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Scuola Universitaria Superiore

Cholesky-Like Preconditioner for Hodge Laplacians via Heavy Collapsible Subcomplex

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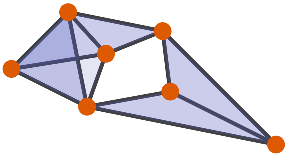
Graphs vs Simplicial Complexes

Graph (classical)
pairwise interactions

↓

Higher-order Models
non-linear relations



hypergraphs, motifs,
simplicial complexes

Definition

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

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

$$\mathcal{K} = \underbrace{\mathcal{V}_0(\mathcal{K})}_{m_0 \text{ nodes}}, \underbrace{\mathcal{V}_1(\mathcal{K})}_{m_1 \text{ edges}}, \underbrace{\mathcal{V}_2(\mathcal{K})}_{m_2 \text{ triangles}}, \ldots$$

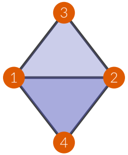
Outline:

Definition

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

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

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



B_1	12	13	14	23	24
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	123	124
12	1	1
13	-1	0
14	0	-1
23	1	0
24	0	1

Higher-Order Laplacian : $L_k = B_k^\top B_k + B_{k+1} B_{k+1}^\top = L_k^\downarrow + L_k^\uparrow$.

Weighted Case: $L_k = W_k B_k^\top W_{k-1}^{-2} B_k W_k + W_k^{-1} B_{k+1} W_{k+1}^2 B_{k+1}^\top W_k^{-1}$.

Linear System with Hodge Laplacian

Linear System for Hodge Laplacians

$$\begin{matrix} L_k \mathbf{x} = \mathbf{f} \\ \mathbf{x}, \mathbf{f} \perp \ker L_k \end{matrix} \quad \Longleftrightarrow \quad \min_{\mathbf{x}} \| L_k \mathbf{x} - \mathbf{f} \|$$

- 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 (complex's topology)
- inside implicit graph neural networks, $\mathbf{x} = \phi\left(W \mathbf{x} L_k + B\right)$
- projections for **gradient** and **curl** components in Hodge decomposition

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*

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

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

Outline:

Consequence

Solution of the "whole" Laplacian system $L_k \mathbf{x} = \mathbf{f}$ can be reduced to solving only up-Laplacian systems $L_k^{\uparrow}\mathbf{x} = B_{k+1} W_k^2 B_{k+1}^\top \mathbf{x} = \mathbf{f}$.

- 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 determined by the **condition number** $\kappa_+(L_k^{\uparrow})$;
- since all Laplacians are naturally singular, we use $\kappa_+(L_k^{\uparrow}) = \frac{\sigma_{\max}^+(L_k^{\uparrow})}{\sigma_{\min}^+(L_k^{\uparrow})}$

Problem

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

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

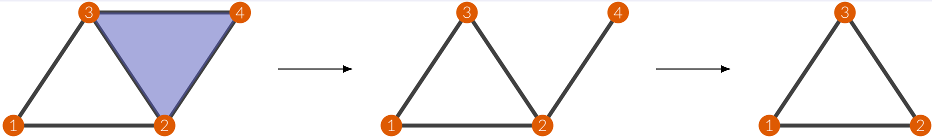
such that the transition is bijective and $C^{\dagger}$ is cheap.

Idea

What are simplicial complexes with fast and efficient Cholesky multipliers for up-Laplacians $L_1^{\uparrow}$?

Definition (Weakly collapsible complex)

A simplicial complex $\mathcal{K}$ restricted to its 2-skeleton is called weakly collapsible, if there exists a collapsing sequence Σ_1 such that the simplicial complex $\mathcal{L} = \mathcal{K} \backslash \Sigma_1$ has no simplices of order 2, i.e. $\mathcal{V}_2(\mathcal{L}) = \varnothing$ and $L_1^{\uparrow}(\mathcal{L}) = 0$.



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

Lemma (Exact Solver for Collapsible Complexes)

Let the simplicial complex $\mathcal{K}$ *be weakly collapsible through the collapsing sequence* Σ *and the corresponding sequence of maximal faces* $\mathbb{T}$*. Let the permutation matrices of the two sequences be* P_Σ *and* $P_\mathbb{T}$*, i.e. such that* $[P_\Sigma]_{ij} = 1 \iff j = \sigma_i$*, and similarly for* $P_\mathbb{T}$*. Then* $C = P_\Sigma \overline{B}_2 P_\mathbb{T}$ *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.

