



DOCTORAL THESIS

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

PHD PROGRAM IN MATHEMATICS: XXXV CYCLE

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Abstract

 Insert here the abstract of the thesis proposal.

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Chapter 1

Introduction

Chapter 2

Simplicial complex as Higher-order Topology Description

2.1 From graph to higher-order models

 graph definition

 graph examples in real life (2 or 3)

 motivation for the transition to the higher order models

 Hypergraphs: definitions and examples

 Motifs: definitions and examples

 somehow relate to the tensor models and tractability simplicial complexes

2.2 Simplicial Complexes

Let $V = \{v_1, v_2, \dots, v_n\}$ be a set of nodes; as discussed above, such set may refer to various interacting entities and agents in the system, e.g. neurons, genes, traffic stops, online actors, publication authors, etc. Then:

Definition 2.1 (Simplicial Complex). The collection of subsets \mathcal{K} of the nodal set V is a (abstract) SC¹ if for each subset $\sigma \in \mathcal{K}$, referred as a simplex, all its subsets σ' , $\sigma' \subseteq \sigma$, referred as faces, enter \mathcal{K} as well, $\sigma' \in \mathcal{K}$.

¹addition of the word “abstract” to the term is more common in the topological setting

A simplex $\sigma \in \mathcal{K}$ on $k + 1$ vertices is said to be of the order k , $\text{ord}(\sigma) = k$. Let $\mathcal{V}_k(\mathcal{K})$ be a set of all k -order simplices in \mathcal{K} and m_k is the cardinality of $\mathcal{V}_k(\mathcal{K})$, $m_k = |\mathcal{V}_k(\mathcal{K})|$; then $\mathcal{V}_0(\mathcal{K})$ is the set of nodes in the simplicial complex \mathcal{K} , $\mathcal{V}_1(\mathcal{K})$ — the set of edges, $\mathcal{V}_2(\mathcal{K})$ — the set of triangles, or 3-cliques, and so on, with $\mathcal{K} = \{\mathcal{V}_0(\mathcal{K}), \mathcal{V}_1(\mathcal{K}), \mathcal{V}_2(\mathcal{K}), \dots\}$. Note that due to the inclusion rule in [Theorem 2.1](#), the number of non-empty $\mathcal{V}_k(\mathcal{K})$ is finite and, moreover, uninterrupted in a sense of the order: if $\mathcal{V}_k(\mathcal{K}) = \emptyset$, then $\mathcal{V}_{k+1}(\mathcal{K})$ is also necessarily empty.

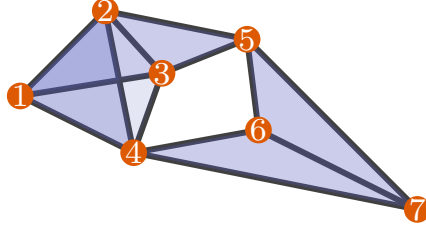


FIGURE 2.1: Example of a simplicial complex

Example 2.1 (Simplicial Complex). *Here we provide the following example of the simplicial complex \mathcal{K} , [Figure 2.1](#): we denote 0-order simplices (vertices) by orange color, 1-order simplices (edges) by black and 2-order simplices (triangles) by blue, where:*

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

$$\mathcal{V}_1(\mathcal{K}) = \{[1, 2], [1, 3], [1, 4], [2, 3], [2, 4], [2, 5], [3, 4], [3, 5], [4, 6], [4, 7], [5, 6], [6, 7]\} \quad (2.1)$$

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

Note that $\mathcal{V}_3(\mathcal{K}) = \emptyset$, so the highest order of simplices in \mathcal{K} is 2. Additionally, edge $[2, 3]$, $[2, 4]$ and $[3, 4]$ are included in \mathcal{K} , but the triangle $[2, 3, 4]$ is not; this does not violate the inclusion rule. Instead, every edge and every vertices of every triangle in $\mathcal{V}_2(\mathcal{K})$ as well as every vertex of every edge in $\mathcal{V}_1(\mathcal{K})$ are contained in \mathcal{K} fullfilling the inclusion principle.

Example 2.2 (Real Life Simplicial Complex). [!\[\]\(cf531ed27e91483460120fcc057b3901_img.jpg\) find a natural example of the simplicial complex with an illustration](#)

Comparing to the general case of the hypergraph described above, it is easy to see that simplicial complex is a special case of a hypergraph where every edge is enclosed with respect to the inclusion. In other words, simplicial complex contains additional structural rigidity which allows to formally describe the topology of \mathcal{K} ; as a result, one is specifically interested in the formal description of the nested inclusion principle achieved through *boundary operators* defined in the subsections below.

2.3 Hodge's Theory

Two linear operators A and B are said to satisfy Hodge's theory if and only if their composition is a null operator,

$$AB = 0 \quad (2.2)$$

which is equivalent to $\text{im } B \subseteq \ker A$.

Definition 2.2. For a pair of operators A and B satisfying Hodge's theory, the *quotient space* \mathcal{H} is defined as follows:

$$\mathcal{H} = \ker A /_{\text{im } B} \quad (2.3)$$

where each element of \mathcal{H} is a manifold $\mathbf{x} + \text{im } B = \{\mathbf{x} + \mathbf{y} \mid \forall \mathbf{y} \in \text{im } B\}$ for $\mathbf{x} \in \ker A$. It follows directly from the definition that \mathcal{H} is an abelian group under addition.

By Theorem 2.2, the quotient space \mathcal{H} is a collection of equivalence classes $\mathbf{x} + \text{im } B$. Then, each class $\mathbf{x} + \text{im } B = \mathbf{x}_H + \text{im } B$ for some $\mathbf{x}_H \perp \text{im } B$ (both $\mathbf{x}, \mathbf{x}_H \in \ker A$); indeed, since the orthogonal component \mathbf{x}_H (referred as *harmonic representative*) of \mathbf{x} with respect to $\text{im } B$ is unique, the map $\mathbf{x}_H \leftrightarrow \mathbf{x} + \text{im } B$ is bijectional.

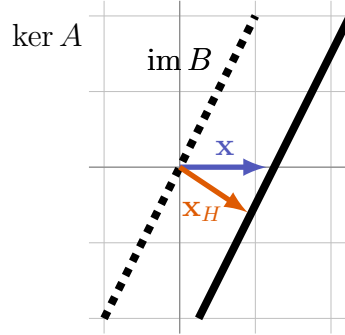


FIGURE 2.2: Illustration of a harmonic representative for an equivalence class

Theorem 2.3 ([1, Thm 5.3]). Let A and B be linear operators, $AB = 0$. Then the homology group \mathcal{H} satisfies:

$$\mathcal{H} = \ker A /_{\text{im } B} \cong \ker A \cap \ker B^\top, \quad (2.4)$$

where \cong denotes the isomorphism.

Proof. One builds the isomorphism through the harmonic representative, as discussed above. It sufficient to note that $\mathbf{x}_H \perp \text{im } B \Leftrightarrow \mathbf{x}_H \in \ker B^\top$ in order to complete the proof. \square

Lemma 2.4 ([1, Thm 5.2]). *Let A and B be linear operators, $AB = 0$. Then:*

$$\ker A \cap \ker B^\top = \ker (A^\top A + BB^\top) \quad (2.5)$$

Proof. Note that if $\mathbf{x} \in \ker A \cap \ker B^\top$, then $\mathbf{x} \in \ker A$ and $\mathbf{x} \in \ker B^\top$, so $\mathbf{x} \in \ker (A^\top A + BB^\top)$. As a result, $\ker A \cap \ker B^\top \subset \ker (A^\top A + BB^\top)$.

On the other hand, let $\mathbf{x} \in \ker (A^\top A + BB^\top)$, then

$$A^\top A\mathbf{x} + BB^\top\mathbf{x} = 0 \quad (2.6)$$

Exploiting $AB = 0$ and multiplying the equation above by B^\top and A one gets the following:

$$\begin{aligned} B^\top BB^\top\mathbf{x} &= 0 \\ AA^\top A\mathbf{x} &= 0 \end{aligned} \quad (2.7)$$

Note that $AA^\top A\mathbf{x} = 0 \Leftrightarrow A^\top A\mathbf{x} \in \ker A$, but $A^\top A\mathbf{x} \in \text{im } A^\top$, so by Fredholm alternative, $A^\top A\mathbf{x} = 0$. Finally, for $A^\top A\mathbf{x} = 0$:

$$A^\top A\mathbf{x} = 0 \implies \mathbf{x}^\top A^\top A\mathbf{x} = 0 \iff \|A\mathbf{x}\|^2 = 0 \implies \mathbf{x} \in \ker A \quad (2.8)$$

Similarly, for the second equation, $\mathbf{x} \in \ker B^\top$ which completes the proof. \square

 Here we need some words about the transitions.

