Spectral graph theory through the eyes of a PDE guy

James Kennedy

Grupo de Física Matemática
Faculdade de Ciências da Universidade de Lisboa

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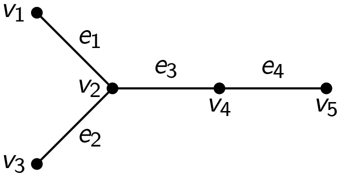
Reminder: graphs

Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where

- $\mathcal{V}$ = set of *vertices* (or *nodes*)
- $\mathcal{E}$ = set of *edges*

Each edge is associated with a pair of vertices.



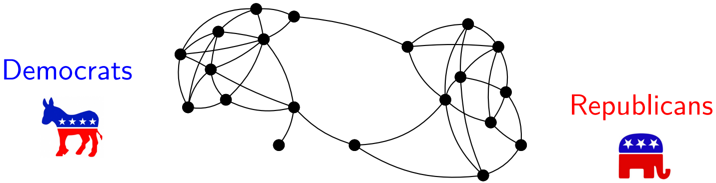
Here:

- $\mathcal{V} = \{v_1, v_2, v_3, v_4, v_5\}$
- $\mathcal{E} = \{e_1, e_2, e_3, e_4\}$
- $e_1 \sim (v_1, v_2)$, $e_2 \sim (v_2, v_3)$
- $e_3 \sim (v_2, v_4)$, $e_4 \sim (v_4, v_5)$

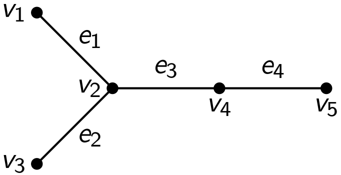
Edges can be *directed*, e.g. $(v_2, v_4) \neq (v_4, v_2)$, or *undirected*.
The *degree* of a vertex v is the number of edges attached to it ("adjacent edges"), e.g., $\deg v_2 = 3$, $\deg v_4 = 2$

Reminder: graphs

- Often used to model *networks*, e.g. social networks:
  - Undirected edges: each node represents a user, each edge represents a “friendship”.
  - Directed edges: each node represents a user or a webpace, each edge represents a follower or a link.
- Plenty of other examples! Electricity circuits, electricity networks, biology, machine learning/data analysis, ...
- Motivating question for us: structure/geometry of the graph: is it “big”? “small”? highly connected? or are there clusters?



Graphs and matrices

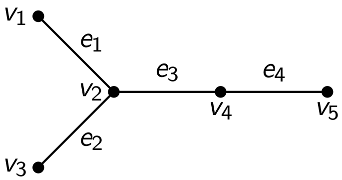


Encode the structure of the graph in matrices:

- The *adjacency matrix* encodes the structure of the graph: the (i,j)-entry is 1 (or weight $w_{ij} > 0$) if v_i and v_j share an edge, or 0 otherwise. It is symmetric if the edges are undirected.
- The *degree matrix* is the diagonal matrix whose (i,i)-entry is the degree of v_i.

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \qquad D = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Graphs, matrices and difference operators



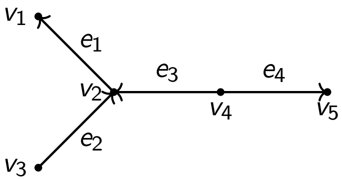
Definition

The *("combinatorial") Laplacian* is the *difference operator* corresponding to the matrix $L := D - A \in \mathbb{R}^{|\mathcal{V}|\times|\mathcal{V}|}$.

Here $L = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 3 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$.

Given a vector $x = (x_1, \dots, x_5)^T$, e.g. $x_4 \mapsto -x_2 + 2x_4 - x_5$.

Observation: $Lx = 0$ iff x has the *mean value property*.



Alternative representation of L via the *(signed) incidence matrix* $\mathcal{I} \in \mathbb{R}^{|\mathcal{V}|\times|\mathcal{E}|}$: given an arbitrary *orientation* of the edges, define

$$\mathcal{I}_{ij} = \begin{cases} 1 & \text{if } e_j \text{ terminates at } v_i \\ -1 & \text{if } e_j \text{ begins at } v_i \\ 0 & \text{otherwise} \end{cases}$$

With this orientation, or any other,

$$\mathcal{I}\mathcal{I}^T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 3 & -1 & -1 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix} = L$$

Matrices and spectra

Proposition

$L = D - A = \mathcal{I}\mathcal{I}^T$ is a symmetric, positive semidefinite matrix.

Consequence

$$a(x, y) = x^T L y = (\mathcal{I}^T x)^T (\mathcal{I}^T y), \qquad x, y \in \mathbb{R}^{|\mathcal{V}|}$$

defines a nonnegative (and continuous, and coercive after a shift) bilinear form, which also characterises the eigenvalues and eigenvectors of L.

