Spectral Theory of Graphs and Hypergraphs
Lecture Notes

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Abstract

These lecture notes accompany the course *Spectral Theory of Graphs and Hypergraphs*, prepared for the PhD students of the BeyondTheEdge MSCA Doctoral Network. The aim of the course is to introduce participants to spectral methods in discrete mathematics, with emphasis on the normalized Laplacian of graphs and hypergraphs, as well as on the non-backtracking Laplacian of graphs. The notes combine classical results with more recent developments (with a focus on the author's own research), and include both introductory exercises and open problems.

While some parts are quite technical, different levels of depth are possible, and students can focus on the aspects that are most relevant to their background and interests. The course follows a flipped classroom format, and in addition to these notes, it is accompanied by recorded video lectures. Dedicated sessions in Marseille (October 2025) will then give students the opportunity to work in groups on the exercises and discuss their findings.

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1 Graph normalized Laplacian

1.1 Historical note

The continuous *Laplace operator* was first introduced and studied by Lagrange (Giuseppe Luigi Lagrangia, 1736 – 1813) [31] for functions on Euclidean spaces, and it is defined by

$$\Delta f := \frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2} + \ldots + \frac{\partial^2 f}{\partial x_n^2}. \tag{1}$$

But it was named after Pierre Simon Laplace (1749 – 1827), who worked on this operator and who focused, in particular, on the Laplace equation

$$\Delta f = 0, \tag{2}$$

whose solutions are called *harmonic functions*. Later on, this Laplacian has also been generalized for Riemannian manifolds.

Can one determine the shape of an object by listening to its vibrations? – this question has been first asked in 1882 by the physicist Arthur Schuster [14] and it can be reformulated as follows: *Can one reconstruct the shape of a mathematical drum form the eigenvalues of its Laplace operator?*. It became famous in 1966, when Mark Kac published the paper *Can one hear the shape of a drum?* [39] and the answer has been given in 1992 by Carolyn Gordon, David L. Webb and Scott Wolper in a paper titled *One cannot hear the shape of a drum* [29]. In other words, one cannot reconstruct the exact shape of an object from the eigenvalues of the Laplacian. Nevertheless, one can infer important information. In 1911, Weyl proved an asymptotic formula for the eigenvalues of a compact Riemmanian manifold that depends on the volume of the manifold [46, 66]. In 1953, Minakshisundaram showed that for a compact Riemmanian manifold without boundary one can hear the dimension, the volume and the total scalar curvature [14, 46].

A discrete version of the Laplace operator in (1) has been used for the first time by Kirchhoff in 1847, for the study of electrical networks [32, 41]. In 1992, Fan Chung [16] introduced the first normalized version of the discrete Laplacian. As already pointed out by Chung when she first introduced the normalized graph Laplacian, two graphs cannot always be distinguished by their spectra (in other words, *we cannot hear the isomorphism class of a graph*), but the spectrum reveals some important properties. *Is the graph bipartite? Is it complete? How many connected components does it have?* – as we shall see, these are all questions that can be answered using the spectrum of the Laplace operator, so even if it does not distinguish the details of graphs, it does partition them into important families. We say, in particular, that two graphs are isospectral if they have the same spectrum. Since, furthermore, the computation of the eigenvalues can be performed with tools from linear algebra, studying the spectrum of these Laplacians is a very common tool in graph theory and data analytics.

1.2 Basic definitions and first properties

Fix a simple graph $G = (V, E)$ with vertices $v_1, \ldots, v_N$. We assume that G has no self-loops and no isolated vertices.

Definition. The *adjacency matrix* of G is the $N \times N$ matrix $A := A(G)$ with entries

$$A_{ij} := \begin{cases} 1 & \text{if } v_i \sim v_j \\ 0 & \text{otherwise.} \end{cases}$$

The *Kirchhoff Laplacian* of G is the matrix

$$K := K(G) := D - A,$$

where $D := D(G) := \operatorname{diag}(\deg v_1, \dots, \deg v_N)$ is the *degree matrix* of G.
The *Chung Laplacian* of G is the matrix

$$\mathcal{L} := \mathcal{L}(G) := \operatorname{Id} - D^{-1/2} A D^{-1/2},$$

where Id denotes the $N \times N$ identity matrix.
The *normalized Laplacian* of G is the matrix

$$L := L(G) := \operatorname{Id} - D^{-1} A.$$

Clearly, there is a 1 : 1 correspondence between graphs and each of these operators, and while exist non-isomorphic graphs with the same spectra, nevertheless such spectra are known to detect many important geometric properties of the graph. Thus, if two graphs are isospectral with respect to a given operator, they have similar structures.

Remark. From the spectral point of view, $\mathcal{L}$ and L are equivalent because $L = D^{-1/2}\mathcal{L}D^{1/2}$, hence the two matrices are similar.

Also, the spectra of all the above operators often encode similar information.

Remark. If G is d-regular, i.e., if $\deg v = d$ for all $v \in V$, then $K = d \cdot \operatorname{Id} - A$ and $\mathcal{L} = L = \frac{1}{d} \cdot K$. Therefore, it is easy to see that, for d-regular graphs,

$$\begin{aligned} \lambda \text{ is an eigenvalue for } K &\iff d - \lambda \text{ is an eigenvalue for } A \\ &\iff \frac{\lambda}{d} \text{ is an eigenvalue for } \mathcal{L} = L. \end{aligned}$$

Remark. The entries of L are

$$L_{ij} = \begin{cases} 1 & \text{if } i = j \\ -\frac{1}{\deg v_i} & \text{if } v_i \sim v_j \\ 0 & \text{otherwise.} \end{cases}$$

In particular, for $v_i \sim v_j$, $-L_{ij}$ is the probability of going from v_i to v_j with a classical random walk on V. This highlights the deep connections between the normalized Laplacian, random walks, and diffusion processes on graphs. For further details, we refer to Chapter 12 in [16].

Remark. Clearly, since L is an $N \times N$ matrix whose trace is N, it has N eigenvalues whose sum is N. Also, since L is isospectral with $\mathcal{L}$, which is real and symmetric, its eigenvalues are real and their algebraic and geometric multiplicities coincide.
We denote the eigenvalues of L by

$$\lambda_1 \leq \ldots \leq \lambda_N.$$

Remark. Let $C(V)$ denote the vector space of functions $f : V \to \mathbb{R}$ and, given $f, g \in C(V)$, let

$$\langle f, g \rangle := \sum_{v \in V} \deg v \cdot f(v) \cdot g(v).$$

We can see L as an operator $C(V) \to C(V)$ such that

$$Lf(v) = f(v) - \frac{1}{\deg v} \sum_{w \sim v} f(w).$$

Also, it is easy to check that L is self-adjoint with respect to the inner product $\langle \cdot, \cdot \rangle$, i.e.,

$$\langle Lf, g \rangle = \langle f, Lg \rangle \quad \forall f, g \in C(V).$$

With the Courant-Fischer-Weyl min-max Principle below, we can characterize the eigenvalues of L.

Theorem 1.1 (Courant-Fischer-Weyl min-max Principle)**.** *Let H be an N-dimensional vector space with a positive definite scalar product $(.,.)$, and let $A : H \to H$ be a self-adjoint linear operator. Let $\mathcal{H}_k$ be the family of all k-dimensional subspaces of H. Then the eigenvalues $\lambda_1 \leq \ldots \leq \lambda_N$ of A can be obtained by*

$$\lambda_k = \min_{H_k \in \mathcal{H}_k} \max_{g(\neq 0) \in H_k} \frac{(Ag,g)}{(g,g)} = \max_{H_{N-k+1} \in \mathcal{H}_{N-k+1}} \min_{g(\neq 0) \in H_{N-k+1}} \frac{(Ag,g)}{(g,g)}. \tag{3}$$

The vectors g_k realizing such a min-max or max-min then are corresponding eigenvectors, and the min-max spaces H_k are spanned by the eigenvectors for the eigenvalues $\lambda_1, \ldots, \lambda_k$, and analogously, the max-min spaces H_{N-k+1} are spanned by the eigenvectors for the eigenvalues $\lambda_k, \ldots, \lambda_N$.
Thus, we also have

$$\lambda_k = \min_{g(\neq 0) \in H, (g,g_j)=0 \text{ for } j=1,\ldots,k-1} \frac{(Ag,g)}{(g,g)} = \max_{g(\neq 0) \in H, (g,g_\ell)=0 \text{ for } \ell=k+1,\ldots,N} \frac{(Ag,g)}{(g,g)}. \tag{4}$$

In particular,

$$\lambda_1 = \min_{g(\neq 0) \in H} \frac{(Ag,g)}{(g,g)}, \qquad \lambda_N = \max_{g(\neq 0) \in H} \frac{(Ag,g)}{(g,g)}. \tag{5}$$

Definition. $\frac{(Ag,g)}{(g,g)}$ is called the *Rayleigh quotient* of g.

According to Theorem 1.1, the eigenvalues of L are given by minimax values of

$$\mathrm{RQ}(f) := \frac{\langle Lf, f \rangle}{\langle f, f \rangle} = \frac{\sum_{v \sim w} \Big(f(v) - f(w) \Big)^2}{\sum_{v \in V} \deg v \cdot f(v)^2}, \quad \text{for } f \in C(V).$$

In particular, let $k \in \{1, \ldots, N\}$ and let g_i be an eigenfunction for λ_i, for each $i \in \{1, \ldots, N\} \setminus \{k\}$. Then,

$$\lambda_k = \min_{\substack{f \in C(V) \setminus \{\mathbf{0}\}: \\ \langle f, g_1 \rangle = \ldots = \langle f, g_{k-1} \rangle = 0}} \mathrm{RQ}(f) = \max_{\substack{f \in C(V) \setminus \{\mathbf{0}\}: \\ \langle f, g_{k+1} \rangle = \ldots = \langle f, g_N \rangle = 0}} \mathrm{RQ}(f),$$

and the functions realizing such a min-max are the corresponding eigenfunctions for λ_k.

Proposition 1.2. *The eigenvalues of L are non-negative. Moreover, the multiplicity of 0 equals the number of connected components of G, and the corresponding eigenfunctions are constant on each connected component.*

Proof. By the min-max principle,

$$\lambda_1 = \min_{f \in C(V) \setminus \{\mathbf{0}\}} \frac{\sum_{v \sim w} \Big(f(v) - f(w) \Big)^2}{\sum_{v \in V} \deg v \cdot f(v)^2}.$$

Clearly, the minimum of the Rayleigh quotient is 0 and it is achieved if and only if $f(v) = f(w)$ for each edge (v, w), that is, f is constant on each connected component of G. The claim follows. □

Exercise 1 (Example)**.** Let K_N be the complete graph with N nodes and all $\frac{N(N-1)}{2}$ possible edges. Show that the spectrum is given by 0, with multiplicity 1, and $\frac{N}{N-1}$, with multiplicity $N-1$.

Definition. A graph $G=(V,E)$ is *bipartite* if there exists a bipartition of the vertex set into two disjoint sets $V=V_1\sqcup V_2$ such that each edge in E has one endpoint in V_1 and one endpoint in V_2.

