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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✎ 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) SC[1] 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, $\sigma' \in \mathcal{K}$.

[1]addition 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, $\operatorname{ord}(\sigma) = k$. 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, uninterupted in a sense of the order: if $\mathcal{V}_k(\mathcal{K}) = \varnothing$, then $\mathcal{V}_{k+1}(\mathcal{K})$ is also necessarily empty.

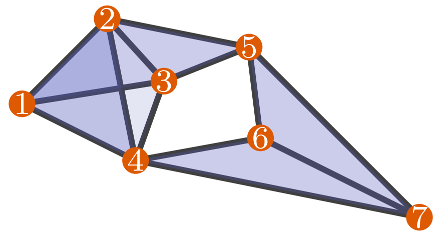

FIGURE 2.1: Example of a simplicial complex

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 simplicies (edges) by black and* 2*-order simplices (triangles) by blue, where:*

$$\begin{aligned}
\mathcal{V}_0(\mathcal{K}) &= \{1, 2, 3, 4, 5, 6, 7\} \\
\mathcal{V}_1(\mathcal{K}) &= \{[1, 2], [1, 3], [1, 4], [2, 3], [2, 4], [2, 5], [3, 4], [3, 5], [4, 6], [4, 7], [5, 6], [6, 7]\} \\
\mathcal{V}_2(\mathcal{K}) &= \{[1, 2, 3], [1, 2, 4], [1, 3, 4], [2, 3, 5], [4, 6, 7], [5, 6, 7]\}
\end{aligned} \tag{2.1}$$

Note that $\mathcal{V}_3(\mathcal{K}) = \varnothing$, 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). ✎ *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 rigidness which allows to formally describe the topology of $\mathcal{K}$; as a result, one is specifically interested in the formal desctiption 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,

$$AB = 0 \tag{2.2}$$

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

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

$$\mathcal{H} = {}^{\ker A}\!/\!_{\operatorname{im} B} \tag{2.3}$$

where each element of $\mathcal{H}$ is a manifold $\mathbf{x} + \operatorname{im} B = \{\mathbf{x} + \mathbf{y} \mid \forall \mathbf{y} \in \operatorname{im} B\}$ 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✎ in a general sense of *equivalence classes* $\mathbf{x} + \operatorname{im} B$. Then, each class $\mathbf{x} + \operatorname{im} B = \mathbf{x}_H + \operatorname{im} B$ for some $\mathbf{x}_H \perp \operatorname{im} B$ (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 $\operatorname{im} B$ is unique, the map $\mathbf{x}_H \leftrightarrow \mathbf{x} + \operatorname{im} B$ is bijectional.

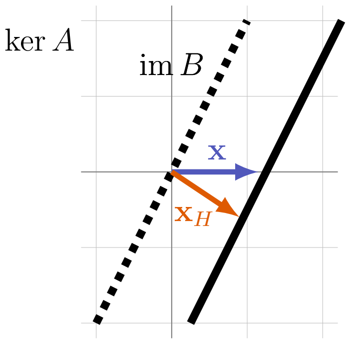

FIGURE 2.2: Illustration of a harmonic representative for an equivalence class

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

$$\mathcal{H} = {}^{\ker A}\!/\!_{\operatorname{im} B} \cong \ker A \cap \ker B^\top, \tag{2.4}$$

where $\cong$ denotes the isomorphism.

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

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

$$\ker A \cap \ker B^\top = \ker \left(A^\top A + BB^\top \right) \tag{2.5}$$

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

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

$$A^\top A\mathbf{x} + BB^\top \mathbf{x} = 0 \tag{2.6}$$

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

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

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

$$A^\top A\mathbf{x} = 0 \Longrightarrow \mathbf{x}^\top A^\top A\mathbf{x} = 0 \iff \|A\mathbf{x}\|^2 = 0 \Longrightarrow \mathbf{x} \in \ker A \tag{2.8}$$

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

✎ Here we need some words about the transitions.

