \subsetneq V$. The conductance (edge expansion) of S is

$$\phi(S) := \frac{e(S, S^c)}{d \cdot |S|}$$

Moreover, the conductance (edge expansion) of the graph G is

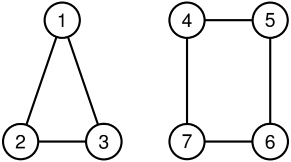
$$\phi(G) := \min_{S \subseteq V:\ 1 \leq |S| \leq n/2} \phi(S)$$

NP-hard to compute!



- $\phi(S) = \frac{5}{9}$
- $\phi(G) \in [0, 1]$ and $\phi(G) = 0$ iff G is disconnected
- If G is a complete graph, then $e(S, V \setminus S) = |S| \cdot (n - |S|)$ and $\phi(G) \approx 1/2$.

λ_2 versus Conductance (1/2)



$$\phi(G) = 0 \quad \Leftrightarrow \quad G \text{ is disconnected} \quad \Leftrightarrow \quad \lambda_2(G) = 0$$

What is the relationship between $\phi(G)$ and $\lambda_2(G)$ for **connected** graphs?

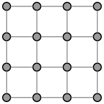
λ_2 versus Conductance (2/2)

1D Grid (Path)

$\lambda_2 \sim n^{-2}$

$\phi \sim n^{-1}$

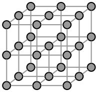
2D Grid



$\lambda_2 \sim n^{-1}$

$\phi \sim n^{-1/2}$

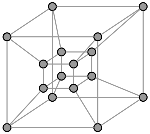
3D Grid



$\lambda_2 \sim n^{-2/3}$

$\phi \sim n^{-1/3}$

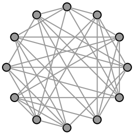
Hypercube



$\lambda_2 \sim (\log n)^{-1}$

$\phi \sim (\log n)^{-1}$

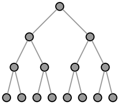
Random Graph (Expanders)



$\lambda_2 = \Theta(1)$

$\phi = \Theta(1)$

Binary Tree



$\lambda_2 \sim n^{-1}$

$\phi \sim n^{-1}$

Relating λ_2 and Conductance

Cheeger's inequality

Let G be a d-regular undirected graph and $\lambda_1 \leq \cdots \leq \lambda_n$ be the eigenvalues of its Laplacian matrix. Then,

$$\frac{\lambda_2}{2} \leq \phi(G) \leq \sqrt{2\lambda_2}.$$

Spectral Clustering:

1. Compute the eigenvector x corresponding to λ_2
2. Order the vertices so that $x_1 \leq x_2 \leq \cdots \leq x_n$ (embed V on $\mathbb{R}$)
3. Try all $n-1$ sweep cuts of the form $(\{1, 2, \ldots, k\}, \{k+1, \ldots, n\})$ and return the one with smallest conductance

- It returns cluster $S \subseteq V$ such that $\phi(S) \leq \sqrt{2\lambda_2} \leq 2\sqrt{\phi(G)}$
- no constant factor worst-case guarantee, but usually works well in practice (see examples later!)
- very fast: can be implemented in $O(|E| \log |E|)$ time

Proof of Cheeger's Inequality (non-examinable)

Proof (of the easy direction):

Optimisation Problem: Embed vertices on a line such that sum of squared distances is minimised

- By the Courant-Fischer Formula,

$$\lambda_2 = \min_{\substack{x \in \mathbb{R}^n \\ x \neq 0, x \perp 1}} \frac{x^T \mathbf{L} x}{x^T x} = \frac{1}{d} \cdot \min_{\substack{x \in \mathbb{R}^n \\ x \neq 0, x \perp 1}} \frac{\sum_{u \sim v} (x_u - x_v)^2}{\sum_u x_u^2}.$$

