



# Topological Stability and Preconditioning of Higher-Order Laplacian Operators on Simplicial Complexes

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- 1.2 Higher-Order Models: Simplicial Complexes
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- 2.2 Principal Spectral Inheritance
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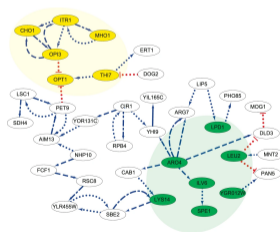
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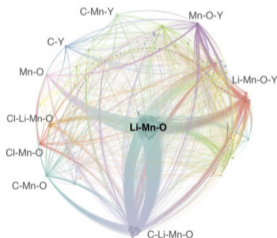
# From Graphs to Simplicial Complexes: Algebra of Boundary Operators and Homology Groups

# Networks of Interactions

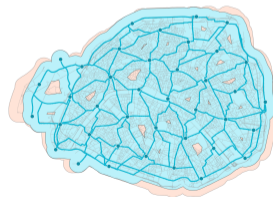
- ◇ **Relational Data** (*multi-agent systems with structured interactions*) are present in biology, neurology, chemistry, transportation and social networks, etc.
- ◇ Structure of the interactions can be induced by the **geometry** of the system or **functionality** of the interactions



(a) gene regulation



(b) chemical reactions



(c) bike paths in Paris

## Outline:

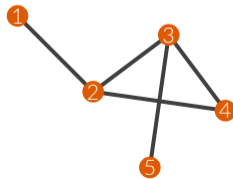
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**Graphs** are widely used models of multi-agent systems restricted to only **dyadic interactions**.

- ◇ graph  $\mathcal{G} = (\mathcal{V}_0, \mathcal{V}_1)$  with  $\mathcal{V}_0$  – set of **nodes** (agents) and  $\mathcal{V}_1 \subseteq \mathcal{V}_0 \times \mathcal{V}_0$  – set of **edges**;
- ◇ associated matrices: *adjacency* (node vs node)  $\mathbf{A}$ , *incidence*  $\mathbf{B}$  (node  $\rightarrow$  edge), *Laplacian*  $\mathbf{L} = \mathbf{B}\mathbf{B}^\top$ , and *degree* matrix  $\mathbf{D}$ , ...

### Used for

- ◇ dynamics on graphs:  $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{y}$
- ◇ random walks:  $\mathbf{p}_{t+1} = \mathbf{D}^{-\frac{1}{2}}\mathbf{L}\mathbf{D}^{-\frac{1}{2}}\mathbf{p}_t$
- ◇ label spreading:  $\min \|\mathbf{y} - \mathbf{x}\| + \alpha \sum A_{ij}|x_i - x_j|^2$
- ◇ centrality measures:  $\mathbf{c} = \frac{1}{\lambda}\mathbf{A}^\top \mathbf{c}$



### Outline:

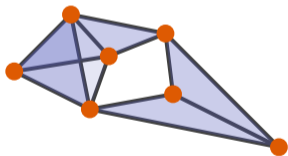
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# Higher-Order Models

Graph (classical)  
pairwise interactions



**Higher-order Models**  
non-linear relations



**motifs**, hypergraphs,  
simplicial complexes

## Definition

**Motifs** are specific repeating subgraphs (e.g. triangles, 4-cycles, etc.).

- ◇ may promote label spreading or synchronization
- ◇ frequency signature for networks' classification
- ◇ require preexisting knowledge of the structures



## Outline:

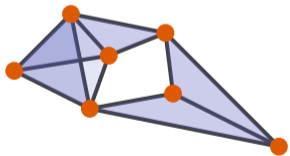
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**Higher-order Models**  
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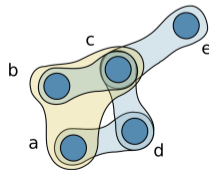


motifs , **hypergraphs**,  
simplicial complexes

## Definition

**Hypergraph** models allows interactions as any possible subset of nodes (**hyperedge**).

- ◇ much more general model
- ◇ lack of structure and restrictions complicate topological analysis
- ◇ may require tensor machinery with worse tractability



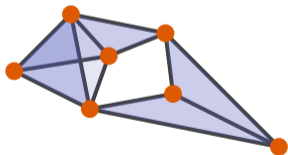
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Graph (classical)  
pairwise interactions



**Higher-order Models**  
non-linear relations



motifs, hypergraphs,  
**simplicial complexes**

## Definition

Simplicial complex  $\mathcal{K} = \{\sigma\}$  is a collection of **nodal simplexes**:

- ◇ each interaction in the system is a nodal simplex;
- ◇ each face of a simplex  $\sigma \in \mathcal{K}$  also lies in  $\mathcal{K}$ .

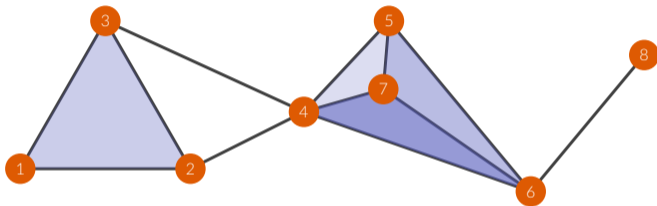
$$\mathcal{K} = \underbrace{\mathcal{V}_0(\mathcal{K})}_{\text{nodes}}, \underbrace{\mathcal{V}_1(\mathcal{K})}_{\text{edges}}, \underbrace{\mathcal{V}_2(\mathcal{K})}_{\text{triangles}}, \dots$$

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# Simplicial Complex Example



$$\mathcal{V}_0(\mathcal{K}) = \{[1], [2], [3], [4], [5], [6], [7], [8]\},$$

$$\mathcal{V}_1(\mathcal{K}) = \{[1, 2], [1, 3], [2, 3], [2, 4], [3, 4], [4, 5], \\ [4, 6], [4, 7], [5, 6], [5, 7], [6, 7], [6, 8]\},$$

$$\mathcal{V}_2(\mathcal{K}) = \{[1, 2, 3], [4, 5, 7], [4, 6, 7], [5, 6, 7]\},$$

$$m_0 = 8$$

$$m_1 = 12$$

$$m_2 = 4$$

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### Definition

Topological properties of the simplicial complex  $\mathcal{K}$  are described via **boundary operators**  $B_k$ :

$$B_k : \text{simplex } \sigma \longrightarrow \text{boundary (faces) of } \sigma$$

**Chain space**  $C_k$  is a linear space of formal sums of simplexes from  $\mathcal{V}_k(\mathcal{K})$ :

- ◇  $C_0$  – space of states of nodes (e.g. labels);
- ◇  $C_1$  – space of edge flows;
- ◇  $C_2$  – space of states of triangles, etc.

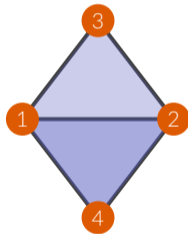
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# Simplicial Complex and Topology

## Boundary operators

$$B_k : C_k \mapsto C_{k-1}, \quad B_k[v_1, \dots, v_{k+1}] = \sum_j (-1)^j [v_1, \dots, v_{j-1}, v_{j+1}, \dots, v_{k+1}]$$



|       |  |    |    |    |    |    |
|-------|--|----|----|----|----|----|
| $B_1$ |  | 1  | 1  | 1  | 2  | 2  |
|       |  | 2  | 3  | 4  | 3  | 4  |
| 1     |  | -1 | -1 | -1 | 0  | 0  |
| 2     |  | 1  | 0  | 0  | -1 | -1 |
| 3     |  | 0  | 1  | 0  | 1  | 0  |
| 4     |  | 0  | 0  | 1  | 0  | 1  |

|       |  |    |    |
|-------|--|----|----|
| $B_2$ |  | 1  | 1  |
|       |  | 2  | 2  |
|       |  | 3  | 4  |
| 12    |  | 1  | 1  |
| 13    |  | -1 | 0  |
| 14    |  | 0  | -1 |
| 23    |  | 1  | 0  |
| 24    |  | 0  | 1  |

**Fundamental Lemma of Topology:**  $B_k B_{k+1} = 0$ .

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Hodge Laplacians on Graphs  
L.H. Lim



### Definition (Homology groups)

Since  $B_k B_{k+1} = 0$ , the **k-th homology group** is defined as

$$\mathcal{H}_k = \ker B_k / \text{im } B_{k+1} \cong \ker B_k \cap \ker B_{k+1}^\top = \ker \underbrace{(B_k^\top B_k + B_{k+1} B_{k+1}^\top)}_{L_k}$$

where  $L_k$  is the **k-th graph Laplacian operator**.

- ◇  $L_0 = B_1 B_1^\top$  – classical graph Laplacian operator
- ◇  $L_1 = B_1^\top B_1 + B_2 B_2^\top$  – 1- (Hodge) Laplacian operator
- ◇  $L_k^\uparrow = B_{k+1} B_{k+1}^\top$  – **up-Laplacian**,  $L_k^\downarrow = B_k^\top B_k$  – **down-Laplacian**

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### Hodge Decomposition ( $k = 1$ ):

$$\mathbb{R}^{m_1} = \underbrace{\text{im } B_1^\top \oplus \text{ker } (B_1^\top B_1 + B_2 B_2^\top)}_{\text{ker } B_1} \oplus \text{im } B_2$$

$\text{ker } B_2^\top$

Each flow  $\mathbf{x} \in C_1$  have three parts in the decomposition,  $\mathbf{x} = \mathbf{y} + \mathbf{z} + \mathbf{h}$ :

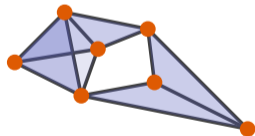
- ◇  $\mathbf{h} \in \text{ker } L_1$  – **harmonic** part;
- ◇ note that the conjugate  $B_1^\top [v_1, v_2] = [v_2] - [v_1]$ , so  $\mathbf{y} \in \text{im } B_1^\top$  – **gradient** part
- ◇ similarly,  $\mathbf{z} \in \text{im } B_2$  – **curl** part

### Outline:

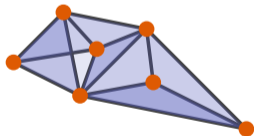
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- ◇ elements of  $\ker L_k$  correspond to the **k-dimensional holes** of  $\mathcal{K}$ ;
- ◇  $\dim \ker L_k =$  number of k-dimensional holes in  $\mathcal{K}$ .

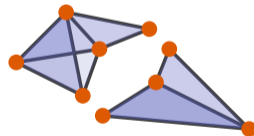
$\ker L_0$  – **connected components**,  $\ker L_1$  – **1D holes**,  $\ker L_2$  – **3D voids**



$$\dim \ker L_0 = 1$$
$$\dim \ker L_1 = 1$$



$$\dim \ker L_0 = 1$$
$$\dim \ker L_1 = 0$$



$$\dim \ker L_0 = 2$$
$$\dim \ker L_1 = 0$$

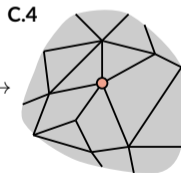
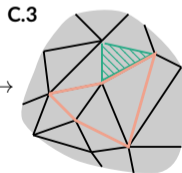
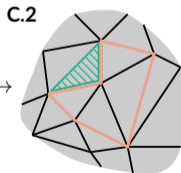
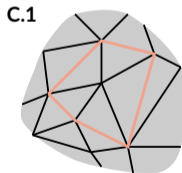
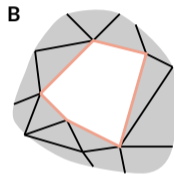
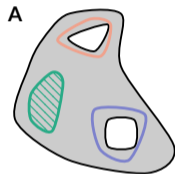
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# Homology Group Illustration



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- ◇ weight function for simplex of  $k$ -th order:  $w_k : C_k \mapsto \mathbb{R}_+$ ;
- ◇ diagonal weight matrix  $W_k = \text{diag} \left( \left\{ \sqrt{w_k(\sigma)} \right\}_{\sigma \in \mathcal{V}_k(\mathcal{K})} \right)$

$$B_k \longrightarrow \bar{B}_k = W_{k-1}^{-1} B_k W_k$$

**Fundamental Lemma of Topology** holds:

$$\bar{B}_k \bar{B}_{k+1} = (W_{k-1}^{-1} B_k W_k) \cdot (W_k^{-1} B_{k+1} W_{k+1}) = 0$$

