The Graph Laplacian

Algebra, Topology, and Hypergraphs

David Marchette

Naval Surface Warfare Center
Q21
david.marchette@navy.mil

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Graph Theory Definition

Definition

A (simple) graph is a pair $G = (V, E)$ such that:

- $V = \{v_1, \ldots, v_n\}$ is a set of vertices.
- E is a collection of unordered pairs of distinct vertices.

If the elements of E are ordered, G is a directed graph.

More Graph Theory Definitions

- We will refer to the number of vertices n as the *order* of the graph, and s, the number of edges, as the *size* of the graph.
- The degree of a vertex is the number of edges incident to it.
- In a directed graph there are in-degrees and out-degrees.
- The (open) neighborhood of a vertex, $N(v)$ is

$$\{w \in V | vw \in E\}.$$

The closed neighborhood $N[v] = N(v) \cup \{v\}$.

Graph Representations

A graph can be represented in several ways:

- As an adjacency matrix $A = (a_{ij})$:

$$a_{ij} = \mathrm{I}\{v_i v_j \in E\}.$$

- As an edge list; either an $s \times 2$ matrix corresponding to the edges or as a list in which the i$^{\text{th}}$ entry is $N(v_i)$.
- As an incidence matrix: an $n \times s$ matrix M whose entries are

$$m_{ij} = \mathrm{I}\{v_i \in e_j\}$$

for $e_j \in E$.

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Hypergraph Definitions

Definition

A (simple) hypergraph is a pair $G = (V, H)$ such that:

- $V = \{v_1, \ldots, v_n\}$ is a set of vertices.
- H (the hyper-edge set) is a collection of distinct sets (containing at least two elements) of distinct vertices.

Hypergraph Definitions

- We will refer to the number of vertices n as the *order* of the hypergraph, and s, the number of hyper-edges, as the *size* of the hypergraph.
- Note that there are other measures we might consider, such as a version of size that weights hyper-edges according to the number of elements in the hyper-edge.
- A hypergraph can be represented using an incidence matrix or as a list of the hyper-edges.

Hypergraphs

- We may relax some of the conditions. For example, when analyzing email using hypergraphs we may allow duplicate hyper-edges (or weight the edges).
- We can define directed hyper-edges in several ways. A “natural” way (with email as an example) is to mark the vertices in a hyper-edge as either “from” or “to”.

Hypergraphs and Graphs

- Given a hypergraph, we can construct a graph several ways, each having different properties:
  - Let the edges be any pair of vertices contained in at least one hyper-edge.
  - Only consider edges that are themselves hyper-edges: retain only the hyper-edges containing two elements.
  - Let the edges be any pair contained in a hyper-edge of at most (at least) k elements.
  - Let the vertices of the graph correspond to the hyper-edges, with an edge in the graph if the hyper-edges intersect. This is the intersection graph defined by the hyper-graph.
  - The bipartite graph defined by the incidence matrix.
- Only the last graph is equivalent to the hypergraph.

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Simplicial Complex Definition

Definition

A simplicial complex is a collection of subsets $\mathcal{S}$ of $\{v_1, \ldots, v_n\}$ such that:

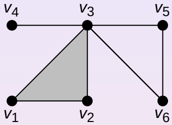
- $\emptyset \in \mathcal{S}$.
- If $A \in \mathcal{S}$ and $B \subset A$ then $B \in \mathcal{S}$.

- An element $s \in \mathcal{S}$ is called a *simplex* of dimension $|s| - 1$, and a subset of a simplex is called a *face*.
- A facet is a $k - 1$ dimensional face of a k-dimensional simplex.

Simplicial Complex Notes

- Note that a hypergraph can be thought of as generating a simplicial complex.
- In order to do this, we must include all subsets of any hyper-edge in the complex.
- There is an implicit ordering to the vertices which results in an orientation to each simplex.
- Thus, for example, we think of the faces (edges) $\{v_1, v_2\}$ and $\{v_2, v_1\}$ as being of opposite orientation and write $\{v_1, v_2\} = -\{v_2, v_1\}$.
- This will be important when we look at the topology of simplicial complexes.