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

$$\begin{aligned} \ker B^\top = \ker B^\top \cap \mathbb{R}^n = \ker B^\top \cap \left(\ker A \oplus \operatorname{im} A^\top \right) = \\ = \left(\ker A \cap \ker B^\top \right) \oplus \left(\operatorname{im} A^\top \cap \ker B^\top \right) \end{aligned} \tag{2.9}$$

Given Theorem 2.4, $\ker A \cap \ker B^\top = \ker \left(A^\top A + BB^\top \right)$ and, since $\operatorname{im} A^\top \subset \ker B^\top$, $\operatorname{im} A^\top \cap \ker B^\top = \operatorname{im} A^\top$, yeilding the decomposition of the whole space:

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

$$\mathbb{R}^n = \overbrace{\operatorname{im} A^\top \oplus \underbrace{\ker \left(A^\top A + BB^\top \right)}_{}}^{\ker B^\top} \underbrace{\oplus \operatorname{im} B}_{\ker A} \tag{2.10}$$

2.4 Boundary and Laplacian Operators

2.4.1 Boundary operators B_k

Each simplicial complex $\mathcal{K}$ has a nested structure of simplicies: 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 $\mathcal{C}_k$

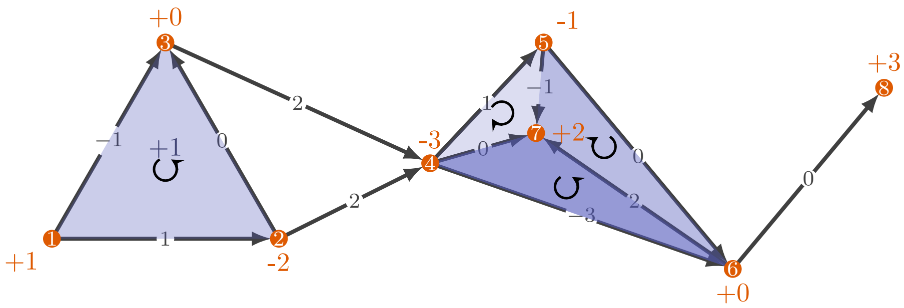

FIGURE 2.3: Example of chains on the simplicial complex

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 evoloving 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. Addiitionally, 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.

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

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

Lemma 2.8 (Fundamental Lemma of Homology)**.**

$$B_k B_{k+1} = 0 \tag{2.12}$$

Proof.

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

□

✎ Examples

2.4.2 Homology group and Hodge Laplacians L_k

2.4.2.1 Homology group as Quontinent 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 Weigthed and Normalised Boundary Operators

✎ definition and motivation of the weighting scheme

Note that, from the definition $\overline{B}_k = W_{k-1}^{-1} B_k W_k$ and (**??**), we immediately have that $\overline{B}_k \overline{B}_{k+1} = 0$. Thus, the group $\overline{\mathcal{H}}_k = \ker \overline{B}_k / \operatorname{im} \overline{B}_{k+1}$ is well defined for any choice of positive weights w_k and is isomorphic to $\ker \overline{L}_k$. 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-simplicies. Precisely, if W_k are positive diagonal matrices, we have*

$$\dim \ker \overline{B}_k = \dim \ker B_k, \quad \dim \ker \overline{B}_k^\top = \dim \ker B_k^\top, \quad \dim \overline{\mathcal{H}}_k = \dim \mathcal{H}_k \,. \tag{2.14}$$

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

Proof. Since W_k is an invertible diagonal matrix,

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

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

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

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

□

✎ 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 $\mathrm{Re}\,[\lambda_i] < 0$ 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 as assume that $X = A + \Delta$ and intead 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 $\overline{L}_k = \overline{L}_k^{down} + \overline{L}_k^{up}$, where $\overline{L}_k^{down} = \overline{B}_k^\top \overline{B}_k$ and $\overline{L}_k^{up} = \overline{B}_{k+1} \overline{B}_{k+1}^\top$. Then:*

