THE GRAPH LAPLACIAN

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These are notes for a lecture given at the topological data analysis seminar held during Fall 2024 at Auburn University. Most of the material is expanded from Hal Schenck's book *Algebraic Foundations for Applied Topology and Data Analysis*.

1. Physics prerequisites

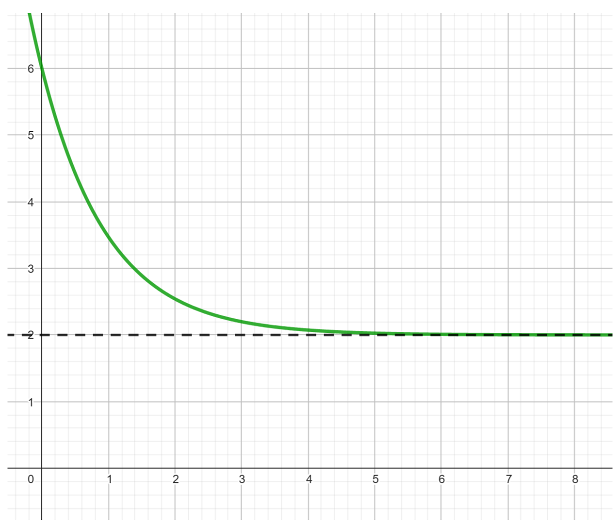
1.1. **Newton's law of cooling.** Let $T(t)$ be the temperature of an object as a function of time, and let T_{env} be the temperature of its surrounding environment, assumed to be constant. Newton's law of cooling states that the speed at which $T(t)$ changes is proportional to the difference $T(t) - T_{env}$ between the temperature of the object and its environment:

$$\frac{dT}{dt} = k(T_{env} - T(t)), \quad k > 0.$$

Solving the ODE using seperation of variables, we obtain

$$T(t) = T_{env} + (T_0 - T_{env})e^{-kt},$$

where $T_0 = T(0)$ is the initial temperature. Notice that $\lim_{t\to\infty} T(t) = T_{env}$. Example graph below.



1.2. **Heat equation.** Let $u(\vec{x}, t)$ be the temperature at a point $\vec{x} \in \mathbb{R}^n$ at time t. The heat equation reads

$$\frac{\partial u}{\partial t} = k\Big(\frac{\partial^2 u}{\partial x_1^2} + \cdots + \frac{\partial^2 u}{\partial x_n^2}\Big) =: k\Delta u, \quad k > 0.$$

The operator Δ is called the Laplacian. In the one-dimensional case, and using one of the finite difference formulas, we have

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} \approx \frac{k}{h^2}[u(x+h,t) - 2u(x,t) + u(x-h,t)]$$

where h is small (we have equality at the limit $h \to 0$). Thus $\partial u/\partial t$ is positive if the temperatures $u(x+h,t)$, $u(x-h,t)$ at the points around x are higher than $u(x,t)$. Similarly, $\partial u/\partial t$ is negative if the temperatures $u(x+h,t)$, $u(x-h,t)$ at the points around x are lower than $u(x,t)$.

2. Graph Laplacian

2.1. **Definitions.** A *graph* $G = (V, E)$ is a 1-dimensional abstract simplicial complex where V is the set of *vertices*, or 0-simplices, and E is the set of *edges*, or 1-simplices. We write the edges as $(v_i, v_j) = \{v_i, v_j\} \in E$, where $v_i, v_j \in V$, even if we do not orient the edges.

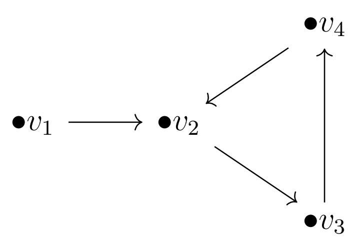
Given a graph G,

- the *adjacency matrix* $A = A(G)$ is the $|V| \times |V|$ matrix defined by

$$A_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

- the *incidence matrix* $B = B(G)$ is the $|V| \times |E|$ matrix representing the boundary map $\partial : C_1(G) \to C_0(G)$ (after choosing an orientation on the edges).
- the *Laplacian matrix* is $L = BB^T$. This does not depend on orientation.

2.2. **An example.** Consider the oriented graph G below.



We calculate the adjacency matrix and the incidence matrix to be

$$A(G) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{array}\!\!\begin{array}{c} \begin{array}{cccc} v_1 & v_2 & v_3 & v_4 \end{array} \\ \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \end{array}, \qquad B(G) = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{array}\!\!\begin{array}{c} \begin{array}{cccc} v_1v_2 & v_2v_3 & v_3v_4 & v_4v_2 \end{array} \\ \begin{pmatrix} -1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix} \end{array}.$$

Then the Laplacian is

$$L = BB^T = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix} = \operatorname{diag}(1,3,2,2) - A.$$

The diagonal matrix $\operatorname{diag}(1,3,2,2)$ is called the *degree matrix* of G. It records the *degree* $\deg(v_i)$ of each vertex v_i, that is, the number of edges $e \in E$ such that $v_i \in e$. It is always true that L is the degree matrix minus the adjacency matrix.

2.3. **Heat diffusion on a graph.** The graph Laplacian is a discrete analog for the Laplace operator Δ. Let us see how.