Example

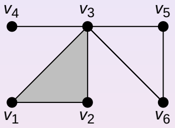


$$d = 0 \qquad \{\{v_1\},\{v_2\},\{v_3\},\{v_4\},\{v_5\},\{v_6\}\}$$

$$d = 1 \qquad \left\{ \begin{array}{l} \{v_1,v_2\},\{v_1,v_3\},\{v_2,v_3\}, \\ \{v_3,v_4\},\{v_3,v_5\},\{v_3,v_6\}, \\ \{v_5,v_6\} \end{array} \right\}$$

$$d = 2 \qquad \{\{v_1,v_2,v_3\}\}.$$

Example: Complex as a Hypergraph



$$V = \{v_1, v_2, v_3, v_4, v_5, v_6\}.$$

$$H = \{\{v_3, v_4\}, \{v_3, v_5\}, \{v_3, v_6\}, \{v_5, v_6\}, \{v_1, v_2, v_3\}\}.$$

Some Notation

- The ordering of the vertices corresponds to an orientation on the simplex.
- We say two k-simplices σ_j, σ_k are *upper adjacent* if they are both faces of some $k+1$ dimensional simplex. We write

$$\sigma_j \frown \sigma_k.$$

- We say two k-simplices σ_j, σ_k are *lower adjacent* if they share a common face, and we write

$$\sigma_j \smile \sigma_k.$$

Some More Notation

- The *lower degree* of a k-simplex σ, denoted $\deg_l(\sigma)$, is the number of faces of σ.
- The *upper degree* of a k-simplex σ, denoted $\deg_u(\sigma)$, is the number of $k+1$-dimensional simplices in which σ is a face.
- If $\sigma_i \frown \sigma_j$ in ζ, and the orientations in ζ induced by these are the same, they are said to be *similarly oriented* with respect to ζ. Otherwise, they are *dissimilarly oriented*.
- We'll write $\sigma_i \smile_s \sigma_j$ for simililarly oriented, $\sigma_i \smile_d \sigma_j$ for dissimilarly oriented. Similarly for $\frown_s$ and $\frown_d$.

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The Laplacian of Calculus

The Laplacian

- The standard definition of the Laplacian is:
  - Let $f : \mathbb{R}^d \to \mathbb{R}$ be sufficiently smooth.
  - The Laplacian is:

$$\Delta f = \nabla^2 f = \nabla \cdot \nabla f = -\sum_{i=1}^{d} \frac{\partial^2 f}{\partial x_i^2}$$

- The minus sign is arbitrary.

The Laplacian of Calculus

Limit Formulation

- We can write the limit definition of the second derivative:

$$\frac{\partial^2 f}{\partial x_i^2} = \lim_{h\to 0} \frac{(f(x_i - h) - f(x_i)) + (f(x_i + h) - f(x_i))}{h^2}$$

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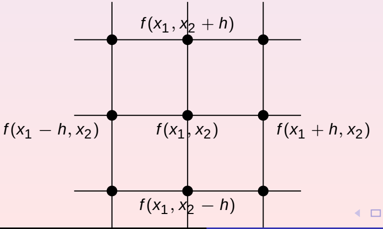
The Discrete Laplacian

Continuous Version

$$\frac{\partial^2 f}{\partial x_i^2} = \lim_{h \to 0} \frac{(f(x_i - h) - f(x_i)) + (f(x_i + h) - f(x_i))}{h^2}$$

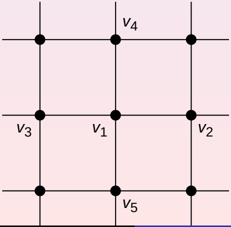
$$\nabla^2 f = -\left(\frac{\partial^2 f}{\partial x_1^2} + \frac{\partial^2 f}{\partial x_2^2}\right)$$