Since $AB = 0$, $B^\top A^\top = 0$ or $\text{im } A^\top \subset \ker B^\top$. Then, exploiting $\mathbb{R}^n = \ker A \oplus \text{im } A^\top$:

$$\begin{aligned} \ker B^\top &= \ker B^\top \cap \mathbb{R}^n = \ker B^\top \cap (\ker A \oplus \text{im } A^\top) = \\ &= (\ker A \cap \ker B^\top) \oplus (\text{im } A^\top \cap \ker B^\top) \end{aligned} \quad (2.9)$$

Given [Theorem 2.4](#), $\ker A \cap \ker B^\top = \ker (A^\top A + BB^\top)$ and, since $\text{im } A^\top \subset \ker B^\top$, $\text{im } A^\top \cap \ker B^\top = \text{im } A^\top$, yielding the decomposition of the whole space:

Theorem 2.5 (Hodge Decomposition). *Let A and B be linear operators, $AB = 0$. Then:*

$$\mathbb{R}^n = \underbrace{\text{im } A^\top \oplus \ker (A^\top A + BB^\top)}_{\ker A} \oplus \text{im } B \quad (2.10)$$

2.4 Boundary and Laplacian Operators

2.4.1 Boundary operators B_k

Each simplicial complex \mathcal{K} has a nested structure of simplices: indeed, if σ is a simplex of order k , $\sigma \in \mathcal{V}_k(\mathcal{K})$, then all of $(k-1)$ -th order faces forming the boundary of σ also belong to \mathcal{K} : for instance, for the triangle $\{1, 2, 3\}$ all the border edges $\{1, 2\}$, $\{1, 3\}$ and $\{2, 3\}$ are also in the simplicial complex, Figure 2.1.

This nested property implies that one can build a formal map from a simplex to its boundary enclosed inside the simplicial complex.

Definition 2.6 (Chain spaces). Let \mathcal{K} be a simplicial complex; then the space C_k of formal sums of simplices from $\mathcal{V}_k(\mathcal{K})$ over real numbers is called a k -th chain space.

 switch to \mathcal{C}_k

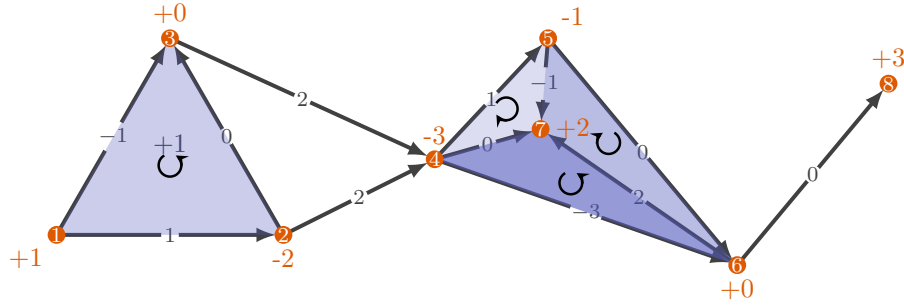



FIGURE 2.3: Example of chains on the simplicial complex

Example 2.3.  add description of the example

Chain spaces on its own are naturally present in the majority of the network models: C_0 is a space of states of vertices (e.g. in the dynamical system $\dot{\mathbf{x}} = A\mathbf{x}$ the evolving vector $\mathbf{x} \in C_0$), C_1 — is a space of (unrestricted) flows on graphs edges, and so on  refs?.


Since C_k is a linear space, versor vectors corresponding to the elements of $\mathcal{V}_k(\mathcal{K})$ is a natural basis of C_k ; in order to proceed with the boundary maps, one needs to fix an order of the simplices inside $\mathcal{V}_k(\mathcal{K})$ (alas one fixes the order of vertices in the graph to form an adjacency matrix) as a matter of bookkeeping. Additionally, since C_k is a space over \mathbb{R} , chains σ and $-\sigma$ naturally introduce the notion of *orientation* of the simplex.

 Simplex orientation and order

 definition of the operators

Definition 2.7.

$$B_k[u_1, u_2, \dots, u_{k+1}] = \sum_{i=1}^{k+1} (-1)^i [u_1, u_2, \dots, u_{i-1}, u_{i+1}, \dots, u_{k+1}] \quad (2.11)$$

 lemma $B_k B_{k+1} = 0$ in general case

Lemma 2.8 (Fundamental Lemma of Homology).

$$B_k B_{k+1} = 0 \quad (2.12)$$

Proof.

$$\begin{aligned} B_k B_{k+1}[u_1, u_2, \dots, u_{k+2}] &= B_k \left(\sum_{i=1}^{k+2} (-1)^i [u_1, u_2, \dots, u_{i-1}, u_{i+1}, \dots, u_{k+2}] \right) = \\ &= \sum_{i=1}^{k+2} (-1)^i B_k [u_1, u_2, \dots, u_{i-1}, u_{i+1}, \dots, u_{k+2}] = \\ &= \sum_{i=1}^{k+2} (-1)^i \left(\sum_{j=1}^{i-1} (-1)^j [u_1, u_2, \dots, u_{j-1}, u_{j+1}, \dots, u_{i-1}, u_{i+1}, \dots, u_{k+2}] + \right. \\ &\quad \left. + \sum_{j=i+1}^{k+2} (-1)^{j-1} [u_1, u_2, \dots, u_{i-1}, u_{i+1}, \dots, u_{j-1}, u_{j+1}, \dots, u_{k+2}] \right) = \\ &= \sum_{i=1}^{k+2} \sum_{j=1}^{i-1} (-1)^{i+j} [u_1, u_2, \dots, u_{j-1}, u_{j+1}, \dots, u_{i-1}, u_{i+1}, \dots, u_{k+2}] + \\ &\quad - \sum_{i=1}^{k+2} \sum_{j=i+1}^{k+2} (-1)^{i+j} [u_1, u_2, \dots, u_{i-1}, u_{i+1}, \dots, u_{j-1}, u_{j+1}, \dots, u_{k+2}] = \\ &= \sum_{\substack{i,j=1 \\ j < i}}^{k+2} (-1)^{i+j} [u_1, u_2, \dots, u_{j-1}, u_{j+1}, \dots, u_{i-1}, u_{i+1}, \dots, u_{k+2}] + \\ &\quad - \sum_{\substack{i,j=1 \\ j > i}}^{k+2} (-1)^{i+j} [u_1, u_2, \dots, u_{i-1}, u_{i+1}, \dots, u_{j-1}, u_{j+1}, \dots, u_{k+2}] = 0 \end{aligned} \quad (2.13)$$

□

 Examples

2.4.2 Homology group and Hodge Laplacians L_k

2.4.2.1 Homology group as Quotient space

2.4.2.2 Elements of the Hodge decomposition as harmonic/vorticity/potential flow

 Maybe we will need here a quick discussion with connection to the continuous case

2.4.2.3 Laplacian operators L_k

2.4.2.4 Classical Laplacian and its kernel elements

2.4.2.5 Kernel elements of L_k

 Some relation to the continuous case

Spreading and balancing as a mechanism of the non-local circulation

2.5 Weighted and Normalised Boundary Operators

 definition and motivation of the weighting scheme

Note that, from the definition $\bar{B}_k = W_{k-1}^{-1} B_k W_k$ and (??), we immediately have that $\bar{B}_k \bar{B}_{k+1} = 0$. Thus, the group $\bar{\mathcal{H}}_k = \ker \bar{B}_k / \text{im } \bar{B}_{k+1}$ is well defined for any choice of positive weights w_k and is isomorphic to $\ker \bar{L}_k$. While the homology group may depend on the weights, we observe below that its dimension does not. Precisely, we have

Proposition 2.9. *The dimension of the homology groups of \mathcal{K} is not affected by the weights of its k -simplices. Precisely, if W_k are positive diagonal matrices, we have*

$$\dim \ker \bar{B}_k = \dim \ker B_k, \quad \dim \ker \bar{B}_k^\top = \dim \ker B_k^\top, \quad \dim \bar{\mathcal{H}}_k = \dim \mathcal{H}_k. \quad (2.14)$$

Moreover, $\ker B_k = W_k \ker \bar{B}_k$ and $\ker B_k^\top = W_{k-1}^{-1} \ker \bar{B}_k^\top$.

Proof. Since W_k is an invertible diagonal matrix,

$$\bar{B}_k \mathbf{x} = 0 \iff W_{k-1}^{-1} B_k W_k \vec{x} = 0 \iff B_k W_k \vec{x} = 0.$$

Hence, if $\vec{x} \in \ker \bar{B}_k$, then $W_k \vec{x} \in \ker B_k$, and, since W_k is bijective, $\dim \ker \bar{B}_k = \dim \ker B_k$. Similarly, one observes that $\dim \ker \bar{B}_k^\top = \dim \ker B_k^\top$.