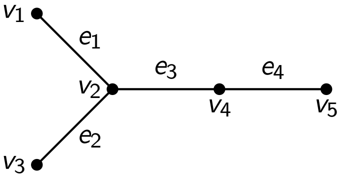
Proposition

L has $n := |\mathcal{V}|$ eigenvalues $0 = \lambda_1 \leq \ldots \leq \lambda_n$, counting multiplicities (the eigenvalue 0 has multiplicity equal to the number of connected components of $\mathcal{G}$, and its eigenvectors are piecewise constant). The eigenvectors can be chosen to form an orthonormal basis of $\mathbb{R}^n$.

There is an alternative normalisation: the *normalised Laplacian*

$$L_{norm} = I - D^{-1/2} A D^{-1/2}$$

has the same basic properties but its $n = |\mathcal{V}|$ eigenvalues lie in the interval $[0, 2]$.



$$L_{norm} = \begin{pmatrix} 1 & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ -\frac{1}{\sqrt{3}} & 1 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{6}} & 0 \\ 0 & -\frac{1}{\sqrt{3}} & 1 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & 0 & 1 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & 1 \end{pmatrix}.$$

Spectra and geometry

The eigenvalues of $L = D - A$ can be characterised *variationally*. For example, supposing $\mathcal{G}$ is connected,

$$0 < \lambda_2 = \min_{0 \neq x \perp \mathbf{1}} \frac{x^T L x}{x^T x} = \min_{0 \neq x \perp \mathbf{1}} \frac{|\mathcal{I}^T x|^2}{|x|^2}$$

(i.e. orthogonal to the span of the first eigenvector), with equality iff x is an eigenvector for λ_2.

$$|\mathcal{I}^T x|^2 = \sum_e |x(e_{\text{terminal}}) - x(e_{\text{initial}})|^2$$

measures (squares of) differences of x at neighbouring vertices.

Definition / Proposition

λ_2 is called the *algebraic connectivity* of $\mathcal{G}$. The corresponding eigenvectors, necessarily sign-changing, are called *Fiedler vectors* and can be chosen to change sign only once (i.e. the sets of vertices where they are positive/negative are both connected).

Spectra and geometry

Theorem (Fiedler, 1973)

Suppose $\mathcal{G}$ has n vertices. Then $\lambda_2(\mathcal{G}) \geq \lambda_2(\mathcal{P}_n)$, where $\mathcal{P}_n$ is a *path graph* on n vertices. 

Actually: Fiedler showed that if $\mathcal{G}$ has *edge connectivity* η, i.e., between any two vertices there are at least η non-edge-overlapping paths, then $\eta + 1 \geq \lambda_2(\mathcal{G}) \geq \eta\lambda_2(\mathcal{P}_n)$.

Heuristic principle

More connected graphs have larger algebraic connectivity λ_2.

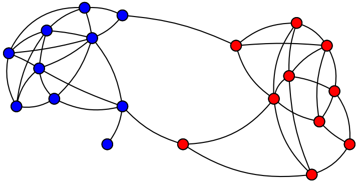
(For a "variational" proof of Fiedler's theorem and a characterisation of equality in the general case see Berkolaiko–K.–Kurasov–Mugnolo, J. Phys. A, 2017.)

$\lambda_2 = \min_{0 \neq x \perp 1} \frac{|\mathcal{I}^T x|^2}{|x|^2}$: deleting an edge lowers $|\mathcal{I}^T x|^2$, leaving $|x|^2$ (and $x \perp 1$) unchanged: thus λ_2 goes down.

Spectra and geometry

Heuristic principle

More connected graphs have larger algebraic connectivity λ_2.



Think of vectors as functions "living" on the vertices, and $\mathcal{I}$ as an operator acting on them.

Choose a *test vector* $y = 1$ at the 10 blue vertices and $y = -1$ at the 10 red ones. Then $y \perp 1$, $\mathcal{I}^T y$ is nonzero only at the two passages from blue to red, and:

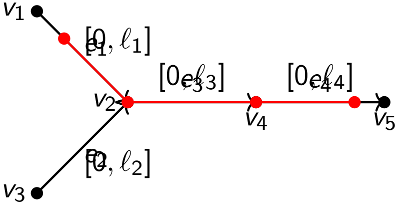
$$\lambda_2 = \min_{0 \neq x \perp 1} \frac{|\mathcal{I}^T x|^2}{|x|^2} \leq \frac{|\mathcal{I}^T y|^2}{|y|^2} \leq \frac{2 \cdot 2^2}{20} = \frac{2}{5}.$$

Comparison: $\lambda_2(\mathcal{P}_{20}) \approx 0.0246$, $\lambda_2(\mathcal{K}_{20}) = 20$.

And now for something completely different ...

Metric graphs:

- Each edge e is identified with an *interval*, say, $[0, \ell]$ for some length $\ell > 0$, or a half-line $[0, \infty)$
- Just as with discrete graphs, the choice of orientation of the edges $\sim$ intervals won't affect the analysis
- "Glue" the intervals together at the vertices: gives rise to a natural metric, the shortest path length between two points (thus hybrid Euclidean/combinatorial)
- Equivalent: *continuous functions* are continuous on each edge (interval), function values at adjacent endpoints must agree
  For example: with this orientation $f(\ell_1) = f(\ell_2) = f(0_{e_3})$



And now for something completely different ...

Natural to consider *differential operators* on the functions. For this we need integration, measures, and derivatives.

Put Lebesgue measure on each edge, the measure on the whole graph is a direct sum. Integrate edgewise:

$$\int_{\mathcal{G}} f(x)\,dx = \sum_{e\in\mathcal{E}} \int_e f(x)\,dx$$

For theoretical reasons, the *Hilbert space* $L^2(\mathcal{G})$ is important:

$$L^2(\mathcal{G}) = \bigoplus_{e\in\mathcal{E}} L^2(e) = \left\{ f : \mathcal{G} \to \mathbb{R} \text{ measurable} : \int_{\mathcal{G}} |f(x)|^2\,dx < \infty \right\}$$

Inner product: $\langle f, g\rangle = \int_{\mathcal{G}} fg\,dx$.

(This space doesn't "see" the vertices, since they have measure 0. The graph structure only appears at the level of continuous functions.)

Smooth functions are also defined edgewise. We're free to impose conditions on the derivatives at the vertices, a common choice is the Kirchhoff-inspired "flow in = flow out" rule $\sum_{e\sim v} \frac{\partial f}{\partial \nu_e}(v) = 0$.

And now for something ~~completely~~ not that different ...

Prototype differential operator: the (metric) Laplacian

$$-\Delta f = -f''$$

acting on continuous functions satisfying Kirchhoff vertex conditions. A triple metric graph + differential operator + vertex conditions is also called a *quantum graph*. Rule of thumb:

$$\left.\begin{array}{r} \text{functions on edges} \\ L^2(\mathcal{G}) \\ \langle f, g\rangle := \displaystyle\int_{\mathcal{G}} fg \\ \text{derivative } f' \end{array}\right\} \text{replace(s)} \begin{cases} \text{vectors on vertices} \\ \mathbb{R}^{|\mathcal{V}|} \\ x^T y \\ \text{difference op. } \mathcal{I}^T x \end{cases}$$

For example, $-\Delta$ is associated with a bilinear form: just as $x^T L x = |\mathcal{I}^T x|^2$, integrating by parts on each edge and using the vertex conditions,

$$\langle f, -\Delta g\rangle = \int_{\mathcal{G}} -fg'' = \int_{\mathcal{G}} f'g' =: a(f, g)$$

Parallels

	combinatorial Lapl. L	metric Lapl. $-\Delta$
Basic	symmetric, pos. semidef.	self-adjoint, pos. semidef.
Form	$x^T L y = (\mathcal{I}^T x)^T (\mathcal{I}^T y)$	$\langle f, -\Delta g \rangle = \int f' g'$
Eigenvalues	$0 = \lambda_1 \leq \lambda_2 \ldots \leq \lambda_n$	$0 = \lambda_1 \leq \lambda_2 \leq \ldots$
Eigenvectors	ONB of $\mathbb{R}^n$	ONB of $L^2(\mathcal{G})$
Char. of λ_2	$\min\limits_{0 \neq x \perp 1} \dfrac{\lvert \mathcal{I}^T x \rvert^2}{\lvert x \rvert^2}$	$\min\limits_{f \neq 0, \int f = 0} \dfrac{\int \lvert \nabla f \rvert^2}{\int f^2}$

Differences? No "explicit" coordinate representation of $-\Delta$ (i.e. no matrices!), use the form and the variational characterisation.

Theorem (von Below, 1985)

Suppose all edges of the metric graph $\mathcal{G}$ have length 1, and suppose that λ_k are the eigenvalues of $-\Delta$. Excluding certain special cases (corresponding to 0 and 2), the eigenvalues of L_{norm} (!!!) are given by $1 - \cos(\sqrt{\lambda_k})$. The values of the eigenvectors correspond to the values of the eigen*functions* at the vertices.

Spectra and geometry

The eigenvalues (and eigenfunctions) of $-\Delta$ also reveal information about the structure/geometry of $\mathcal{G}$.

Heuristic principle

More connected graphs have larger λ_2.

Suppose $\mathcal{G}$ is connected, so $\lambda_2 > 0$. Denote by L the total length (sum of edge lengths) of $\mathcal{G}$.

Theorem (Nicaise, 1987)

Let $\mathcal{P}$ be the path graph ($=$ interval!) of the same total length L, then

$$\lambda_2(\mathcal{G}) \geq \lambda_2(\mathcal{P}) = \frac{\pi^2}{L^2},$$

with equality iff $\mathcal{G}$ is a path.

Other proofs and extensions by Friedlander (2005), Kurasov–Naboko (2013), Band–Lévy (2017), Berkolaiko–K.–Kurasov–Mugnolo (2019), ...

Thank you
for your attention!