The Discrete Laplacian

Discrete Version

$$\begin{aligned}\nabla^2 f &= f(v_1) - f(v_2) + \\ &\quad f(v_1) - f(v_3) + \\ &\quad f(v_1) - f(v_4) + \\ &\quad f(v_1) - f(v_5)\end{aligned}$$



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The Graph Laplacian

$$\begin{aligned}
\nabla^2 f(v_1) &= f(v_1) - f(v_2) + \\
&\quad f(v_1) - f(v_3) + \\
&\quad f(v_1) - f(v_4) + \\
&\quad f(v_1) - f(v_5) \\
&= 4f(v_1) - f(v_2) - f(v_3) - f(v_4) - f(v_5) \\
&= \text{degree}(v_1) f(v_1) - f(N(v_1)) \\
&= \begin{pmatrix} 4 & \text{-1} & \text{-1} & \text{-1} & \text{-1} & 0 & 0 & \dots & 0 \end{pmatrix} \begin{pmatrix} f(v_1) \\ f(v_2) \\ f(v_3) \\ \vdots \end{pmatrix}
\end{aligned}$$

- So, the graph Laplacian is:

$$L = D - A$$

where D is the diagonal matrix of degrees.

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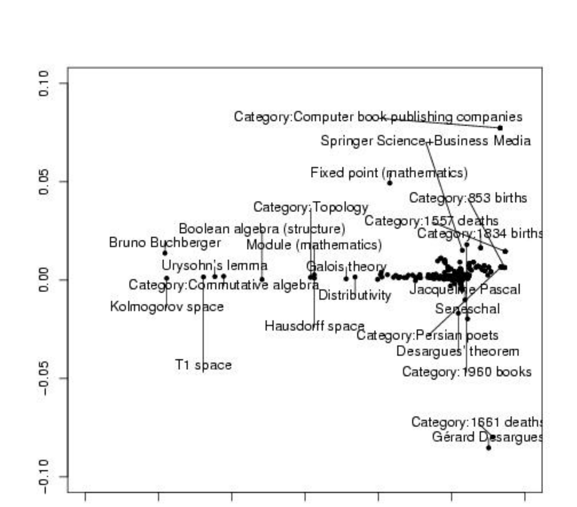
Projecting the Graph with the Laplacian

- Given L, we can compute the spectrum and use this to project the graph into $\mathbb{R}^d$.
- Note that the eigenvalues are positive and the multiplicity of the 0 eigenvalue is the number of components of the graph.
  - Compute the non-zero eigenvalues Λ (ordered in increasing value) and corresponding eigenvectors U of L.
  - Let U_d denote the first d columns of U. Set $X = U_d\sqrt{\Lambda}$ (here we are thinking of Λ as the diagonal matrix).
  - Plot X or perform inference on X.
- Note that this will only work if the graph is connected:
  - in effect, each component is mapped to a subspace that is orthogonal to the other components.
  - We need to operate on each component separately.

Example: Wikipedia Algebraic Geometry Graph



Outline

Pseudoinverse

We first need to know about the Moore-Penrose pseudoinverse:

Definition

A psedoinverse A^+ of an $m \times n$ matrix A is the unique $n \times m$ matrix satisfying (A^* is the conjugate transpose):

1. $AA^+A = A$.
2. $A^+AA^+ = A^+$.
3. $(AA^+)^* = AA^+$.
4. $(A^+A)^* = A^+A$.

Since our matrices are always real, we'll just use transpose from now on.

Computing the Pseudoinverse

- The pseudoinverse of A can be computed using the SVD:
  - Let $A = U\Sigma V'$. Σ is the diagonal matrix of singular values.
  - Let Σ^+ be the diagonal matrix in which the non-zero elements of Σ are replaced with their inverses.
  - Then $A^+ = V\Sigma^+ U'$.
- The Moore-Penrose pseudoinverse is implemented in R in the MASS library as ginv.