Lemma 2.1. *For any graph G, the Laplacian is symmetric, singular, and positive semidefinite (has no negative eigenvalues).*

Proof. L is singular since $(1, 1, \dots, 1)^\top \in \ker L$. Also, $L = BB^\top$ so L is symmetric. By the spectral theorem, L is orthogonally diagonalizable with real eigenvalues. Choose eigenvectors w_i with corresponding eigenvalues λ_i such that $1 = \|w_i\|^2 = w_i^\top w_i$. Then

$$\lambda_i = \lambda_i w_i^\top w_i = w_i^\top L w_i = w_i^\top BB^\top w_i = (B^\top w_i)^\top (B^\top w_i) = \|B^\top w_i\|^2 \geq 0,$$

thus L is positive semidefinite. □

Suggested exercise: Show that the dimension of $\ker L$ is the number of connected components of G.

Let G be a graph with vertices $V = \{v_i\}_{i=1}^n$ and let $u_i(t)$ be the temperature at the vertex v_i. By Newton's law of cooling,

$$\begin{aligned}
\frac{du_i}{dt} &= \sum_{j \text{ such that } (i,j) \in E} k(u_j - u_i) \\
&= \sum_{j=1}^{n} A_{ij} k(u_j - u_i) \\
&= -k \sum_{j=1}^{n} A_{ij}(u_i - u_j) \\
&= -k\Big(\sum_{j=1}^{n} A_{ij} u_i - \sum_{j=1}^{n} A_{ij} u_j\Big) \\
&= -k(\deg(v_i) u_i - \sum_{j=1}^{n} A_{ij} u_j) \\
&= -k(\sum_{j=1}^{n} L_{ij} u_j).
\end{aligned}$$

It follows that $\mathbf{u}' = -kL\mathbf{u}$, where $\mathbf{u} = (u_1, \dots, u_n)^\top$ and $\mathbf{u}' = (u_1', \dots, u_n')^\top$. Compare this with the heat equation $\partial u / \partial t = k \Delta u$.

To solve for the functions u_i we use the diagonalization of the Laplacian $L = P^\top D P$, where D is diagonal and P is orthogonal. Then set $\mathbf{y} = P\mathbf{u}$. Differentiating both sides, $\mathbf{y}' = P\mathbf{u}'$. Then we have $\mathbf{u}' = -kL\mathbf{u} = -kP^\top DP\mathbf{u}$. Multiplying by P on both sides, we obtain $P\mathbf{u}' = -kDP\mathbf{u}$ or $\mathbf{y}' = -kD\mathbf{y}$. Then $y_i' = -k\lambda_i y_i$ which gives $y_i = c_i e^{-k\lambda_i t}$ for some constant c_i. This gives the solution $\mathbf{u} = P^\top \mathbf{y}$. The c_i's are determined by the initial conditions since $\mathbf{y} = P\mathbf{u}$ implies $\mathbf{c} = P\mathbf{u}_0$, where $\mathbf{c} = (c_1, \dots, c_n)^\top$ and $\mathbf{u}_0 = (u_1(0), \dots, u_n(0))^\top$.

Going back to our example graph, one can calculate

$$D = \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 3 & \\ & & & 4 \end{pmatrix}, \quad \text{and} \quad P^\top = \frac{1}{6} \begin{pmatrix} 3 & 2\sqrt{6} & 0 & \sqrt{3} \\ 3 & 0 & 0 & -3\sqrt{3} \\ 3 & -\sqrt{6} & -3\sqrt{2} & \sqrt{3} \\ 3 & -\sqrt{6} & 3\sqrt{2} & \sqrt{3} \end{pmatrix}.$$

Assuming $k = 1$, we get

$$\begin{aligned}
u_1(t) &= \frac{1}{2}c_1 + \frac{\sqrt{6}}{3}c_2e^{-t} + \frac{\sqrt{3}}{6}c_4e^{-4t},\\
u_2(t) &= \frac{1}{2}c_1 - \frac{\sqrt{3}}{2}c_4e^{-4t},\\
u_3(t) &= \frac{1}{2}c_1 - \frac{\sqrt{6}}{6}c_2e^{-t} - \frac{\sqrt{2}}{2}c_3e^{-3t} + \frac{\sqrt{3}}{6}c_4e^{-4t},\\
u_4(t) &= \frac{1}{2}c_1 - \frac{\sqrt{6}}{6}c_2e^{-t} + \frac{\sqrt{2}}{2}c_3e^{-3t} + \frac{\sqrt{3}}{6}c_4e^{-4t},
\end{aligned}$$

where

$$\begin{aligned}
c_1 &= \frac{1}{2}u_1(0) + \frac{1}{2}u_2(0) + \frac{1}{2}u_3(0) + \frac{1}{2}u_4(0),\\
c_2 &= \frac{\sqrt{6}}{3}u_1(0) - \frac{\sqrt{6}}{6}u_3(0) - \frac{\sqrt{6}}{6}u_4(0),\\
c_3 &= -\frac{\sqrt{2}}{2}u_3(0) + \frac{\sqrt{2}}{2}u_4(0),\\
c_4 &= \frac{\sqrt{3}}{6}u_1(0) - \frac{\sqrt{3}}{2}u_2(0) + \frac{\sqrt{3}}{6}u_3(0) + \frac{\sqrt{3}}{6}u_4(0).
\end{aligned}$$

I made an animation of this family of solutions on desmos.com. You can control the initial conditions $u_i(0)$ and the time t with the sliders.