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

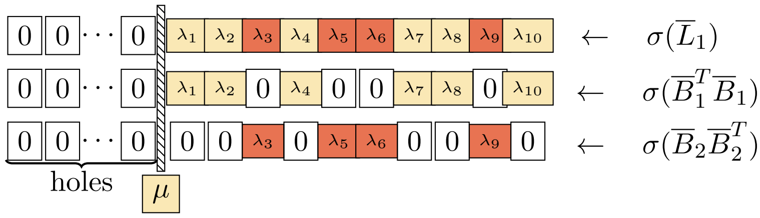

FIGURE 3.1: Illustration for the principal spectrum inheritance (Theorem 3.1) in case $k = 0$: spectra of $\overline{L}_1$, $\overline{L}_1^{\downarrow}$ and $\overline{L}_1^{\downarrow}$ are shown. Colors signify the splitting of the spectrum, $\lambda_i > 0 \in \sigma(\overline{L}_1)$; all yellow eigenvalues are inherited from $\sigma_+(\overline{L}_0)$; 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* $\mu \in \sigma_+(\overline{L}_k)$ *with an eigenvector* $\mathbf{u} \in \ker \overline{L}_k^{up}$*, and* $\nu \in \sigma_+(\overline{L}_{k+1})$ *with an eigenvector* $\mathbf{u} \in \ker \overline{L}_{k+1}^{down}$*, such that:*

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

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

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 $\overline{L}_{k+1}^{down}$ inherits the positive part of the spectrum from the up-term of $\overline{L}_k^{up}$; the eigenvectors corresponding to the inherited positive part of the spectrum lie in the kernel of $\overline{L}_{k+1}^{up}$; at the same time, the "new" up-term $\overline{L}_{k+1}^{up}$ 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 $\overline{L}_0 = \overline{L}_0^{up}$, the theorem yields $\sigma_+(\overline{L}_0) = \sigma_+(\overline{L}_1^{down}) \subseteq \sigma_+(\overline{L}_1)$. In other terms, the positive spectrum of the $\overline{L}_0$ is inherited by the spectrum of $\overline{L}_1$ and the remaining (non-inherited) part of $\sigma_+(\overline{L}_1)$ coincides with $\sigma_+(\overline{L}_1^{up})$. Figure 3.1 provides an illustration of the statement of Theorem 3.1 for $k = 0$.

3.3.2 Example with inheritted disconnectedness

3.3.3 Example with faux edges (different weighting scheme)

3.4 Functional, derivative and alternating scheme

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3.4.3 Constrained gradient

3.4.4 Alternating scheme

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Chapter 4

Preconditioning

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

4.1 Preconditioning 101

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✎ Transition to collapsibility

4.4 Collapsible simplicial complexes

4.4.1 Classical collapsiblity

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 (inlusion-wise) maximal face of simplex $\sigma \in \mathcal{K}$ if τ is maximal by inlusion simplex such that $\sigma \subseteq \tau$ and $\mathrm{ord}\,(\sigma) < \mathrm{ord}\,(\tau)$. For instance, in Figure 4.1

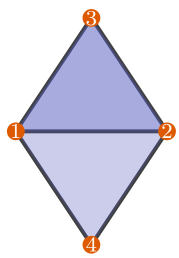

FIGURE 4.1: Example of a simplicial complex: free simplices and maximal faces.

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 $\mathcal{K}\backslash\{\sigma\}$ 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, $\mathcal{K} \to \mathcal{K}' = \mathcal{K} - \sigma - \tau$; 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 $\Sigma = \{\sigma_1, \sigma_2, \ldots\}$ 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. $\Sigma = \{\sigma_1, \sigma_2, \ldots\}$ is a collapsing sequence if σ_1 is free in $\mathcal{K}$ and each σ_i, $i > 1$, is free at $\mathcal{K}^{(i)} = \mathcal{K}^{(i-1)}\backslash\{\sigma_i\}$, $\mathcal{K}^{(1)} = \mathcal{K}$. The collapse of $\mathcal{K}$ to a new complex $\mathcal{L}$ at Σ is denoted by $\mathcal{L} = \mathcal{K}\backslash\Sigma$.

By the definition, every collapsing sequence Σ has a corresponding sequence $\mathbb{T} = \{\tau(\sigma_1), \tau(\sigma_2), \ldots\}$ 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, $\mathcal{K}\backslash\Sigma = \{v\}$.

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 embeded into the triangulation of the d-dimensional unit sphere, [4]. Naturally restricting the collapses to the case of d-collapses (such that $\operatorname{ord}(\sigma)_i \leq d-1$), 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 $\mathcal{K}\backslash\Sigma$ 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 $\mathcal{K}\backslash\Sigma$ 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, $\operatorname{ord}(\sigma) = d-1$, 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.

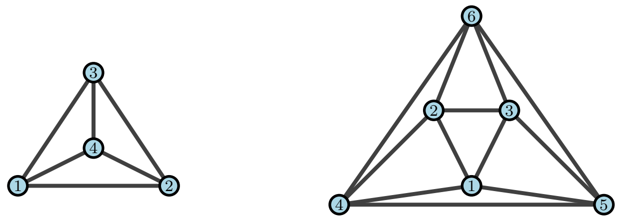

FIGURE 4.2: 2-Core, examples.

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

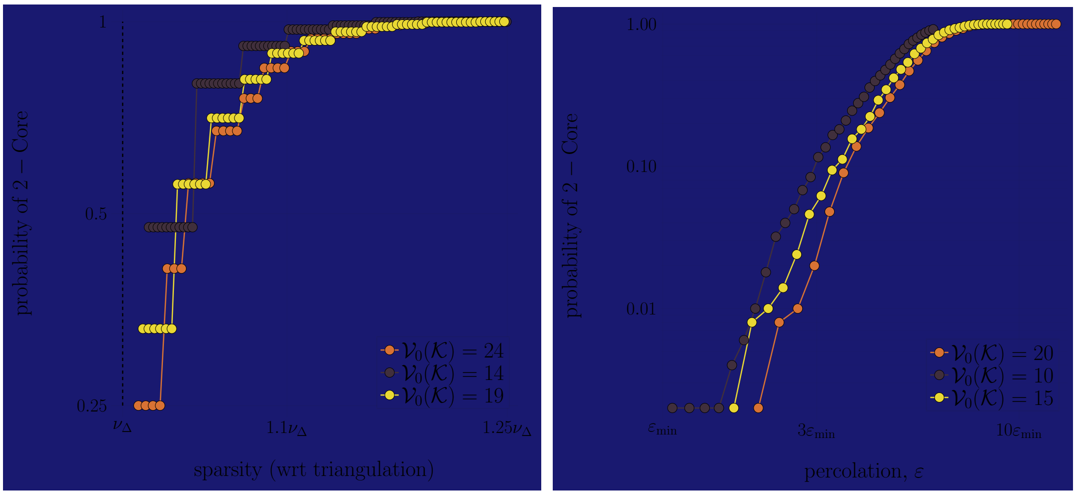

FIGURE 4.3: The probability of the 2-Core in richer-than-triangulation simplicial complexes: triangulation of random points modified to have $\left[\nu \frac{|\mathcal{V}_0(\mathcal{K})|\cdot(|\mathcal{V}_0(\mathcal{K})|-1)}{2}\right]$ edges on the left; random sensor networks with ε-percolation on the 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 $\mathcal{K}\backslash\Sigma_1 = \mathcal{L}$ eliminates all the triangles in the complex, $\mathcal{V}_2(\mathcal{L}) = \varnothing$; otherwise, the whole sequence Σ is not collapsing $\mathcal{K}$ to a single vertex. Since $\mathcal{V}_2(\mathcal{L}) = \varnothing$, 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 $\mathcal{L} = \mathcal{K}\backslash\Sigma_1$ has no simplices of order 2, $\mathcal{V}_2(\mathcal{L}) = \varnothing$ 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.*