Theorem 1.3. *The largest eigenvalue satisfies*

$$\frac{N}{N-1}\leq \lambda_N\leq 2.$$

Also, $\lambda_N=\frac{N}{N-1}$ *if and only if* G *is the complete graph* K_N*, while* $\lambda_N=2$ *if and only if at least one connected component of* G *is bipartite.*

Proof. Observe that

$$\lambda_N\geq \frac{1}{N-1}\left(\sum_{i=2}^{N}\lambda_i\right)=\frac{N}{N-1},$$

with equality if and only if $\lambda_i=\frac{N}{N-1}$, for all $i=2,\dots,N$, and we already know that this holds for the complete graph.
Now, if G is not complete, then there exist $v_1,v_2\in V$ that are not connected by any edge. Let $g\in C(V)$ be such that $g(v_1)\neq 0$, $g(v_2)\neq 0$, $g=0$ otherwise and

$$\deg v_1\cdot g(v_1)+\deg v_2\cdot g(v_2)=0.$$

Then, by the min-max principle,

$$\lambda_2=\min_{\substack{f\in C(V)\setminus\{\mathbf{0}\}:\\ \sum_{v\in V}\deg v\cdot f(v)=0}}\mathrm{RQ}(f)\leq \mathrm{RQ}(g)=1<\frac{N}{N-1}.$$

Hence, if G is not complete, $\lambda_2<\frac{N}{N-1}$, implying that $\lambda_N>\frac{N}{N-1}$. This proves the claim for the lower bound.

In order to prove the last claim we use the fact that, given two real numbers a and b,

$$(a-b)^2\leq 2a^2+2b^2,$$

with equality if and only if $a=-b$. This implies that, given an eigenfunction f for λ_N,

$$\lambda_N=\frac{\sum_{v\sim w}\Big(f(v)-f(w)\Big)^2}{\sum_{v\in V}\deg v\cdot f(v)^2}\leq\frac{\sum_{v\sim w}\left(2f(v)^2+2f(w)^2\right)}{\sum_{v\in V}\deg v\cdot f(v)^2}=\frac{2\cdot\sum_{v\in V}\deg v\cdot f(v)^2}{\sum_{v\in V}\deg v\cdot f(v)^2}=2,$$

with equality if and only if $f(v)=-f(w)$ for each edge (v,w). Since $f\neq\mathbf{0}$, this is possible if and only if at least one connected component of G is bipartite. □

From Theorem 1.3 we have that $\lambda_N>\frac{N}{N-1}$ for non-complete graphs. But Das and Sun [20] proved that for all non-complete graphs we also have

$$\lambda_N\geq\frac{N+1}{N-1},$$

with equality if and only if the complement graph (that is, the graph that connects precisely those vertices that are not neighbors in the graph under consideration) is a single edge or a complete bipartite graph with both parts of size $\frac{N-1}{2}$. More precise results in this direction can be found in [36]. As a consequence, not only we have that complete graphs K_N are completely determined by their spectrum, but additionally, we also know that there do not even exist graphs whose spectrum is very close to that of K_N.

Exercise 2 (Open problem)**.** What is the third smallest possible value of λ_N, and for which graphs is it achieved?

Exercise 3 (Open problem)**.** What is the second largest possible value of λ_N, and for which graphs is it achieved?

1.3 Cheeger-type estimates

Cheeger constants and Cheeger inequalities have a long history. The now-called *Cheeger constant* of a simple graph $G = (V, E)$ was introduced in 1951 by George Pólya and Gábor Szegő [57], who called it the *isoperimetric constant* and defined it as

$$h(G) := \min_{\emptyset \neq S \subsetneq V} \frac{|E(S, \bar{S})|}{\min\{\mathrm{vol}(S), \mathrm{vol}(\bar{S})\}},$$

where $E(S, \bar{S})$ denotes the set of edges between S and its complement $\bar{S} := V \setminus S$, while the *volume* of S, denoted $\mathrm{vol}(S)$, is the sum of the vertex degrees in S. Finding a set S realizing the Cheeger constant means finding a small *edge cut* $E(S, \bar{S})$ such that, if removed from G, it divides the graph into two disconnected components that have roughly equal volume (Figure 1). Therefore, h measures how different G is from a disconnected graph, and it is largest for the complete graph.

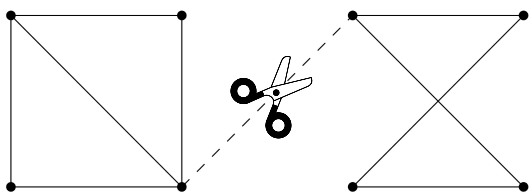

Figure 1: The Cheeger cut on a simple graph

The continuous analogue of $h(G)$ was then defined by Jeff Cheeger [15] in 1970, in the context of spectral geometry, as follows. Given a compact n-dimensional manifold M, let

$$h(M) := \inf_{D} \frac{\mathrm{vol}_{n-1}(\delta D)}{\mathrm{vol}_n(D)},$$

where $D \subset M$ is a smooth n-submanifold with boundary δD and $0 < \mathrm{vol}_n(D) \leq \mathrm{vol}(M)/2$. Cheeger proved that the first nonvanishing eigenvalue $\lambda_{\min}(M)$ of the Laplace-Beltrami operator is such that

$$\lambda_{\min}(M) \geq \frac{1}{4} h^2(M)$$

and, as shown by Peter Buser [12] in 1978, for each compact manifold there exist Riemannian metrics for which the inequality becomes sharp. In a later work in 1982, Buser [13] also proved that, if the Ricci curvature of a compact unbordered Riemannian n-manifold M is bounded below by $-(n-1)a^2$, for some $a \geq 0$, then

$$\lambda_{\min}(M) \leq 2a(n-1)h + 10h^2.$$

Therefore, $h(M)$ can be used to estimate $\lambda_{\min}(M)$ and vice versa.
In 1984-5, Jozef Dodziuk [22] and Noga Alon with Vitali Milman [2] derived analogous estimates for the graph Cheeger constant and for the first non-vanishing eigenvalue of the Kirchhoff Laplacian associated to a connected graph. Similarly, in 1992, Fan Chung [16] proved the Cheeger inequalities for the normalized Laplacian of a connected graph:

Theorem 1.4. *If G is a connected graph, then*

$$\frac{1}{2}h^2 \leq \lambda_2 \leq 2h.$$

Proof of the upper bound. Fix $S, \bar{S} \subseteq V$ that realize the Cheeger constant and assume, without loss of generality, that $\mathrm{vol}(S) \leq \mathrm{vol}(\bar{S})$, so that $h = \frac{|E(S,\bar{S})|}{\mathrm{vol}(S)}$. Let $\alpha := \frac{\mathrm{vol}(S)}{\mathrm{vol}(\bar{S})} \in (0,1]$ and let $f \in C(V)$ be such that $f := 1$ on S and $f := -\alpha$ on $\bar{S}$. Then, $\sum_{v \in V} \deg v \cdot f(v) = 0$. Therefore, by the min-max principle,

$$\begin{aligned}
\lambda_2 \leq \mathrm{RQ}(f) &= \frac{\sum_{v\sim w}\Big(f(v)-f(w)\Big)^2}{\sum_{v\in V}\deg v\cdot f(v)^2} \\
&= \frac{|E(S,\bar{S})|\cdot(1+\alpha)^2}{\mathrm{vol}(S)+\alpha^2\,\mathrm{vol}(\bar{S})} = \frac{|E(S,\bar{S})|(1+\alpha)}{\mathrm{vol}(S)} \leq 2h,
\end{aligned}$$

where we have used the fact that $\alpha\,\mathrm{vol}(\bar{S}) = \mathrm{vol}(S)$ and $\alpha \leq 1$. ☐

In the proof of the lower bound, we will need the following observation.
Remark. Given $g : V \to \mathbb{R}$, let

$$g_+(v) := \begin{cases} g(v), & \text{if } g(v) \geq 0 \\ 0, & \text{if } g(v) < 0 \end{cases}$$

and let

$$g_-(v) := \begin{cases} |g(v)|, & \text{if } g(v) \leq 0 \\ 0, & \text{if } g(v) > 0. \end{cases}$$

Then, $g(v) = g_+(v) - g_-(v)$, $g(v)^2 = g_+(v)^2 + g_-(v)^2$, and

$$\sum_{v\sim w}\Big(g(v)-g(w)\Big)^2 \geq \sum_{v\sim w}\left[\Big(g_+(v)-g_+(w)\Big)^2 + \Big(g_-(v)-g_-(w)\Big)^2\right].$$

Therefore,

$$\begin{aligned}
\mathrm{RQ}(g) &= \frac{\sum_{v\sim w}\Big(g(v)-g(w)\Big)^2}{\sum_{v\in V}\deg v\cdot g(v)^2} \\
&\geq \frac{\sum_{v\sim w}\left[\Big(g_+(v)-g_+(w)\Big)^2 + \Big(g_-(v)-g_-(w)\Big)^2\right]}{\sum_{v\in V}\deg v\cdot (g_+(v)^2+g_-(v)^2)}
\end{aligned}$$

$$\geq \min\{\mathrm{RQ}(g_+), \mathrm{RQ}(g_-)\},$$

since $\frac{a+b}{c+d} \geq \min\{\frac{a}{c}, \frac{b}{d}\}$.

Proof of the lower bound. Let $\phi : V \to \mathbb{R}_{\geq 0}$ be a function, and let $M := \max \phi(v)^2$. We put, for $\tau \geq 0$,

$$\Phi_v(\tau) := \begin{cases} 1 & \text{if } \phi(v) \geq \tau \\ 0 & \text{else.} \end{cases}$$

Let also $V_\phi^+(\tau) := \{v \in V : \phi(v) \geq \tau\} = \{v \in V : \Phi_v(\tau) = 1\}$. Then, for every $t \geq 0$,

$$\sum_{u \sim v} \left| \Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t}) \right| = \left| E\left(V_\phi^+(\sqrt{t}), \overline{V_\phi^+(\sqrt{t})} \right) \right|.$$

Thus,

$$\begin{aligned} \int_0^M \sum_{u \sim v} \left| \Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t}) \right| dt &= \int_0^M \left| E\left(V_\phi^+(\sqrt{t}), \overline{V_\phi^+(\sqrt{t})} \right) \right| dt \\ &\geq \inf_{t>0} \frac{\left| E\left(V_\phi^+(\sqrt{t}) \right), \overline{V_\phi^+(\sqrt{t})} \right) \right|}{\sum_{v:\, \phi(v) \geq \sqrt{t}} \deg(v)} \int_0^M \sum_{v:\, \phi(v) \geq \sqrt{\tau}} \deg(v) d\tau \\ &= \inf_{t>0} \frac{\left| E\left(V_\phi^+(\sqrt{t}) \right), \overline{V_\phi^+(\sqrt{t})} \right) \right|}{\sum_{v:\, \phi(v) \geq \sqrt{t}} \deg(v)} \sum_v \deg(v) \phi(v)^2, \end{aligned} \tag{6}$$

where the inequality follows from the fact that

$$\frac{\int_0^M \left| E\left(V_\phi^+(\sqrt{t}), \overline{V_\phi^+(\sqrt{t})} \right) \right| dt}{\int_0^M \sum_{v:\, \phi(v) \geq \sqrt{\tau}} \deg(v) d\tau} \geq \inf_{t>0} \frac{\left| E\left(V_\phi^+(\sqrt{t}) \right), \overline{V_\phi^+(\sqrt{t})} \right) \right|}{\sum_{v:\, \phi(v) \geq \sqrt{t}} \deg(v)}$$

while the last equality in (6) follows from the fact that

$$\int \sum_{v:\, \phi(v) \geq \sqrt{\tau}} \deg(v) d\tau = \sum_v \deg(v) \int_{\tau:\, 0 \leq \tau \leq \phi(v)^2} 1 d\tau = \sum_v \deg(v) \phi(v)^2.$$

We now let

$$\mathcal{C}(\phi) := \inf_{t>0} \frac{\left| E\left(V_\phi^+(\sqrt{t}) \right), \overline{V_\phi^+(\sqrt{t})} \right) \right|}{\mathrm{vol}(V_\phi^+(\sqrt{t}))}.$$

From (6), together with the fact that

$$\sum_{v:\, \phi(v) \geq \sqrt{t}} \deg(v) = \sum_{v \in V_\phi^+(\sqrt{t})} \deg(v) = \mathrm{vol}(V_\phi^+(\sqrt{t})),$$

we then obtain

$$\mathcal{C}(\phi) \leq \frac{\int_0^M \sum_{u \sim v} \left| \Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t}) \right| dt}{\sum_v \deg(v) \phi(v)^2}. \tag{7}$$

Now, fix $v \sim u$ and assume that $\phi(v) \leq \phi(u)$. Then, $\left|\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})\right| = 1$ if and only if $\phi(v) < \sqrt{t} \leq \phi(u)$, while $\left|\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})\right| = 0$ otherwise. Hence,

$$\begin{aligned}\int_0^M \left|\Phi_u(\sqrt{t}) - \Phi_v(\sqrt{t})\right| dt &= \int_{t\in[0,M]\,:\,\phi(v)<\sqrt{t}\leq\phi(u)} 1dt \\ &= \phi(u)^2 - \phi(v)^2 \\ &= \big(|\phi(u) - \phi(v)|\big)\big(|\phi(u) + \phi(v)|\big). \end{aligned} \tag{8}$$

From (7) and (8), we obtain

$$\begin{aligned}\mathcal{C}(\phi) &\leq \frac{\sum_{u\sim v}\big(|\phi(u) - \phi(v)|\big)\big(|\phi(u) + \phi(v)|\big)}{\sum_v \deg(v)\phi(v)^2} \\ &\leq \frac{\sqrt{\sum_{u\sim v}|\phi(u) - \phi(v)|^2}\sqrt{\sum_{u\sim v}(\phi(u) + \phi(v))^2}}{\sum_v \deg(v)\phi(v)^2} \\ &\leq \frac{\sqrt{\sum_{u\sim v}|\phi(u) - \phi(v)|^2}\sqrt{2\sum_u \deg(u)\phi(u)^2}}{\sum_v \deg(v)\phi(v)^2},\end{aligned}$$

where the second inequality follows from the fact that, by the Cauchy–Schwarz Inequality, $\sum_i |a_i||b_i| \leq \sqrt{\sum_i a_i^2}\sqrt{\sum_i b_i^2}$, while the last inequality follows from $(a+b)^2 \leq 2a^2+2b^2$, which implies that

$$\sum_{u\sim v}(\phi(u) + \phi(v))^2 \leq 2\sum_u \deg(u)\phi(u)^2.$$

Hence, by using $\frac{\sqrt{a}}{a} = \frac{1}{\sqrt{a}}$, we obtain that

$$\mathcal{C}(\phi) \leq \sqrt{\frac{2\sum_{u\sim v}|\phi(u) - \phi(v)|^2}{\sum_v \deg(v)\phi(v)^2}}, \tag{9}$$

for all $\phi : V \to \mathbb{R}_{\geq 0}$.

We then consider an eigenfunction f for the eigenvalue λ_2. Since f is orthogonal to the constant functions, the eigenfunction for λ_1, we have $\sum_v \deg(v)f(v) = 0$. Thus, f attains both positive and negative values, and the function

$$\begin{aligned}p(t) :&= \sum_{v\in V} \deg v\,(f(v) - t)^2 \\ &= \sum_{v\in V} \deg v\,\big(f(v)^2 + t^2 - 2tf(v)\big) \\ &= \sum_{v\in V} \deg v f(v)^2 + t^2\sum_{v\in V}\deg v - 2t\sum_{v\in V}\deg v f(v) \\ &= \sum_{v\in V} \deg v f(v)^2 + t^2\sum_{v\in V}\deg v\end{aligned}$$

attains its minimum at $t = 0$.

Now, reorder the vertices so that

$$f(v_1) \leq \ldots \leq f(v_N).$$

Let k be the largest integer such that $\sum_{i=1}^k \deg(v_i) \leq \mathrm{vol}(V)/2$, and let $c := f(v_{k+1})$. Then,

$$\mathrm{vol}(\{v \in V : f(v) < c\}) \leq \sum_{i=1}^{k} \deg(v_i) \leq \frac{\mathrm{vol}(V)}{2}$$

and, since k is the largest integer such that $\sum_{i=1}^k \deg(v_i) \leq \mathrm{vol}(V)/2$, we have that $\sum_{i=1}^{k+1} \deg(v_i) > \mathrm{vol}(V)/2$, therefore $\sum_{i=k+2}^{N} \deg(v_i) \leq \mathrm{vol}(V)/2$, implying that

$$\mathrm{vol}(\{v \in V : f(v) > c\}) \leq \sum_{i=k+2}^{N} \deg(v_i) \leq \frac{\mathrm{vol}(V)}{2}.$$

Therefore,

$$\max\{\mathrm{vol}(\{v \in V : f(v) > c\}), \mathrm{vol}(\{v \in V : f(v) < c\})\} \leq \frac{\mathrm{vol}(V)}{2}.$$

Hence, by letting

$$g(v) := f(v) - c \quad \text{for } v \in V,$$

we get that

$$\max\{\mathrm{vol}(\{v \in V : g(v) > 0\}), \mathrm{vol}(\{v \in V : g(v) < 0\})\} \leq \frac{\mathrm{vol}(V)}{2}. \tag{10}$$

Now, since we observed that the function $p(t) = \sum_{v\in V} \deg v\,(f(v) - t)^2$ attains its minimum at $t = 0$, we have that

$$\sum_{v\in V} \deg v f(v)^2 \leq \sum_{v\in V} \deg v g(v)^2.$$

Moreover, it is easy to check that

$$\sum_{u\sim v} |f(u) - f(v)|^2 = \sum_{u\sim v} |g(u) - g(v)|^2.$$

This implies that

$$\mathrm{RQ}(f) = \frac{\sum_{u\sim v} |f(u) - f(v)|^2}{\sum_v \deg(v) f(v)^2} \geq \frac{\sum_{u\sim v} |g(u) - g(v)|^2}{\sum_v \deg(v) g(v)^2} = \mathrm{RQ}(g).$$

Now, let ϕ be either g_+ or g_-, such that (by Remark 1.3)

$$\mathrm{RQ}(g) \geq \min\{\mathrm{RQ}(g_+), \mathrm{RQ}(g_-)\} = \mathrm{RQ}(\phi).$$

Let $S := \{v \in V : \phi(v) > 0\}$ and note that, by (10), $\mathrm{vol}\, S \leq \mathrm{vol}\, \bar{S}$.

Now, fix $t > 0$ that realizes the infimum in the definition of $\mathcal{C}(\phi)$ ($t > 0$ exists because ϕ attains finitely many values), and let $T := V_\phi^+(\sqrt{t})$, so that

$$\mathcal{C}(\phi) = \frac{|E(T, \overline{T})|}{\mathrm{vol}\, T}.$$

Then, since

$$T = V_\phi^+(\sqrt{t}) = \{v \in V : \phi(v) \geq \sqrt{t}\} \subseteq \{v \in V : \phi(v) > 0\} = S,$$

we have that $\operatorname{vol} T \leq \operatorname{vol} S \leq \operatorname{vol} \bar{S} \leq \operatorname{vol} \bar{T}$, therefore, by (9),

$$h \leq \frac{|E(T,\bar{T})|}{\operatorname{vol} T} = \mathcal{C}(\phi) \leq \sqrt{\frac{2\sum_{u\sim v}|\phi(u)-\phi(v)|^2}{\sum_v \deg(v)\phi(v)^2}}.$$

Since we chose ϕ such that $\mathrm{RQ}(\phi) \leq \mathrm{RQ}(g) \leq \mathrm{RQ}(f)$, we have

$$\frac{\sum_{u\sim v}|\phi(u)-\phi(v)|^2}{\sum_v \deg(v)\phi(v)^2} \leq \frac{\sum_{u\sim v}|f(u)-f(v)|^2}{\sum_v \deg(v)f(v)^2}. \tag{11}$$

It follows that

$$h \leq \sqrt{\frac{2\sum_{u\sim v}|f(u)-f(v)|^2}{\sum_v \deg(v)f(v)^2}} = \sqrt{2\lambda_2}.$$

We therefore obtain the desired eigenvalue estimate

$$\frac{1}{2}h^2 \leq \lambda_2.$$

□

As a consequence of the latter result, λ_2 can be used to approximate the Cheeger constant. Moreover, the corresponding eigenfunctions can be used to approximate the Cheeger cut by considering the sets $\{v \in V : f(v) \geq 0\}$ and $\{v \in V : f(v) < 0\}$.

Similarly to h, the *dual Cheeger constant* bounds the largest eigenvalue [5, 6]. It is defined as

$$\bar{h} := \max_{\text{partitions } V=V_1\sqcup V_2\sqcup V_3} \frac{2\cdot|E(V_1,V_2)|}{\operatorname{vol}(V_1)+\operatorname{vol}(V_2)},$$

and it satisfies $\bar{h} \leq 1$, with equality if and only if G is bipartite [6]. The dual Cheeger constant bounds the largest eigenvalue above and below, as follows:

$$2\bar{h} \leq \lambda_N \leq 1 + \sqrt{1-(1-\bar{h})^2}.$$

Moreover, the two constants h and $\bar{h}$ are also related to each other [6].

Exercise 4 (Open problem)**.** For a bipartite graph, λ is an eigenvalue if and only if $2-\lambda$ is an eigenvalue. In particular, $\lambda_{n-1} = 2-\lambda_2$ and we can therefore bound λ_{n-1} both above and below in terms of the Cheeger constant. Can we generalize this to all graphs?

1.4 Petals and books

A graph is called *singular* if its adjacency matrix is singular, i.e., if and only if 0 is an eigenvalue of A, hence if and only if 1 is an eigenvalue of L. A complete characterization of singular graphs is given in [59]. For instance, graphs with *duplicate vertices* are singular:

Definition. Given a vertex v, we let $\mathcal{N}(v) := \{w \in V : w \sim v\}$ denote the neighborhood of v. Two vertices v_i and v_j are *duplicates* of each other if $\mathcal{N}(v_i) = \mathcal{N}(v_j)$.

In particular, if v_i and v_j are duplicates, then they are not neighbors, and the corresponding rows/columns of the adjacency matrix are the same, that is,

$$A_{il} = A_{jl} \quad \text{for each } l = 1, \ldots, N.$$

Lemma 1.5. *If G has k vertices that are duplicate of each other, then 0 is an eigenvalue for A with multiplicity at least $k-1$, or equivalently, 1 is an eigenvalue for L with multiplicity at least $k-1$.*

Proof. Assume, without loss of generality, that $v_1, \dots, v_k$ are duplicates. Then, the first k rows/columns of the adjacency matrix are identical. Now, for $i = 2, \dots, k$, consider the function $f_i : V \to \mathbb{R}$ that has value 1 on v_1, -1 on v_i, and 0 otherwise. Then, $Af_i(v_l) = A_{l1} - A_{li} = 0$ for all $l = 1, \dots, N$, that is, $Af_i = \mathbf{0}$. Hence, the f_i's are $k-1$ eigenfunctions of A for the eigenvalue 0, and they are linearly independent. This proves the claim. □

Example 1.1. The *star graph* S_k on $k+1$ nodes is given by k peripheral vertices $v_1, \dots, v_k$ that are connected to one central vertex v_{k+1}. Since the k peripheral vertices are duplicates, 1 is an eigenvalue of L with multiplicity (at least) $k-1$. But we also know that 0 is an eigenvalue, and 2 is also an eigenvalue since the graph is bipartite. Hence, this gives the entire spectrum of S_k.

Example 1.2. More generally, the *complete bipartite graph* $K_{n,m}$ is the bipartite graph such that $V = V_1 \sqcup V_2$, $|V_1| = n$, $|V_2| = m$ and

$$E = \{(v, w) : v \in V_1 \text{ and } w \in V_2\}.$$

Clearly, 0 and 2 are eigenvalues in this case. Moreover, since the n vertices of V_1 are duplicate of each other, they produce the eigenvalue 1 with multiplicity $n-1$. Similarly, the m vertices of V_2 produce the eigenvalue 1 with multiplicity $m-1$. This gives the entire spectrum of $K_{n,m}$. In particular, all complete bipartite graphs on N nodes (including the star graph) are isospectral to each other.

Definition (Petal graph, $N \geq 3$ odd)**.** Given $m \geq 1$, the *m–petal graph* is the graph on $N = 2m+1$ nodes such that (Figure 2):

- $V = \{x, v_1, \dots, v_m, w_1, \dots, w_m\}$;
- $E = \{(x, v_i)\}_{i=1}^m \cup \{(x, w_i)\}_{i=1}^m \cup \{(v_i, w_i)\}_{i=1}^m$.

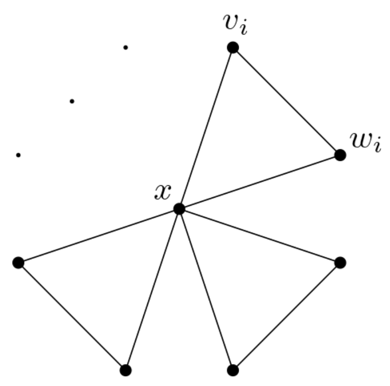

Figure 2: The petal graph

Exercise 5. For the petal graph on $N = 2m+1$ vertices, the eigenvalues are 0, $\frac{1}{2}$ (with multiplicity $m-1$) and $\frac{3}{2}$ (with multiplicity $m+1$).

Petal graphs are also called *Dutch windmill graphs*, *fan graphs* or *friendship graphs*, and they are well-known because of the famous Friendship Theorem of Paul Erdős, Alfréd Rényi and Vera T. Sós from 1966.

Theorem 1.6 (Friendship Theorem)**.** *The finite graphs with the property that every two vertices have exactly one neighbor in common are exactly the petal graphs.*

Informally, the theorem states that if a group of people has the property that every pair of people has exactly one friend in common, then there must be one person who is friend with everyone else.

The analogue of the petal graph for N even is the book graph:

Definition (Book graph, $N \geq 4$ even)**.** Given $m \geq 1$, the *m–book graph* is the graph on $N = 2m + 2$ nodes such that (Figure 3):

- $V = \{x, y, v_1, \dots, v_m, w_1, \dots, w_m\}$;
- $E = \{(x, v_i)\}_{i=1}^m \cup \{(y, w_i)\}_{i=1}^m \cup \{(v_i, w_i)\}_{i=1}^m$.

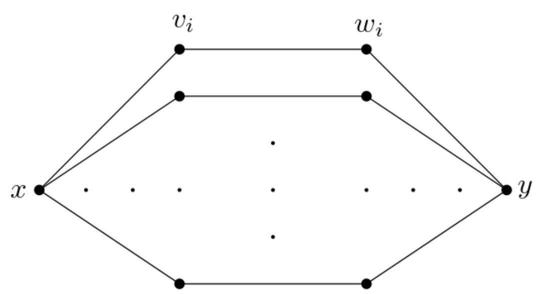

Figure 3: The book graph

Exercise 6. For the book graph on $N = 2m + 2$ nodes, 0 and 2 are eigenvalues with multiplicity 1, and $\lambda = 1 \pm \frac{1}{2}$ are eigenvalues with multiplicity m each.

We now define the *spectral gap at* 1 as

$$\varepsilon := \min_i |1 - \lambda_i|.$$

We have

Theorem 1.7. *For any connected graph G on $N \geq 3$ nodes,*

$$\varepsilon \leq \frac{1}{2}.$$

Moreover, equality is achieved if and only if G is either a petal graph (for N odd) or a book graph (for N even).

We now give a brief idea of the proof of Theorem 1.7, and we refer to [38] for a complete proof and discussion.

The following lemma allows us to characterize ε for any graph.

Lemma 1.8. *For any graph G,*

$$\varepsilon^2 = \min_{f\in C(V)\setminus\{\mathbf{0}\}} \frac{\sum\limits_{w\in V} \frac{1}{\deg w}\left(\sum\limits_{v\in\mathcal{N}(w)} f(v)\right)^2}{\sum\limits_{w\in V} \deg w \cdot f(w)^2}.$$

Proof. We observe that the values $(1-\lambda_1)^2, \dots, (1-\lambda_N)^2$ are exactly the eigenvalues of the symmetric matrix $M := (D^{-\frac{1}{2}}AD^{-\frac{1}{2}})^2$ whose entries are

$$M_{vu} = \sum_{w\in\mathcal{N}(v)\cap\mathcal{N}(u)} \frac{1}{\deg w\sqrt{\deg u\cdot\deg v}}, \qquad \text{for } v,u\in V,$$

In particular, ε^2 is the smallest eigenvalue of M. Therefore, by the Courant–Fischer–Weyl min-max principle applied to the Euclidean inner product $(\cdot,\cdot)$, we can write

$$\begin{aligned}
\varepsilon^2 &= \min_{f\in C(V)\setminus\{\mathbf{0}\}} \frac{(Mf,f)}{(f,f)}\\
&= \min_{f\in C(V)\setminus\{\mathbf{0}\}} \frac{\sum\limits_{v\in V} Mf(v)f(v)}{\sum\limits_{w\in V} f(w)^2}\\
&= \min_{f\in C(V)\setminus\{\mathbf{0}\}} \frac{\sum\limits_{v\in V}\sum\limits_{u\in V} M_{vu}f(u)\cdot f(v)}{\sum\limits_{w\in V} f(w)^2}\\
&= \min_{f\in C(V)\setminus\{\mathbf{0}\}} \frac{\sum\limits_{v\in V}\sum\limits_{u\in V}\sum\limits_{w\in\mathcal{N}(u)\cap\mathcal{N}(v)} \frac{1}{\deg w\sqrt{\deg u\cdot\deg v}}f(u)\cdot f(v)}{\sum\limits_{w\in V} f(w)^2}.
\end{aligned}$$

Now, observe that the numerator can be rewritten as

$$\begin{aligned}
\sum_{v\in V}\sum_{u\in V}\sum_{w\in\mathcal{N}(u)\cap\mathcal{N}(v)} \frac{f(u)\cdot f(v)}{\deg w\sqrt{\deg u\cdot\deg v}} &= \sum_{w\in V}\frac{1}{\deg w}\sum_{v\in\mathcal{N}(w)}\sum_{u\in\mathcal{N}(w)}\frac{f(u)\cdot f(v)}{\sqrt{\deg u\cdot\deg v}}\\
&= \sum_{w\in V}\frac{1}{\deg w}\left(\sum_{v\in\mathcal{N}(w)}\frac{f(v)}{\sqrt{\deg v}}\right)^2.
\end{aligned}$$

It follows that

$$\begin{aligned}
\varepsilon^2 &= \min_{f\in C(V)\setminus\{\mathbf{0}\}} \frac{\sum\limits_{w\in V}\frac{1}{\deg w}\left(\sum\limits_{v\in\mathcal{N}(w)}\frac{f(v)}{\sqrt{\deg v}}\right)^2}{\sum\limits_{w\in V} f(w)^2}\\
&= \min_{f\in C(V)\setminus\{\mathbf{0}\}} \frac{\sum\limits_{w\in V}\frac{1}{\deg w}\left(\sum\limits_{v\in\mathcal{N}(w)} f(v)\right)^2}{\sum\limits_{w\in V}\deg w\cdot f(w)^2}.
\end{aligned}$$

□

As a consequence of Lemma 1.8, we have that a graph on $N \geq 3$ nodes with $\varepsilon > \frac{1}{2}$ would satisfy

$$\sum_{w \in V} \frac{1}{\deg w} \left(\sum_{v \in \mathcal{N}(w)} f(v) \right)^2 > \frac{1}{4} \sum_{w \in V} \deg w \cdot f(w)^2, \quad \forall f \in C(V) \setminus \{\mathbf{0}\}. \tag{12}$$

This allows us, as shown in [38], to prove several properties that such graph should satisfy, and to arrive to a contradiction, which implies that $\varepsilon \leq \frac{1}{2}$. Similarly, in order to prove that equality is achieved if and only if G is either a petal graph or a book graph, once can study and analyze the structural constraints that a graph with $\varepsilon = \frac{1}{2}$ should have, again as a consequence of the characterization in Lemma 1.8.

Examples of properties that can be inferred from (12) are given by the following lemmas.

Lemma 1.9. *Let G be a connected graph on $N \geq 3$ nodes such that $\varepsilon > \frac{1}{2}$. Then, for any $v \in V$, there exists $w \in \mathcal{N}(v)$ such that* $\deg w \leq 3$.

Proof. Let f be such that $f(v) := 1$ and $f(u) := 0$ for all $u \neq v$. Then, (12) implies

$$\sum_{w \in \mathcal{N}(v)} \frac{1}{\deg w} > \frac{1}{4} \deg v.$$

Now, if $\deg w \geq 4$ for all $w \in \mathcal{N}(v)$, then

$$\sum_{w \in \mathcal{N}(v)} \frac{1}{\deg w} \leq \sum_{w \in \mathcal{N}(v)} \frac{1}{4} = \frac{1}{4} \deg v,$$

which is a contradiction. □

Given two vertices u and v, we let

$$\mathcal{N}(u) \triangle \mathcal{N}(v) := \big(\mathcal{N}(u) \cup \mathcal{N}(v)\big) \setminus \big(\mathcal{N}(u) \cap \mathcal{N}(v)\big)$$

be the *symmetric difference* of $\mathcal{N}(u)$ and $\mathcal{N}(v)$.

Lemma 1.10. *Let G be a connected graph on $N \geq 3$ nodes such that $\varepsilon > \frac{1}{2}$. If $\mathcal{N}(u) \cap \mathcal{N}(v) \neq \emptyset$, then $\mathcal{N}(u) \triangle \mathcal{N}(v) \neq \emptyset$ and*

$$\sum_{w \in \mathcal{N}(u) \triangle \mathcal{N}(v)} \left(\frac{1}{\deg w} - \frac{1}{4} \right) > \frac{1}{2}.$$

Proof. Let f be such that $f(v) := 1$, $f(u) := -1$ and $f(w) := 0$ for all $w \in V \setminus \{u, v\}$. Then, by (12),

$$\sum_{w \in \mathcal{N}(u) \triangle \mathcal{N}(v)} \frac{1}{\deg w} > \frac{1}{4} (\deg v + \deg u),$$

which also implies $\mathcal{N}(u) \triangle \mathcal{N}(v) \neq \emptyset$. Moreover, since

$$\deg v + \deg u = \mathcal{N}(u) \triangle \mathcal{N}(v) + 2 |\mathcal{N}(u) \cap \mathcal{N}(v)|,$$

the above inequality can be rewritten as

$$\sum_{w\in\mathcal{N}(u)\triangle\mathcal{N}(v)}\left(\frac{1}{\deg w}-\frac{1}{4}\right)>\frac{1}{4}\cdot 2|\mathcal{N}(u)\cap\mathcal{N}(v)|.$$

Since $\mathcal{N}(u)\cap\mathcal{N}(v)\neq\emptyset$, we have that $|\mathcal{N}(u)\cap\mathcal{N}(v)|\geq 1$, implying that

$$\sum_{w\in\mathcal{N}(u)\triangle\mathcal{N}(v)}\left(\frac{1}{\deg w}-\frac{1}{4}\right)>\frac{1}{2}.$$

□

It has long been an open question whether petal graphs can be characterized by the eigenvalues of some operators. In 2015 it has been proved that, among connected graphs, petal graphs are uniquely determined by the eigenvalues of the adjacency matrix [17]. And as a consequence of Theorem 1.7, we can say that petal graphs are completely characterized by the spectrum of the normalized Laplacian.