Moreover, since $\bar{B}_k \bar{B}_{k+1} = 0$, then $\text{im } \bar{B}_{k+1} \subseteq \ker \bar{B}_k$ and $\text{im } \bar{B}_k^\top \subseteq \ker \bar{B}_{k+1}^\top$. This yields $\ker \bar{B}_k \cup \ker \bar{B}_{k+1}^\top = \mathbb{R}^{\mathcal{V}_k} = \ker B_k \cup \ker B_{k+1}^\top$. Thus, for the homology group it holds:

$$\begin{aligned} \dim \bar{\mathcal{H}}_k &= \dim \left(\ker \bar{B}_k \cap \ker \bar{B}_{k+1}^\top \right) = \\ &= \dim \ker \bar{B}_k + \dim \ker \bar{B}_{k+1}^\top - \dim \left(\ker \bar{B}_k \cup \ker \bar{B}_{k+1}^\top \right) = \\ &= \dim \ker B_k + \dim \ker B_{k+1}^\top - \dim \left(\ker B_k \cup \ker B_{k+1}^\top \right) = \dim \mathcal{H}_k \end{aligned}$$

□

 normalisation theorem

Chapter 3

Topological Stability as MNP

3.1 General idea of the topological stability

3.1.1 Alternative with a persistent homology



3.1.2 Transition to the spectral properties

3.2 101 on Spectral Matrix Nearness Problems

definition

Generally speaking, for a given matrix A a *matrix nearness problem* consists of finding the closest possible matrix X among the admissible set with a number of desired properties. For instance, one may search for the closest (in some metric) symmetric positive/negative definite matrix, unitary matrix or the closest graph Laplacian.

Motivated by the topological meaning of the *kernel* of Hodge Laplacians L_k , we assume the specific case of *spectral* MNPs: here one aims for the target matrix X to have a specific spectrum $\sigma(X)$. For instance in the stability study of the dynamical system $\dot{\mathbf{x}} = A\mathbf{x}$ one can search for the closest Hurwitz matrix such that $\text{Re}[\lambda_i] < 0$ for all $\lambda_i \in \sigma(X)$; similarly, assuming given matrix A is a graph Laplacian, one can search for the closest disconnected graph (so the algebraic connectivity $\lambda_2 = 0$).

Here we recite the optimization framework developed by REFREFREF  [fix it](#) for the class of the spectral matrix nearness problems; one should note, however, that this is by far not the only approach to the task, REFREFREF  [also fix it with Nicholas and others, I guess?](#).

3.2.1 Functional and Gradient Flow

Let us assume that $X = A + \Delta$ and instead of searching for X , we search for the perturbation matrix Δ ; additionally, we assume that Ω is the admissible set containing all possible perturbations Δ .

3.2.2 Transition to the gradient flow

 Derivative

3.2.3 Constraint gradient flow

3.2.4 Sparsity pattern and rank-1 optimizers

3.2.5 Idea of two level optimization

3.3 Direct approach: failure and discontinuity problems

3.3.1 Principal spectral inheritance

Before moving on to the next section, we recall here a relatively direct but important spectral property that connects the spectra of the k -th and $(k+1)$ -th order Laplacians.

Theorem 3.1 (HOL's spectral inheritance). *Let L_k and L_{k+1} be higher-order Laplacians for the same simplicial complex \mathcal{K} . Let $\bar{L}_k = \bar{L}_k^{\text{down}} + \bar{L}_k^{\text{up}}$, where $\bar{L}_k^{\text{down}} = \bar{B}_k^\top \bar{B}_k$ and $\bar{L}_k^{\text{up}} = \bar{B}_{k+1} \bar{B}_{k+1}^\top$. Then:*

1. $\sigma_+(\bar{L}_k^{\text{up}}) = \sigma_+(\bar{L}_{k+1}^{\text{down}})$, where $\sigma_+(\cdot)$ denotes the positive part of the spectrum;
2. if $0 \neq \mu \in \sigma_+(\bar{L}_k^{\text{up}}) = \sigma_+(\bar{L}_{k+1}^{\text{down}})$, then the eigenvectors are related as follows:
 - (a) if \mathbf{x} is an eigenvector for \bar{L}_k^{up} with the eigenvalue μ , then $\mathbf{y} = \frac{1}{\sqrt{\mu}} \bar{B}_{k+1}^\top \mathbf{x}$ is an eigenvector for $\bar{L}_{k+1}^{\text{down}}$ with the same eigenvalue;
 - (b) if \mathbf{u} is an eigenvector for $\bar{L}_{k+1}^{\text{down}}$ with the eigenvalue μ and $\mathbf{u} \notin \ker \bar{B}_{k+1}$, then $\mathbf{v} = \frac{1}{\sqrt{\mu}} \bar{B}_{k+1} \mathbf{u}$ is an eigenvector for \bar{L}_k^{up} with the same eigenvalue;
3. for each Laplacian \bar{L}_k : if $\mathbf{v} \notin \ker \bar{L}_k^{\text{down}}$ is the eigenvector for \bar{L}_k^{down} , then $\mathbf{v} \in \ker \bar{L}_k^{\text{up}}$; vice versa, if $\mathbf{u} \notin \ker \bar{L}_k^{\text{up}}$ is the eigenvector for \bar{L}_k^{up} , then $\mathbf{v} \in \ker \bar{L}_k^{\text{down}}$;

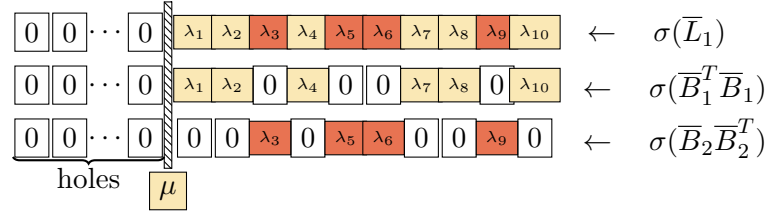


FIGURE 3.1: Illustration for the principal spectrum inheritance (Theorem 3.1) in case $k = 0$: spectra of \bar{L}_1 , \bar{L}_1^\top and \bar{L}_1^\top are shown. Colors signify the splitting of the spectrum, $\lambda_i > 0 \in \sigma_+(\bar{L}_1)$; all yellow eigenvalues are inherited from $\sigma_+(\bar{L}_0)$; red eigenvalues belong to the non-inherited part. Dashed barrier μ signifies the penalization threshold (see the target functional in ??) preventing homological pollution (see ??).

4. consequently, there exist $\mu \in \sigma_+(\bar{L}_k)$ with an eigenvector $\mathbf{u} \in \ker \bar{L}_k^{up}$, and $\nu \in \sigma_+(\bar{L}_{k+1})$ with an eigenvector $\mathbf{u} \in \ker \bar{L}_{k+1}^{down}$, such that:

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

Proof. For (2a) it is sufficient to note that $\bar{L}_{k+1}^{down} \mathbf{y} = \bar{B}_{k+1}^\top \bar{B}_{k+1} \frac{1}{\sqrt{\mu}} \bar{B}_{k+1}^\top \mathbf{x} = \frac{1}{\sqrt{\mu}} \bar{B}_{k+1}^\top \bar{L}_k^{up} \mathbf{x} = \sqrt{\mu} \bar{B}_{k+1}^\top \mathbf{x} = \mu \mathbf{y}$. Similarly, for (2b): $\bar{L}_k^{up} \mathbf{v} = \bar{B}_{k+1} \bar{B}_{k+1}^\top \frac{1}{\sqrt{\mu}} \bar{B}_{k+1} \mathbf{u} = \frac{1}{\sqrt{\mu}} \bar{B}_{k+1} \bar{L}_{k+1}^{down} \mathbf{u} = \mu \mathbf{v}$; joint 2(a) and 2(b) yield (1). Hodge decomposition immediately yields the strict separation of eigenvectors between \bar{L}_k^{up} and \bar{L}_k^{down} , (3); given (3), all the inherited eigenvectors from (2a) fall into the $\ker \bar{L}_{k+1}^{down}$, thus resulting into (4). \square

In other words, the variation of the spectrum of the k -th Laplacian when moving from one order to the next one works as follows: the down-term \bar{L}_{k+1}^{down} inherits the positive part of the spectrum from the up-term of \bar{L}_k^{up} ; the eigenvectors corresponding to the inherited positive part of the spectrum lie in the kernel of \bar{L}_{k+1}^{up} ; at the same time, the “new” up-term \bar{L}_{k+1}^{up} has a new, non-inherited, part of the positive spectrum (which, in turn, lies in the kernel of the $(k+2)$ -th down-term).

In particular, we notice that for $k = 0$, since $B_0 = 0$ and $\bar{L}_0 = \bar{L}_0^{up}$, the theorem yields $\sigma_+(\bar{L}_0) = \sigma_+(\bar{L}_1^{down}) \subseteq \sigma_+(\bar{L}_1)$. In other terms, the positive spectrum of the \bar{L}_0 is inherited by the spectrum of \bar{L}_1 and the remaining (non-inherited) part of $\sigma_+(\bar{L}_1)$ coincides with $\sigma_+(\bar{L}_1^{up})$. Figure 3.1 provides an illustration of the statement of Theorem 3.1 for $k = 0$.

3.3.2 Example with inherited disconnectedness

3.3.3 Example with faux edges (different weighting scheme)

3.4 Functional, derivative and alternating scheme

3.4.1 Target Functional

3.4.2 Free gradient calculation

3.4.3 Constrained gradient

3.4.4 Alternating scheme

3.4.5 Implementation

3.4.5.1 Algorithms

3.4.5.2 Computation of the first non-zero eigenvalue

3.4.5.3 Preconditioning in the eigen-phase

3.5 Benchmarking

3.5.1 Toy example

3.5.2 Triangulation

 Preconditioning of the LS as a way forward


3.5.3 Cities

Cities	network			β_1	logarithmic weights		
	m_0	m_1	m_2		time	ε	p
Bologna	60	175	171	2	2.43s [11, 47] (4^{th} smallest)	0.65	0.003
Anaheim	38	159	221	1	5.39s [10, 29] (11^{th} smallest)	0.57	0.003
Berlin-Tiergarten	26	63	55	0	2.46s [6, 16] (20^{th} smallest)	1.18	0.015
Berlin-Mitte	98	456	900	1	127s [57, 87] (6^{th}), [58, 87], (17^{th})	0.887	0.0016

TABLE 3.1: Topological instability of the transportation networks: filtered zone networks with the corresponding perturbation norm ε and its percentile among $w_1(\cdot)$ profile. For each simplicial complex the number of nodes, edges and triangles in $\mathcal{V}_2(\mathcal{K})$ are provided alongside the initial number of holes β_1 . The results of the algorithm consist of the perturbation norm, ε , computation time, and approximate percentile p .

Chapter 4

Preconditioning

 Here we need to say general words about how we need an efficient preconditioning scheme.

4.1 Preconditioning 101

4.1.1 why do we care about the condition number?

4.1.2 Iterative methods

4.1.3 CG and convergence

 CGLS

4.1.4 Zoo of preconditioners

 Reinforced diagonal

 Cholesky  Incomplete Cholesky

4.2 LSq problem for the whole Laplacian -¿ up-Laplacian

4.3 Preconditioning on the up-Laplacian

4.3.1 Sparsification (Spielman/Osting)

4.3.2 Cholesky preconditioning for classical graphs

4.3.2.1 Stochastic Cholesky preconditioning

4.3.2.2 Schur complements

4.3.3 Problem with Schur complements in the case of L_1

 [Transition to collapsibility](#)

4.4 Collapsible simplicial complexes

4.4.1 Classical collapsibility

In this section we borrow the terminology from [2]; additionally, let us assume that considered simplicial complex \mathcal{K} is restricted to its 2-skeleton, so \mathcal{K} consists only of nodes, edges, and triangles, $\mathcal{K} = \mathcal{V}_0(\mathcal{K}) \cup \mathcal{V}_1(\mathcal{K}) \cup \mathcal{V}_2(\mathcal{K})$.

Simplex $\tau \in \mathcal{K}$ is called an (inclusion-wise) maximal face of simplex $\sigma \in \mathcal{K}$ if τ is maximal by inclusion simplex such that $\sigma \subseteq \tau$ and $\text{ord}(\sigma) < \text{ord}(\tau)$. For instance, in [Figure 4.1](#)

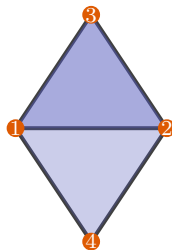


FIGURE 4.1: Example of a simplicial complex: free simplices and maximal faces.

the edge $\{1, 2\}$ and nodes $\{1\}$ and $\{2\}$ have two maximal faces, $\{1, 2, 3\}$ and $\{1, 2, 4\}$, while all the other edges and nodes have unique maximal faces — their corresponding triangles. Note that in the case of the node $\{1\}$, there are bigger simplices containing it besides the triangles (e.g. the edge $\{1, 2\}$), but they are not maximal by inclusion.

Definition 4.1 (Free simplex). The simplex $\sigma \in \mathcal{K}$ is free if it has exactly one maximal face τ , $\tau = \tau(\sigma)$. F.i. edges $\{1, 3\}$, $\{1, 4\}$, $\{2, 3\}$ and $\{2, 4\}$ are all free in Figure 4.1.

The collapse $\mathcal{K} \setminus \{\sigma\}$ of \mathcal{K} at a free simplex σ is the transition from the original simplicial complex \mathcal{K} to a smaller simplicial complex \mathcal{L} without the free simplex σ and the corresponding maximal face τ , $\mathcal{K} \rightarrow \mathcal{K}' = \mathcal{K} - \sigma - \tau$; namely, one can eliminate a simplex τ if it has an accessible (not included in another simplex) face σ .

Naturally, one can perform several consequent collapses at $\Sigma = \{\sigma_1, \sigma_2, \dots\}$ assuming σ_i is free in collapse simplicial complex from the previous stage; Σ is called the collapsing sequence. Formally:

Definition 4.2 (Collapsing sequence). Let \mathcal{K} be a simplicial complex. $\Sigma = \{\sigma_1, \sigma_2, \dots\}$ is a collapsing sequence if σ_1 is free in \mathcal{K} and each σ_i , $i > 1$, is free at $\mathcal{K}^{(i)} = \mathcal{K}^{(i-1)} \setminus \{\sigma_i\}$, $\mathcal{K}^{(1)} = \mathcal{K}$. The collapse of \mathcal{K} to a new complex \mathcal{L} at Σ is denoted by $\mathcal{L} = \mathcal{K} \setminus \Sigma$.

By the definition, every collapsing sequence Σ has a corresponding sequence $\mathbb{T} = \{\tau(\sigma_1), \tau(\sigma_2), \dots\}$ of maximal faces being collapsed at every step.

Definition 4.3 (Collapsible simplicial complex, [2]). The simplicial complex \mathcal{K} is collapsible if there exists a collapsing sequence Σ such that \mathcal{K} collapses to a single vertex at Σ , $\mathcal{K} \setminus \Sigma = \{v\}$.

Determining whether the complex is collapsible is in general *NP-complete*, [3], but can be almost linear for a set of specific families of \mathcal{K} , e.g. if the simplex can be embedded into the triangulation of the d -dimensional unit sphere, [4]. Naturally restricting the collapses to the case of d -collapses (such that $\text{ord}(\sigma)_i \leq d - 1$), one arrive at the notion of d -collapsibility, [5].

Definition 4.4 (d -Core). A d -Core is a subcomplex of \mathcal{K} such that every simplex of order $d - 1$ belongs to at least 2 simplices of order d . E.g. 2-Core is such a subcomplex of the original 2-skeleton \mathcal{K} that every edge from $\mathcal{V}_1(\mathcal{K})$ belong to at least 2 triangles from $\mathcal{V}_2(\mathcal{K})$.

Lemma 4.5 ([6]). \mathcal{K} is d -collapsible if and only if it does not contain a d -core.

Proof. The proof of the lemma above naturally follows from the definition of the core. Assume Σ is a d -collapsing sequence, and $\mathcal{K} \setminus \Sigma$ consists of more than a single vertex and has no free simplices of order $\leq d - 1$ (“collapsing sequence gets stuck”). Then, each simplex of order $d - 1$ is no free but belongs to at least 2 simplices of order d , so $\mathcal{K} \setminus \Sigma$ is a d -Core.

Conversely if a d -Core exists in the complex, the collapsing sequence should necessarily include its simplices of order $d - 1$ which can not become free during as a result of a sequence of collapses. Indeed, for σ from d -Core, $\text{ord}(\sigma) = d - 1$, to become free, one needs to collapse at least one of σ 's maximal faces for d -Core, all of whose faces are, in turn, contained in the d -Core (since d -Core is a simplicial complex). As a result one necessarily needs a prior collapse inside the d -Core to perform the first collapse in the d -Core, which is impossible. \square

In the case of the classical graph model, the 1-Core is a subgraph where each vertex has a degree at least 2; in other words, 1-Core cannot be a tree and necessarily contains a simple cycle. Hence, the collapsibility of a classical graph coincides with the acyclicity. The d -Core is the generalization of the cycle for the case of 1-collapsibility of the classical graph; additionally, the d -Core is very dense due to its definition. In the case of 2-Core, we provide simple exemplary structures on Figure 4.2 which imply various possible configurations for a d -Core, $d \geq 2$, hence a search for d -Core inside \mathcal{K} is neither trivial, no computationally cheap.

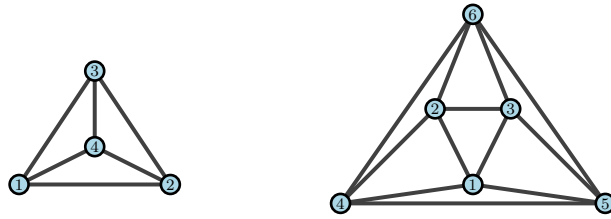


FIGURE 4.2: 2-Core, examples.

Additionally, we demonstrate that an arbitrary simplicial complex \mathcal{K} tends to contain 2-Cores as long as \mathcal{K} is denser than a trivially collapsible case. Assume the complex formed by triangulation of m_0 random points on the unit square with a sparsity pattern ν ; the triangulation itself with the corresponding ν_Δ is collapsible, but a reasonably small addition of edges already creates a 2-Core (since it is local), Figure 4.3, left. Similarly, sampled sensor networks, where $\exists \sigma \in \mathcal{V}_1(\mathcal{K}) : \sigma = [v_1, v_2] \iff \|v_1 - v_2\|_2 < \varepsilon$ for a chosen percolation parameter $\varepsilon > 0$, quickly form a 2-Core upon the densifying of the network.

However, in the following, we observe that a weaker condition is enough to efficiently design a preconditioner for any “sparse enough” simplicial complex.

4.4.2 Weak collapsibility

Let the complex \mathcal{K} be restricted up to its 2-skeleton, $\mathcal{K} = \mathcal{V}_0(\mathcal{K}) \cup \mathcal{V}_1(\mathcal{K}) \cup \mathcal{V}_2(\mathcal{K})$, and \mathcal{K} is collapsible. Then the collapsing sequence Σ necessarily involves collapses at

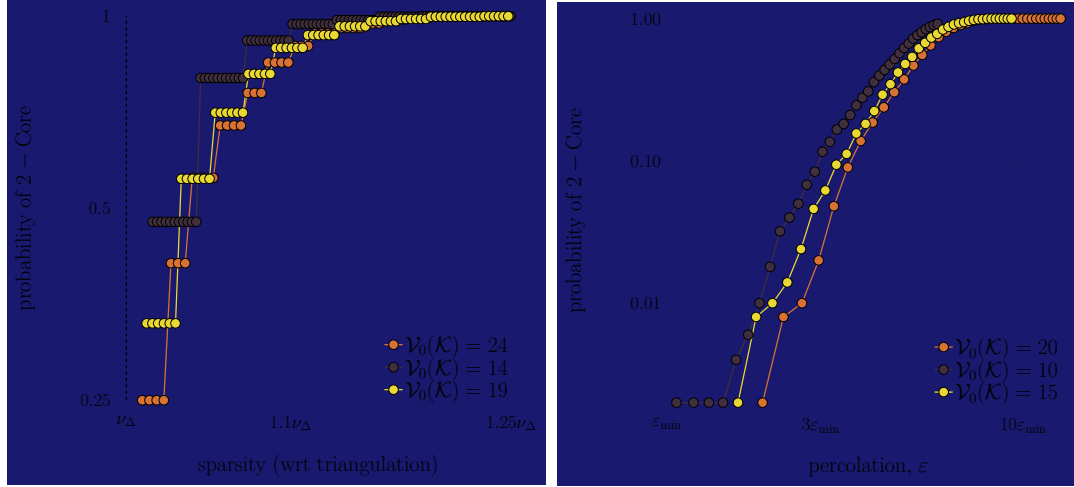


FIGURE 4.3: The probability of the 2-Core in richer-than-triangulation simplicial complexes: triangulation of random points modified to have $\left\lceil \nu \frac{|\mathcal{V}_0(\mathcal{K})| \cdot (|\mathcal{V}_0(\mathcal{K})| - 1)}{2} \right\rceil$ edges on the left; random sensor networks with ε -percolation on the right. ν_Δ defines the initial sparsity of the triangulated network; $\varepsilon_{\min} = \mathbb{E} \min_{x,y \in [0,1]^2} \|x - y\|_2$ is the minimal possible percolation parameter.

simplices σ_i of different orders: at edges (eliminating *edges* and *triangles*) and at vertices (eliminating *vertices* and *edges*). One can show that for a given collapsing sequence Σ there is a reordering $\tilde{\Sigma}$ such that $\dim \tilde{\sigma}_i$ are non-increasing, [4, Lemma 2.5]. Namely, if such a complex is collapsible, then there is a collapsible sequence $\Sigma = \{\Sigma_1, \Sigma_0\}$ where Σ_1 contains all the collapses at edges first and Σ_0 is composed of collapses at vertices. Note that the partial collapse $\mathcal{K} \setminus \Sigma_1 = \mathcal{L}$ eliminates all the triangles in the complex, $\mathcal{V}_2(\mathcal{L}) = \emptyset$; otherwise, the whole sequence Σ is not collapsing \mathcal{K} to a single vertex. Since $\mathcal{V}_2(\mathcal{L}) = \emptyset$, the associated up-Laplacian $L_1^\uparrow(\mathcal{L}) = 0$.

Definition 4.6 (Weakly collapsible complex). 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 $\mathcal{L} = \mathcal{K} \setminus \Sigma_1$ has no simplices of order 2, $\mathcal{V}_2(\mathcal{L}) = \emptyset$ and $L_1^\uparrow(\mathcal{L}) = 0$.

Example 4.1. Note that a collapsible complex is necessarily weakly collapsible; the opposite does not hold. Consider the following example in Figure 4.4: the initial complex is weakly collapsible either by a collapse at $[3, 4]$ or at $[2, 4]$. After this, the only available collapse is at the vertex $[4]$ leaving the uncollapsible 3-vertex structure.

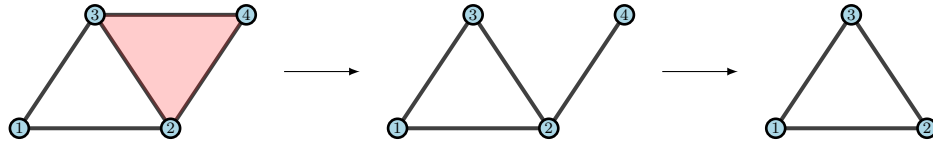


FIGURE 4.4: Example of weakly collapsible but not collapsible simplicial complex

Theorem 4.7. Weak collapsibility of 2-skeleton \mathcal{K} is polynomially solvable.

Proof. The *greedy algorithm* for the collapsing sequence intuitively operates as follows: at each iteration perform any of possible collapses; in the absence of free edges, the complex should be considered not collapsible, [Algorithm 1](#). Clearly, such an algorithm runs polynomially with respect to the number of simplexes in \mathcal{K} .

The failure of the greedy algorithm indicates the existence of a weakly collapsible complex \mathcal{K} such that the greedy algorithm gets stuck at a 2-Core, which is avoidable for another possible order of collapses. Among all the counter exemplary complexes, let \mathcal{K} be a minimal one with respect to the number of triangles m_2 . Then there exist a free edge $\sigma \in \mathcal{V}_1(\mathcal{K})$ such that $\mathcal{K} \setminus \{\sigma\}$ is *collapsible* and another $\sigma' \in \mathcal{V}_2(\mathcal{K})$ such that $\mathcal{K} \setminus \{\sigma'\}$ is *not collapsible*.

Note that if \mathcal{K} is minimal then for any pair of free edges σ_1 and σ_2 belong to the same triangle: $\tau(\sigma_1) = \tau(\sigma_2)$. Indeed, for any $\tau(\sigma_1) \neq \tau(\sigma_2)$, $\mathcal{K} \setminus \{\sigma_1, \sigma_2\} = \mathcal{K} \setminus \{\sigma_2, \sigma_1\}$. Let $\tau(\sigma_1) \neq \tau(\sigma_2)$ for at least one pair of σ_1 and σ_2 ; in our assumption, either both $\mathcal{K} \setminus \{\sigma_1\}$ and $\mathcal{K} \setminus \{\sigma_2\}$, only $\mathcal{K} \setminus \{\sigma_1\}$ or none are collapsible. In the former case either $\mathcal{K} \setminus \{\sigma_1\}$ or $\mathcal{K} \setminus \{\sigma_2\}$ is a smaller example of the complex satisfying the assumption, hence, violating the minimality. If only $\mathcal{K} \setminus \{\sigma_1\}$ is collapsible, then $\mathcal{K} \setminus \{\sigma_2, \sigma_1\}$ is not collapsible; hence, $\mathcal{K} \setminus \{\sigma_1, \sigma_2\}$ is not collapsible, so $\mathcal{K} \setminus \{\sigma_1\}$ is a smaller example of a complex satisfying the assumption. Finally, if both $\mathcal{K} \setminus \{\sigma_1\}$ and $\mathcal{K} \setminus \{\sigma_2\}$ are collapsible, then for known σ' such that $\mathcal{K} \setminus \{\sigma'\}$ is not collapsible, $\tau(\sigma') \neq \tau(\sigma_1)$ or $\tau(\sigma') \neq \tau(\sigma_2)$, which revisits the previous point.

As a result, for σ ($\mathcal{K} \setminus \{\sigma\}$ is collapsible) and for σ' ($\mathcal{K} \setminus \{\sigma'\}$ is not collapsible) it holds that $\tau(\sigma) = \tau(\sigma') \Rightarrow \sigma \cap \sigma' = \{v\}$, so after collapses $\mathcal{K} \setminus \{\sigma\}$ and $\mathcal{K} \setminus \{\sigma'\}$ we arrive at two identical simplicial complexes modulo the hanging vertex irrelevant for the weak collapsibility. A simplicial complex can not be simultaneously collapsible and not collapsible, so the question of weak collapsibility can always be resolved by the greedy algorithm which has polynomial complexity. \square

4.4.3 Computational cost of the greedy algorithm

Let \mathcal{K} be a 2-skeleton; let Δ_σ be a set of triangles of \mathcal{K} containing the edge σ , $\Delta_\sigma = \{t \mid t \in \mathcal{V}_2(\mathcal{K}) \text{ and } \sigma \in t\}$. Then the edge σ is free iff $|\Delta_\sigma| = 1$ and $F = \{\sigma \mid |\Delta_\sigma| = 1\}$ is a set of all free edges. Note that $|\Delta_e| \leq m_0 - 2 = \mathcal{O}(m_0)$.

The complexity of [Algorithm 1](#) rests upon the precomputed $\sigma \mapsto \Delta_\sigma$ structure that de-facto coincides with the boundary operator B_2 (assuming B_2 is stored as a sparse matrix, the adjacency structure describes its non-zero entries). Similarly, the initial F set can be computed alongside the construction of B_2 matrix. Another concession is

Algorithm 1 GREEDY_COLLAPSE(\mathcal{K}): greedy algorithm for the weak collapsibility

Require: initial set of free edges F , adjacency sets $\{\Delta_{\sigma_i}\}_{i=1}^{m_1}$

- 1: $\Sigma = [], \mathbb{T} = []$ ▷ initialize the collapsing sequence
- 2: **while** $F \neq \emptyset$ **and** $\mathcal{V}_2(\mathcal{K}) \neq \emptyset$ **do**
- 3: $\sigma \leftarrow \text{pop}(F), \tau \leftarrow \tau(\sigma)$ ▷ pick a free edge σ
- 4: $\mathcal{K} \leftarrow \mathcal{K} \setminus \{\sigma\}, \Sigma \leftarrow [\Sigma \ \sigma], \mathbb{T} \leftarrow [\mathbb{T} \ \tau]$ ▷ τ is a triangle being collapsed;
 $\tau = [\sigma, \sigma_1, \sigma_2]$
- 5: $\Delta_{\sigma_1} \leftarrow \Delta_{\sigma_1} \setminus \tau, \Delta_{\sigma_2} \leftarrow \Delta_{\sigma_2} \setminus \tau$ ▷ remove τ from adjacency lists
- 6: $F \leftarrow F \cup \{\sigma_i \mid i = 1, 2 \text{ and } |\Delta_{\sigma_i}| = 1\}$ ▷ update F if any of σ_1 or σ_2 has become free
- 7: **end while**
- 8: **return** $\mathcal{K}, \Sigma, \mathbb{T}$

needed for the complexity of the removal of elements from Δ_{σ_i} and F , which may vary from $\mathcal{O}(1)$ on average up to guaranteed $\log(|\Delta_{\sigma_i}|)$. As a result, given a pre-existing B_2 operator, [Algorithm 1](#) runs linearly, $\mathcal{O}(m_1)$, or almost linearly depending on the realisation, $\mathcal{O}(m_1 \log m_1)$.

 [Picture](#)

4.5 HeCS preconditioning

Given ??, a weakly collapsible simplicial complex \mathcal{K} immediately yields an exact Cholesky decomposition for its up-Laplacian:

Lemma 4.8. *Assume \mathcal{K} , 2-skeleton simplicial complex, is weakly collapsible through the collapsing sequence Σ with the corresponding sequence of maximal faces \mathbb{T} . Let B_2W_2 be a weighted boundary operator for \mathcal{K} . Then*

$$C = P_\Sigma B_2 W_2 P_\mathbb{T} \quad \text{is an exact Cholesky multiplier for} \quad P_\Sigma L_1^\uparrow(\mathcal{K}) P_\Sigma^\top,$$

i.e. $P_\Sigma L_1^\uparrow(\mathcal{K}) P_\Sigma^\top = C C^\top$, where P_Σ and $P_\mathbb{T}$ are permutation matrices for each sequence ($[P_\Sigma]_{ij} = 1 \iff j = \sigma_i$).

Proof. Note that the sequences Σ and \mathbb{T} (and the multiplication by the corresponding permutation matrices) impose only the reordering of $\mathcal{V}_1(\mathcal{K})$ and $\mathcal{V}_2(\mathcal{K})$ respectively; after such reordering the i -th edge collapses the i -triangle. Hence, the first $(i - 1)$ entries of the i -th columns of the matrix B_2W_2 ($[B_2W_2]_{\cdot i} = \sqrt{w(t_i)} \mathbf{e}_{t_i}$) are zeros, otherwise one of the previous edges is not free. As a result, C is lower-triangular and by the direct computation $C C^\top = P_\Sigma L_1^\uparrow(\mathcal{K}) P_\Sigma^\top$. □

An arbitrary simplicial complex \mathcal{K} is generally not weakly collapsible (see Figure 4.2). Specifically, weak collapsibility is a property of sparse simplicial complexes with the sparsity being measured by the number of triangles m_2 (in the weakly collapsible case $m_2 < m_1$); hence, the removal of triangles from $\mathcal{V}_2(\mathcal{K})$ can potentially destroy the 2-Core structure inside \mathcal{K} and make the complex weakly collapsible.

As a result, the original ?? may be reduced to the search for a collapsible subcomplex \mathcal{L} inside the original complex \mathcal{K} , in order to use an exact Cholesky multiplier of \mathcal{L} as an approximate Cholesky preconditioner for $L_1^\uparrow(\mathcal{K})$. Specifically:

Problem 1. Let \mathcal{K} be a 2-skeleton simplicial complex, $\mathcal{K} = \mathcal{V}_0(\mathcal{K}) \cup \mathcal{V}_1(\mathcal{K}) \cup \mathcal{V}_2(\mathcal{K})$ with the corresponding triangle weight matrix $W_2(\mathcal{K})$. Find the subcomplex \mathcal{L} such that:

- (1) it has the same set of 0- and 1-simplices, $\mathcal{V}_0(\mathcal{L}) = \mathcal{V}_0(\mathcal{K})$ and $\mathcal{V}_1(\mathcal{L}) = \mathcal{V}_1(\mathcal{K})$;
- (2) triangles in \mathcal{L} are subsampled, $\mathcal{V}_2(\mathcal{L}) \subseteq \mathcal{V}_2(\mathcal{K})$;
- (3) \mathcal{L} has the same 1-homology as \mathcal{K} ;
- (4) \mathcal{L} is weakly collapsible through some collapsing sequence Σ and corresponding sequence of maximal faces \mathbb{T} ;
- (5) the Cholesky multiplier $C = P_\Sigma B_2(\mathcal{L}) W_2(\mathcal{L}) P_\mathbb{T}$ improves the conditionality of $L_1^\uparrow(\mathcal{K})$:

$$\kappa_+(L_1^\uparrow(\mathcal{K})) \gg \kappa_+(C^\dagger P_\Sigma L_1^\uparrow(\mathcal{K}) P_\Sigma^\top C^{\dagger\top})$$

Conditions (1) and (2) imply that a subcomplex \mathcal{L} is obtained from \mathcal{K} through the elimination of triangles.

Remark 4.9 (On the conservation of the 1-homology). Since one transitions between the systems $L_1^\uparrow(\mathcal{K})\mathbf{x} = \mathbf{f}$ and $(C^\dagger P_\Sigma L_1^\uparrow(\mathcal{K}) P_\Sigma^\top C^{\dagger\top}) C^\top P_\Sigma \mathbf{x} = C^\dagger P_\Sigma \mathbf{f}$, it is necessary to have $\ker C^\top = \ker L_1^\uparrow(\mathcal{K}) = \ker W_2 B_2^\top$ so the transition is bijective (assuming $\mathbf{x} \perp \ker L_1^\uparrow(\mathcal{K})$).

Due to ?? and the spectral inheritance principle, [?, Thm. 2.7], $\ker L_k^\uparrow(\mathcal{X}) = \ker L_k(\mathcal{X}) \oplus B_k^\top \cdot \text{im } L_{k-1}^\uparrow$. The second part, $B_k^\top \cdot \text{im } L_{k-1}^\uparrow$, consists of the action of B_k^\top on non-zero related eigenvectors of L_{k-1}^\uparrow and is not dependent on $\mathcal{V}_{k+1}(\mathcal{K})$ (triangles, in case $k = 1$), hence remains conserved in the subcomplex from Problem 1. As a result, the conservation of 1-homology is sufficient to converse the kernels $\ker L_1^\uparrow(\mathcal{K}) = \ker L_1^\uparrow(\mathcal{L})$. Moreover, one can show that the subcomplex \mathcal{L} can only extend the kernel: $\ker L_1(\mathcal{K}) \subseteq \ker L_1(\mathcal{L})$. Indeed, the elimination of the triangle $t \in \mathcal{V}_2(\mathcal{K})$ lifts the restriction $\mathbf{e}_t^\top \mathbf{x} = 0$ for $\mathbf{x} \in \ker L_1(\mathcal{K})$; hence, if $\mathbf{x} \in \ker L_1(\mathcal{K})$, then $\mathbf{x} \in \ker L_1(\mathcal{L})$.

Definition 4.10 (Subsampling matrix). Assume \mathcal{K} be a 2-skeleton simplicial complex; let \mathbb{T} be a subset of triangles, $\mathbb{T} \subset \mathcal{V}_2(\mathcal{K})$ (so forming the subcomplex $\mathcal{L} = \mathcal{V}_0(\mathcal{K}) \cup \mathcal{V}_1(\mathcal{K}) \cup \mathbb{T}$). Then Π is a subsampling matrix if

- Π is diagonal;
- $(\Pi)_{ii} = 1 \iff i \in \mathbb{T}$; otherwise, $(\Pi)_{ii} = 0$.