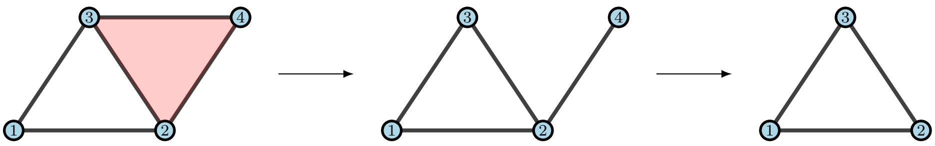

FIGURE 4.4: Example of weakly collapsible but not collapsible simplicial complex

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 $\mathcal{K}\backslash\{\sigma\}$ is *collapsible* and another $\sigma' \in \mathcal{V}_2(\mathcal{K})$ such that $\mathcal{K}\backslash\{\sigma'\}$ 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 $\tau(\sigma_1) \neq \tau(\sigma_2)$, $\mathcal{K}\backslash\{\sigma_1, \sigma_2\} = \mathcal{K}\backslash\{\sigma_2, \sigma_1\}$. Let $\tau(\sigma_1) \neq \tau(\sigma_2)$ for at least one pair of σ_1 and σ_2; in our assumption, either both $\mathcal{K}\backslash\{\sigma_1\}$ and $\mathcal{K}\backslash\{\sigma_2\}$, only $\mathcal{K}\backslash\{\sigma_1\}$ or none are collapsible. In the former case either $\mathcal{K}\backslash\{\sigma_1\}$ or $\mathcal{K}\backslash\{\sigma_2\}$ is a smaller example of the complex satisfying the assumption, hence, violating the minimality. If only $\mathcal{K}\backslash\{\sigma_1\}$ is collapsible, then $\mathcal{K}\backslash\{\sigma_2, \sigma_1\}$ is not collapsible; hence, $\mathcal{K}\backslash\{\sigma_1, \sigma_2\}$ is not collapsible, so $\mathcal{K}\backslash\{\sigma_1\}$ is a smaller example of a complex satisfying the assumption. Finally, if both $\mathcal{K}\backslash\{\sigma_1\}$ and $\mathcal{K}\backslash\{\sigma_2\}$ are collapsible, then for known σ' such that $\mathcal{K}\backslash\{\sigma'\}$ 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 ($\mathcal{K}\backslash\{\sigma\}$ is collapsible) and for σ' ($\mathcal{K}\backslash\{\sigma'\}$ is not collapsible) it holds that $\tau(\sigma) = \tau(\sigma') \Rightarrow \sigma \cap \sigma' = \{v\}$, so after collapses $\mathcal{K}\{\sigma\}$ and $\mathcal{K}\backslash\{\sigma'\}$ 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. □

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 $F = \{\sigma \mid |\Delta_e| = 1\}$ 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 $\{\Delta_{\sigma_i}\}_{i=1}^{m_1}$

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

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 though 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*

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

i.e. $P_\Sigma L_1^{\uparrow}(\mathcal{K}) P_\Sigma^\top = CC^\top$, 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 $CC^\top = P_\Sigma L_1^{\uparrow}(\mathcal{K}) P_\Sigma^\top$. □

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 $\left(C^\dagger P_\Sigma L_1^\uparrow(\mathcal{K}) P_\Sigma^\top C^{\dagger\top}\right) C^\top P_\Sigma \mathbf{x} = C^\dagger P_\Sigma \mathbf{f}$, 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], $\ker L_k^\uparrow(\mathcal{X}) = \ker L_k(\mathcal{X}) \oplus B_k^\top \cdot \operatorname{im} L_{k-1}^\uparrow$. The second part, $B_k^\top \cdot \operatorname{im} L_{k-1}^\uparrow$, 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:

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

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 $\frac{d}{dt}\sigma_1 \left(L_1^{\uparrow}(\mathcal{L}) - L_1^{\uparrow}(\mathcal{K}) \right)$:

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

By projecting onto the diagonal structure of the weight perturbation,

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

Note that $\operatorname{diag}\left(\Pi B_2^\top\mathbf{x}\mathbf{x}^\top B_2\Pi \right)_{ii} = |\Pi B_2^\top\mathbf{x}|_i^2$; 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 $\Delta W \equiv 0$. □

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 $\Pi = \Pi^2$, $\ker L_1^\uparrow = \ker W_2 B_2^\top$ and $\ker\left(B_2 W_2 \Pi W_2 B_2^\top\right) = \ker\left(\Pi W_2 B_2^\top\right)$. Additionally, $\ker W_2 B_2^\top \subseteq \ker\left(\Pi W_2 B_2^\top\right)$, so $\ker\left(B_2 W_2 \Pi W_2 B_2^\top\right) \neq \ker\left(B_2 W_2^2 B_2^\top\right) \iff$ there exists $\mathbf{y} \in \operatorname{im} W_2 B_2^\top$ 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 $\operatorname{im} W_2 B_2^\top \cap \ker \Pi = \{0\}$.

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 $L_1^\uparrow(\mathcal{L})$ defined as in Theorem 4.8. 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 of $\operatorname{im} W_2 B_2^\top$.

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 $P_\Sigma L_1^\uparrow P_\Sigma^\top$; then the preconditioned matrix is given by:

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

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

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

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

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

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

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

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

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

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

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

$$\sigma^+_{\min \setminus \max} = \min_{\mathbf{y}} \setminus \max \frac{\left\|\left(S_1 V_1^\top \Pi\right)^\dagger S_1 \mathbf{y}\right\|}{\|\mathbf{y}\|} \underset{\mathbf{z}=S_1\mathbf{y}}{=} \min_{\mathbf{z}} \setminus \max \frac{\left\|\left(S_1 V_1^\top \Pi\right)^\dagger \mathbf{z}\right\|}{\left\|S_1^{-1}\mathbf{z}\right\|}$$

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

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

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

$\square$

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 $\operatorname{span} V_1 = \operatorname{im} W_2 B_2^\top = W_2 \operatorname{im} B_2^\top$, 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: $\mathcal{L} \to \mathcal{L} \cup \{t\}$[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

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

```
ℒ ← ∅, 𝕋 ← ∅                                          ▷ initial empty subcomplex
while there is unprocessed triangle in 𝒱₂(𝒦) do
    t ← nextHeaviestTriangle(𝒦, W₂)   ▷ e.g. iterate through 𝒱₂(𝒦) sorted by weight
    if ℒ ∪ {t} is weakly collapsible then      ▷ run GREEDY_COLLAPSE(ℒ ∪ {t})
(Algorithm 1)
        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
```

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

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

[2] algebraically, 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 GREEDY_COLLAPSE($\mathcal{K}$) reduces the complex to a smaller 2-Core $\mathcal{K}'$ with faster 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).

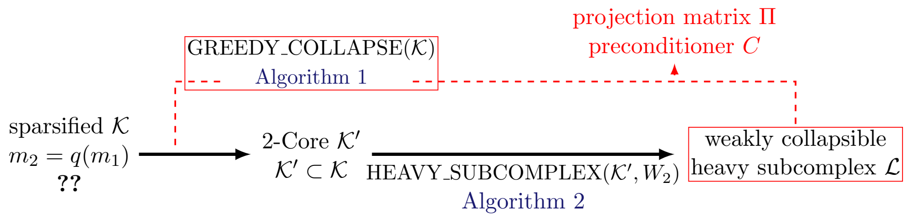

FIGURE 4.5: The scheme of the simplicial complex transformation: from the original $\mathcal{K}$ to the heavy weakly collapsible subcomplex $\mathcal{L}$.

We refer to the preconditioner built according to Figure 4.5 via Algorithm 1 and Algorithm 2 as a *heavy collapsbile 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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