**Lemma (Weight impact on  $\mathcal{H}_k$ )**

*The dimension of the homology groups of  $\mathcal{K}$  is not affected by the weights of its  $k$ -simplices:*

$$\dim \ker \bar{B}_k = \dim \ker B_k, \quad \dim \ker \bar{B}_k^T = \dim \ker B_k^T, \quad \dim \bar{\mathcal{H}}_k = \dim \mathcal{H}_k$$

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# Simplicial Complex and Topology

## Generalisation to the Weighted Case

- ◇ weight function for simplex of  $k$ -th order:  $w_k : C_k \mapsto \mathbb{R}_+$ ;
- ◇ diagonal weight matrix  $W_k = \text{diag} \left( \{ \sqrt{w_k(\sigma)} \}_{\sigma \in \mathcal{V}_k(\mathcal{K})} \right)$

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Common choices:

- ◇ **min-rule**: the weight of the triangle is the minimal weight of adjacent edges,  $w_2(\tau) = \min\{w_1(\sigma_1), w_1(\sigma_2), w_1(\sigma_3)\}$
- ◇ **product**: the weight of the triangle is the product of weights of adjacent edges,  $w_2(\tau) = \sqrt[3]{w_1(\sigma_1)w_1(\sigma_2)w_1(\sigma_3)}$

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# Topological Instability of Simplicial Complexes via Matrix Nearness Problems

## Problem Statement

Find the **smallest (in weight) set of edges** to eliminate in  $\mathcal{K}$  such that:

$$\dim \overline{\mathcal{H}}_1(\tilde{\mathcal{K}}) \geq \dim \overline{\mathcal{H}}_1(\mathcal{K}) + 1$$

create another hole in  $\overline{\mathcal{H}}_1(\mathcal{K})$



create another dimension in  $\ker \overline{L}_1$



push the smallest positive  $\lambda_+ \in \sigma(\overline{L}_1)$  to 0

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# Stability of the Homology Group

## Principal Spectral Inheritance

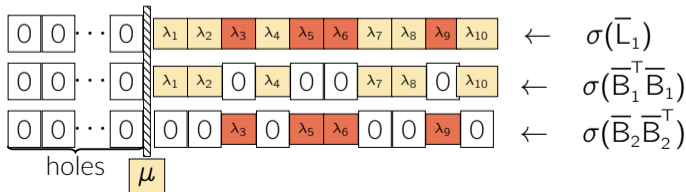
### Theorem (HOL's spectral inheritance)

Let  $\bar{L}_k^{\text{down}} = \bar{B}_k^T \bar{B}_k$  and  $\bar{L}_k^{\text{up}} = \bar{B}_{k+1} \bar{B}_{k+1}^T$  (so  $\bar{L}_k = \bar{L}_k^{\text{down}} + \bar{L}_k^{\text{up}}$ ). Then:

1.  $\sigma_+(\bar{L}_k^{\text{up}}) = \sigma_+(\bar{L}_{k+1}^{\text{down}})$ , where  $\sigma_+(\cdot)$  denotes the set of positive eigenvalues;
2. for any  $\mu \in \sigma_+(\bar{L}_k)$ , either  $\mu \in \sigma_+(\bar{L}_k^{\text{up}})$  or the corresponding eigenvector  $\vec{v} \in \ker \bar{L}_k^{\text{up}}$ .

Similarly, for any  $\nu \in \sigma_+(\bar{L}_{k+1})$ , either  $\nu \in \sigma_+(\bar{L}_{k+1}^{\text{down}})$  or the corresponding eigenvector  $\vec{u} \in \ker \bar{L}_{k+1}^{\text{down}}$ , and

$$\bar{B}_k^T \bar{B}_k \vec{v} = \mu \vec{v}, \quad \bar{B}_{k+2} \bar{B}_{k+2}^T \vec{u} = \nu \vec{u}.$$



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# Stability of the Homology Group

## Problem Statement

Creating another hole in  $\overline{\mathcal{H}}_1 \iff$  push  $\lambda_+ \in \sigma(\overline{L}_1^{\text{up}}) \rightarrow 0$ , and avoid **homological pollution**.

### combinatorial approach

find edges  $E^- \subset \mathcal{V}_1(\mathcal{K})$  to eliminate such that

$$\dim \overline{\mathcal{H}}_1(\tilde{\mathcal{K}}) \geq \dim \overline{\mathcal{H}}_1(\mathcal{K}) + 1 \quad \longrightarrow$$

with

$$\sum_{e \in E^-} w_1(e) \rightarrow \min$$

### continuous approach

perturb edges' weights

$$W_1 \rightarrow W_1 + \delta W_1$$

such that  $\lambda_+(\delta W_1) = 0$  with  $\|\delta W_1\| \rightarrow \min$

**spectral matrix nearness problem**

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**Problem:** find *smallest*  $X$  such that  $A + X$  has desired spectral properties.

**Target eigenvalue** and **functional:** for example, right-most eigenvalue  $\lambda_{\max}(A + X)$  or first non-zero eigenvalue  $\lambda_+(A + X)$  with  $F(X) = \frac{1}{2}\lambda_{\max}^2(A + X)$ .

**Gradient flow:** Integrate in the direction of anti-gradient of the target functional.

**Lemma (Derivative of the eigenvalue)**

$A(\tau)$  has a unique eigenvalue  $\lambda(\tau)$  that is analytic in a neighborhood of  $\tau_0$ , with  $\lambda(\tau_0) = \lambda_0$

$$\dot{\lambda}(\tau_0) = \frac{1}{\mathbf{y}_0^* \mathbf{x}_0} \mathbf{y}_0^* \dot{A}(\tau_0) \mathbf{x}_0$$

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# Stability of the Homology Group

## Weight update

The edges' weight perturbation  $W_1 \rightarrow W_1 + \delta W_1$  triggers a weight update for **nodes' weights**  $W_0$  and **triangles weights**  $W_2$ :

◇ edge elimination ( $w_1(e) + \delta w_1(e) = 0$ ) should trigger the elimination of all adjacent triangles, e.g. for  $\mathbf{t} = [e_1, e_2, e_3]$

$$w_2(\mathbf{t}) \sim \min \{w_1(e_1) + \delta w_1(e_1), w_1(e_2) + \delta w_1(e_2), w_1(e_3) + \delta w_1(e_3)\}$$

◇ vertex isolation should not trigger its elimination, e.g.

$$w_0(v) \sim \rho + \sum_{v \in e} (w_1(e) + \delta w_1(e)), \quad \rho > 0$$

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# Gradient Flow for Topological Stability

Let  $\delta W_1 = \varepsilon E$ , where  $\varepsilon$  is the **perturbation size** and  $E$ ,  $\|E\| = 1$ , is the **perturbation shape**.

**Target functional:**

$$F(\varepsilon, E) = \underbrace{\frac{1}{2} \lambda_+(\varepsilon, E)^2}_{\text{extend } \mathcal{H}_1} + \underbrace{\frac{\alpha}{2} \max\left(0, 1 - \frac{\mu_2(\varepsilon, E)}{\mu}\right)^2}_{\text{prevent pollution}}$$

where  $\lambda_+(\varepsilon, E)$  is the smallest positive eigenvalue of perturbed  $\bar{L}_1^{\text{up}}(\varepsilon, E)$  and  $\mu_2(\varepsilon, E)$  is the algebraic connectivity of perturbed  $\bar{L}_0(\varepsilon, E)$ .

## Gradient Flow for Steepest Descent

Let  $E = E(t)$ . Then:

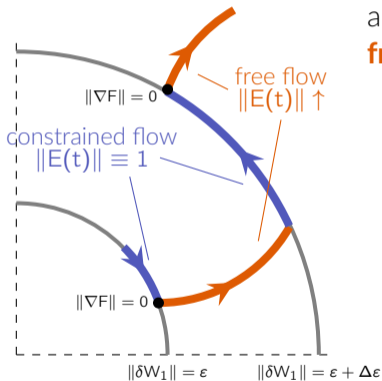
$$\frac{d}{dt} F(\varepsilon, E(t)) = \varepsilon \langle \nabla_E F(\varepsilon, E(t)), \dot{E} \rangle \implies \text{steepest } \mathbf{monotone} \text{ descent} \\ \dot{E} = -\nabla_E F(\varepsilon, E(t))$$

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# Gradient Flow for Topological Stability

## Free and Constrained Stages



Given the intricate landscape of  $F(\varepsilon, E)$ , we alternate **constrained**, norm-preserving, and **free** gradient flows:

◇ **constrained**:

$\dot{E} = -\nabla_E F(e, E(t)) + \kappa E(t)$  where  $\kappa$  is given by  $\langle \dot{E}, E \rangle$ ;

◇ **free** flow:  $\dot{E} = -\nabla_E F(e, E(t))$  until  $\|\varepsilon E(t)\| = \varepsilon + \Delta\varepsilon$ ;

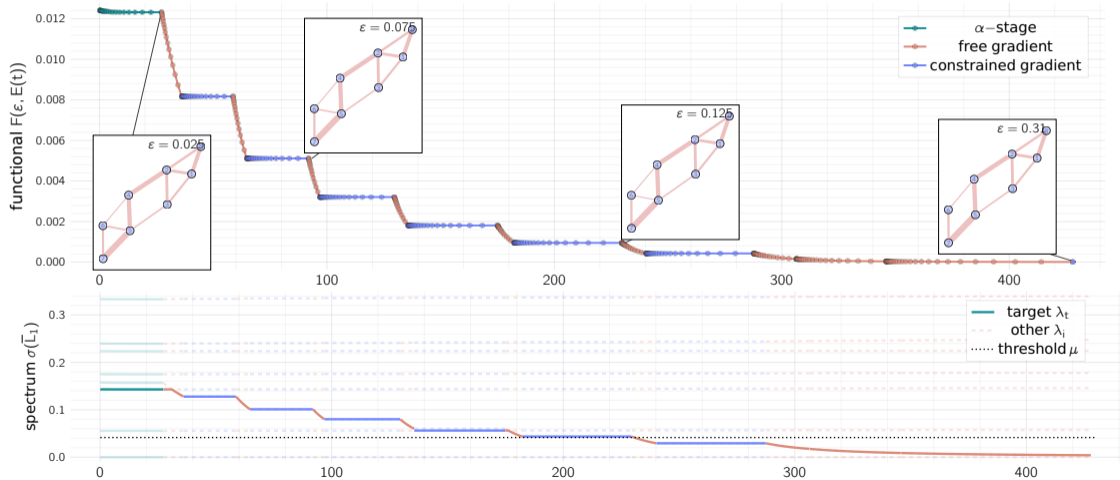
◇ both flows use non-negativity projector  $\mathbb{P}_+$  to avoid negative weights;

◇ the functional  $F(\varepsilon, E)$  monotonically decreases.

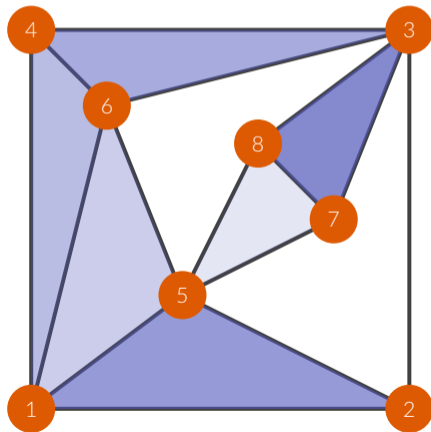
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- **Stability of Homology Group**
  - Spectral inheritance and homological pollution
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  - Gradient Flow for Perturbation
  - Free and Constrained Stages**
  - Numerical experiments
- HeCS-preconditioning