- Let $S \subseteq V$ be the subset for which $\phi(G)$ is minimised. Define $y \in \mathbb{R}^n$ by:

$$y_u = \begin{cases} \frac{1}{|S|} & \text{if } u \in S, \\ -\frac{1}{|V \setminus S|} & \text{if } u \in V \setminus S. \end{cases}$$

- Since $y \perp 1$, it follows that

$$\lambda_2 \leq \frac{1}{d} \cdot \frac{\sum_{u \sim v} (y_u - y_v)^2}{\sum_u y_u^2} = \frac{1}{d} \cdot \frac{|E(S, V \setminus S)| \cdot (\frac{1}{|S|} + \frac{1}{|V \setminus S|})^2}{\frac{1}{|S|} + \frac{1}{|V \setminus S|}}$$

$$= \frac{1}{d} \cdot |E(S, V \setminus S)| \cdot \left(\frac{1}{|S|} + \frac{1}{|V \setminus S|} \right)$$

$$\leq \frac{1}{d} \cdot \frac{2 \cdot |E(S, V \setminus S)|}{|S|} = 2 \cdot \phi(G). \qquad \square$$

Outline

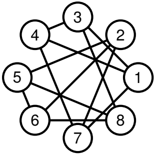
Conductance, Cheeger's Inequality and Spectral Clustering

Illustrations of Spectral Clustering and Extension to Non-Regular Graphs

Appendix: Relating Spectrum to Mixing Times (non-examinable)

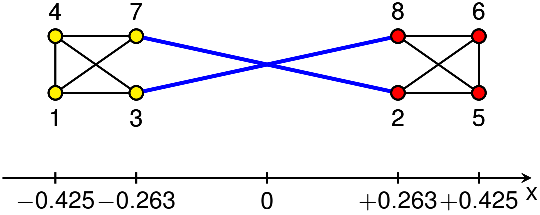
Illustration on a small Example

$$\mathbf{A} = \begin{pmatrix} 0&0&1&1&0&0&1&0\\ 0&0&0&0&1&1&1&0\\ 1&0&0&1&0&0&0&1\\ 1&0&1&0&0&0&1&0\\ 0&1&0&0&0&1&0&1\\ 0&1&0&0&1&0&0&1\\ 1&1&0&1&0&0&0&0\\ 0&0&1&0&1&1&0&0 \end{pmatrix} \qquad \mathbf{L} = \begin{pmatrix} 1&0&-\frac{1}{3}&-\frac{1}{3}&0&0&-\frac{1}{3}&0\\ 0&1&0&0&-\frac{1}{3}&-\frac{1}{3}&-\frac{1}{3}&0\\ -\frac{1}{3}&0&1&-\frac{1}{3}&0&0&0&-\frac{1}{3}\\ -\frac{1}{3}&0&-\frac{1}{3}&1&0&0&-\frac{1}{3}&0\\ 0&-\frac{1}{3}&0&0&1&-\frac{1}{3}&0&-\frac{1}{3}\\ 0&-\frac{1}{3}&0&0&-\frac{1}{3}&1&0&-\frac{1}{3}\\ -\frac{1}{3}&-\frac{1}{3}&0&-\frac{1}{3}&0&0&1&0\\ 0&0&-\frac{1}{3}&0&-\frac{1}{3}&-\frac{1}{3}&0&1 \end{pmatrix}$$



$$\lambda_2 = 1 - \sqrt{5}/3 \approx 0.25$$

$$v = (-0.425, +0.263, -0.263, -0.425, +0.425, +0.425, -0.263, +0.263)^T$$



Sweep: 4

Conductance: 0.166

Physical Interpretation of the Minimisation Problem

- For each edge $\{u, v\} \in E(G)$, add spring between pins at x_u and x_v
- The potential energy at each spring is $(x_u - x_v)^2$
- Courant-Fisher characterisation:

$$\lambda_2 = \min_{\substack{x \in \mathbb{R}^n \setminus \{\mathbf{0}\} \\ x \perp \mathbf{1}}} \frac{x^T \mathbf{L} x}{x^T x} = \frac{1}{d} \cdot \min_{\substack{x \in \mathbb{R}^n \\ \|x\|_2^2 = 1, x \perp \mathbf{1}}} (x_u - x_v)^2$$