Resistive Distance

Definition

Let L be the Laplacian and Γ the Moore-Penrose inverse of L. Then the resistive distance between v_i and v_j is:

$$\Omega_{ij} = \Gamma_{ii} + \Gamma_{jj} - \Gamma_{ij} - \Gamma_{ji}$$

Note that the resistive distance is defined for directed graphs. For an undirected graph, $\Gamma_{ij} = \Gamma_{ji}$ and we have

$$\Omega_{ij} = \Gamma_{ii} + \Gamma_{jj} - 2\Gamma_{ij}.$$

Properties of the Resistive Distance

Let $G = (V, E)$ be a simple connected graph on n vertices, $V = [n]$, with Laplacian L.

- For any $n \times n$ matrix M,

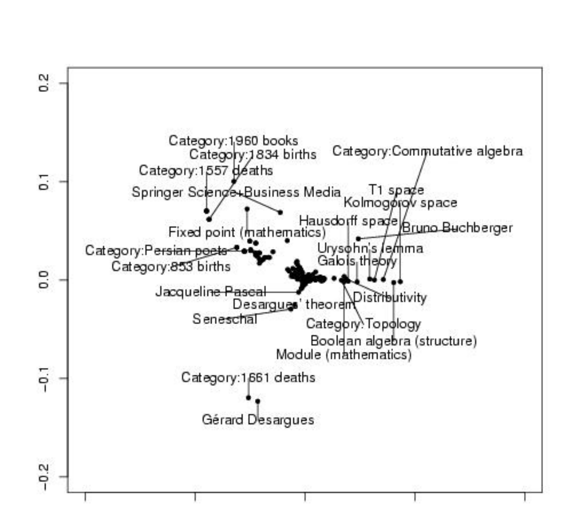
$$\sum_{ij \in E} (LML)_{ij} \Omega_{ij} = -2\text{tr}(ML).$$

- $\sum_{ij \in E} \Omega_{ij} = n - 1$.
- $\sum_{i<j \in V} \Omega_{ij} = n \sum_{k=1}^{n-1} \lambda_k^{-1}$, where λ_k is the k^{th} non-zero eigenvalue of L.

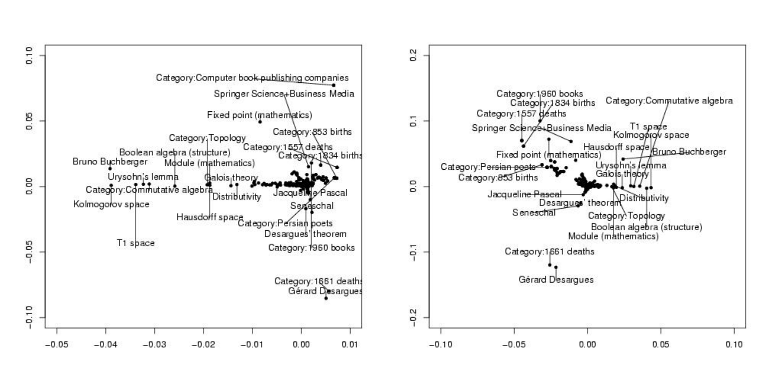
Properties of the Resistive Distance

- Let T be the number of spanning trees of G. If $ij \notin E$, set $E' = E \cup \{ij\}$, otherwise set $E' = E$. Let T^{ij} be the number of spanning trees in the graph $G' = (V, E')$ which contain the edge ij. Then
$$\Omega_{ij} = \frac{T^{ij}}{T}.$$
- Write $\Gamma = KK^T$. We can do this since Γ is symmetric and positive semi-definite. Then
$$\Omega_{ij} = (K_i - K_j)^2,$$
so resistive distance is squared Euclidean distance in the space spanned by K.

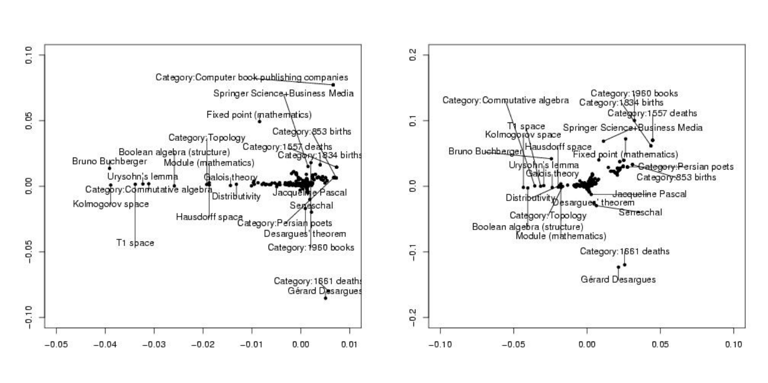
Example: Wikipedia Algebraic Geometry Graph



Example: Wikipedia Algebraic Geometry Graph



Example: Wikipedia Algebraic Geometry Graph



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Chain Complex

Definition

A chain complex $(C_\bullet, \partial_\bullet)$ is a sequence of modules and homomorphisms (boundary operators) such that $\partial_n \partial_{n+1} = 0$ for all n.

The picture is:

$$\ldots C_n \xrightarrow{\partial_n} C_{n-1} \xrightarrow{\partial_{n-1}} \ldots \xrightarrow{\partial_3} C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0 \xrightarrow{\partial_0} 0.$$

Simplicial Homology

Definition

C_n is (the free abelian group) generated by the n-simplices in the complex: $\sigma = \{v_0, \ldots, v_n\}$ with boundary map:

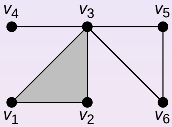
$$\partial_n : C_n \to C_{n-1}$$

defined by:

$$\partial_n \sigma = \sum_{i=0}^{n} (-1)^i \sigma_{(-i)}$$

where $\sigma_{(-i)}$ is σ with the i^{th} element removed.

Examples



$$
\begin{aligned}
\partial_2\{v_1, v_2\} &= v_2 - v_1 \\
\partial_3\{v_1, v_2, v_3\} &= \{v_1, v_3\} - \{v_1, v_2\} - \{v_2, v_3\} \\
\partial_2\partial_3\{v_1, v_2, v_3\} &= \partial_2(\{v_1, v_3\} - \{v_1, v_2\} - \{v_2, v_3\}) \\
&= (v_3 - v_1) - (v_2 - v_1) - (v_3 - v_2) \\
&= 0
\end{aligned}
$$

Simplicial Homology

- Note: $\partial^2 = 0$ means that the image of ∂_{n+1} is contained in the kernel of ∂_n.
- This means that “the boundary of a boundary is 0” – boundaries do not themselves have boundaries.

Definition

Simplicial homology is defined as

$$H_n(X) = \ker\partial_n / \mathrm{im}\partial_{n+1}.$$

Co-Chain Complex

Definition

A co-chain complex $(C^\bullet, \delta^\bullet)$ is a sequence of modules and homomorphisms (boundary operators) such that $\delta^{n+1}\delta^n = 0$ for all n.

The picture is:

$$0 \xrightarrow{\delta_0} C^0 \xrightarrow{\delta_1} C^1 \xrightarrow{\delta^2} C^2 \xrightarrow{\delta^3} \ldots \xrightarrow{\delta^n} C^n \xrightarrow{\delta^{n+1}} C^{n+1} \ldots .$$

Chains and Co-Chains

- Given a chain complex $(C_\bullet, \partial_\bullet)$ we construct a co-chain complex $(C^\bullet, \delta^\bullet)$ as:
  - $C^n = \text{Hom}(C_n, R)$.
- Here, R is any ring (say, $\mathbb{R}$ or $\mathbb{Z}$).
- These are the homomorphisms from C_n to R.

Chains and Co-Chains

- Now, let $R = \mathbb{R}$. A member of C^i is completely determined by its value on each simplex.
- We identify C^i with C_i via the inner product:
  - C_i and C^i are vector spaces, and C^i is dual to C_i:
  - Define the map $\Phi : C_i \to C^i$ as $\Phi(\sigma)(\tau) = <\sigma, \tau>$.
  - Everything is finite dimensional here, so Φ is an isomorphism.
- Thus we can think of these as the same.
- δ is dual to ∂: if we represent ∂ as a matrix, δ is it's transpose.

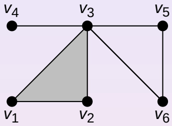
Simplicial Cohomology

Definition

Simplicial cohomology is defined as the homology of the co-chain complex:

$$H^n(X) = \ker\delta^{n+1}/\mathrm{im}\,\delta^n.$$

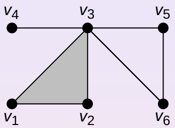
Example: A Simplicial Complex



$$C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0$$

$$\{\{v_1, v_2, v_3\}\} \qquad \left\{ \begin{array}{c} \{v_1, v_2\} \\ \{v_1, v_3\} \\ \{v_2, v_3\} \\ \{v_3, v_4\} \\ \{v_3, v_5\} \\ \{v_3, v_6\} \\ \{v_5, v_6\} \end{array} \right\} \qquad \left\{ \begin{array}{c} \{v_1\} \\ \{v_2\} \\ \{v_3\} \\ \{v_4\} \\ \{v_5\} \\ \{v_6\} \end{array} \right\}$$

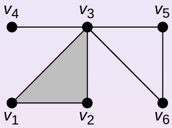
Example: A Simplicial Complex



$$C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0$$

$$\begin{bmatrix} -1 \\ 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad \begin{bmatrix} -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

Example: A Simplicial Complex



$$C_2 \overset{\delta^2}{\longleftarrow} C_1 \overset{\delta^1}{\longleftarrow} C_0$$

$$\begin{bmatrix} -1 & 1 & -1 & 0 & 0 & 0 & 0 \end{bmatrix} \qquad \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

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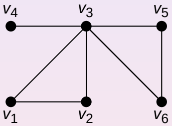
Example: The Simplicial Complex as a Graph



$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{bmatrix}$$

$$\partial_1 \delta^1 = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 5 & -1 & -1 & -1 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 2 & -1 \\ 0 & 0 & -1 & 0 & -1 & 2 \end{bmatrix} = D - A = L$$

Higher Order Laplacian

- Note that for graphs, there are only chains in dimensions 0 and 1.
- Define the k-th order Laplacian as:

$$L_k = \partial_{k+1}\delta^{k+1} + \delta^k\partial_k.$$

- We saw that this agreed with the graph Laplacian in our example.
- This is the generalized Laplacian, and can be applied to any simplicial complex, in particular to the complex defined by a hypergraph.

Example: Simplicial Complex

$$L_0 = \partial_1 \delta^1 + 0 = \begin{bmatrix} -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

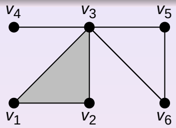
$$= \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 5 & -1 & -1 & -1 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 2 & -1 \\ 0 & 0 & -1 & 0 & -1 & 2 \end{bmatrix}$$

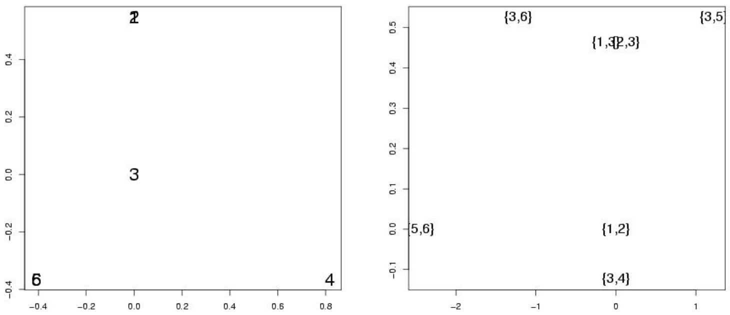
$$
\begin{aligned}
L_1 &= \partial_2\delta^2+\delta^1\partial_1 = \begin{bmatrix} -1 & 1 & -1 & 0 & 0 & 0 & 0 \end{bmatrix}' \begin{bmatrix} -1 & 1 & -1 & 0 & 0 & 0 & 0 \end{bmatrix} \\
&+ \begin{bmatrix} -1 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{bmatrix}
\begin{bmatrix} -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix} \\
&= \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & -1 & -1 & -1 & 0 \\ 0 & 0 & 3 & -1 & -1 & -1 & 0 \\ 0 & -1 & -1 & 2 & 1 & 1 & 0 \\ 0 & -1 & -1 & 1 & 2 & 1 & -1 \\ 0 & -1 & -1 & 1 & 1 & 2 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 2 \end{bmatrix}
\end{aligned}
$$

$$L_2 = 0 + \delta^2 \partial_2$$

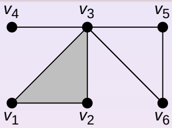
$$= \begin{bmatrix} -1 & 1 & -1 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -1 \\ 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \end{bmatrix}$$

Example: Simplicial Complex





Example: Simplicial Complex



- L_0 is the graph Laplacian and has 1 zero eigenvalue (there is 1 component to the complex).
- L_1 has 1 zero eigenvalue (there is one "empty cycle": induced cycle with no chords or filling-in).
- L_2 has no zero eigenvalues (no higher-dimensional structure).
- Note that the homology of the complex is 0 except for H_0 and H_1, both of rank 1.
- This is not a coincidence.

Notes on Higher Order Laplacians

- L_0 is the graph Laplacian that maps the vertices into $\mathbb{R}^d$.
- L_1 maps the edges.
- L_2 maps the triangles (hyper-edges with three elements).
- Each level gives different information about the hypergraph.
- The Laplacian looks at the dimensions above and below: looks at σ's faces and those simplices for which σ is a face.
- That is, it looks at $\sigma \smile \tau$ and $\sigma \frown \tau$.

Notes on Higher Order Laplacians

- We can think of $\{L_0, \ldots, L_k\}$ as a multi-scale representation of a graph or hypergraph.
- Each element provides information about the (hyper)graph at a different resolution (dimension).
- Something to think about: what if we convert a graph into a hypergraph? Several ways to do this. For example, let the k-dimensional hyper-edges be one of:
  - the induced k-cliques.
  - the induced empty (no chords) k-cycles.
  - the paths of length k.
- This might be a fruitful area to explore.

Formulae for Higher Order Laplacians

Let $\sigma_1, \ldots, \sigma_{n_k}$ be the oriented k-simplices of the complex, $k > 0$.

$$(\partial_{k+1}\delta^{k+1})_{ij} = \begin{cases} \deg_u(\sigma_i) & \text{if } i = j \\ 1 & \text{if } i \neq j, \sigma_i \frown_d \sigma_j \\ -1 & \text{if } i \neq j, \sigma_i \frown_s \sigma_j \\ 0 & \text{otherwise} \end{cases}$$

$$(\delta^k \partial_k)_{ij} = \begin{cases} k+1 & \text{if } i = j \\ 1 & \text{if } i \neq j, \sigma_i \smile_s \sigma_j \\ -1 & \text{if } i \neq j, \sigma_i \smile_d \sigma_j \\ 0 & \text{otherwise} \end{cases}$$

Formulae for Higher Order Laplacians

Let $\sigma_1, \ldots, \sigma_n$ be the oriented k-simplices of the complex, $k > 0$.

$$(L_k)_{ij} = \begin{cases} \deg_u(\sigma_i) + k + 1 & \text{if } i = j \\ 1 & \text{if } i \neq j, \sigma_i \not\frown \sigma_j \text{ and } \sigma_i \smile_s \sigma_j \\ -1 & \text{if } i \neq j, \sigma_i \not\frown \sigma_j \text{ and } \sigma_i \smile_d \sigma_j \\ 0 & \text{otherwise} \end{cases}$$

Note, whenever $\sigma_i \frown \sigma_j$ the contributions are of opposite signs, and hence cancel, so we need only consider those cases where $\sigma_i \not\frown \sigma_j$.