Lemma 4.11 (Optimal weight choice for the subcomplex). *Let \mathcal{K} be a simplicial complex and \mathcal{L} be its subcomplex, satisfying [Problem 1](#), with fixed corresponding subsampling matrix Π . Then in order to obtain the closest up-Laplacian $L_1^\uparrow(\mathcal{L})$ to the original $L_1^\uparrow(\mathcal{K})$, one should choose the weight matrix $W_2(\mathcal{L})$ as follows:*

$$W_2(\mathcal{L}) = W_2(\mathcal{K})\Pi$$

Proof. Let $W_2^2(\mathcal{K}) = W$; then $L_1^\uparrow(\mathcal{K}) = B_2 W B_2^\top$. Then $\widehat{W}\Pi$ is the diagonal matrix of weights of subsampled triangles (in case $t \notin \mathbb{T}$, the entry $(\widehat{W}\Pi)_{tt} = 0$). Note that $\Pi\widehat{W} = \widehat{W}\Pi = \Pi\widehat{W}\Pi$; then, ignoring the reordering of the edges, $L_1^\uparrow(\mathcal{L}) = B_2 \Pi \widehat{W} \Pi B_2^\top$ barring several zero columns and rows corresponding to some of the eliminated triangles.

Generally speaking, weights \widehat{W} of sampled triangles \mathbb{T} differ from the original weights W . Let $\widehat{W} = W + \Delta W$, where ΔW is still diagonal, but entries are not necessarily positive. Then one can formulate the question of the optimal weight redistribution as the optimization problem:

$$\min_{\Delta W} \left\| L_1^\uparrow(\mathcal{L}) - L_1^\uparrow(\mathcal{K}) \right\| = \min_{\Delta W} \left\| B_2 [\Pi(W + \Delta W)\Pi - W] B_2^\top \right\|$$

Let $\Delta W = \Delta W(t)$ where t is a virtual time parametrization; then one can compute the gradient $\nabla_{\Delta W} \sigma_1 \left(L_1^\uparrow(\mathcal{L}) - L_1^\uparrow(\mathcal{K}) \right)$ through the time derivative $\frac{d}{dt} \sigma_1 \left(L_1^\uparrow(\mathcal{L}) - L_1^\uparrow(\mathcal{K}) \right)$:

$$\begin{aligned} \dot{\sigma}_1 &= \mathbf{x}^\top B_2 \Pi \Delta \dot{W} \Pi B_2^\top \mathbf{x} = \left\langle B_2 \Pi \Delta \dot{W} \Pi B_2^\top, \mathbf{x} \mathbf{x}^\top \right\rangle = \text{Tr} \left(B_2 \Pi \Delta \dot{W} \Pi B_2^\top \mathbf{x} \mathbf{x}^\top \right) = \\ &= \left\langle \Pi B_2^\top \mathbf{x} \mathbf{x}^\top B_2 \Pi, \Delta \dot{W} \right\rangle = \left\langle \nabla_{\Delta W} \sigma_1, \Delta \dot{W} \right\rangle \end{aligned}$$

By projecting onto the diagonal structure of the weight perturbation,

$$\nabla_{\text{diag } \Delta W} \sigma_1 = \text{diag} \left(\Pi B_2^\top \mathbf{x} \mathbf{x}^\top B_2 \Pi \right).$$

Note that $\text{diag} \left(\Pi B_2^\top \mathbf{x} \mathbf{x}^\top B_2 \Pi \right)_{ii} = |\Pi B_2^\top \mathbf{x}|_i^2$; then the stationary point is characterized by $\Pi B_2^\top \mathbf{x} = 0 \iff \mathbf{x} \in \ker L_1^\uparrow$. The latter is impossible since \mathbf{x} is the eigenvector corresponding to the largest eigenvalue; hence, since $\Pi(W + \Delta W)\Pi \neq W$, the optimal perturbation is $\Delta W \equiv 0$. \square

Remark 4.12. Given [Problem 1](#) and the optimal conserved triangle wait from [Theorem 4.11](#), one aims to preserve the kernel of subsampled Laplacian

$$\ker \left(B_2 W_2 \Pi W_2 B_2^\top \right) = \ker \left(B_2 W_2^2 B_2^\top \right)$$

Since $\Pi = \Pi^2$, $\ker L_1^\dagger = \ker W_2 B_2^\top$ and $\ker (B_2 W_2 \Pi W_2 B_2^\top) = \ker (\Pi W_2 B_2^\top)$. Additionally, $\ker W_2 B_2^\top \subseteq \ker (\Pi W_2 B_2^\top)$, so $\ker (B_2 W_2 \Pi W_2 B_2^\top) \neq \ker (B_2 W_2^2 B_2^\top) \iff$ there exists $\mathbf{y} \in \text{im } W_2 B_2^\top$ such that $W_2 B_2^\top \mathbf{y} \neq 0$ and $W_2 B_2^\top \mathbf{y} \in \ker \Pi$. Then in order to preserve the kernel, one needs $\text{im } W_2 B_2^\top \cap \ker \Pi = \{0\}$.

Theorem 4.13 (Conditionality of the 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 $L_1^\dagger(\mathcal{L})$ defined as in Theorem 4.8. Then the conditioning of the symmetrically preconditioned L_1^\dagger is given by:*

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

where V_1 forms the orthonormal basis of $\text{im } W_2 B_2^\top$.

Proof. By Theorem 4.11, $W_2(\mathcal{L}) = \Pi W_2$; then let us consider the lower-triangular preconditioner $C = P_\Sigma B_2 W_2 \Pi P_\mathbb{T}$ for $P_\Sigma L_1^\dagger P_\Sigma^\top$; then the preconditioned matrix is given by:

$$\begin{aligned} C^\dagger \left(P_\Sigma L_1^\dagger P_\Sigma^\top \right) C^{\top\dagger} &= (P_\Sigma B_2 W_2 \Pi P_\mathbb{T})^\dagger \left(P_\Sigma L_1^\dagger P_\Sigma^\top \right) (P_\Sigma B_2 W_2 \Pi P_\mathbb{T})^{\top\dagger} = \\ &= P_\mathbb{T}^\top (B_2 W_2 \Pi)^\dagger L_1^\dagger (B_2 W_2 \Pi)^{\top\dagger} P_\mathbb{T} \end{aligned}$$

Note that $P_\mathbb{T}$ is unitary, so $\kappa_+(P_\mathbb{T} X P_\mathbb{T}^\top) = \kappa_+(X)$, hence the principle matrix is $(B_2 W_2 \Pi)^\dagger L_1^\dagger (B_2 W_2 \Pi)^{\top\dagger} = (B_2 W_2 \Pi)^\dagger (B_2 W_2) (B_2 W_2)^\top (B_2 W_2 \Pi)^{\top\dagger}$. Since $\kappa_+(X^\top X) = \kappa_+^2(X)$, then in fact one needs to consider

$$\kappa_+ \left((B_2 W_2 \Pi)^\dagger (B_2 W_2) \right)$$

Let us consider the SVD-decomposition for $B_2 W_2 = U S V^\top$; more precisely,

$$B_2 W_2 = U S V^\top = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} S_1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^\top \\ V_2^\top \end{pmatrix} = U_1 S_1 V_1^\top$$

where S_1 is a diagonal invertible matrix. Note that U and U_1 have orthonormal columns and S_1 is diagonal and invertible, so

$$(B_2 W_2 \Pi)^\dagger B_2 W_2 = \left(S V^\top \Pi \right)^\dagger S V^\top = \left(S_1 V_1^\top \Pi \right)^\dagger S_1 V_1^\top$$

By the definition of the condition number κ_+ , one needs to compute σ_{\min}^+ and σ_{\max}^+ where:

$$\sigma_{\min \setminus \max}^+ = \min_{\mathbf{x} \perp \ker \left((S_1 V_1^\top \Pi)^\dagger S_1 V_1^\top \right)} \max \frac{\left\| (S_1 V_1^\top \Pi)^\dagger S_1 V_1^\top \mathbf{x} \right\|}{\|\mathbf{x}\|}$$

Note that $\text{im } W_2 B_2^\top = \text{im } V_1 = \text{im } V_1 S_1$, so by [Theorem 4.12](#), $\ker \Pi \cap \text{im } V_1 S_1 = \{0\}$, hence $\ker \Pi V_1 S_1 = \ker V_1 S_1$. Since $\ker V_1 S_1 \cap \text{im } S_1 V_1^\top = \{0\}$, one gets $\ker \Pi V_1 S_1 \cap \text{im } S_1 V_1^\top = \{0\}$. By the properties of the pseudo-inverse $\ker \Pi V_1 S_1 = \ker (S_1 V_1^\top \Pi)^\top = \ker (S_1 V_1^\top \Pi)^\dagger$; as a result, $\ker \left((S_1 V_1^\top \Pi)^\dagger S_1 V_1^\top \right) = \ker S_1 V_1^\top$. Since S_1 is invertible, $\ker \left((S_1 V_1^\top \Pi)^\dagger S_1 V_1^\top \right) = \ker V_1^\top$.

