University of Edinburgh

INFR11156: Algorithmic Foundations of Data Science (2025)

Lecture 8: Graphs versus Matrices

Graphs are one of the most fundamental objects to represent the relations of data items and are ubiquitous in every research field of computer science. Among many techniques studying graphs, spectral graph theory investigates the algebraic properties of the matrices associated with graphs, which has had a tremendous impact in computer science. In particular, spectral techniques have been successfully used to overcome fundamental barriers faced by combinatorial algorithms, and key concepts developed in algorithmic spectral graph theory have led to many breakthroughs in designing fast algorithms in data science. In the upcoming five lectures, we will study algebraic properties of graphs: we will see how basic graph properties can be derived from the eigenvalues of a graph matrix, and how algebraic techniques will be applied to design faster graph algorithms.

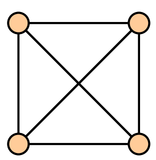
We assume that $G = (V, E)$ is an undirected and unweighted graph with n vertices. The set of neighbours of vertex u is represented by $N(u)$, and its degree is $d_u = |N(u)|$. For simplicity, we write $u \sim v$ if $\{u, v\}$ is an edge of G. For any set $S \subseteq V$, let $\mathrm{vol}(S) = \sum_{u \in S} d_u$. In particular, let $\mathrm{vol}(G) = \sum_{u \in V[G]} d_u$.

1 Graph Laplacians

We first define the matrices used in the lecture. Let $D \in \mathbb{R}^{n \times n}$ be the diagonal matrix where $D_{u,u} = d_u$ for any vertex u. The **adjacency matrix** of graph G is the matrix A defined by $A_{u,v} = 1$ if $u \sim v$, and $A_{u,v} = 0$ otherwise. In particular, we write $A_{u,u} = 1$ if there is a self-loop of vertex u. The **Laplacian matrix** of G is defined by $L = D - A$, where A is the **adjacency matrix** of G. The **normalised Laplacian matrix** of G is defined by

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

Hence, it holds that $\mathcal{L} = I - (1/d) \cdot A$ if G is d-regular, see Figure 1 for example. For matrix $\mathcal{L}$, we denote its n eigenvalues with $\lambda_1 \leq \ldots \leq \lambda_n$ with corresponding orthonormal eigenvectors $f_1, \ldots, f_n$. The set of n eigenvalues $\{\lambda_i\}_{i=1}^n$ together with their multiplicities is called the **spectrum** of G.



$$L_G = \begin{pmatrix} 1 & -1/3 & -1/3 & -1/3 \\ -1/3 & 1 & -1/3 & -1/3 \\ -1/3 & -1/3 & 1 & -1/3 \\ -1/3 & -1/3 & -1/3 & 1 \end{pmatrix}$$

Figure 1: The normalised Laplacian matrix of a complete graph with 4 vertices.

Lemma 1. *It holds that* $\lambda_1(\mathcal{L}) = 0$ *with the associated eigenvector* $D^{1/2} \cdot \mathbf{1}$.

Proof. Let $x \in \mathbb{R}^n$ be any vector. Then it holds that

$$\begin{aligned} x^\intercal \mathcal{L} x &= \sum_u x_u^2 - \sum_{u\sim v} \frac{2x_u x_v}{\sqrt{d_u d_v}} \\ &= \sum_u d_u \left(\frac{x_u}{\sqrt{d_u}}\right)^2 - \sum_{u\sim v} \frac{2x_u x_v}{\sqrt{d_u d_v}} \\ &= \sum_{u\sim v} \left(\frac{x_u}{\sqrt{d_u}} - \frac{x_v}{\sqrt{d_v}}\right)^2, \end{aligned}$$

which implies that

$$\frac{x^\intercal \mathcal{L} x}{x^\intercal x} \geq 0$$

holds for any $x \in \mathbb{R}^n$. Since

$$\lambda_1 = \min_{x \in \mathbb{R}^n, x \neq 0} \frac{x^\intercal \mathcal{L} x}{x^\intercal x} \geq 0,$$

and $\left(D^{1/2}\mathbf{1}\right)^\intercal \mathcal{L} \left(D^{1/2}\mathbf{1}\right) = 0$, the statement holds. □

Among the n eigenvalues, λ_2 plays a central role in studying many properties of a graph. Here, we present some simple bounds.

Theorem 2. *It holds that*

$$\lambda_2 = \min_{f \perp D\mathbf{1}} \frac{\sum_{u\sim v} (f_u - f_v)^2}{\sum_u d_u \cdot f_u^2}.$$

Proof. The statement follows from the proof of Lemma 1 and the fact that, for any $g = D^{1/2} f \in \mathbb{R}^n$ orthogonal to $D^{1/2}\mathbf{1}$, we have that

$$\langle g, D^{1/2}\mathbf{1}\rangle = 0 \Leftrightarrow \langle D^{1/2} f, D^{1/2}\mathbf{1}\rangle = 0 \Leftrightarrow \langle f, D\mathbf{1}\rangle = 0.$$ □

Execrise 3. $\lambda_2 \leq n/(n-1)$, *and* $\lambda_2 = n/(n-1)$ *iff* G *is a complete graph.*

Lemma 4. *If* G *is not a complete graph, then* $\lambda_2 \leq 1$.