# Illustrative example



# Numerical benchmark Triangulation

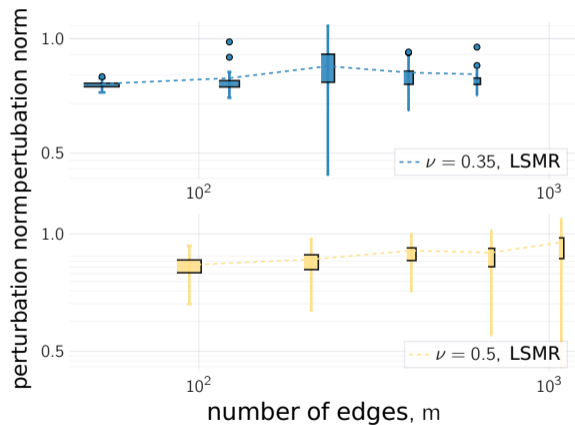
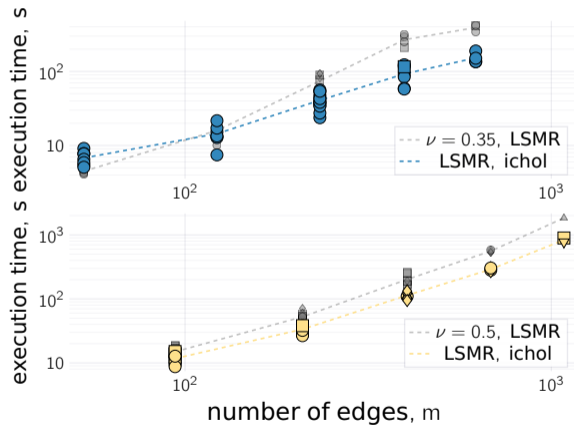


- ◇  $(n - 4)$  points are randomly thrown on the unit square;
- ◇ Delaunay triangulation of sampled and corner points is calculated;
- ◇ edges randomly added or removed to reach the target sparsity  $\nu$ ;
- ◇ weights of the edges are randomly sampled,  $w_i \sim \mathcal{U}[\frac{1}{4}, \frac{3}{4}]$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

## Outline:

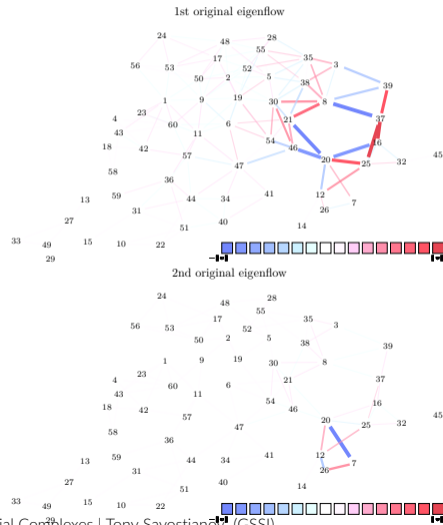
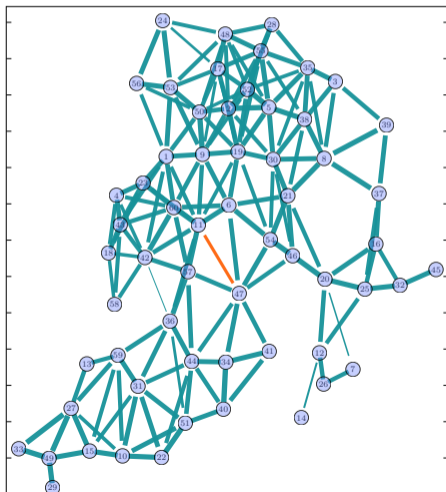
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# Numerical benchmark Triangulation



# Real data example Transportation Network

## Bologna: Regional Network



# Cholesky-like Preconditioning via Heavy Collapsible Subcomplex for Laplacian Systems

## Linear System for Hodge Laplacians

$$\begin{array}{l} L_k \mathbf{x} = \mathbf{f} \\ \mathbf{x}, \mathbf{f} \perp \ker L_k \end{array} \iff \min_{\mathbf{x}} \|L_k \mathbf{x} - \mathbf{f}\|$$

- ◇ inside simplicial dynamics  $\dot{\mathbf{x}} = L_k \mathbf{x} - \mathbf{f}$  (stationary point and implicit integrators)
- ◇ iterative solutions  $\mathbf{x}_l = L_k \mathbf{x}_{l-1}$  for spectrum computations
- ◇ inside implicit graph neural networks,  $\mathbf{x} = \phi(W\mathbf{x}L_k + B)$
- ◇ projections for **gradient** and **curl** components in **Hodge decomposition**

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### Theorem (Joint k-Laplacian solver)

The least-square problem  $L_k \mathbf{x} = \mathbf{f}$  can be reduced to a sequence of consecutive least-square problems for isolated up-Laplacians. Precisely,  $\mathbf{x}$  is a solution of

$$L_k \mathbf{x} = \mathbf{f} \quad \text{s. t.} \quad \mathbf{x}, \mathbf{f} \perp \ker L_k$$

if and only if it can be written as  $\mathbf{x} = B_k^\top \mathbf{u} + \mathbf{x}_2$ , where:

$$\hat{\mathbf{u}} = \arg \min_{\mathbf{z}} \left\| L_{k-1}^\uparrow \mathbf{z} - B_k \mathbf{f}_1 \right\|, \quad \mathbf{u} = \arg \min_{\mathbf{z}} \left\| L_{k-1}^\uparrow \mathbf{z} - \hat{\mathbf{u}} \right\|,$$
$$\mathbf{x}_2 = \arg \min_{\mathbf{y}} \left\| L_k^\uparrow \mathbf{y} - \mathbf{f}_2 \right\|$$

and  $\mathbf{f} = \mathbf{f}_1 + \mathbf{f}_2$  with  $\mathbf{f}_1 = B_k^\top \mathbf{z}_1$ ,  $\mathbf{z}_1 = \arg \min_{\mathbf{z}} \left\| L_{k-1}^\uparrow \mathbf{z} - B_k \mathbf{f} \right\|$ .

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### Consequence

Solution of the “whole” Laplacian system  $L_k \mathbf{x} = \mathbf{f}$  can be reduced to solving only up-Laplacian systems  $L_k^\uparrow \mathbf{x} = \mathbf{f}$ .

- ◇ both  $L_k$  and  $L_k^\uparrow$  are sparse, so iterative solvers (CGLS, LSMR, etc.) can benefit from fast `matvec` operation;
- ◇ convergence of such methods are primarily determined by the **condition number**  $\kappa_+(L_k^\uparrow)$ , or, specifically:

$$\|\mathbf{x}_N - \mathbf{x}^*\|_{L_k^\uparrow} \leq 2 \left( \frac{\sqrt{\kappa_+(L_k^\uparrow)} - 1}{\sqrt{\kappa_+(L_k^\uparrow)} + 1} \right)^N \|\mathbf{e}_0\|_{L_k^\uparrow}$$

- ◇ since all Laplacians are naturally singular, we use  $\kappa_+(L_k^\uparrow) = \frac{\sigma_{\max}^+(L_k^\uparrow)}{\sigma_{\min}^+(L_k^\uparrow)}$

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## Definition (Sparse Simplicial Complex)

We assume  $\mathcal{K}$  to be a **sparse simplicial complex** (in comparison with always sparse Laplacian operators) at the  $k$ -th order, if

$$m_k = \mathcal{O}(m_{k-1} \log m_{k-1})$$

analogously to the standard graph case.

## Problem

In order to reduce  $\kappa_+(L_k^\dagger)$ , we want to move:

$$\min_{\mathbf{x}} \|L_k^\dagger \mathbf{x} - \mathbf{f}\| \longrightarrow \min_{\mathbf{x}} \|(C^\dagger L_k^\dagger C^{\top\dagger})(C^\top \mathbf{x}) - C^\dagger \mathbf{f}\|$$

such that the transition is bijective and  $C^\dagger$  is cheap.

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If  $C$  is lower-triangular, the pseudo-inverse is cheap and  $C$  is known as **Cholesky preconditioner**. It is computed along **Schur complements**:

$$S_i = S_{i-1} - \frac{1}{\alpha_i} S_{i-1} \delta_i \delta_i^T S_{i-1}^T$$

$$\mathbf{c}_i = \frac{1}{\sqrt{\alpha_i}} S_{i-1} \delta_i$$

$$\alpha_i = \delta_i^T S_{i-1} \delta_i$$

With these definitions, the Cholesky factor  $C$  such that  $A = CC^T$  is formed by the columns  $\mathbf{c}_i$ , namely

$$C = [\mathbf{c}_1 \ \mathbf{c}_2 \ \dots \ \mathbf{c}_n]$$

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# Cholesky Preconditioner

## Exact computation problem

- ◇ computation of exact Schur complements  $S_i$  is expensive
- ◇ one aims to leverage underlying simplicial complex  $\mathcal{K}$  to speed it up

**Lemma (Rank-1 decomp.):**  $L_k^\uparrow = \sum_{t \in \mathcal{V}_k(\mathcal{K})} L_k^\uparrow(t) = \sum_{t \in \mathcal{V}_k(\mathcal{K})} w(t) \mathbf{e}_t \mathbf{e}_t^\top$

- ◇  $w(t) = [W_k^2]_{tt}$  is the weight of the simplex  $t$
- ◇  $\mathbf{e}_t$  is the  $t$ -th column of the matrix  $B_k$

Then, for  $L_1^\uparrow$ :

$$S_1 = \underbrace{\sum_{t|1 \notin t} w(t) \mathbf{e}_t \mathbf{e}_t^\top}_{\text{remainder of } L_1^\uparrow \text{ without edge } 1} + \underbrace{\frac{1}{2\Omega_{\{1\}|\emptyset}} \sum_{\substack{t_1|1 \in t_1 \\ t_2|1 \in t_2}} w(t_1)w(t_2) [\mathbf{e}_{t_1} - \mathbf{e}_{t_2}][\mathbf{e}_{t_1} - \mathbf{e}_{t_2}]^\top}_{\text{clique term not a Laplacian}}$$

### Outline:

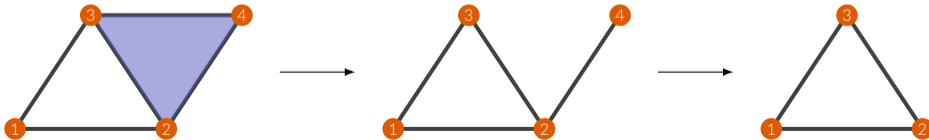
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# Collapsibility of Simplicial Complexes

The simplex  $\sigma \in \mathcal{K}$  is **free** if it is a face of exactly one simplex  $\tau = \tau(\sigma) \in \mathcal{K}$  of higher order (maximal face).

The **collapse**  $\mathcal{K} \setminus \{\sigma\}$  of  $\mathcal{K}$  at a free simplex  $\sigma$  is the operation of reducing  $\mathcal{K}$  to  $\mathcal{K}'$ , where  $\mathcal{K}' = \mathcal{K} - \sigma - \tau$ .

Simplex  $\mathcal{K}$  is called **collapsible** if it can be reduced to a single node.



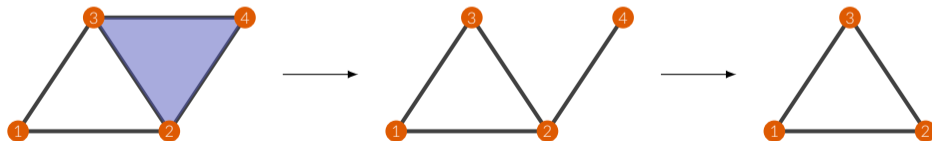
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General collapsibility is *NP-hard* and too demanding for our purposes (to eliminate cyclic terms).

## Definition (Weakly collapsible complex)

A simplicial complex  $\mathcal{K}$  restricted to its 2-skeleton is called **weakly collapsible**, if there exists a collapsing sequence  $\Sigma_1$  such that the simplicial complex  $\mathcal{L} = \mathcal{K} \setminus \Sigma_1$  has no simplices of order 2, i.e.  $\mathcal{V}_2(\mathcal{L}) = \emptyset$  and  $L_1^\uparrow(\mathcal{L}) = 0$ .



**Weak collapsibility** can be consistently checked by **GREEDY ALGORITHM** and polynomially solvable ( $\mathcal{O}(m_1)$ ).

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## Lemma (Exact Solver for Collapsible Complexes)

Let the simplicial complex  $\mathcal{K}$  be weakly collapsible through the collapsing sequence  $\Sigma$  and the corresponding sequence of maximal faces  $\mathbb{T}$ . Let the permutation matrices of the two sequences be  $P_\Sigma$  and  $P_\mathbb{T}$ , i.e. such that  $[P_\Sigma]_{ij} = 1 \iff j = \sigma_i$ , and similarly for  $P_\mathbb{T}$ . Then  $C = P_\Sigma \bar{B}_2 P_\mathbb{T}$  is an *exact Cholesky multiplier* for  $P_\Sigma L_1^\uparrow(\mathcal{K}) P_\Sigma^\top$ , i.e.  $P_\Sigma L_1^\uparrow(\mathcal{K}) P_\Sigma^\top = CC^\top$ .

### Idea

Find a weakly collapsible **subcomplex**  $\mathcal{L} \subseteq \mathcal{K}$  and use its Cholesky multiplier  $C$  as preconditioner.

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# Preconditioning by Subcomplex

## How to find the best subcomplex?

### Definition (Subsampling Matrix)

Diagonal matrix  $\Pi$  is called **subsampling matrix** if  $\Pi_{ii} = 1$  only if the  $i$ -th triangle is included in subcomplex  $\mathcal{L}$ .

### Lemma (Optimal Weight Choice)

*Triangles should be sampled in  $\mathcal{L}$  with the same weight as the original  $\mathcal{K}$ .*

### Theorem (Preconditioning by Subcomplex)

Let  $\mathcal{L}$  be a weakly collapsible subcomplex of  $\mathcal{K}$  defined by the subsampling matrix  $\Pi$  and let  $C$  be a Cholesky multiplier of  $L_1^\uparrow(\mathcal{L})$ . Then the conditioning of the symmetrically preconditioned  $L_1^\uparrow$  is given by:

$$\kappa_+ \left( C^\dagger P_\Sigma L_1^\uparrow P_\Sigma^\top C^{\dagger\top} \right) = \left( \kappa_+ \left( (S_1 V_1^\top \Pi)^\dagger S_1 \right) \right)^2 = (\kappa_+(\Pi V_1))^2,$$

where  $V_1$  forms the orthonormal basis on  $\text{im } \bar{B}_2^\top$ .

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# Preconditioning by Subcomplex

## How to find the best weakly collapsible subcomplex?

Preconditioning quality is determined by  $\kappa_+(\Pi V_1)$ :

- ◇ Note that  $\text{im } V_1 = W_2 \text{im } B_2^\top$
- ◇ Rows in  $V_1$  are scaled by the weights of the triangles
- ◇ Multiplication by  $\Pi$  cancels rows in  $V_1$  for the eliminated triangles
- ◇ Good choice of  $\Pi$ : *eliminate triangles with the smallest edges*

Subcomplex  $\mathcal{L}$  should:

1. have the same set of nodes and edges;
2. subsample triangles,  $\mathcal{V}_2(\mathcal{L}) \subseteq \mathcal{V}_2(\mathcal{K})$ ;
3. be weakly collapsible through some collapsing sequence  $\Sigma$  and sequence of maximal faces  $\mathbb{T}$ ;
4. have the same 1-homology as  $\mathcal{K}$ , that is  $\ker L_1(\mathcal{K}) = \ker L_1(\mathcal{L})$  (bijectivity);
5. have the highest possible total weight to improve preconditioning.

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# Preconditioning by Subcomplex

## Heavy Collapsible Subcomplex

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**Algorithm 5** HEAVY\_SUBCOMPLEX( $\mathcal{K}, W_2$ ): construction a heavy collapsible subcomplex

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**Require:** the original complex  $\mathcal{K}$ , weight matrix  $W_2$

```
1:  $\mathcal{L} \leftarrow \emptyset, \mathbb{T} \leftarrow \emptyset$  ▷ initial empty subcomplex
2: while there is unprocessed triangle in  $\mathcal{V}_2(\mathcal{K})$  do
3:    $t \leftarrow \text{nextHeaviestTriangle}(\mathcal{K}, W_2)$  ▷ e.g. iterate through
    $\mathcal{V}_2(\mathcal{K})$  sorted by weight
4:   if  $\mathcal{L} \cup \{t\}$  is weakly collapsible then ▷ run
   GREEDY_COLLAPSE( $\mathcal{L} \cup \{t\}$ ) (Algorithm 4)
5:      $\mathcal{L} \leftarrow \mathcal{L} \cup \{t\}, \mathbb{T} \leftarrow [\mathbb{T} \ t]$  ▷ extend  $\mathcal{L}$  by  $t$ 
6:   end if
7: end while
8: return  $\mathcal{L}, \mathbb{T}, \Sigma$  ▷ here  $\Sigma$  is the collapsing sequence of  $\mathcal{L}$ 
```

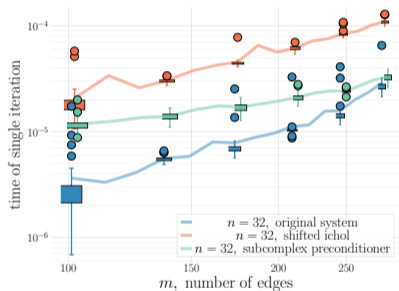
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- ◇ we assume  $\mathcal{K}$  to be sparse,  $m_2 = \mathcal{O}(m_1 \log m_1)$ ;
- ◇  $\mathcal{K}$  has a **disbalanced weight profile** for triangles (e.g. generated `minrule`), so a dominating heavy subcomplex is more probable;
- ◇ algorithmic complexity of **HeCS** preconditioning is  $\mathcal{O}(m_1 m_2)$ .

