Graph Topological Stability via Matrix Differential Equations

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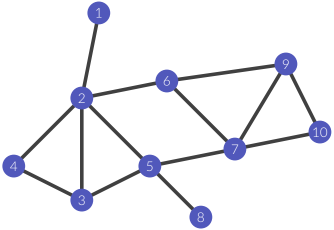
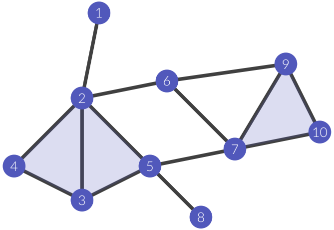
Graph $\mathcal{G}$ is a pair of sets, $\mathcal{G} = (V, E)$:

- V is the set of vertices, $|V| = n$
- $\mathcal{E}$ is the set of edges, $\mathcal{E} \subseteq V, \times V, |\mathcal{E}| = m$



Pairwise Interactions



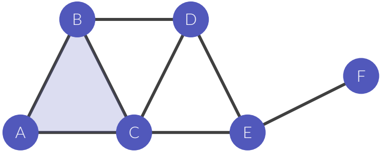
Higher-order relations

Outline:

There is a number of ways to introduce higher-order interactions in the network: hypergraphs, motifs, etc.; we focus on:

Definition

For a given set V, a family X of its subsets is called a simplicial complex if for any set S in X, every $S' \subseteq S$ also belongs to X.



Example of simplicial complex X

$$\begin{aligned}\{ \\ &[A, B, C], - \text{2-simplices}, \; K_2(X) \\ &[A, B], [A, C], [B, C], [B, D], \\ &[C, D], [C, E], [D, E], [E, F], - \text{1-simplices}, \; K_1(X) \\ &[A], [B], [C], [D], [E], [F] - \text{0-simplices}, \; K_0(X) \\ \}\end{aligned}$$

Inside the simplicial complex X, simplexes of different orders are connected through the **boundary relation** ∂_k.

$$[1,2,3] \xrightarrow{\partial_2} [1,2]-[1,3]+[2,3]$$

Formal linear **Chain Spaces** are spanned by the simplexes σ_i of the same cardinality ($\sigma_i \in K_k(X)$):

$$C_k(X) = \mathrm{span}(\sigma_1, \dots, \sigma_{|K_k(X)|})$$

Examples of Chain Spaces

- $C_0(X)$ – states of vertices;
- $C_1(X)$ – edge flows;
- $\dots$

Outline:

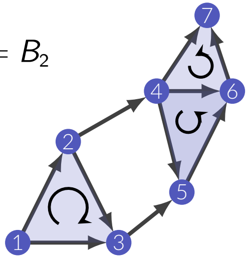
Definition

The boundary operator $\partial_k : C_k(X) \to C_{k-1}(X)$

$$\partial_k[v_0, v_1, \dots, v_p] = \sum_{j=0}^{k} (-1)^j [v_0, \dots, v_{j-1}, v_{j+1}, \dots, v_k]$$

∂_2	$\begin{bmatrix}1\\2\\3\end{bmatrix}$	$\begin{bmatrix}4\\5\\6\end{bmatrix}$	$\begin{bmatrix}4\\6\\7\end{bmatrix}$
[1, 2]	1	0	0
[1, 3]	−1	0	0
[2, 3]	1	0	0
[2, 4]	0	0	0
[3, 5]	0	0	0
[4, 5]	0	1	0
[4, 6]	0	−1	1
[4, 7]	0	0	−1
[5, 6]	0	1	0
[6, 7]	0	0	1

$= B_2$



B_1
||

∂_1	$\begin{bmatrix}1\\2\end{bmatrix}$	$\begin{bmatrix}1\\3\end{bmatrix}$	$\begin{bmatrix}2\\3\end{bmatrix}$	$\begin{bmatrix}2\\4\end{bmatrix}$	$\begin{bmatrix}3\\5\end{bmatrix}$	$\begin{bmatrix}4\\5\end{bmatrix}$	$\begin{bmatrix}4\\6\end{bmatrix}$	$\begin{bmatrix}4\\7\end{bmatrix}$	$\begin{bmatrix}5\\6\end{bmatrix}$	$\begin{bmatrix}6\\7\end{bmatrix}$
[1]	−1	−1	0	0	0	0	0	0	0	0
[2]	1	0	−1	−1	0	0	0	0	0	0
[3]	0	1	1	0	−1	0	0	0	0	0
[4]	0	0	0	1	0	−1	−1	−1	0	0
[5]	0	0	0	0	1	1	0	0	−1	0
[6]	0	0	0	0	0	0	1	0	1	−1
[7]	0	0	0	0	0	0	0	1	0	1

Outline:

Fundamental Lemma of Homology

$\partial_k \partial_{k+1} = 0$

The conjugate map ∂_k^* (B_k^T) is called a co-boundary operator.

$$(\partial_1^* f)[v_1, v_2] = f(v_2) - f(v_1) \quad \leftrightarrow \quad \nabla f(x) = \frac{1}{\Delta x}\left(f(x + \Delta x) - f(x)\right)$$

Definition

Analogous to the continuous Laplacian operator, $L = \nabla^T \nabla$, one defines the classical graph Laplacian or connecting Laplacian:

$$L_0 = B_1 B_1^T, \qquad L_0 \in Mat_{n \times n}$$

- $L_0 = \mathrm{diag}(A\mathbb{1}) - A$, where A is the graph adjacency matrix;
- L_0 is s.p.d

Hodge Laplacians on Graphs
L.H. Lim

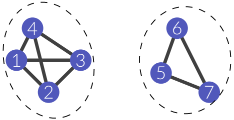
Definition

The higher-order graph Laplacian is given by:

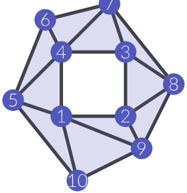
$$L_k = B_k^T B_k + B_{k+1} B_{k+1}^T$$

In case $k = 1$, $L_1 = B_1^T B_1 + B_2 B_2^T$ is called a Hodge Laplacian, $L_1 \in Mat_{m \times m}$

$\dim \ker L_0 =$ number of connected components



$\dim \ker L_1 =$ number of 1-dim. holes



Cheeger constant, Fiedler vector

Outline:

Hodge Laplacians on Graphs
L.H. Lim

Problem Statement

Let us assume **weighted generalizations** of the **boundary** operators:

$$B_1 \mapsto D_v^+ B_1 W, \qquad B_2 \mapsto W^+ B_2 D_t$$

- W is the diagonal matrix of weights of *edges*;
- $D_v(W)$ is the diagonal matrix of weights of *vertices*;
- $D_t(W)$ is the diagonal matrix of weights of *triangles*.

Probem Statement

Given the weighted connected graph $\mathcal{G}$ with the simplicial complex $X = (\mathcal{V}, \mathcal{E}, \mathcal{T})$ and k one-dimensional holes, find the **smallest perturbation** ΔW of edges' weights that **increases the number of 1-dimensional holes** in the graph $\mathcal{G}$.

Outline:

$\mathcal{T}$ – set of triangles in X, $\mathcal{T} = \mathcal{K}_2(X)$

Consider the perturbation $\Delta W = \varepsilon E$:

- $\varepsilon \geq 0$, $\|E\| = 1$;
- $W + \varepsilon E \geq 0$.

The target functional:

$$F_k(\varepsilon, E) = \underbrace{\frac{1}{2}\sum_{i=1}^{k+1} \lambda_i^2}_{\text{control } \ker L_1} + \underbrace{\frac{\alpha}{2} \max\left(0, 1 - \frac{\mu_2}{\mu}\right)^2}_{\text{connectedness}}$$

where $\lambda_i \in \sigma(L_1(W + \varepsilon E))$,
$\mu_2 \in \sigma(L_0(W + \varepsilon E))$.

Why connectedness?

- $\sigma(L_1)$ contains non-zero part of $\sigma(L_0)$;
- due to W^+, L_1 can be discontinuous upon complete edge elimination;
- complete edge elimination = dimensionality reduction.

Outline:

$\|E\| = \sqrt{\langle E, E \rangle_F}$
$\langle A, B \rangle_F = \mathrm{Tr}(A^T B)$

$\sigma(A)$ = ordered by magnitude spectrum of A

The optimization task:

$$\operatorname{argmin}_{\varepsilon} F_k(\varepsilon, E), \qquad \text{where } \|E\| = 1, \; W + \varepsilon E \succeq 0$$

Optimization: Inner Iteration

Assume ε is fixed, then one optimizes for E:

$$\begin{array}{ll|} \min & F_k(\varepsilon, E) \\ & \|E\| = 1 \\ & W + \varepsilon E \succeq 0 \end{array} \quad \longrightarrow \quad \begin{array}{l} \dot{E}(t) = -\nabla_E F_k(\varepsilon, E(t)) \\ \|E\| = 1 \\ W + \varepsilon E \succeq 0 \end{array}$$

For the case of simple eigenvalue $\lambda(t)$ with corresponding unit eigenvector x, we use the derivative formula:

$$\frac{d}{dt}\lambda(t) = \left\langle \frac{d}{dt} L(t), xx^T \right\rangle$$

Constrained graph partitioning via matrix differential equations
E. Andreotti, D. Edelmann, N. Guglielmi, and C. Lubich,

Gradient Flow Approach
Inner and Outer Iterations

Constraints are taken in the account through projections to corresponding manifolds (in Frobenius norm):

- $W + \varepsilon E \geq 0 \leftrightarrow \mathbb{P}_+$ – non-negativity projector;
- $\|E\| = 1 \leftrightarrow \dot{E}(t) = -\nabla_E F_k(\varepsilon, E(t)) + \kappa E(t)$ – trajectory's projection on the unit sphere.