Definition (Subsampling Matrix)

Diagonal matrix Π 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 Π 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:

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

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

Preconditioning by Subcomplex
How to find the best weakly collapsible subcomplex?

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

- Note that $\mathbf{im}\, V_1 = W_2\, \mathbf{im}\, B_2^\top$
- Rows in V_1 are scaled by the weights of the triangles
- Multiplication by Π cancels rows in V_1 for the eliminated triangles
- Good choice of Π: *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 Σ 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.

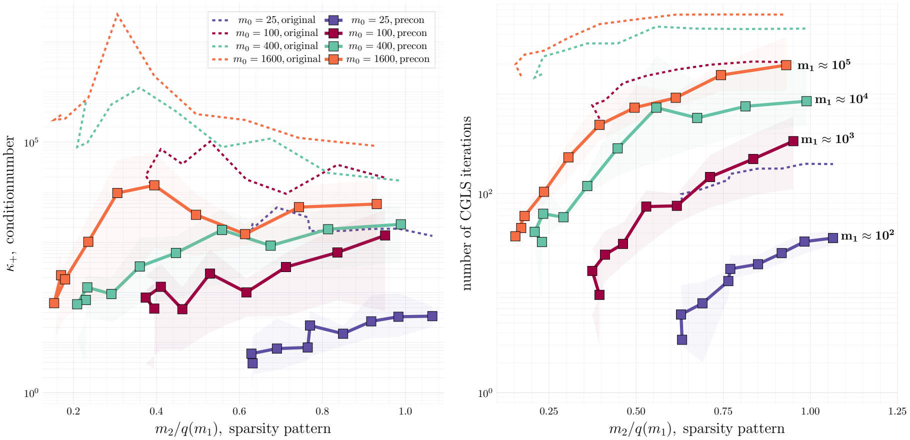
Outline:

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

```
Require: the original complex K, weight matrix W_2
L ← ∅, T ← ∅                                          ▷ initial empty subcomplex
while there is unprocessed triangle in V_2(K) do
    t ← nextHeaviestTriangle(K, W_2)       ▷ e.g. iterate through V_2(K) sorted by weight
    if L ∪ {t} is weakly collapsible then   ▷ run GREEDY_COLLAPSE(L ∪ {t}) (Algorithm 4)
        L ← L ∪ {t}, T ← [T t]                        ▷ extend L by t
    end if
end while
return L, T, Σ                      ▷ here Σ is the collapsing sequence of L
```

- 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 $\mathcal{O}(m_1 m_2)$.

Numerical Experiments



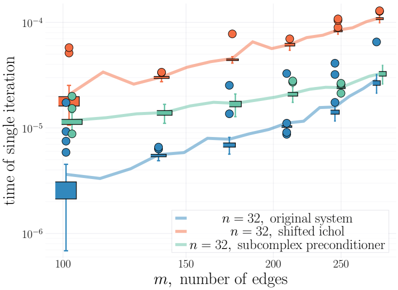
Outline:

Thank you for attention!

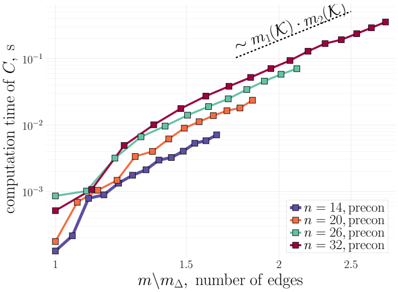
paper on arXiV

code on Github

Personal Page: further materials on https://antsav.me/
Comp@GSSI: our group at https://num-gssi.github.io/



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

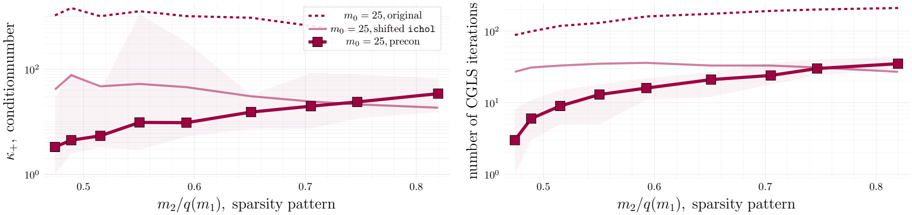


(b) Computation time for the heavy subcomplex preconditioner in case of enriched triangulations on m_0 vertices

Outline:

HeCS
Shifted `ichol` comparison

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



U can be formed directly using the vectors $B_1^{\top}\mathbf{x}$, $\mathbf{x} \in (\mathbf{1})^{\perp}$, when $\mathcal{K}$ has trivial 0- and 1-homology.

Outline: