CS5275 – The Algorithm Designer's Toolkit (S2 AY2025/26)

Lecture 4:

Expanders – spectral graph theory

Matrix representation of graphs

- Let $G = (V, E)$ be a graph, with $V = \{1,2, \ldots, n\}$.

The adjacency matrix $\boldsymbol{A}$ is an $(n \times n)$-matrix:

$$\boldsymbol{A}[i,j] = \begin{cases} 0, & \{i,j\} \notin E \\ 1, & \{i,j\} \in E \end{cases}$$

The degree matrix $\boldsymbol{D}$ is an $(n \times n)$-matrix:

$$\boldsymbol{D}[i,j] = \begin{cases} \deg(i), & i = j \\ 0, & i \neq j \end{cases}$$

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The <u>Laplacian matrix</u>: $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A}$

The <u>normalized Laplacian matrix</u>: $\boldsymbol{N} = \boldsymbol{D}^{-1/2}\boldsymbol{L}\boldsymbol{D}^{-1/2}$

Connection to cuts

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The Laplacian matrix: $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A}$

The normalized Laplacian matrix: $\boldsymbol{N} = \boldsymbol{D}^{-1/2}\boldsymbol{L}\boldsymbol{D}^{-1/2}$

Let $\boldsymbol{x} \in \mathbb{R}^n$ be a column vector.

$$\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x} = \sum_{\{u,v\}\in E} (x_u - x_v)^2$$

If $\boldsymbol{x} = \boldsymbol{1}_S$ is the indicator vector for a cut $S \subseteq V$, then $\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x} = |E(S, V \setminus S)|$ is the size of the cut.

Regular graphs

- Let $G = (V, E)$ be a d-regular graph, with $V = \{1,2,\dots,n\}$.

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The degree matrix $\boldsymbol{D}$ is an $(n \times n)$-matrix:

$$\boldsymbol{D}[i,j] = d\boldsymbol{I} = \begin{cases} d, & i = j \\ 0, & i \neq j \end{cases}$$

The Laplacian matrix:

$$\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{A} = d\boldsymbol{I} - \boldsymbol{A}$$

The normalized Laplacian matrix:

$$\boldsymbol{N} = \boldsymbol{D}^{-1/2}\boldsymbol{L}\boldsymbol{D}^{-1/2} = \boldsymbol{I} - \frac{1}{d}\boldsymbol{A}$$

For simplicity, we restrict our attention to regular graphs, noting that all results extend to general graphs.

$$\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x} = \sum_{\{u,v\} \in E} (x_u - x_v)^2$$

$$\boldsymbol{x}^\top \boldsymbol{N}\boldsymbol{x} = \frac{1}{d}\sum_{\{u,v\} \in E} (x_u - x_v)^2$$

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For simplicity, we restrict our attention to regular graphs, noting that all results extend to general graphs.

All four types of matrices $\boldsymbol{A}, \boldsymbol{D}, \boldsymbol{L}, \boldsymbol{N}$ are symmetric.
We start by reviewing some basic facts about such matrices.

Symmetric real matrices

- Let $\boldsymbol{M}$ be a real symmetric $(n \times n)$-matrix.

$\boldsymbol{M}[i,j] \in \mathbb{R}$ $\quad\quad$ $\boldsymbol{M}[i,j] = \boldsymbol{M}[j,i]$

Symmetric real matrices

- Let $\boldsymbol{M}$ be a real symmetric $(n \times n)$-matrix.

Theorem: There exist
- $\lambda_1, \lambda_2, \dots, \lambda_n \in \mathbb{R}$ (they are called <u>eigenvalues</u>)
- Orthonormal vectors $\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_n \in \mathbb{R}^n$ (they are called <u>eigenvectors</u>)

such that:

$$\boldsymbol{M} = \sum_{i=1}^{n} \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i^\top$$

Which implies: (for all i)

$$\boldsymbol{M}\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$$

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Which implies: (for all i)

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If we change the axes of the Euclidean space $\mathbb{R}^n$ to the eigenvectors $v_1, \dots, v_n$, then the matrix $\boldsymbol{M}$ becomes diagonal, with $\lambda_1, \dots, \lambda_n$ on the diagonal.