Optimization: Inner Iteration

$$\dot{E}(t) = -\nabla_E \mathbb{P}_+ F_k(\varepsilon, E(t)) + \kappa \mathbb{P}_+ E(t)$$

$$\text{minimizer } E^*(\varepsilon) = \lim_{t \to \infty} E(t)$$

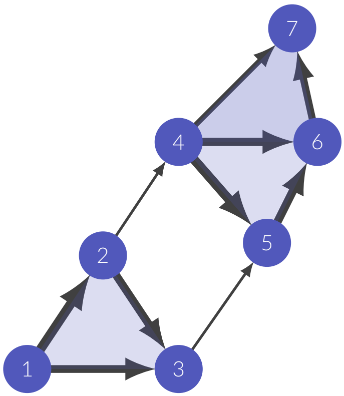
- if $\mathbb{P}_+$ support is conserved, $F_k(\varepsilon, E(t))$ monotonically decreases;
- $\mathbb{P}_+$ limits the control of the rank of the minimizer $E^*(\varepsilon)$.

Outline:

Constrained graph partitioning via matrix differential equations
E. Andreotti, D. Edelmann, N. Guglielmi, and C. Lubich,

- inner iteration is Euler integrated conserving monotonicity;
- inner iteration converges to a local minimizer $E^*(\varepsilon)$;
- outer iteration conducts a search for the minimal ε such that $F_k(\varepsilon, E^*(\varepsilon)) = 0$;
- due to the intrinsic structure of the target functional:
  - outer iteration is started with small ε;
  - quasi-homotopic transition: the minimizer $E^*(\varepsilon)$ is used as an initial point in Euler integration for the inner iteration when ε is modified to a nearby value;
  - forward phase: increase ε until $F_k(\varepsilon, E^*(\varepsilon)) = 0$;
  - backward phase: decrease ε while $F_k(\varepsilon, E^*(\varepsilon)) = 0$ holds.

Illustrative Example

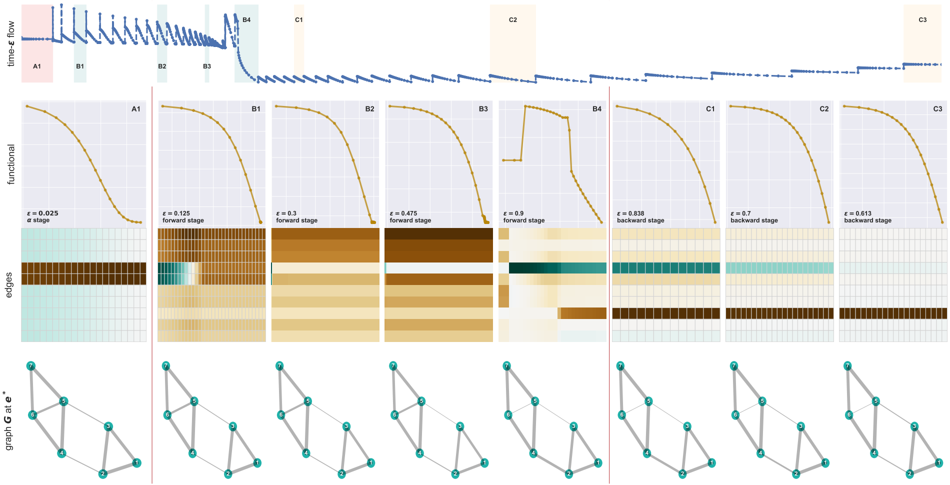


- the set of triangles T in the simplicial complex consists of 3 triangles, $[1,2,3]$, $[4,5,6]$ and $[4,6,7]$;
- weights of the edges are randomly sampled, $w_i \sim U\left[\frac{1}{4}, \frac{3}{4}\right]$;
- weight of the vertex in matrix D_v equals the sum of all adjacent edges;
- weight of the triangle is a minimal weight of included edges:

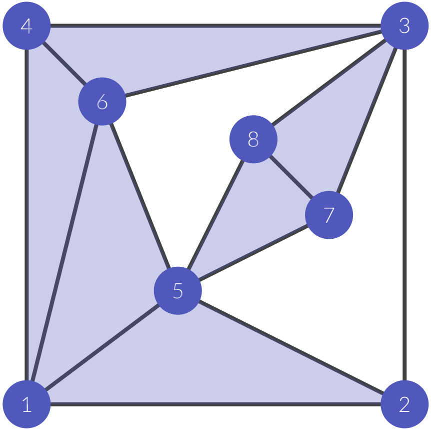
$$w([i,j,k]) = \min\{w_{[i,j]}, w_{[i,k]}, w_{[j,k]}\}$$