1.5 Coloring the normalized Laplacian

We start with a historical note on graph coloring taken from [50].

Historical note

While graph theory was born in 1736, when Leonard Euler solved the Königsberg Seven Bridges Problem [25], the history of graph coloring started in 1852, when the South African mathematician and botanist Francis Guthrie formulated the Four Color Problem [33, 44, 65, 67]. Francis Guthrie noticed that, when coloring a map of the counties of England, one needed at least four distinct colors if two regions sharing a common border could not have the same color. Moreover, he conjectured (and tried to prove) that four colors were sufficient to color any map in this way. His brother, Frederick Guthrie, supported him by sharing his work with Augustus De Morgan, of whom he was a student at the time, and De Morgan immediately showed his interest for the problem [30]. On October 23, 1852, De Morgan presented Francis Guthrie's conjecture in a letter to Sir William Rowan Hamilton, in which he wrote:

The more I think of it the more evident it seems.

But Hamilton replied:

I am not likely to attempt your quaternion of color very soon.

De Morgan then tried to get other mathematicians interested in the conjecture, and it eventually became one of the most famous open problems in graph theory and mathematics for more than a century. After several failed attempts in solving the problem, Francis Guthrie's conjecture was proved to be true in 1976, by Kenneth Appel and Wolfgang Haken, with the first major computer-assisted proof in history [3].

The Four Color Theorem can be equivalently described in the language of graph theory as follows. Let $G=(V,E)$ be a simple graph. A *k-coloring of the vertices* is a function $c:V\to\{1,\dots,k\}$, and it is *proper* if $v\sim w$ implies $c(v)\neq c(w)$. The *vertex coloring number* $\chi=\chi(G)$ is the minimum k such that there exists a proper k-coloring of the vertices. Moreover, the graph G is called *planar* if it can be embedded in the plane, that is, it can be drawn on the plane in such a way that its edges intersect only at their endpoints.

Theorem 1.11 (Four Color Theorem, 1976)**.** *If G is a planar simple graph, then $\chi \leq 4$.*

Despite the huge importance of this result, quoting William Thomas Tutte [64],

> *The Four Color Theorem is the tip of the iceberg, the thin end of the wedge and the first cuckoo of Spring.*

In fact, the study of the vertex coloring number χ has shown to be interesting also for several other problems in graph theory, as well as for applications to partitioning problems. Moreover, other notions of coloring have been introduced, and each of them has led to numerous challenging problems, many of which are beautifully summarized in [33, 64].

Graph coloring problems also raise important computational challenges, since determining whether a graph can be colored with k is NP-complete for every $k \geq 3$. For discussions of algorithmic and complexity aspects of graph coloring, we refer to [26, 45].

Relationship between χ and λ_N

Let G be a connected graph.

It is well-known (and easy to check) that $\chi = 2$ if and only if G is bipartite, while $\chi = N - 1$ if and only if G is the complete graph K_N. Similarly, Theorem 1.3 shows that $\lambda_N = 2$ if and only if G is bipartite, while $\lambda_N = \frac{N}{N-1}$ if and only if G is the complete graph K_N. Interestingly, in both the bipartite and the complete case we have

$$\lambda_N = \frac{\chi}{\chi - 1}.$$

It is therefore natural to ask what happens in the general case.

The following result was first proved by Elphick and Wocjan (2015) [23] (Equation 20) as a consequence of Theorem 1 in Nikiforov (2007) [56]. Alternative proofs and related results were later given by Coutinho, Grandsire and Passos (2019) [18] (Lemma 6) and by Sun and Das (2020) [61] (Theorem 3.1). We refer to [7] for a detailed discussion and further results.

Theorem 1.12. *Let G be a connected simple graph. Then,*

$$\lambda_N \geq \frac{\chi}{\chi - 1}.$$

Exercise 7. Find a family of graphs satisfying

$$\lambda_N = \frac{\chi}{\chi - 1}.$$

Exercise 8 (Open problem)**.** Determine all connected finite graphs satisfying

$$\lambda_N = \frac{\chi}{\chi - 1}.$$

2 Hypergraph normalized Laplacian(s)

2.1 Introduction

Hypergraphs (Figure 6) are a generalization of graphs in which edges are sets of vertices of any cardinality:

Definition. A *hypergraph* is a pair $G = (V, E)$, where

- $V := \{v_1, \ldots, v_N\}$ is the set of *vertices*,
- $E := \{e_1, \ldots, e_M\}$ is the multiset of *edges*, and $\emptyset \neq e_j \subseteq V$ for each j.

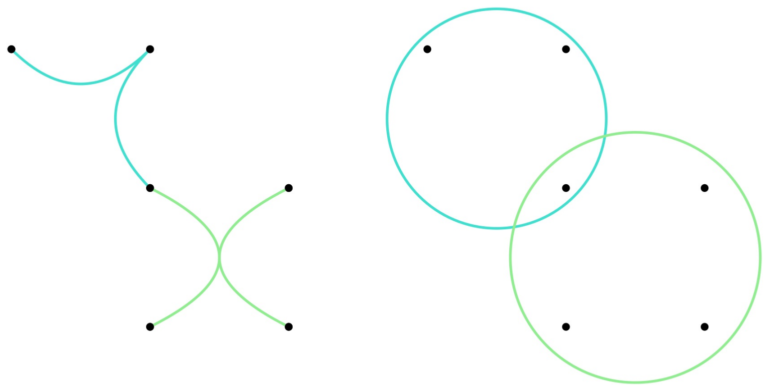

Figure 4: Two ways of drawing the same hypergraph on six vertices and two edges.

Hypergraphs can represent communities of elements of any size. For instance, in a collaboration network, vertices represent authors, and an edge connects all authors of a given paper. Such a representation naturally captures collaborations involving more than two people, which ordinary graphs can only model indirectly by introducing multiple pairwise connections.

Historically, while graphs were born in 1736, hypergraphs were probably born in 1931. In fact, in a 1994 paper [24], Erdős wrote:

> As far as I know, the subject of hypergraphs was first mentioned by T. Gallai in a conversation with me in 1931. He remarked that hypergraphs should be studied as a generalization of graphs. The subject really came to life only with the work of Berge.

This probably happened in front of the Statue of Anonymous, at the City Park of Budapest, where some of the greatest graph theorists in history like Paul Erdős, Tibor Gallai, Paul Turán, Vera Sós and their collaborators used to meet regularly.

In this section, we do not present proofs. The arguments are typically longer and more technical versions of those already seen for graphs in the previous section, while the underlying ideas remain similar. Instead, our focus is on providing an overview of the main results.

We consider a few generalizations of classical hypergraphs, as well as their spectral properties with respect to a specific type of generalized Laplacian matrix. We also discuss alternative approaches (such as the use of tensors) and one application to biology.

For the results in this section, we refer to [1, 8, 9, 34, 47–49, 52, 54].

Before proceeding, we give the following basic definitions.

Definition. The *degree* of a vertex $v \in V$ is

$$\deg v := |\{e \in E : v \in e\}|.$$

The *cardinality* of an edge $e \in E$ is

$$|e| := |\{v \in V : e \ni v\}|.$$

A hypergraph is *d-regular* if all vertices have the same degree d.
A hypergraph is *k-uniform* if all edges have the same cardinality k.

In particular, graphs are 2-regular hypergraphs.

2.2 Oriented hypergraphs

Oriented hypergraphs were introduced by Shi in [60] as a generalization of classical hypergraphs in which a plus or minus sign is assigned to each vertex–edge incidence. Since their introduction, such hypergraphs have received a lot of attention. The adjacency and Kirchhoff Laplacian matrices of oriented hypergraphs were introduced by Reff and Rusnak [58], while the normalized Laplacian was introduced in [34].

Definition. An *oriented hypergraph* (Figure 5) is a triple $G = (V, E, \varphi)$, where

- (V, E) is a hypergraph, and
- $\varphi : V \times E \to \{-1, 0, +1\}$ is such that

$$\varphi(v, e) \neq 0 \iff v \in e.$$

If $\varphi(v, e) = 1$ (resp. $\varphi(v, e) = -1$), v is said to be an *output* (resp. *input*) for e. If $v \neq v'$ and

$$\varphi(v, e) = \varphi(v', e) \neq 0 \quad (\text{resp. } \varphi(v, e) = -\varphi(v', e) \neq 0),$$

the vertices v and v' are *co-oriented* (resp. *anti-oriented*) in e.

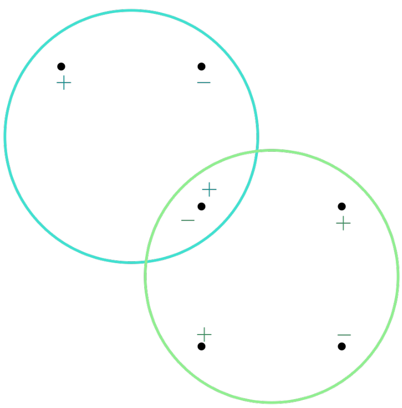

Figure 5: An oriented hypergraph on six vertices and two edges. Plus signs represent inputs, and minus signs represent outputs.

Let $G = (V, E, \varphi)$ be an oriented hypergraph on N vertices and M edges, with no vertices of degree 0.

Definition. The *degree matrix* of G is the $N \times N$ diagonal matrix

$$D := \mathrm{diag}(\deg v_1, \ldots, \deg v_N).$$

The *incidence matrix* of G is the $N \times M$ matrix $\mathcal{I} := (\varphi(v_i, e_j))_{ij}$.
The *adjacency matrix* of G is he $N \times N$ matrix $A := (A_{ij})_{ij}$, where $A_{ii} := 0$ for each $i = 1, \ldots, N$ and, for $i \neq j$,

$$\begin{aligned} A_{ij} := &\left|\{\text{edges in which } v_i \text{ and } v_j \text{ are anti-oriented}\}\right| \\ &- \left|\{\text{edges in which } v_i \text{ and } v_j \text{ are co-oriented}\}\right|. \end{aligned}$$

The *normalized Laplacian* of G is the $N \times N$ matrix

$$L := \mathrm{Id} - D^{-1}A = D^{-1}\mathcal{I}\mathcal{I}^{\top}.$$

Remark. A simple graph can be seen as oriented hypergraph in which E is a set (and not a multiset), all edges have cardinality 2, and each edge has one input and one output. In this case, independently of the choice of the edge orientations, we have that $A_{ij} = 1$ for $v_i \sim v_j$. Hence, in particular, L coincides with the graph normalized Laplacian.

Remark. Unlike in the graph case, $-L_{ij}$ is not always the transition probability from v_i to v_j in a random walk on V. One can define hypergraph Laplacians that do encode random walks, but these depend on *pairwise* transition probabilities between vertices, which can always be represented by an ordinary weighted graph. As discussed in [53], this may be seen as a drawback if one wishes to capture higher-order structure that is unique to hypergraphs.