In other words, symmetric matrices stretch space independently along orthogonal directions.

Variational characterizations

- Let $\boldsymbol{M}$ be a real symmetric $(n \times n)$-matrix.
  - Eigenvalues: $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$
  - Eigenvectors $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n$

Rayleigh quotient of $\boldsymbol{x}$ with respect to $\boldsymbol{M}$:

$$R_{\boldsymbol{M}}(\boldsymbol{x}) = \frac{\boldsymbol{x}^\top \boldsymbol{M}\boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}}$$

Related to cuts

$$\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x} = \sum_{\{u,v\}\in E} (x_u - x_v)^2$$

$$\boldsymbol{x}^\top \boldsymbol{N}\boldsymbol{x} = \frac{1}{d} \sum_{\{u,v\}\in E} (x_u - x_v)^2$$

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$$\boldsymbol{x}^\top \boldsymbol{N}\boldsymbol{x} = \frac{1}{d} \sum_{\{u,v\}\in E} (x_u - x_v)^2$$

Theorem:

$$\lambda_k = \min_{k-\text{dim space } \mathcal{V}} \max_{\boldsymbol{x}\in\mathcal{V}\setminus\{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$$

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Theorem:

$$\lambda_k = \min_{k-\text{dim space } \mathcal{V}} \max_{\boldsymbol{x} \in \mathcal{V} \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$$

Proof $(\geq)$**:**

Consider $\mathcal{V} = \text{span}\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_k\}$

- Write $\boldsymbol{x} \in \mathcal{V}$ as $\boldsymbol{x} = \sum_{i=1}^{k} \alpha_i \boldsymbol{v}_i$.
- $R_{\boldsymbol{M}}(\boldsymbol{x}) = \frac{\sum_{i=1}^{k} \alpha_i^2 \lambda_i}{\sum_{i=1}^{k} \alpha_i^2}$.
- $\max_{\boldsymbol{x} \in V \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x}) = \lambda_k$.
- $\lambda_k \geq \min_{k-\text{dim space } \mathcal{V}} \max_{\boldsymbol{x} \in V \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$.

Variational characterizations

Rayleigh quotient of $\boldsymbol{x}$ with respect to $\boldsymbol{M}$:

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Theorem:

$$\lambda_k = \min_{k-\text{dim space } \mathcal{V}} \max_{\boldsymbol{x} \in \mathcal{V} \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$$

Proof $(\le)$**:**

Consider any k-dimensional space $\mathcal{V}$.

- $\exists \boldsymbol{x} \in \mathcal{V} \cap \operatorname{span}\{\boldsymbol{v}_k, \dots, \boldsymbol{v}_n\} \setminus \{\boldsymbol{0}\}$.
  - $\boldsymbol{x} = \sum_{i=k}^n \alpha_i \boldsymbol{v}_i$.
  - $R_{\boldsymbol{M}}(\boldsymbol{x}) = \frac{\sum_{i=k}^n \alpha_i^2 \lambda_i}{\sum_{i=k}^n \alpha_i^2} \ge \lambda_k$.
- $\lambda_k \le \min_{k-\text{dim space } \mathcal{V}} \max_{\boldsymbol{x} \in \mathcal{V} \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$.

Variational characterizations

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$$\lambda_k = \min_{k-\text{dim space } \mathcal{V}} \max_{\boldsymbol{x} \in \mathcal{V} \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$$

$$\lambda_1 = \min_{\boldsymbol{x} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$$

Moreover, any minimizer $\boldsymbol{x}$ is a corresponding eigenvector.

Consider $-\boldsymbol{M}$.

$$\lambda_n = \max_{\boldsymbol{x} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$$

Moreover, any maximizer $\boldsymbol{x}$ is a corresponding eigenvector.