$U[a,b]$ — uniform distribution on $[a,b]$ segment

Example: Flow

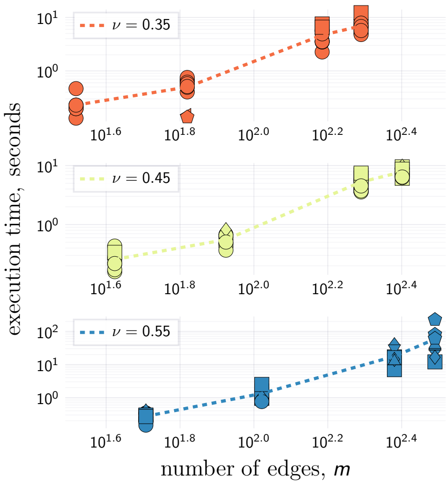


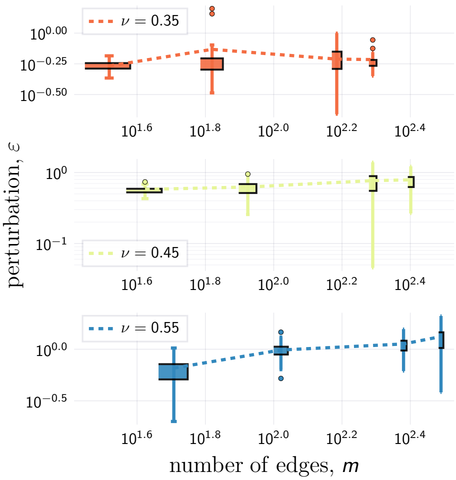
Outline:



- $(n-4)$ points are randomly thrown on the unit square;
- Delauney triangulation of sampled and corner points is calculated;
- edges randomly added or removed to reach the target sparsity ν;
- weights of the edges are randomly sampled, $w_i \sim U\left[\frac{1}{4}, \frac{3}{4}\right]$.

Example
Triangulation





Outline:

Thank you for attention

Theorem (HOL's Inheritance of the Spectrum)

Given the Classical Laplacian L_0 *and the Hodge Laplacian* L_1 *for graph* $\mathcal{G}$, *one gets:*

1. $\sigma_+(L_0) \subseteq \sigma_+(L_1)$;
2. *if* $0 \neq \mu \in \sigma_+(L_0) \subseteq \sigma_+(L_1)$, *then eigenvectors are related as follows:*
   1. *if* x *is an eigenvector for* L_0 *with* μ*-eigenvalue, then* $y = \frac{1}{\sqrt{\mu}} B_1^T x$ *is an eigenvector for* L_1 *with the same eigenvalue*
   2. *if* u *is an eigenvector for* L_1 *with* μ*-eigenvalue and* $u \notin \ker B_1$, *then* $v = \frac{1}{\sqrt{\mu}} B_1 u$ *is an eigenvector for* L_0 *with the same eigenvalue*
3. $\mu \in \sigma_+(L_1)$ *and* $\mu \notin \sigma_+(L_0)$, *then its corresponding eigenvector* u *is in* $\ker B_1$ *and the eigen-properties hold for the second term in the* L_1:

$$B_2 B_2^T u = \mu u$$

Outline:

$\sigma_+(\cdot)$ denotes the positive part of the spectrum

Inheritance of the Spectrum

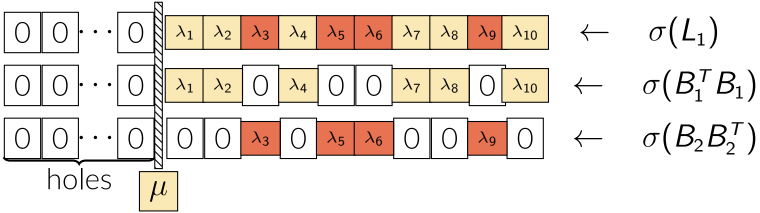


Figure: Illustration for the Combinatorial Spectrum Inheritance

Outline:

Th-Limit to the Continuous Case

One can show the convergence of the discrete L_1 to the continuous L_1 as $|V| \to \infty$ for:

- $w([i,j]) = \mathrm{d}(x_i, x_j)$
- $w([i]) = \sum_{[i,j]\in\mathcal{E}} w([i,j])$
- $w([i,j,k]) = w([i,j])w([i,k])w([j,k])$

Note:

The elimination of the edge here eliminates also triangle and vertex. Such setup is less sensible for the current work's topological stability definition.

Helmholtzian Eigenmap: Topological feature discovery & edge flow learning from point cloud data
Y.-C. Chen, M. Meila, I.G. Kevrekidis