Proof. Since G is not a complete graph, there are vertices u, v which are not connected by an edge. Define a vector $f \in \mathbb{R}^n$ such that

$$f_w = \begin{cases} d_u & \text{if } w = v, \\ -d_v & \text{if } w = u, \\ 0 & \text{otherwise.} \end{cases}$$

Notice that $f \perp D\mathbf{1}$. By Theorem 2, it holds that

$$\lambda_2 \leq \frac{\sum_{u\sim v} (f_u - f_v)^2}{\sum_u d_u \cdot f_u^2} = 1.$$ □

Execrise 5. G *has* k *connected components iff* $\lambda_k = 0$ *and* $\lambda_{k+1} > 0$. *In particular,* G *is connected iff* $\lambda_2 > 0$.

Lemma 6. *It holds that* $\lambda_n \leq 2$. *In particular,* $\lambda_n = 2$ *iff a connected component of* G *is a non-empty bipartite graph.*

Proof. Let $g \in \mathbb{R}^n$ be any vector. From the proof of Lemma 1, it holds that

$$\frac{\langle g, \mathcal{L}g \rangle}{\langle g, g \rangle} = \frac{\sum_{u\sim v}(f_u - f_v)^2}{\sum_u d_u \cdot f_u^2} \leq \frac{\sum_{u\sim v} 2(f_u^2 + f_v^2)}{\sum_u d_u \cdot f_u^2} = \frac{2 \cdot \sum_u d_u \cdot f_u^2}{\sum_u d_u \cdot f_u^2} = 2. \tag{1}$$

Moreover, by (1) we know that $\lambda_n = 2$ iff the eigenvector associated with λ_n satisfies

$$\sum_{u\sim v}(f_u - f_v)^2 = \sum_{u\sim v} 2(f_u^2 + f_v^2),$$

i.e., $\sum_{u\sim v}(f_u + f_v)^2 = 0$, which is equivalent to say that

$$f_u = -f_v, \quad \text{for every } u \sim v. \tag{2}$$

Since f is an eigenvector, there is at least one coordinate $f_u \neq 0$. Based on this and (2), the sign of each $f_v \neq 0$ gives the partition of a connected component of G. □

We have seen that some of a graph's properties can be obtained by its graph spectrum. To summarise our discussion, let us look at several examples.

Example 7. *Let the spectrum of a graph G be*

$$0, \quad 2/3, \quad 2/3, \quad 2/3, \quad 2/3, \quad 2/3, \quad 5/3, \quad 5/3, \quad 5/3, \quad 5/3.$$

From this sequence, we know that (i) G has 10 vertices; (2) G is connected; (3) G is not bipartite.

Example 8. *Let the spectrum of a graph G be*

$$0, \quad 0, \quad 0.69, \quad 0.69, \quad 1.5, \quad 1.5, \quad 1.8, \quad 1.8.$$

From this sequence, we know that (i) G has 8 vertices; (2) G is disconnected, and has 2 connected components; (3) none of G's connected component is bipartite.

Finally, we show some examples of the spectra for specific graphs.

- For the complete graph K_n on n vertices, the eigenvalues are 0 and $n/(n-1)$ with multiplicity $n-1$.
- For the star S_n on n vertices, the eigenvalues are 0, 1 with multiplicity $n-2$, and 2.
- For the path P_n on n vertices, the eigenvalues are $1 - \cos\left(\frac{\pi k}{n-1}\right)$ for $k = 0, 1, \ldots, n-1$.

2 Expander Mixing Lemma

Let $\lambda = \max_{i\geq 2} |1 - \lambda_i|$ the **spectral expansion** of G.

Theorem 9 (Expander Mixing Lemma)**.** *Let G be a graph, and $X, Y \subset V$ be sets of vertices. Then, it holds that*

$$\left| |E(X,Y)| - \frac{\operatorname{vol} X \cdot \operatorname{vol} Y}{\operatorname{vol} G} \right| \leq \lambda \cdot \sqrt{\operatorname{vol} X \operatorname{vol} Y}. \tag{3}$$

Notice that $\operatorname{vol} X \cdot \operatorname{vol} Y / \operatorname{vol} G$ is the expected value of $|E(X,Y)|$ in a random graph of edge density $\operatorname{vol} G/n^2$. Hence, the left side of (3) is the difference between $|E(X,Y)|$ and its expected value in a random graph. So, a smaller value of λ shows that the graph is more close to be a random graph. Before proving the expander mixing lemma, we look at its applications in analysing combinatorial properties of a graph.