Remark. While there is a 1 : 1 correspondence between graphs and each of their associated $N \times N$ matrices, this is not true for oriented hypergraphs. An alternative representation is via tensors, which offer a 1 : 1 correspondence with the hypergraph but at the cost of a much harder spectral theory, as the tensor eigenvalue problem is NP-hard. For a detailed discussion of spectral hypergraph theory via tensors, see [27].

Summarizing the main spectral properties of the normalized Laplacian L for oriented hypergraphs:

- L has N real, non-negative eigenvalues $\lambda_1 \leq \cdots \leq \lambda_N$, which sum to N and lie in the interval $[0, N]$.
- In contrast to the graph case, 0 is not necessarily an eigenvalue, and if it is, the corresponding eigenfunctions are not necessarily constant.
- The notion of bipartite graph and the bounds for λ_N in Theorem 1.3 have been generalized to the case of oriented hypergraphs [48].
- Cheeger inequalities have been generalized for uniform oriented hypergraphs [47].
- Spectral bounds on the chromatic number (including a generalization of Theorem 1.12) are discussed in [1, 8].

2.3 A biology application

We conclude this section with an application of spectral hypergraph theory to biology, taken from [51]. In this context, we consider an even more general class of hypergraphs, namely the *hypergraphs with real coefficients* that were introduced in [35], in which real coefficients can be assigned to the vertex-edge incidences (Figure 6).

Definition. A *hypergraph with real coefficients* is a triple $G = (V, E, \varphi)$, where

- (V, E) is a hypergraph, and
- $\varphi : V \times E \to \mathbb{R}$ is such that

$$\varphi(v, e) \neq 0 \iff v \in e.$$

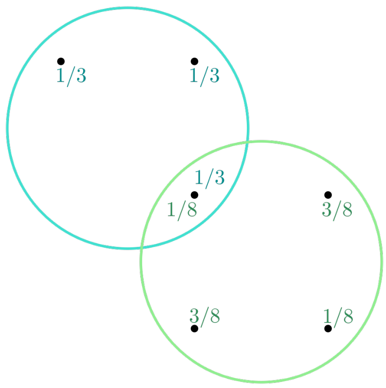

Figure 6: A hypergraph with real coefficients in $[0, 1]$.

Let G be a hypergraph with real coefficients. We define the following matrices, which generalize those used for oriented hypergraphs.

Definition. The *incidence matrix* of G is the $N \times M$ matrix $\mathcal{I}$ with entries $\mathcal{I}_{ij} := \varphi(v_i, e_j)$.

The *degree matrix* of G is the $N \times N$ matrix $D := \operatorname{diag}(\deg v_1, \dots, \deg v_N)$, where

$$\deg v_i := \sum_{j=1}^{M} \varphi(v_i, e_j)^2.$$

The *normalized Laplacian* is the $N \times N$ matrix

$$L := D^{-1} \mathcal{I} \mathcal{I}^\top.$$

Remark. The square in the above definition ensures that the degree depends only on the magnitude of the incidence coefficients, regardless of their sign, and that it generalizes the notion of degree for oriented hypergraphs.

Given a dataset of gene expression with N cells and M genes, we model it as a hypergraph with real coefficients on N nodes and M edges in which each vertex v represents a cell, each edge e represents a gene, and each coefficient $\varphi(v, e)$ represents the fraction of transcripts in cell v mapping to gene e. We assume that the coefficients are normalized with respect to cells, so that

$$\sum_{e} \varphi(v, e) = 1 \quad \text{for each } v.$$

Such normalization is the norm in RNA-seq analysis [21, 43, 63].

Remark. Because the edges of a hypergraph form a multiset, we can have distinct edges that contain the same vertices. In the context of gene expression networks, this allows us to model different genes that are expressed in exactly the same set of cells.

In the setting described above, let $\lambda_1 \leq \ldots \leq \lambda_N$ denote the eigenvalues of the normalized Laplacian L of the hypergraph with real coefficients. The following result (Corollary 2.6 in [51]) characterizes the extremal cases of the largest eigenvalue.

Theorem 2.1. *In the above setting, $1 \leq \lambda_N \leq N$ and, moreover,*

- $\lambda_N = 1$ *if and only if each edge has cardinality* 1*;*
- $\lambda_N = N$ *if and only if all edges have cardinality N and, for each edge e and for all vertices $v_i \neq v_j$,*
$$\varphi(v_i, e) = \varphi(v_j, e).$$

In the context of gene expression networks, Theorem 2.1 can be interpreted as follows. The largest eigenvalue λ_N attains its minimum value 1 precisely when each gene is concentrated in a single cell. Conversely, $\lambda_N = N$ exactly when each gene is uniformly distributed among all cells, a situation corresponding to complete cellular redundancy. In general, larger values of λ_N indicate greater cellular redundancy. Following [51], it is convenient to consider the normalized quantity $\mathcal{R} = \lambda_N/N$ as a measure of redundancy, making it independent of the number of cells. The interpretation of $\mathcal{R}$ as an estimate of cellular redundancy is supported by analyses of both simulated and real gene expression datasets in [51].

Exercise 9. Hypergraphs are also used in mathematical neuroscience to model neural networks, where vertices represent neurons and edges group together neurons that fire simultaneously. In this context, hypergraphs are often called *neural codes* [19]. Can you find a way to apply spectral methods in this setting, similarly to the biology applications above?

3 Graph non-backtracking Laplacian

"The non-backtracking operators have made their way into my dreams."

Joe Geraci

3.1 Basic definitions

This section is mainly based on [37].

Fix now a simple graph $G = (V, E)$ with vertices $v_1, \ldots, v_N$ and minimum degree ≥ 2. Choosing an *orientation* for an edge means letting one of its endpoints be its *input* and the other one be its *output*. We let $e = [v, w]$ denote the oriented edge whose input is v and whose output is w. In this case, we write $\mathrm{in}(e) \coloneqq v$ and $\mathrm{out}(e) \coloneqq w$. Moreover, we let $e^{-1} \coloneqq [w, v]$.

From now on, we fix an orientation for each edge of G. We let $e_1, \ldots, e_M$ denote the edges of G with this fixed orientation and we let

$$e_{M+1} \coloneqq e_1^{-1}, \ldots, e_{2M} \coloneqq e_M^{-1}$$

denote the edges with the inverse orientation.

Definition. A *non-backtracking random walk* on G is a discrete-time Markov process on the oriented edges such that the probability of going from e_i to e_j is

$$\mathbb{P}(e_i \to e_j) = \begin{cases} \frac{1}{\deg(\mathrm{out}(e_i))-1} & \text{if } \mathrm{out}(e_i) = \mathrm{in}(e_j) \text{ and } \mathrm{in}(e_i) \neq \mathrm{out}(e_j) \\ 0 & \text{otherwise.} \end{cases}$$

Equivalently, a non-backtracking random walk on $G = (V, E)$ can also be seen as a process on V, in which the probability that a random walker goes from a vertex v to a vertex w depends on where she was before arriving at v. However, this process is not Markovian, which is why it is convenient to study it from the point of view of the oriented edges.

Definition. The matrix $B \coloneqq B(G)$ is the $2M \times 2M$ matrix with $(0, 1)$–entries such that

$$B_{ij} = 1 \iff \text{out}(e_i) = \text{in}(e_j) \text{ and } \text{in}(e_i) \neq \text{out}(e_j).$$

The *non-backtracking matrix* of G is $B^\top$, the transpose matrix of B.

From now on, we also fix a directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ on $\mathcal{N}$ nodes and $\mathcal{M}$ edges that has no vertices of outdegree 0. If $\mathcal{G}$ has an edge from a vertex v to a vertex w, we write $v \to w$ and we denote such an edge by $(v \to w)$.

Remark. Note that, although both oriented edges and directed edges are defined as ordered pairs of vertices, these two definitions are conceptually different. In fact, while directions are intrinsic of the chosen graph, orientations are not. This is what motivates us to use two different notations for oriented and directed edges.

Definition. The *degree* of a vertex v is

$$\deg v \coloneqq \deg_{\mathcal{G}} v \coloneqq |\{w \in \mathcal{V} : (v \to w) \in \mathcal{E}\}|.$$

The *degree matrix* of $\mathcal{G}$ is the $\mathcal{N} \times \mathcal{N}$ diagonal matrix $\mathcal{D} \coloneqq \mathcal{D}(\mathcal{G}) \coloneqq (\mathcal{D}_{vw})_{v,w \in \mathcal{V}}$ whose diagonal entries are

$$\mathcal{D}_{vv} \coloneqq \deg v.$$

The *adjacency matrix* of $\mathcal{G}$ is the $\mathcal{N} \times \mathcal{N}$ matrix $\mathcal{A} \coloneqq \mathcal{A}(\mathcal{G}) \coloneqq (\mathcal{A}_{vw})_{v,w \in \mathcal{V}}$ defined by

$$\mathcal{A}_{vw} \coloneqq \begin{cases} 1 & \text{if } v \to w \\ 0 & \text{otherwise.} \end{cases}$$

Remark. Note that the degree counts the number of outgoing edges from a node, and therefore it is also often called the outdegree.

Definition. A *random walk* on $\mathcal{G}$ is a discrete-time Markov process on $\mathcal{V}$ such that the probability of going from a vertex v to a vertex w is

$$\mathbb{P}(v \to w) = \begin{cases} \frac{1}{\deg v} & \text{if } v \to w \\ 0 & \text{otherwise.} \end{cases}$$

Definition. The *normalized Laplacian* of $\mathcal{G}$ is the $\mathcal{N} \times \mathcal{N}$ matrix

$$\mathcal{L}(\mathcal{G}) \coloneqq \text{Id} - \mathcal{D}^{-1}\mathcal{A}.$$

Definition. The *non-backtracking graph* or *Hashimoto graph* of G is the directed graph $\mathcal{NB}(G)$ on vertices $e_1, \ldots, e_{2M}$, that has B as adjacency matrix.

Example 3.1. If G is the cycle graph on N nodes, then $\mathcal{NB}(G)$ is given by two disconnected directed cycles on N nodes (Figure 7).

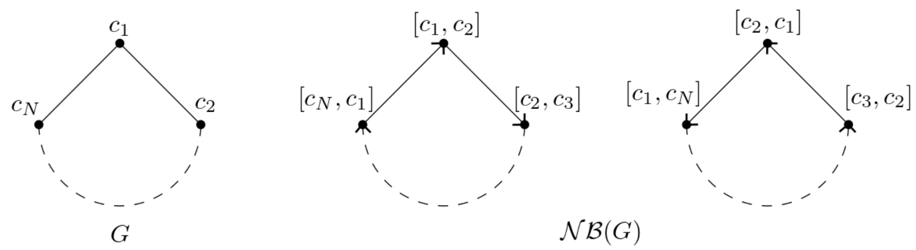

Figure 7: The cycle graph G and its non-backtracking graph $\mathcal{NB}(G)$.

Clearly, a random walk on the directed graph $\mathcal{NB}(G)$ is equivalent to a non-backtracking random walk on G. Moreover, for each oriented edge e_i,

$$\deg_{\mathcal{G}} e_i = \deg_G(\text{out}(e_i)) - 1.$$

As a consequence, we have that G is $k+1$–*regular* (meaning that all its vertices have constant degree $k+1$) if and only if $\mathcal{NB}(G)$ is k–regular. Similarly, G is bipartite if and only if $\mathcal{NB}(G)$ is bipartite, since G has odd-length cycles if and only if $\mathcal{NB}(G)$ has odd-length cycles.

Exercise 10. Let $G = (V, E)$ be a simple graph on N nodes and M edges, and let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be its non-backtracking graph. Then, $\mathcal{G}$ has $2M$ nodes and $\sum_{v \in V}(\deg_G v)^2 - 2M$ edges.

Definition. The *non-backtracking Laplacian* of G, denoted by $\mathcal{L} := \mathcal{L}(G)$, is the normalized Laplacian $\mathcal{L}(\mathcal{NB}(G))$ of $\mathcal{NB}(G)$.

3.2 First properties

In Example 3.1 we saw that, if G is a cycle graph, then its non-backtracking graph is given by two disconnected cycles. The next theorem shows that this is the only case in which a connected simple graph has a disconnected non-backtracking graph.

Theorem 3.1. *Let $G = (V, E)$ be a simple connected graph on N nodes and M edges, with minimum degree ≥ 2, and let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be its non-backtracking graph. Then, the following are equivalent:*

1. *G is not the cycle graph;*
2. *G has at least two cycles;*
3. *$\mathcal{G}$ is weakly connected;*
4. *$\mathcal{G}$ is strongly connected.*

Proof. Clearly, since the minimum degree in G is ≥ 2, the first two conditions are equivalent to each other. Moreover, 4 clearly implies 3 and, by Example 3.1, 3 implies 1. Hence, if we prove that 1 implies 4, we are done.

Assume that G is not the cycle graph and fix two distinct elements $[v, w], [x, y] \in \mathcal{V}$. We want to show that there exists a directed path, in $\mathcal{G}$, from $[v, w]$ to $[x, y]$.
Since G is connected, there exists a path, in G, of the form

$$(w, p_1), (p_1, p_2), \ldots, (p_{k-1}, p_k), (p_k, x)$$

which is non-backtracking, i.e., such that $p_2 \neq w$, $p_{k-1} \neq x$ and $p_i \neq p_{i+2}$ for $i = 1, \dots, k-2$. This gives a directed path, in $\mathcal{G}$, of the form

$$[w, p_1] \to [p_1, p_2] \to \dots \to [p_{k-1}, p_k] \to [p_k, x].$$

If $p_1 \neq v$ and $p_k \neq y$, then $\mathcal{G}$ has also the directed path

$$[v, w] \to [w, p_1] \to [p_1, p_2] \to \dots \to [p_{k-1}, p_k] \to [p_k, x] \to [x, y],$$

hence the claim holds in this case.
If $p_1 = v$ and $p_k \neq y$, then by the assumptions that G is not the cycle graph and each vertex in G has degree ≥ 2, it follows that there exists a non-backtracking path in G of the form (Figure 8)

$$(v, w), (w = q_1, q_2), \dots, (q_{r-1}, q_r = c_1), \dots, (c_{s-1}, c_s = c_1),$$

for some $r \geq 1$ and $s \geq 3$.

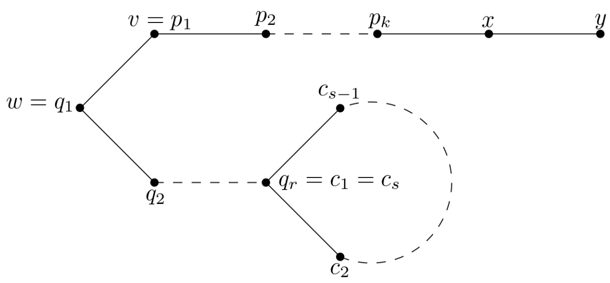

Figure 8: An illustration of the proof of Theorem 3.1.

In this case, there exists a directed path from $[v, w]$ to $[x, y]$, in $\mathcal{G}$, of the form

$$\begin{aligned}
&[v, w] \to [w, q_2] \to \dots \to [q_{r-1}, q_r = c_1] \to \dots \to [c_{s-1}, c_s = c_1] \\
&\to [c_1 = q_r, q_{r-1}] \to \dots \to [q_2, w] \to [w, v] \\
&\to [v, p_2] \to \dots \to [p_k, x] \to [x, y].
\end{aligned}$$

If either $p_1 \neq v$ and $p_k = y$, or $p_1 \neq v$ and $p_k \neq y$, the claim follows in a similar way. This shows that, if G is not the cycle graph, then $\mathcal{G}$ is strongly connected. □

We now consider a directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ on $\mathcal{N}$ nodes and $\mathcal{M}$ edges that has no vertices of degree 0 and which is not, necessarily, the non-backtracking graph of a simple graph. We observe that its normalized Laplacian $\mathcal{L}$ can be seen as an operator

$$\mathcal{L} : \{f : \mathcal{V} \to \mathbb{C}\} \to \{f : \mathcal{V} \to \mathbb{C}\}$$

such that, given $f : \mathcal{V} \to \mathbb{C}$ and $\omega \in \mathcal{V}$,

$$\mathcal{L}f(\omega) = f(\omega) - \frac{1}{\deg \omega} \left(\sum_{\omega \to \tau} f(\tau) \right).$$

In particular, a pair (λ, f) with $\lambda \in \mathbb{C}$ and $f : \mathcal{V} \to \mathbb{C}$ is an eigenpair for $\mathcal{L}$ if and only if, for each $\omega \in \mathcal{V}$,

$$(1 - \lambda) f(\omega) = \frac{1}{\deg \omega} \left(\sum_{\omega \to \tau} f(\tau) \right).$$

The following observations have been proved by Bauer in [4].

Remark. Clearly, for any directed graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ on $\mathcal{N}$ nodes, its normalized Laplacian $\mathcal{L}$ has $\mathcal{N}$ eigenvalues (counted with algebraic multiplicity) that sum to $\mathcal{N}$, since $\mathcal{L}$ is an $\mathcal{N} \times \mathcal{N}$ matrix that has trace $\mathcal{N}$. Moreover, by Proposition 3.2 in [4], the spectrum of $\mathcal{L}$ is contained in the complex disc $D(1,1)$. In particular, the real eigenvalues are contained in $[0,2]$. Also, by Proposition 3.1 in [4], 0 is an eigenvalue for $\mathcal{L}$ and the constant functions $f : \mathcal{V} \to \mathbb{C}$ are the corresponding eigenfunctions. As a consequence, from the spectrum of $\mathcal{L}$ we can derive the number of connected components of $\mathcal{G}$. Notably, this does not hold for the adjacency matrix $\mathcal{A}$ of $\mathcal{G}$.

Now, for a simple undirected graph G, the following are equivalent [11, 16]:

1. G is bipartite;
2. The spectrum of the normalized Laplacian $L(G)$ is symmetric with respect to the line $x = 1$;
3. 2 is an eigenvalue of $L(G)$;
4. The spectrum of the adjacency matrix $A(G)$ is symmetric with respect to the line $x = 0$.

In the next proposition we prove that, for a directed graph $\mathcal{G}$, condition 1 above implies 2, 3 and 4. However, as shown in Example 3.2 below, these conditions are not equivalent.

Proposition 3.2. *If $\mathcal{G}$ is a directed bipartite graph, then the spectra of both its normalized Laplacian $\mathcal{L}$ and its adjacency matrix $\mathcal{A}$ are symmetric. Hence, in particular, 2 is an eigenvalue for $\mathcal{L}$.*

Proof. Without loss of generality, we only prove the first claim for the normalized Laplacian, the other case being similar. The proof follows the same idea as the proof for the undirected case in [16, Lemma 1.8].
If $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is bipartite, $\mathcal{V}_1 \sqcup \mathcal{V}_2$ is a corresponding bipartition and (λ, f) is an eigenpair for $\mathcal{L}$, then also $(2 - \lambda, \tilde{f})$ is an eigenpair, where

$$\tilde{f} := \begin{cases} f & \text{on } \mathcal{V}_1 \\ -f & \text{on } \mathcal{V}_2. \end{cases}$$

As an immediate consequence, 2 is an eigenvalue for $\mathcal{L}$, since 0 is always an eigenvalue. □

The next example shows a directed graph that is not bipartite but is such that 2 is an eigenvalue for its normalized Laplacian.

Example 3.2. Consider the connected graph $\mathcal{G}$ in Figure 9, where the numbers on the vertices indicate the values of a function f. Then, $\mathcal{G}$ is not bipartite, and f is an eigenfunction for $\mathcal{L}(G)$ with eigenvalue 2, since it satisfies

$$-f(\omega) = \frac{1}{\deg \omega} \left(\sum_{\omega \to \tau} f(\tau) \right), \quad \forall \omega \in \mathcal{V}.$$

Remark. For any directed graph $\mathcal{G}$, its normalized Laplacian $\mathcal{L}$ and its adjacency matrix $\mathcal{A}$ satisfy:

- $(f, 0)$ is an eigenpair for $\mathcal{A}$ if and only if $(f, 1)$ is an eigenpair for $\mathcal{L}$;

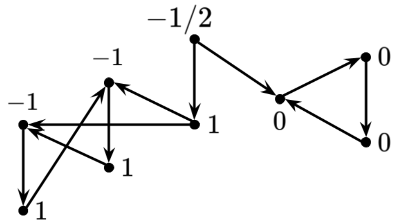

Figure 9: The directed graph in Example 3.2.

- If $\mathcal{G}$ is k–regular, then (f, λ) is an eigenpair for $\mathcal{A}$ if and only if $(f, 1 - \frac{\lambda}{k})$ is an eigenpair for $\mathcal{L}$.

The properties of the normalized Laplacian that we investigated so far hold for any directed graph. For the next observations and results, we focus on the case of non-backtracking graphs. As before, we fix a simple graph $G = (V, E)$ on N nodes and M edges that has minimum degree ≥ 2. For simplicity, we denote its non-backtracking graph by $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. We let $\mathcal{A}$ denote the adjacency matrix of $\mathcal{G}$ (equivalently, the transpose of the non-backtracking matrix of G) and we let $\mathcal{L}$ denote the normalized Laplacian of $\mathcal{G}$ (equivalently, the non-backtracking Laplacian of G). Similarly, we let A and L denote the adjacency matrix and the normalized Laplacian of G, respectively.

Remark. We observed that G is regular if and only if $\mathcal{G}$ is regular. In this case, by Remark 3.2, the spectral properties of $\mathcal{L}$ and $\mathcal{A}$ are equivalent to each other, and similarly also the spectral properties of L and A are equivalent to each other. But since it is known that, in the regular case, the eigenvalues of $\mathcal{A}$ can be recovered by those of A [40, 42], it follows that in this case also the spectral theory of $\mathcal{L}$ can be recovered from the one of A or, equivalently, of L.

Before stating next theorem, we define the $2M \times 2M$ matrix

$$P := \begin{pmatrix} 0 & \mathrm{Id} \\ \mathrm{Id} & 0 \end{pmatrix} \tag{13}$$

and we observe that $P^\top = P$, while $P^2 = \mathrm{Id}$.
Moreover, given $\mathbf{x}, \mathbf{y} \in \mathbb{C}^{2M}$, we let $\langle \mathbf{x}, \mathbf{y} \rangle := \overline{\mathbf{x}}^\top \mathbf{y}$ be the usual complex inner product, and we define their *P-product* as

$$(\mathbf{x}, \mathbf{y})_P := \langle \mathbf{x}, P\mathbf{y} \rangle = \overline{\mathbf{x}}^\top P \mathbf{y}.$$

The next theorem also holds for the adjacency matrix of $\mathcal{G}$ (equivalently, the transpose of the non-backtracking matrix of G). The proofs are analogous.

Theorem 3.3. *Let $\mathcal{L}$ be the non-backtracking Laplacian of a graph. Then,*

1. *$\mathcal{L}^\top = P\mathcal{L}P$;*
2. *$\mathcal{L}$ is self-adjoint with respect to the P-product;*
3. *If $(\lambda, \mathbf{x})$ is an eigenpair for $\mathcal{L}$ and $\lambda \in \mathbb{C}$ is not real, then*

$$\sum_{[v,w]} \overline{x_{[v,w]}} \cdot x_{[w,v]} = \sum_{i=1}^{m} \left(\overline{x_i} \cdot x_{i+M} + \overline{x_{i+M}} \cdot x_i \right) = 0.$$

Proof. 1. We have that, for $i \neq j$ with $i, j \leq M$,

$$(\mathcal{L}^\top)_{ij} = \mathcal{L}_{ji} = -\mathbb{P}(e_j \to e_i) = -\mathbb{P}(e_i^{-1} \to e_j^{-1}) = \mathcal{L}_{i+M,j+M} = (P\mathcal{L}P)_{ij}.$$

This allows us to write

$$\mathcal{L}^\top = P\mathcal{L}P.$$

2. Since $P^\top = P$ and $P^2 = \mathrm{Id}$, we have that

$$\begin{aligned}(\mathbf{x}, \mathcal{L}\mathbf{y})_P &= \langle \mathbf{x}, P\mathcal{L}\mathbf{y}\rangle = \langle P\mathbf{x}, \mathcal{L}\mathbf{y}\rangle = \langle \mathcal{L}^\top P\mathbf{x}, \mathbf{y}\rangle \\ &= \langle P\mathcal{L}P^2\mathbf{x}, \mathbf{y}\rangle = \langle P\mathcal{L}\mathbf{x}, \mathbf{y}\rangle = \langle \mathcal{L}\mathbf{x}, P\mathbf{y}\rangle = (\mathcal{L}\mathbf{x}, \mathbf{y})_P.\end{aligned}$$

Therefore, $\mathcal{L}$ is self-adjoint with respect to the P-product.

3. The second claim implies that, if $(\lambda, \mathbf{x})$ is an eigenpair for $\mathcal{L}$, then

$$\lambda(\mathbf{x}, \mathbf{x})_P = (\mathbf{x}, \lambda\mathbf{x})_P = (\mathbf{x}, \mathcal{L}\mathbf{x})_P = (\mathcal{L}\mathbf{x}, \mathbf{x})_P = (\lambda\mathbf{x}, \mathbf{x})_P = \overline{\lambda}(\mathbf{x}, \mathbf{x})_P.$$

Hence, if $\lambda \neq \overline{\lambda}$, i.e., λ is not real, then $(\mathbf{x}, \mathbf{x})_P = 0$, that is, $\overline{\mathbf{x}}^\top P\mathbf{x} = 0$, which can be re-written as

$$\sum_{[v,w]} \overline{x_{[v,w]}} \cdot x_{[w,v]} = \sum_{i=1}^{m} (\overline{x_i} \cdot x_{i+M} + \overline{x_{i+M}} \cdot x_i) = 0.$$

□

Following the terminology in [10], the first condition in Theorem 3.3 can be reformulated by saying that $\mathcal{L}$ is *PT-symmetric* (where PT stands for parity-time). Moreover, following the terminology in [28], the second condition in Theorem 3.3 can be reformulated by saying that $\mathcal{L}$ is *P-self adjoint.*

3.3 Cospectrality and spectral gap from 1

As before, we fix a simple graph $G = (V, E)$ that has minimum vertex degree $\delta \geq 2$. We let Δ denote the maximum vertex degree of G, and we let $\mathcal{G}$ denote the non-backtracking graph of G. We also let A be the adjacency matrix of G, we let L be the normalized Laplacian of G, we let $\mathcal{A}$ be the adjacency matrix of $\mathcal{G}$ (equivalently, the transpose of the non-backtracking matrix of G), we let $\mathcal{D}$ denote the degree matrix of $\mathcal{G}$, and we let $\mathcal{L} = \mathrm{Id} - \mathcal{D}^{-1}\mathcal{A}$ denote the normalized Laplacian of $\mathcal{G}$ (equivalently, the non-backtracking Laplacian of G).
Moreover, given any operator $\mathcal{O}$, we let $\sigma(\mathcal{O})$ denote its spectrum and we let $\rho(\mathcal{O})$ denote its spectral radius, i.e., the largest modulus of its eigenvalues.

Cospectrality

Our computations for graphs with small number of nodes suggest that the non-backtracking Laplacian has nicer cospectrality properties than all other operators. We show the outcome in Table 1 and Table 2 below. Interestingly, we can observe that the number of $\mathcal{L}$–cospectral graphs as a function of the number of edges M is in progression:

$$4, 8, 16, 24, 26, 26, 14, 16, 8, 4;$$

N	#graphs	A	L	$\mathcal{A}$	$\mathcal{L}$
≤6	76	0	2	0	0
7	510	26	4	0	0
8	7 459	744	11	2	0
9	197 867	32 713	243	6	0
10	9 808 968	1 976 884	16 114	10 130	156
total	10 014 880	2 010 367	16 374	10 138	156

Table 1: Graphs with minimum degree ≥ 2 not determined by their spectrum, by number of nodes N.

see right-most column of Table 2. We hypothesize this is not an accident but part of a larger pattern.

Spectral gap from 1

It is known that $0 \in \sigma(\mathcal{A}^\top) = \sigma(\mathcal{A})$ if and only if G contains nodes of degree 1 [62]. Since $\delta \geq 2$, this implies that $1 \notin \sigma(\mathcal{L})$. Hence, the spectral gap from 1 for $\mathcal{L}$,

$$\varepsilon := \min_{\lambda \in \sigma(\mathcal{L})} |1 - \lambda| = \min_{\lambda \in \sigma(\mathcal{D}^{-1}\mathcal{A})} |\lambda|,$$

is non-zero.

In Theorem 3.4 below, we give a lower bound for ε, and we prove that the bound is sharp. We refer to [55] for a sharp upper bound.

Theorem 3.4. *Let G be a simple graph with maximum vertex degree Δ. Then, the spectral gap from 1 for the non-backtracking Laplacian $\mathcal{L}$ of G satisfies*

$$\varepsilon \geq \frac{1}{\Delta - 1}.$$

Moreover, the bound is sharp.

Proof. We follow the notations in the beginning of this section. We observe that, since $0 \notin \sigma(\mathcal{A})$, the matrix $\mathcal{A}$ is invertible. Therefore, we can write

$$\varepsilon^{-1} = \max_{\lambda \in \sigma(\mathcal{D}\mathcal{A}^{-1})} |\lambda| = \rho(\mathcal{D}\mathcal{A}^{-1}).$$

Further, it is known that any sub-multiplicative norm $\|\cdot\|$ satisfies

$$\rho\left(\mathcal{D}\mathcal{A}^{-1}\right) \leq \|\mathcal{D}\mathcal{A}^{-1}\| \leq \|\mathcal{D}\| \cdot \|\mathcal{A}^{-1}\|.$$

Take for example the spectral norm $\|\cdot\|_2$, defined by

$$\|M\|_2 := \sqrt{\max_{\lambda \in \sigma(M^* M)} |\lambda|},$$

and note that $\|\mathcal{D}\|_2 = \Delta - 1$. Also note that $\|\mathcal{A}^{-1}\|_2^2$ equals the largest magnitude among the eigenvalues of $\left(\mathcal{A}^{-1}\right)^* \mathcal{A}^{-1}$. But we have $\mathcal{A}^* = P\mathcal{A}P$, hence $(\mathcal{A}^{-1})^* = P\mathcal{A}^{-1}P$ and thus

$$\|\mathcal{A}^{-1}\|_2^2 = \max_{\lambda \in \sigma(P\mathcal{A}^{-1}P\mathcal{A}^{-1})} |\lambda| = \max_{\lambda \in \sigma(P\mathcal{A}^{-1})} |\lambda|^2 = \frac{1}{\min_{\lambda \in \sigma(\mathcal{A}P)} |\lambda|^2} = 1,$$

M	#graphs	$\mathcal{A}$	$\mathcal{L}$
0	0	0	0
1	0	0	0
2	0	0	0
3	0	0	0
4	1	0	0
5	2	0	0
6	6	0	0
7	10	0	0
8	25	0	0
9	68	0	0
10	182	0	0
11	532	0	0
12	1 679	0	0
13	5 218	4	0
14	15 437	14	0
15	41 126	26	0
16	96 274	62	0
17	197 433	162	0
18	355 986	364	4
19	567 827	634	8
20	807 284	983	16
21	1 029 639	1 329	24
22	1 184 688	1 492	26
23	1 235 599	1 490	26
24	1 172 658	1 333	24
25	1 015 663	989	16
26	804 863	628	8
27	584 762	368	4
28	390 136	166	0
29	239 514	60	0
30	135 636	26	0
31	71 025	8	0
32	34 559	0	0
33	15 734	0	0
34	6 745	0	0
35	2 764	0	0
36	1 101	0	0
$\geq$37	704	0	0
total	10 014 880	10 138	156

Table 2: Graphs with minimum degree ≥ 2 and $4 \leq N \leq 10$ not determined by their spectrum, by number of edges M.

where we have used that the smallest magnitude among eigenvalues of $\mathcal{A}P$ is 1 [37]. Therefore,

$$\varepsilon^{-1} = \rho\left(\mathcal{D}\mathcal{A}^{-1}\right) \leq \|\mathcal{D}\|_2 \cdot \|\mathcal{A}^{-1}\|_2 = \Delta - 1.$$

Thus, the spectral gap ε is at least $(\Delta - 1)^{-1}$.
To prove that the lower bound is sharp, use the fact that $\pm 1 \in \sigma(\mathcal{A})$ [42]. If G is Δ–regular, this implies that $1 \pm \frac{1}{\Delta - 1}$ are eigenvalues of $\mathcal{L}$. Thus, $\varepsilon = \frac{1}{\Delta-1}$ in this case. □

Remark. For the normalized Laplacian of simple graphs, the result in Theorem 3.4 does not hold. In fact, as we have seen in Section 1.4, 1 can be an eigenvalue.

In the proof of Theorem 3.4 we have shown that, if G is Δ–regular, then $1 \pm \frac{1}{\Delta-1}$ are two real eigenvalues of $\mathcal{L}$. A natural question is whether regular graphs are the only graphs for which $\varepsilon = \frac{1}{\Delta-1}$, but the answer is no. As shown in [37], also the presence of a Δ–regular cycle in the graph G produces the eigenvalues $1 \pm \frac{1}{\Delta-1}$ for $\mathcal{L}$.

3.4 More exercises

We conclude with a few further exercises. The open questions below are theoretical, but exploring examples numerically could already give valuable insight and provide intuition for possible results. These questions were formulated by Raffaella Mulas and Leo Torres in the course of their joint work on [37] and their lecture series on *Non-backtracking operators of graphs* at the Max Planck Institute for Mathematics in the Sciences.

Given two undirected graphs, they are said to be *X–cospectral*, *X-cospectral mates* or simply *X-mates* if the eigenvalue spectrum of their respective matrices X is the same, including multiplicities.

Exercise 11 (Conjecture)**.** Almost all graphs with minimum degree ≥ 2 are determined by the spectrum of their non-backtracking Laplacian $\mathcal{L}$.

Exercise 12 (Open problem)**.** Prove interlacing results for $\mathcal{L}$, i.e., establish inequalities that relate the eigenvalues of the non-backtracking Laplacian of a graph G to those of a subgraph of G.

Exercise 13 (Conjecture)**.** Prove that the number of real eigenvalues of $\mathcal{L}$ is at least $2M - 2N$.

Exercise 14. How would you generalize the non-backtracking Laplacian to hypergraphs?

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