Formulae for Higher Order Laplacians

Let A_u, A_l denote the upper and lower adjacency matrices between the n_k k-simplices, $k > 0$.

$$\begin{aligned}
(L_k)(\sigma_i) &= (\deg_u(\sigma_i) + k + 1)\sigma_i + \\
&\sum_{\sigma_i \smile_s \sigma_j} \sigma_j - \sum_{\sigma_i \smile_d \sigma_j} \sigma_j + \sum_{\sigma_i \frown_d \sigma_j} \sigma_j - \sum_{\sigma_i \frown_s \sigma_j} \sigma_j \\
L_k &= D + (k+1)I_{n_k} + A_l - A_u, \text{ for } k > 0 \\
L_0 &= D - A_u
\end{aligned}$$

Here

$$D = \operatorname{diag}(\deg_u(\sigma_1), \ldots, \deg_u(\sigma_{n_k})).$$

Example: Simplicial Complex

$$L_1 = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & -1 & -1 & -1 & 0 \\ 0 & 0 & 3 & -1 & -1 & -1 & 0 \\ 0 & -1 & -1 & 2 & 1 & 1 & 0 \\ 0 & -1 & -1 & 1 & 2 & 1 & -1 \\ 0 & -1 & -1 & 1 & 1 & 2 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 & 2 \end{bmatrix}, \quad \sigma \in \left\{ \begin{array}{c} \{v_1, v_2\} \\ \{v_1, v_3\} \\ \{v_2, v_3\} \\ \{v_3, v_4\} \\ \{v_3, v_5\} \\ \{v_3, v_6\} \\ \{v_5, v_6\} \end{array} \right\}$$

k+1=2

$$C_2 = < \{v_1, v_2, v_3\} >$$

Outline

Hodge Theory

- It turns out that there is an isomorphism:

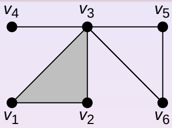
$$\mathrm{ker} L_k \cong H_k(X).$$

- So the higher order Laplacians provide a way to compute homology.
- Since the homology is related to the “holes” in X, the Laplacian also tells us about “holes”.
- There is also a deep connection between L_k and harmonic analysis.

Hodge Theory

- We can use the higher order Laplacian to not only determine the rank of the homologies, but their generators:
  - The number of zero eigenvalues of L_k corresponds to the rank of H_k.
  - The associated eigenvectors are the generators (under the isomorphism).
- We can learn quite a bit about the complex (graph, hypergraph) by looking at these eigenvectors.

Example: Simplicial Complex



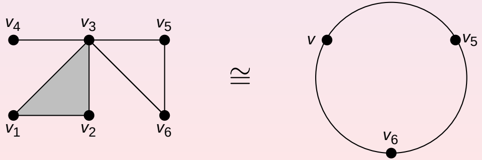
- L_0 has one zero eigenvalue whose eigenvector is $(1, 1, 1, 1, 1, 1)$.
  - The sum of the vertices: the graph component.
- L_1 has one zero eigenvalue whose eigenvector is

$$(0, 0, 0, 0, 0.5773505, -0.5773505, 0.5773505)$$
$$\frac{1}{\sqrt{3}}(0, 0, 0, 0, 1, -1, 1)$$

  - The cycle $(v_6, v_3) + (v_3, v_5) + (v_5, v_6)$.
- L_2 has no zero eigenvalues, so the homology vanishes.

Example: Simplicial Complex

- Note that we can compute the homology of this complex easily.
- The complex is contractible to the circle, whose homology is well-known.
- The Laplician provides the generators of the homology groups in terms of the simplices in the complex.



Outline