Corollary 10. *The volume of any independent set in G is at most $\lambda \cdot \operatorname{vol} G$.*

Proof. Let $X = Y$ be an independent set of G. Then $|E(X, X)| = 0$. We apply Theorem 9 and obtain that

$$\left| \frac{(\operatorname{vol} X)^2}{\operatorname{vol} G} \right| \leq \lambda \cdot \operatorname{vol} X,$$

which implies that $\operatorname{vol} X \leq \lambda \cdot \operatorname{vol} G$. Hence, the volume of any independent set in G is at most $\lambda \cdot \operatorname{vol} G$. For the case of regular graphs, the number of vertices in an independent set is at most $\lambda \cdot n$. □

Corollary 11. *Let G be a regular graph. Then the chromatic number of G is at least $1/\lambda$.*

Proof. Let $c : V \to \{1, \ldots, k\}$ be a colouring of G. Then, for every $1 \leq i \leq k$, $c^{-1}(i)$ is an independent set. Since the number of vertices in an independent set is at most λn, the chromatic number is at least $1/\lambda$. □

Proof of Theorem 9. For any set $S \subset V$, let χ_S be the indicator vector of set S, i.e., $\chi_S(u) = 1$ if $u \in S$, and $\chi_S(u) = 0$ otherwise. Then, we have that

$$|E(X, Y)| = \langle \chi_X, A\chi_Y \rangle = \chi_X^\intercal D^{1/2}(I - \mathcal{L})D^{1/2}\chi_Y.$$

Without loss of generality, we write

$$D^{1/2}\chi_X = \sum_{i=1}^{n} a_i f_i$$

and

$$D^{1/2}\chi_Y = \sum_{i=1}^{n} b_i f_i,$$

where $f_1, \ldots, f_n$ are orthonormal eigenvectors of $\mathcal{L}$, and $f_1 = D^{1/2}\mathbf{1}/\sqrt{\operatorname{vol} G}$. Hence, we have that $a_1 = \operatorname{vol} X/\sqrt{\operatorname{vol} G}$ and $b_1 = \operatorname{vol} Y/\sqrt{\operatorname{vol} G}$. With this, it holds that

$$\begin{aligned}
\left| |E(X,Y)| - \frac{\operatorname{vol} X \cdot \operatorname{vol} Y}{\operatorname{vol} G} \right| &= \left| \chi_X^\intercal D^{1/2}(I - \mathcal{L})D^{1/2}\chi_Y - a_1 b_1 \right| \\
&= \left| \left(\sum_{i=1}^{n} a_i f_i^\intercal \right) (I - \mathcal{L}) \left(\sum_{i=1}^{n} b_i f_i \right) - a_1 b_1 \right| \\
&= \left| \sum_{i=2}^{n} (1 - \lambda_i) \cdot a_i b_i \right| \\
&\leq \lambda \sqrt{\sum_{i=2}^{n} a_i^2} \sqrt{\sum_{i=2}^{n} b_i^2} \\
&\leq \lambda \cdot \frac{\sqrt{\operatorname{vol} X \operatorname{vol} \bar{X} \operatorname{vol} Y \operatorname{vol} \bar{Y}}}{\operatorname{vol}(G)},
\end{aligned}$$

where $\operatorname{vol} \bar{X} = \operatorname{vol}(V \setminus X)$, the second last inequality follows by the Cauchy-Schwarz inequality, and the last inequality follows by the fact that

$$\sum_{i=1}^{n} a_i^2 = \left(\sum_{i=1}^{n} a_i f_i^\intercal \right) \left(\sum_{i=1}^{n} a_i f_i \right) = \langle \chi_X^\intercal D^{1/2}, D^{1/2}\chi_X \rangle = \operatorname{vol} X,$$

and

$$\sum_{i=2}^{n} a_i^2 = \operatorname{vol} X - \frac{(\operatorname{vol} X)^2}{\operatorname{vol} G} = \operatorname{vol} X \operatorname{vol} \bar{X} / \operatorname{vol} G \leq \operatorname{vol} X.$$

□

Remark 12. *We remark that the proof above actually shows a stronger version of the expander mixing lemma, i.e., it holds for any* $X, Y \subset V$ *that*

$$\left| |E(X,Y)| - \frac{\operatorname{vol} X \cdot \operatorname{vol} Y}{\operatorname{vol} G} \right| \leq \lambda \cdot \frac{\sqrt{\operatorname{vol} X \operatorname{vol} \bar{X} \operatorname{vol} Y \operatorname{vol} \bar{Y}}}{\operatorname{vol}(G)}.$$

From the expander mixing lemma, we know that a small value of λ implies that G behaves more like a random graph. Hence a natural question is to study a lower bound of λ. Alon and Boppana showed that, for any constant $\varepsilon > 0$, every sufficiently large d-regular graph has $\lambda \geq 2\sqrt{d-1}/d - \varepsilon$. We call a d-regular graph G **Ramanujan** if $\lambda(G) \leq 2\sqrt{d-1}/d$. For any fixed constant d, constructing an infinite family of d-regular Ramanujan graphs is a major open question in theoretical computer science.