Variational characterizations

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A natural extension

$$\lambda_2 = \min_{\boldsymbol{x}\neq\boldsymbol{0},\ \boldsymbol{x}\perp\boldsymbol{v}_1} R_{\boldsymbol{M}}(\boldsymbol{x})$$

Consider $-\boldsymbol{M}$.

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Theorem: We omit the proof.
$$\lambda_k = \min_{\boldsymbol{x} \neq \boldsymbol{0},\ \boldsymbol{x} \perp \operatorname{span}\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{k-1}\}} R_{\boldsymbol{M}}(\boldsymbol{x})$$

Spectral graph theory

- The eigenvalues of $\boldsymbol{A}$ (adjacency), $\boldsymbol{L}$ (Laplacian), and $\boldsymbol{N}$ (normalized Laplacian) reveal information about:
  - Average density of cuts.
  - Bipartiteness.
  - Chromatic number.
  - Conductance.
  - Hamiltonicity.
  - Size of a maximum independent set.
  - Size of a maximum matching.
  - Toughness of a graph.
  - Number of connected components.

https://adga-workshop.org/2025/tijn.pdf

Application 1: Spectral embedding

Data

Graph

Embedding the vertices to $\mathbb{R}^k$ by taking the eigenvectors corresponding to the first k non-zero eigenvalues.

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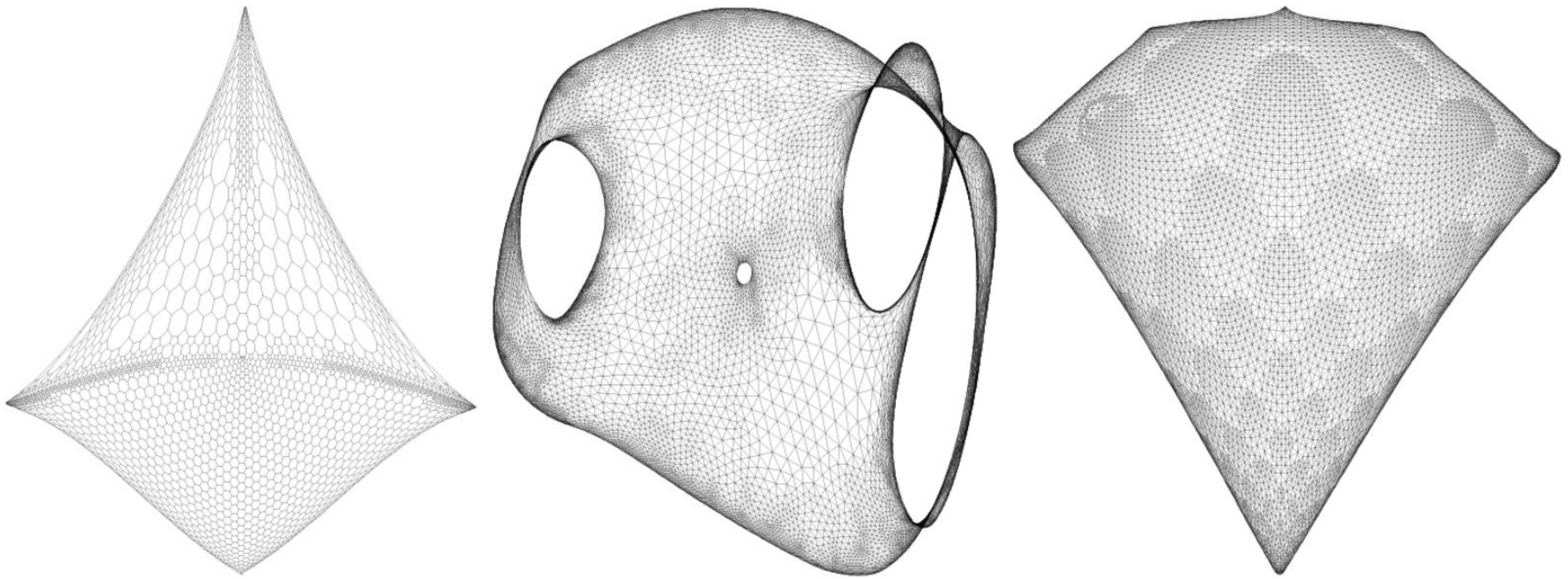
Graph

Embedding the vertices to $\mathbb{R}^k$ by taking the eigenvectors corresponding to the first k non-zero eigenvalues.