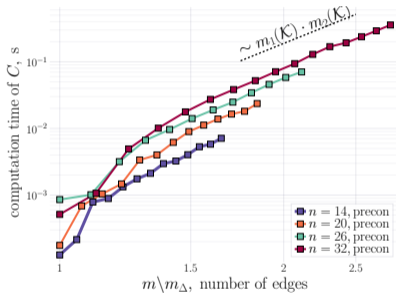
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# Numerical Experiments Timings



(a) Single iteration timing: the average time of `matvec` computation for the original system (blue), shifted `ichol` (orange) and HeCS preconditioner (green).

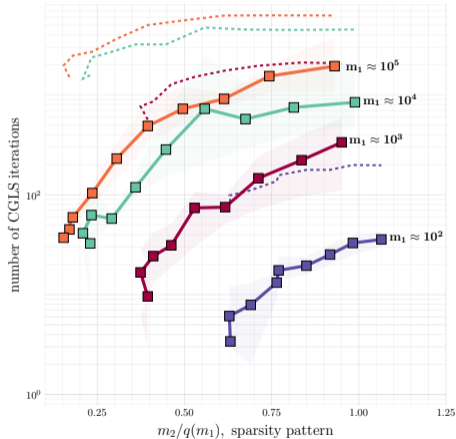
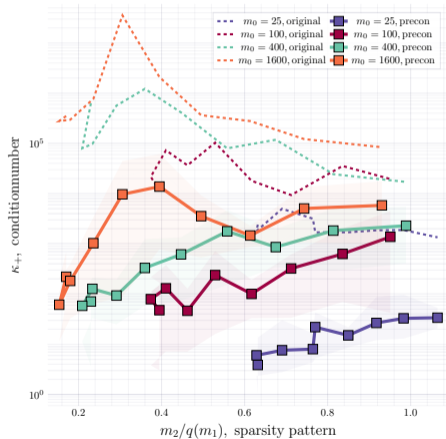


(b) Computation time for the heavy subcomplex preconditioner in case of enriched triangulations on  $m_0$  vertices

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# Thank you for attention!

Topological  
Stability



paper on arXiv



code on Github

HeCS -  
Preconditioning



paper on arXiv



code on Github

Personal Page: further materials on <https://antsav.me/>

Comp@GSSI: our group at <https://num-gssi.github.io/>

Break the screen in case of ...  
Well, just break it,  
we will figure it out later!

- ◇ main computational load: first non-zero eigenvalue of both  $\bar{L}_1^\uparrow(\varepsilon, E)$  and  $\bar{L}_0(\varepsilon, E)$
- ◇ both operators are of form  $A^\top A$  (with  $A = \bar{B}_2$  or  $A = \bar{B}_1^\top$ );
- ◇ corresponding optimization problem:  $\min_{\mathbf{x} \perp \ker A} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|}$
- ◇ requires sparse singular value solver based on a Krylov subspace scheme for the pseudo inverse of  $A^\top A$

**L-Sq Problems** (solve with **preconditioned LSMR**):

$$\min_{\mathbf{x}} \|\bar{L}_1^{\text{up}}(\varepsilon, E)\mathbf{x} - \mathbf{b}\|, \quad \min_{\mathbf{x}} \|\bar{L}_0(\varepsilon, E)\mathbf{x} - \mathbf{b}\|,$$

**Idea:** fix the preconditioner along the flow.

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## Theorem (Simplicial Sparsification)

For any  $\varepsilon > 0$ , a sparse simplicial complex  $\mathcal{L}$  can be sampled from  $\mathcal{K}$  as follows:

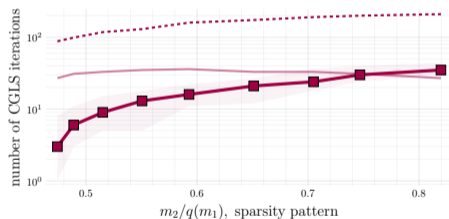
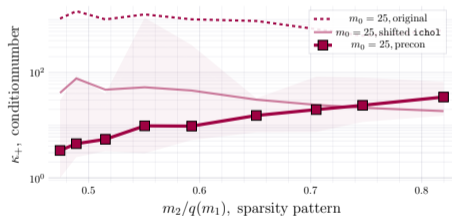
1. compute the probability measure  $\mathbf{p}$  on  $\mathcal{V}_{k+1}(\mathcal{K})$  proportional to the generalized resistance vector  $\mathbf{r} = \text{diag} \left( \mathbf{B}_{k+1}^\top (\mathbf{L}_k^\uparrow)^\dagger \mathbf{B}_{k+1} \right)$ ;
2. sample  $q$  simplices  $\tau_i$  from  $\mathcal{V}_{k+1}(\mathcal{K})$  according to the probability measure  $\mathbf{p}$ , where  $q$  is chosen so that  $q(m_k) \geq 9C^2 m_k \log(m_k/\varepsilon)$ , for some absolute constant  $C > 0$ ;
3. form a sparse simplicial complex  $\mathcal{L}$  with all the sampled simplexes of order  $k$  and all its faces with the weight  $\frac{w_{k+1}(\tau_i)}{q(m_k)\mathbf{p}(\tau_i)}$ ; weights of repeated simplices are accumulated.

Then, with probability at least  $1/2$ , the up-Laplacian of the sparsifier  $\mathcal{L}$  is  $\varepsilon$ -close to the original one, i.e. it holds  $\mathbf{L}_k^\uparrow(\mathcal{L}) \approx_\varepsilon \mathbf{L}_k^\uparrow(\mathcal{K})$ .

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Assuming  $\mathbf{U}$  is an orthogonal basis of  $\ker L_1^\uparrow$ , one can move to  $L_1^\uparrow \rightarrow L_1^\uparrow + \alpha \mathbf{U} \mathbf{U}^\top$ , which can be preconditioned by non-singular methods. Specifically, we use  $\mathbf{C}_\alpha = \text{ichol}(L_1^\uparrow + \alpha \mathbf{U} \mathbf{U}^\top)$ .



$\mathbf{U}$  can be formed directly using the vectors  $\mathbf{B}_1^\top \mathbf{x}$ ,  $\mathbf{x} \in (\mathbf{1})^\perp$ , when  $\mathcal{K}$  has trivial 0- and 1-homology.

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