- In our example, we found out that $\lambda_2 \approx 0.25$
- The eigenvector x on the last slide is normalised (i.e., $\|x\|_2^2 = 1$). Hence,

$$\lambda_2 = \frac{1}{3} \cdot \left((x_1 - x_3)^2 + (x_1 - x_4)^2 + (x_1 - x_7)^2 + \cdots + (x_6 - x_8)^2 \right) \approx 0.25$$

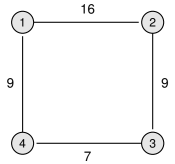
Let us now look at an example of a non-regular graph!

The Laplacian Matrix (General Version)

The (normalised) Laplacian matrix of $G = (V, E, w)$ is the n by n matrix

$$\mathbf{L} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$$

where $\mathbf{D}$ is a diagonal $n \times n$ matrix such that $\mathbf{D}_{uu} = deg(u) = \sum_{v\colon \{u,v\}\in E} w(u,v)$, and $\mathbf{A}$ is the weighted adjacency matrix of G.



$$\mathbf{L} = \begin{pmatrix} 1 & -16/25 & 0 & -9/20 \\ -16/25 & 1 & -9/20 & 0 \\ 0 & -9/20 & 1 & -7/16 \\ -9/20 & 0 & -7/16 & 1 \end{pmatrix}$$

- $\mathbf{L}_{uv} = -\frac{w(u,v)}{\sqrt{d_u d_v}}$ for $u \neq v$
- $\mathbf{L}$ is symmetric
- If G is d-regular, $\mathbf{L} = \mathbf{I} - \frac{1}{d} \cdot \mathbf{A}$.

Conductance and Spectral Clustering (General Version)

Conductance (General Version)

Let $G = (V, E, w)$ and $\emptyset \subsetneq S \subsetneq V$. The conductance (edge expansion) of S is

$$\phi(S) := \frac{w(S, S^c)}{\min\{\mathrm{vol}(S), \mathrm{vol}(S^c)\}},$$

where $w(S, S^c) := \sum_{u \in S, v \in S^c} w(u, v)$ and $\mathrm{vol}(S) := \sum_{u \in S} d(u)$. Moreover, the conductance (edge expansion) of G is

$$\phi(G) := \min_{\emptyset \neq S \subsetneq V} \phi(S).$$

Spectral Clustering (General Version):

1. Compute the eigenvector x corresponding to λ_2 **and** $y = \mathbf{D}^{-1/2}x$.
2. Order the vertices so that $y_1 \leq y_2 \leq \cdots \leq y_n$ (embed V on $\mathbb{R}$)
3. Try all $n-1$ sweep cuts of the form $(\{1, 2, \ldots, k\}, \{k+1, \ldots, n\})$ and return the one with smallest conductance

Stochastic Block Model and 1D-Embedding

Stochastic Block Model

$G = (V, E)$ with clusters $S_1, S_2 \subseteq V$, $0 \leq q < p \leq 1$

$$\mathbf{P}[\{u, v\} \in E] = \begin{cases} p & \text{if } u, v \in S_i, \\ q & \text{if } u \in S_i, v \in S_j, i \neq j. \end{cases}$$

Here:

- $|S_1| = 80$, $|S_2| = 120$
- $p = 0.08$
- $q = 0.01$

```
Number of Vertices: 200
Number of Edges:  919
Eigenvalue  1  :  -1.1968431479565368e-16
Eigenvalue  2  :  0.1543784937248489
Eigenvalue  3  :  0.37049909753568877
Eigenvalue  4  :  0.39770640242147404
Eigenvalue  5  :  0.4316114413430584
Eigenvalue  6  :  0.44379221120189777
Eigenvalue  7  :  0.4564011652684181
Eigenvalue  8  :  0.4632911204500282
Eigenvalue  9  :  0.474638606357877
Eigenvalue  10  :  0.4814019607292904
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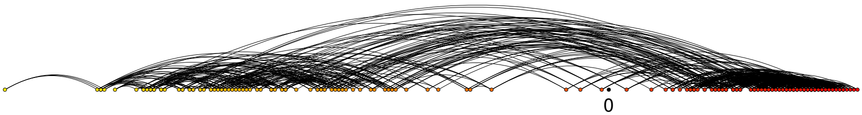
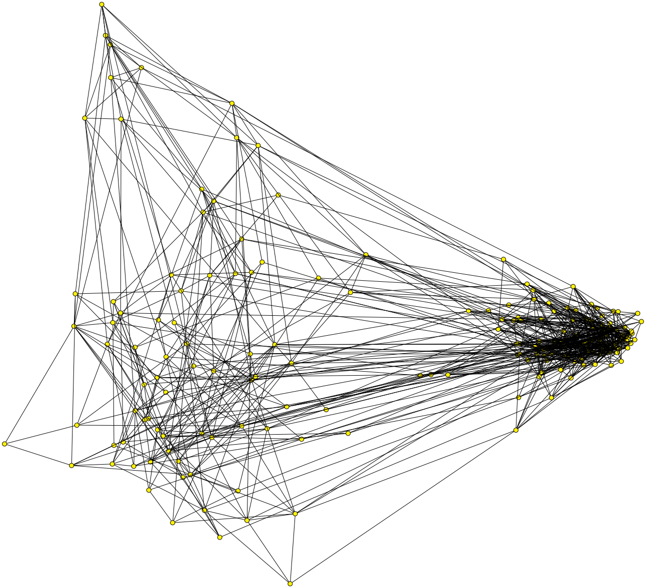
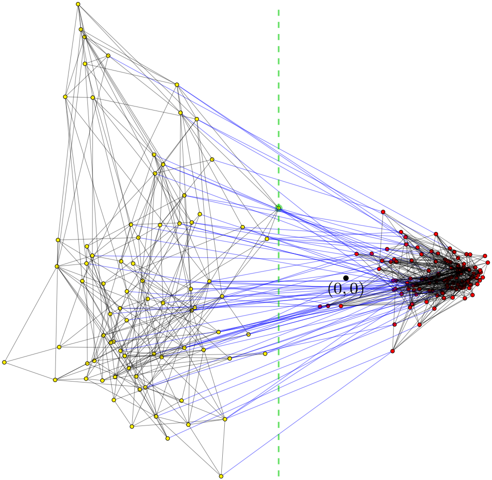


Drawing the 2D-Embedding

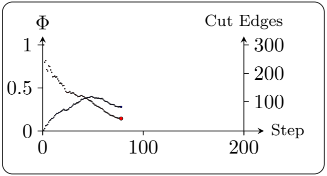


Best Solution found by Spectral Clustering

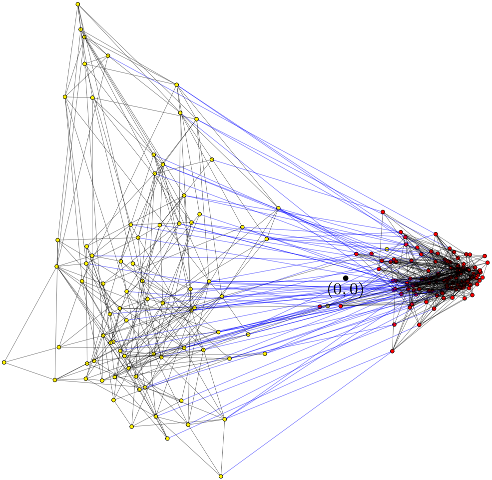
For the complete animation, see the full slides.



- Step: 78
- Threshold: −0.0336
- Partition Sizes: 78/122
- Cut Edges: 84
- Conductance: 0.1448



Clustering induced by Blocks



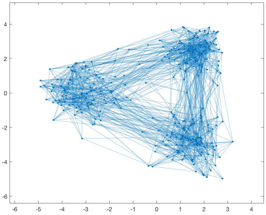
- Step: –
- Threshold: –
- Partition Sizes: 80/120
- Cut Edges: 88
- Conductance: 0.1486

Additional Example: Stochastic Block Models with 3 Clusters

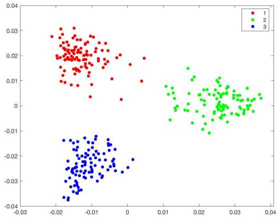
Graph $G = (V, E)$ with clusters
$S_1, S_2, S_3 \subseteq V; \quad 0 \leq q < p \leq 1$

$$\mathbf{P}[\{u, v\} \in E] = \begin{cases} p & u, v \in S_i \\ q & u \in S_i, v \in S_j, i \neq j \end{cases}$$

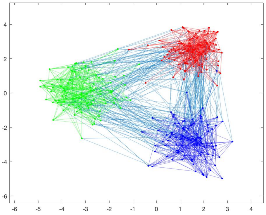
$|V| = 300, |S_i| = 100$
$p = 0.08, q = 0.01.$



Spectral embedding



Output of Spectral Clustering



How to Choose the Cluster Number k

- If k is unknown:
  - small λ_k means there exist k sparsely connected subsets in the graph (recall: $\lambda_1 = \ldots = \lambda_k = 0$ means there are k connected components)
  - large λ_{k+1} means all these k subsets have "good" inner-connectivity properties (cannot be divided further)

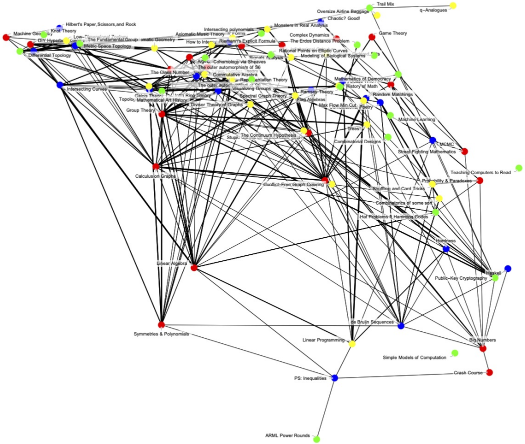
  $\Rightarrow$ choose smallest $k \geq 2$ so that the spectral gap $\lambda_{k+1} - \lambda_k$ is "large"

- In the latter example $\lambda = \{0, 0.20, 0.22, 0.43, 0.45, \ldots\} \implies k = 3$.

- In the former example $\lambda = \{0, 0.15, 0.37, 0.40, 0.43, \ldots\} \implies k = 2$.

- For $k = 2$ use sweep-cut extract clusters. For $k \geq 3$ use embedding in k-dimensional space and apply k-means (geometric clustering)

Another Example



(many thanks to Kalina Jasinska)

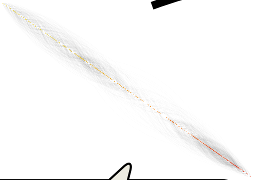
- nodes represent math topics taught within 4 weeks of a Mathcamp
- node colours represent to the week in which they thought
- teachers were asked to assign weights in $0 - 10$ indicating how closely related two classes are

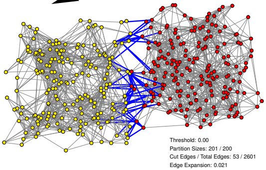
Summary: Spectral Clustering

Spectral Embedding onto Line

Compute Sweep Cuts

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$





$$\min_{\substack{x \in \mathbb{R}^n \setminus \{\mathbf{0}\} \\ x \perp \mathbf{1}}} \frac{\sum_{u \sim v} (x_u - x_v)^2}{\sum_u x_u^2}$$

- Given any graph (adjacency matrix)
- Graph Spectrum (computable in poly-time)
  - λ_2 (relates to connectivity)
  - λ_n (relates to bipartiteness)

  ...

- Cheeger's Inequality
  - relates λ_2 to conductance
  - unbounded approximation ratio
  - effective in practice

Outline

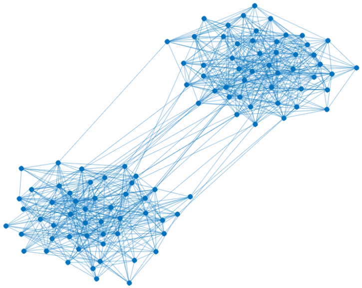
Conductance, Cheeger's Inequality and Spectral Clustering

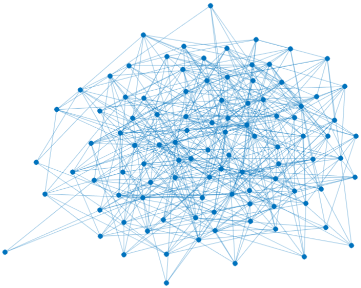
Illustrations of Spectral Clustering and Extension to Non-Regular Graphs

Appendix: Relating Spectrum to Mixing Times (non-examinable)

Relation between Clustering and Mixing (non-examinable)

- Which graph has a "cluster-structure"?
- Which graph mixes faster?





Convergence of Random Walk (non-examinable)

Recall: If the underlying graph G is connected, undirected and d-regular, then the random walk converges towards the stationary distribution $\pi = (1/n, \ldots, 1/n)$, which satisfies $\pi \mathbf{P} = \pi$.

Here all vector multiplications (including eigenvectors) will always be from the left!

Lemma

Consider a lazy random walk on a connected, undirected and d-regular graph. Then for any initial distribution x,

$$\left\| x\mathbf{P}^t - \pi \right\|_2 \leq \lambda^t,$$

with $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ as eigenvalues and $\lambda := \max\{|\lambda_2|, |\lambda_n|\}$.

$\Rightarrow$ This implies for $t = \mathcal{O}\left(\frac{\log n}{\log(1/\lambda)}\right) = \mathcal{O}\left(\frac{\log n}{1-\lambda}\right)$,

$$\left\| x\mathbf{P}^t - \pi \right\|_{tv} \leq \frac{1}{4}.$$

due to laziness, $\lambda_n \geq 0$

Proof of Lemma (non-examinable)

- Express x in terms of the orthonormal basis of $\mathbf{P}$, $v_1 = \pi, v_2, \ldots, v_n$:

$$x = \sum_{i=1}^{n} \alpha_i v_i.$$

- Since x is a probability vector and all $v_i \geq 2$ are orthogonal to π, $\alpha_1 = 1$.

$\Rightarrow$

$$\begin{aligned}
\|x\mathbf{P} - \pi\|_2^2 &= \left\| \left(\sum_{i=1}^{n} \alpha_i v_i \right) \mathbf{P} - \pi \right\|_2^2 \\
&= \left\| \pi + \sum_{i=2}^{n} \alpha_i \lambda_i v_i - \pi \right\|_2^2 \\
&= \left\| \sum_{i=2}^{n} \alpha_i \lambda_i v_i \right\|_2^2 \\
&= \sum_{i=2}^{n} \|\alpha_i \lambda_i v_i\|_2^2 \\
&\leq \lambda^2 \sum_{i=2}^{n} \|\alpha_i v_i\|_2^2 = \lambda^2 \left\| \sum_{i=2}^{n} \alpha_i v_i \right\|_2^2 = \lambda^2 \|x - \pi\|_2^2
\end{aligned}$$

since the v_i's are orthogonal

since the v_i's are orthogonal

- Hence $\|x\mathbf{P}^t - \pi\|_2^2 \leq \lambda^{2t} \cdot \|x - \pi\|_2^2 \leq \lambda^{2t} \cdot 1.$

$\|x - \pi\|_2^2 + \|\pi\|_2^2 = \|x\|_2^2 \leq 1$

Some References on Spectral Graph Theory and Clustering

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The End...

Thank you and Best Wishes for the Exam!