For $\mathbf{x} \in \ker V_1^\top \Rightarrow \mathbf{x} \in \text{im } V_1$, so $\mathbf{x} = V_1 \mathbf{y}$. Since $V_1^\top V_1 = I$, $\|\mathbf{x}\| = \|V_1 \mathbf{y}\|$ and:

$$\sigma_{\min \setminus \max}^+ = \min_y \setminus \max_y \frac{\left\| (S_1 V_1^\top \Pi)^\dagger S_1 \mathbf{y} \right\|}{\|\mathbf{y}\|} \stackrel{\mathbf{z} = S_1 \mathbf{y}}{=} \min_z \setminus \max_z \frac{\left\| (S_1 V_1^\top \Pi)^\dagger \mathbf{z} \right\|}{\|S_1^{-1} \mathbf{z}\|}$$

Note that $\mathbf{v} = (S_1 V_1^\top \Pi)^\dagger \mathbf{z} \iff \begin{cases} S_1 V_1^\top \Pi \mathbf{v} = \mathbf{z} \\ \mathbf{v} \perp \ker S_1 V_1^\top \Pi \end{cases}$ and $\ker S_1 V_1^\top \Pi = \ker V_1^\top \Pi$, so:

$$\sigma_{\min \setminus \max}^+ = \min_{\mathbf{v} \perp \ker V_1^\top \Pi} \setminus \max_{\mathbf{v} \perp \ker V_1^\top \Pi} \frac{\|\mathbf{v}\|}{\|V_1^\top \Pi \mathbf{v}\|}$$

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

□

Proposition 4.14. *The structure of the matrix ΠV_1 from [Theorem 4.13](#) provides a strategy for optimizing subsampling quality. Note that by the definition, the subsampling matrix Π is diagonal and binary, hence the best conditioning is achieved at $\Pi = I$ with $\kappa_+^2(V_1) = 1$, so one should minimize the distance between ΠV_1 and V_1 . Since $\text{span } V_1 = \text{im } W_2 B_2^\top = W_2 \text{im } B_2^\top$, V_1 is naturally scaled by the weight matrix W_2 , i.e. i -th row of V_1 is scaled by $w(t_i)$. Similarly, the subsampling matrix Π multiplies each row of V_1 either by 1 or 0; as a result, in order to close the distance between V_1 and ΠV_1 , one may aim to align 0s in the diagonal of Π with smallest weights in W_2 . In other words, one should search for heavier collapsible subcomplexes \mathcal{L} to achieve better preconditioning quality.*

4.5.1 Constructing Heavy Subcomplex out of 2-Core

Given [Theorem 4.13](#) and [Theorem 4.14](#), we search for a weakly collapsible subcomplex with a high total weight:

$$\max_{\mathcal{L} \in \Omega_{\mathcal{K}}} \|W \Pi(\mathcal{L})\|_F \quad \text{where} \quad \Omega_{\mathcal{K}} = \{\mathcal{L} \mid \mathcal{L} \subseteq \mathcal{K} \text{ and } \mathcal{L} \text{ is weakly collapsible}\}.$$

The [Algorithm 2](#) works as follows: start with an empty subcomplex \mathcal{L} ; then, at each step try to extend \mathcal{L} with the heaviest unconsidered triangle t : $\mathcal{L} \rightarrow \mathcal{L} \cup \{t\}$ ¹. If the extension $\mathcal{L} \cup \{t\}$ is weakly collapsible, it is accepted as the new \mathcal{L} , otherwise t is rejected; in either case triangle t is not considered for the second time.

Algorithm 2 HEAVY_SUBCOMPLEX(\mathcal{K}, W_2): construction a heavy collapsible subcomplex

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 1)
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  $\mathcal{L}$ 

```

Remark 4.15 (Validity of [Algorithm 2](#)). The subcomplex \mathcal{L} sampled with [Algorithm 2](#) satisfies [Problem 1](#): indeed, $\mathcal{V}_0(\mathcal{K}) = \mathcal{V}_0(\mathcal{L})$, $\mathcal{V}_1(\mathcal{K}) = \mathcal{V}_1(\mathcal{L})$ and \mathcal{L} is weakly collapsible by construction. It is less trivial to show that the subsampling \mathcal{L} does not increase the dimensionality of 1-homology.

Assuming the opposite, the subcomplex \mathcal{L} cannot have any additional 1-dimensional holes in the form smallest-by-inclusion cycles of more than 3 edges: since this cycle is not present in \mathcal{K} , it is “covered” by at least one triangle t which necessarily has a free edge, so \mathcal{L} can be extended by t and remain weakly collapsible. Alternatively, if the only additional hole correspond to the triangle t not present in \mathcal{L} ; then, reminiscent of the proof for [Theorem 4.7](#), let us consider the minimal by inclusion simplicial complex \mathcal{K} for which it happens. Then the only free edges in \mathcal{L} are the edges of t , otherwise \mathcal{K} is not minimal. At the same time, in such setups t is not registered as a hole since it is an outer boundary of the complex \mathcal{L} , e.g. consider the exclusion of exactly one triangle in the tetrahedron case, [Figure 4.2](#)², which proves that \mathcal{L} cannot extend the 1-homology of \mathcal{K} .

The complexity of [Algorithm 2](#) is $\mathcal{O}(m_1 m_2)$ at worst which could be considered comparatively slow: the algorithm passes through every triangle in $\mathcal{V}_2(\mathcal{K})$ and performs collapsibility check via [Algorithm 1](#) on \mathcal{L} which never has more than m_1 triangles since it is weakly collapsible. Note that [Algorithm 2](#) and [Theorem 4.13](#) do not depend on \mathcal{K} being

¹here the extension implies the addition of the triangle t with all its vertices and edges to the complex \mathcal{L}

²algebraically, this fact is extremely dubious: due to the lack of free edges, there is a “path” between any two triangles in \mathcal{L} adjacent to t through adjacent triangles in \mathcal{L} , which reduces degrees of freedom in the circulation of the flow around t and brings it to $\ker B_2^\top$.

a 2-Core; moreover, the collapsible part of a generic \mathcal{K} is necessarily included in the subcomplex \mathcal{L} produced by [Algorithm 2](#). Hence a prior pass of $\text{GREEDY_COLLAPSE}(\mathcal{K})$ reduces the complex to a smaller 2-Core \mathcal{K}' with faster $\text{HEAVY_SUBCOMPLEX}(\mathcal{K}', W_2)$ since $\mathcal{V}_1(\mathcal{K}') \subset \mathcal{V}_1(\mathcal{K})$ and $\mathcal{V}_2(\mathcal{K}') \subset \mathcal{V}_2(\mathcal{K})$.

We summarise the whole procedure in [Figure 4.5](#): in order to construct the preconditioner C , one reduces a generic simplicial complex \mathcal{K} to a 2-Core \mathcal{K}' through the collapsing sequence Σ_1 and the corresponding sequence of maximal faces \mathbb{T}_1 ; then, a heavy weakly connected subcomplex \mathcal{L} is sampled from \mathcal{K}' with the collapsing sequence Σ_2 and the corresponding sequence of maximal faces \mathbb{T}_2 . The preconditioner C is formed by the subset of triangles $\mathbb{T}_1 \cup \mathbb{T}_2$ (that produces the projection matrix Π) with collapsing sequence (Σ_1, Σ_2) .

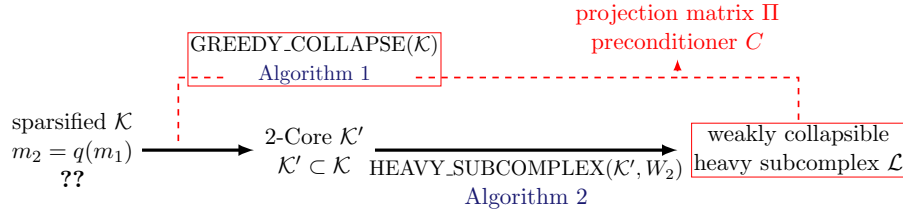


FIGURE 4.5: The scheme of the simplicial complex transformation: from the original \mathcal{K} to the heavy weakly collapsible subcomplex \mathcal{L} .

We refer to the preconditioner built according to [Figure 4.5](#) via [Algorithm 1](#) and [Algorithm 2](#) as a *heavy collapsible subcomplex* (HeCS) preconditioner.

4.5.2 Cholesky decomposition for weakly collapsible subcomplex

4.5.3 Problem: precondition by subcomplex

4.5.4 Optimal weights for subsampling

4.5.5 Theorem on conditionality of a subcomplex

4.5.6 The notion of the heavy collapsible subcomplex

4.5.7 Algorithm and complexity

4.6 Benchmarking: triangulation

4.6.1 Timings of algorithm and preconditioned application

4.6.2 Conditionality and iterations

4.6.3 Compare with shifted ichol

Chapter 5

Conclusion and future prospects

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