- Useful for: Minimizing $\boldsymbol{x}^\top \boldsymbol{L}\boldsymbol{x} = \sum_{\{u,v\}\in E}(x_u - x_v)^2$ leads to natural drawings.
  - **Visualization**



https://www.mathe2.uni-bayreuth.de/axel/papers/koren:on_spectral_graph_drawing.pdf

Application 1: Spectral embedding

Data

Graph

Embedding the vertices to $\mathbb{R}^k$ by taking the eigenvectors corresponding to the first k non-zero eigenvalues.

- Useful for:
  - Visualization
  - **Clustering + dimension reduction** https://en.wikipedia.org/wiki/Spectral_clustering

- Spectral embedding turns high-dimensional data into points in a low-dimensional space where clusters become visible.
- Eigenvectors can capture many features of the data that many traditional clustering methods fail to detect.

Already many theoretical evidences

Application 2: Network analysis

The eigenvector equation

$$\boxed{\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}}$$

$$\boxed{x_v = \frac{1}{\lambda} \sum_{u \in N(v)} x_u}$$

- Intuitively, an eigenvector $\boldsymbol{x}$ captures the influence of nodes in a network:

Connections to influential nodes enhance your own influence.

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Some applications:

- Eigenvector centrality is the unique measure satisfying certain natural axioms for a **ranking system**.
- In **neuroscience**, the eigenvector centrality of a neuron in a model neural network has been found to correlate with its relative firing rate.
- Eigenvector centrality and related concepts have been used to model **opinion influence in sociology and economics**.
- **Google's PageRank** is based on a variant of Eigenvector centrality.

https://en.wikipedia.org/wiki/Eigenvector_centrality

The smallest eigenvalue λ_1

- Consider the normalized Laplacian $\boldsymbol{N}$ of a graph $G = (V, E)$.
  - Eigenvalues: $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$

Theorem:

- $\lambda_1 = 0$, with $\mathbf{1}$ being a corresponding eigenvector.

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$\lambda_1 \geq 0$

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$$\lambda_1 = \min_{\boldsymbol{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}} R_{\boldsymbol{N}}(\boldsymbol{x}) \leq R_{\boldsymbol{N}}(\mathbf{1}) = \frac{\sum_{\{u,v\} \in E} (1-1)^2}{d \sum_{v \in V} 1^2} = 0$$

$\lambda_1 \leq 0$

The eigenvalue λ_k

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Theorem:
- $\lambda_k = 0$ if and only if G has at least k connected components.

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if and only if

For every connected component S,
$x_u = x_v \quad \forall u, v \in S$

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$$R_N(\boldsymbol{x}) = \frac{\boldsymbol{x}^\top \boldsymbol{N} \boldsymbol{x}}{\boldsymbol{x}^\top \boldsymbol{x}} = \frac{\sum_{\{u,v\} \in E} (x_u - x_v)^2}{d \sum_{v \in V} {x_v}^2} = 0$$

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Theorem:
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G has at least k connected components $S_1, \dots, S_k$. $\rightarrow$ Set $\mathcal{V} = \mathrm{span}\{\mathbf{1}_{S_1}, \dots, \mathbf{1}_{S_k}\}$.
- $\forall \boldsymbol{x} \in \mathcal{V} \setminus \{\mathbf{0}\},\ R_N(\boldsymbol{x}) = \mathbf{0}$

$\xrightarrow{\lambda_k = \min_{k\text{-dim space } \mathcal{V}} \max_{\boldsymbol{x} \in \mathcal{V} \setminus \{\mathbf{0}\}} R_N(\boldsymbol{x})}$ $\lambda_k = 0$

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if and only if

For every connected component S,
$x_u = x_v \quad \forall u, v \in S$

Theorem:
- $\lambda_k = 0$ if and only if G has at least k connected components.

$k =$ dimension of $\mathcal{V} \leq$ the number of connected components.

$\lambda_k = 0$

There is a k-dimensional subspace $\mathcal{V}$ of $\mathbb{R}^n$ such that:
- $\forall \boldsymbol{x} \in \mathcal{V} \setminus \{\boldsymbol{0}\},\ R_{\boldsymbol{N}}(\boldsymbol{x}) = \boldsymbol{0}$

The value of $\boldsymbol{x}$ is constant within each connected component.

The largest eigenvalue λ_n

- Consider the normalized Laplacian $\boldsymbol{N}$ of a graph $G = (V, E)$.
  - Eigenvalues: $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$

Theorem:
- $\lambda_n \leq 2$.
- $\lambda_n = 2$ if and only if G has a bipartite connected component.

$$\lambda_n = \max_{\boldsymbol{x} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{N}}(\boldsymbol{x})$$

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$$\lambda_n = \max_{\boldsymbol{x} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}} R_{\boldsymbol{N}}(\boldsymbol{x}) = 2 - \min_{\boldsymbol{x} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}} \frac{\sum_{\{u,v\} \in E} (x_u + x_v)^2}{d \sum_{v \in V} {x_v}^2} \leq 2$$

$$R_{\boldsymbol{N}}(\boldsymbol{x}) = \frac{\sum_{\{u,v\} \in E} (x_u - x_v)^2}{d \sum_{v \in V} {x_v}^2}$$

$$= \frac{2 \sum_{\{u,v\} \in E} (x_u^2 + x_v^2) - \sum_{\{u,v\} \in E} (x_u + x_v)^2}{d \sum_{v \in V} {x_v}^2}$$

$$= 2 - \frac{\sum_{\{u,v\} \in E} (x_u + x_v)^2}{d \sum_{v \in V} {x_v}^2}$$

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$$\lambda_n = 2 - \min_{\boldsymbol{x} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}} \frac{\sum_{\{u,v\} \in E} (x_u + x_v)^2}{d \sum_{v \in V} {x_v}^2}$$

- Suppose G has a bipartite connected component S with bipartition $S = A \cup B$.
- Setting $\boldsymbol{x} = \mathbf{1}_A - \mathbf{1}_B$ makes $\frac{\sum_{\{u,v\} \in E} (x_u + x_v)^2}{d \sum_{v \in V} {x_v}^2} = 0$.
- Therefore, $\lambda_n = 2$.

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- Suppose $\lambda_n = 2$.
- There exists $\boldsymbol{x} \in \mathbb{R}^n \setminus \{\boldsymbol{0}\}$ such that $\frac{\sum_{\{u,v\} \in E} (x_u + x_v)^2}{d \sum_{v \in V} {x_v}^2} = 0$.
- Define:
  - $A = \{v \in V \mid x_v > 0\} \neq \emptyset$
  - $B = \{v \in V \mid x_v < 0\} \neq \emptyset$
- $A \cup B$ is a union of bipartite connected components.

Outlook

- **Next:** We will show that:

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

Cheeger's inequality

where λ_2 is the second eigenvalue of the normalized Laplacian $\boldsymbol{N}$ of G.

Moreover, given the eigenvector $\boldsymbol{v}_2$, we can obtain a cut of conductance at most $\sqrt{2\lambda_2}$ in polynomial time.

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

Cheeger's inequality

where λ_2 is the second eigenvalue of the normalized Laplacian $\boldsymbol{N}$ of G.

Moreover, given the eigenvector $\boldsymbol{v}_2$, we can obtain a cut of conductance at most $\sqrt{2\lambda_2}$ in polynomial time.

- **Next:** $\underbrace{\text{Efficient eigenvector computation.}}_{\text{Useful in many applications, both in practice and in theory.}}$

References

- **Main reference:**
  - Lecture 4.1 of https://sites.google.com/site/thsaranurak/teaching/Expander
  - Chapters 1, 2, and 3 of https://lucatrevisan.github.io/books/expanders-2016.pdf