Spectral relaxations of persistent rank invariants

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Abstract

Using the fact that the persistent rank invariant determines the persistence diagram and vice versa, we introduce a framework for constructing families of continuous relaxations of the persistent rank invariant for persistence modules indexed over the real line. Like the rank invariant, these families obey inclusion-exclusion, are derived from simplicial boundary operators, and encode all the information needed to construct a persistence diagram. Unlike the rank invariant, these spectrally-derived families enjoy a number of stability and continuity properties typically reserved for persistence diagrams, such as smoothness and differentiability. By leveraging its relationship with combinatorial Laplacian operators, we find the non-harmonic spectra of our proposed relaxation encode valuable geometric information about the underlying space, prompting several avenues for geometric data analysis. As these Laplacian operators are trace-class operators, we also find the corresponding relaxation can be efficiently approximated with a randomized algorithm based on the stochastic Lanczos quadrature method. We investigate the utility of our relaxation with applications in topological data analysis and machine learning, such as parameter optimization and shape classification.

1 Introduction

Persistent homology [17] (PH) is the most widely deployed tool for data analysis and learning applications within the topological data analysis (TDA) community. Persistence-related pipelines often follow a common pattern: given a data set X as input, construct a simplicial complex K and an order-preserving function $f : K \to \mathbb{R}$ such that useful topological/geometric information may be gleaned from its *persistence diagram*—a multiset summary of f formed by pairs $(a, b) \in \mathbb{R}^2$ exhibiting non-zero *multiplicity* $\mu_p^{a,b} \in \mathbb{Z}_+$:

$$\mathrm{dgm}_p(K, f) \triangleq \{\, (a, b) : \mu_p^{a,b} \neq 0 \,\}, \qquad \mu_p^{a,b} \triangleq \min_{\delta > 0} \left(\beta_p^{a+\delta,b-\delta} - \beta_p^{a+\delta,b+\delta}\right) - \left(\beta_p^{a-\delta,b-\delta} - \beta_p^{a-\delta,b+\delta}\right) \tag{1.1}$$

where $\beta_p^{a,b}$ is the rank of the linear map in homology induced by the inclusion $f^{-1}(-\infty, a] \hookrightarrow f^{-1}(-\infty, b]$. The surprising and essential quality of persistence is that these pairings exist, are unique, and are stable under additive perturbations [12]. Whether for shape recognition [8], dimensionality reduction [33], or time series analysis [29], persistence is the de facto connection between homology and the application frontier.

Though theoretically sound, diagrams suffer from many practical issues: they are sensitive to outliers, far from injective, and expensive both to compute *and* compare. Towards ameliorating these issues, practitioners have equipped diagrams with additional structure by way of maps to function spaces; examples include persistence images [1], persistence landscapes [6], and template functions [30]. Tackling the issue of injectivity, Turner et al. [35] propose an injective shape statistic of directional diagrams associated to a data set $X \subset \mathbb{R}^d$, sparking both an inverse theory for persistence and a mathematical foundation for metric learning. Despite the potential these extensions have in learning applications, diagrams can still be expensive to obtain. The severity of this issue is compounded in the parameterized setting, where adaptations of the persistence computation has proven non-trivial [31].

We seek to shift the computational paradigm on persistence while retaining its application potential: rather than following a construct-then-vectorize approach, we devise a spectral method that performs both steps, simultaneously and approximately. Our strategy is motivated both by a technical observation that suggests advantages exist for the rank invariant computation (section 2.1) and by measure-theoretic results on $\mathbb{R}$-indexed persistence modules [7, 9], which generalize (1.1) to rectangles $R = [a, b] \times [c, d]$ in the plane:

$$\mu_p^R(K, f) \triangleq \mathrm{card}\left(\mathrm{dgm}_p(K, f)\big|_R\right) = \beta_p^{b,c} - \beta_p^{a,c} - \beta_p^{b,d} + \beta_p^{a,d} \tag{1.2}$$

Notably, our approach not only avoids explicitly constructing diagrams, but is in fact *matrix-free*, circumventing the reduction algorithm from [16] entirely. Additionally, the relaxation is computable in linear space and quadratic time, can be iteratively approximated, and requires no complicated data structures or maintenance procedures to implement.

Contributions: Our primary contribution is the introduction of several families of spectral approximations to the rank invariants—μ_p and β_p**??**—all of which are Lipshitz continuous**??**, stable under relative perturbations**??**, and differentiable on the positive semi-definite cone**??**. By a reduction to spectral methods for Laplacian operators**??**, we also show these approximations are computable in $\approx O(m)$ memory and $\approx O(mn)$ time, where n, m are the number of $p, p+1$ simplices in K, respectively (see section 4). Moreover, both relaxations admit iterative $(1-\epsilon)$-approximation schemes**??**, and in both cases are recovered exactly when the parameters ϵ and τ made small enough**??**.

Outline: We now outline the proposed relaxation, leaving the rest of the paper to discuss theoretical and practical details. Informally, we study a family of vector-valued mappings over a *parameter space* $\mathcal{A} \subset \mathbb{R}^d$:

$$(X_\alpha, \mathcal{R}, \tau, \epsilon) \mapsto \mathbb{R}^h \tag{1.3}$$

where X_α is an $\mathcal{A}$-parameterized input data set, $\mathcal{R} \subset \Delta_+ = \{(a,b) \in \mathbb{R}^2 : a \leq b\}$ is a region which decomposes as a disjoint union of rectangles $R_1 \cup \ldots \cup R_h$—we will call such a set a *sieve*—and $(\tau, \epsilon) \in \mathbb{R}^2_+$ are smoothness/approximation parameters, respectively. The intuition is that $\mathcal{R}$ is used to filter and summarize the topological and geometric behavior exhibited by X_α for all $\alpha \in \mathcal{A}$, thereby *sifting* the diagrams in the space $\mathcal{A} \times \Delta_+$. The steps to produce this mapping are as follows:

1. Let K denote a fixed simplicial complex constructed from the data set X. Select a parameter space $\mathcal{A} \subset \mathbb{R}^d$ which indexes a family of filter functions $\{ f_\alpha : K \to \mathbb{R} : \alpha \in \mathcal{A} \}$ of K, where:

$$f_\alpha(\tau) \leq f_\alpha(\sigma) \;\forall\, \tau \subseteq \sigma \in K \quad \text{and} \quad f_\alpha(\sigma) \text{ is continuous in } \alpha \in \mathcal{A} \text{ for every } \sigma \in K \tag{1.4}$$

   Exemplary choices of f_α include filtrations geometrically realized from methods that themselves are have parameters, such as density filtrations or time-varying filtrations over dynamic metric spaces [22].

2. Select a *sieve* $\mathcal{R} = R_1 \cup \ldots \cup R_h \subset \Delta_+$. This choice is application-dependent and typically requires a priori knowledge, though in section 5 we give evidence that, when $\mathcal{R}$ is unknown, random sampling may be sufficient for vectorization or data exploration purposes.

3. Fix a homology dimension $p \geq 0$ and parameters $(\tau, \epsilon) \in \mathbb{R}^2_+$ representing how *smoothly* and *accurately* the relaxation $\hat{\mu}_p^{\mathcal{R}}$ (defined in step 5 below) should model the quantity:

$$\mu_p^{\mathcal{R}}(K, f_\alpha) \triangleq \mathrm{card}\left(\mathrm{dgm}_p(f_\alpha)\big|_{\mathcal{R}} \right) \tag{1.5}$$

4. Choose an $\mathcal{A}$-parameterized Laplacian operator $\mathcal{L}_p^{a,b} : \mathcal{A} \times C^p(K_b, K_a; \mathbb{R}) \to C^p(K_b, K_a; \mathbb{R})$ on the relative p-cochains of (K_b, K_b) and a τ-parameterized continuous function $\phi(\cdot, \tau) : \mathbb{R} \to \mathbb{R}_+$ which converges to sgn_+ as $\tau \to 0$. The choice of $\mathcal{L}$ (e.g. Kirchoff, random walk) determines the kind of geometric/topological information to extract from (K, f_α), while ϕ determines how that information is encoded.

5. Denote by $\Lambda(\mathcal{L}_{a,b}(\alpha))$ the spectrum of $\mathcal{L}_{a,b}$ at any $\alpha \in \mathcal{A}$ ordered in non-increasing order. Our relaxation approximates (1.5) by $(1 \pm \epsilon)$-approximating μ_p at each corner point (a,b) in the boundary of $\mathcal{R}$:

$$\mu_p^{\mathcal{R}}(\alpha) \overset{\epsilon}{\approx} \hat{\mu}_p^{\mathcal{R}}(\alpha) \triangleq \sum_{(a,b)} s_{a,b} \cdot \|\Phi_\tau(\mathcal{L}_p^{a,b}(\alpha))\|_*$$

   where $\Phi_\tau(\cdot)$ is a τ-parameterized matrix function induced by ϕ (see section 3). In section 3.4, we show that letting both $\tau \to 0$ and $\epsilon \to 0$ yields the multiplicity function $\mu_p^{\mathcal{R}}$ exactly.

The remaining steps of the relaxation depend on the application in mind. Applications looking to vectorize persistence information over random and highly structured complexes may benefit from the concentration of mass phenomenon known to occur their spectra; examples include topology-guided image denoising [32], shape classification under metric invariants [8], bifurcation detection in dynamical systems [30], and so on. The differentiability of our relaxation also suggests it may be used in topological optimization applications, i.e. optimization problems whose loss functions incorporate persistence information [27].

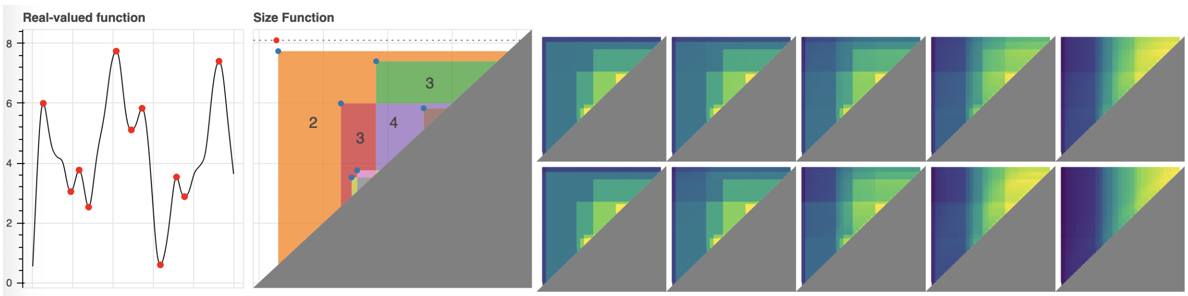


Figure 1: (left) Vineyards analogy depicting diagrams as ‘snapshots’ over time; (middle) visualization of a rectangular sieve $\mathcal{R} \subset \Delta_+$ (orange) intersecting vines collapsed onto Δ_+; (right) the integer-valued multiplicity function $\mu_p^{\mathcal{R}}(\alpha)$ as a function of time $\alpha \in \mathbb{R}$ (top) and a real-valued spectral relaxation (bottom)

2 Notation & Background

A *simplicial complex* $K \subseteq \mathcal{P}(V)$ over a finite set $V = \{v_1, v_2, \ldots, v_n\}$ is a collection of simplices $\{\, \sigma : \sigma \in \mathcal{P}(V) \,\}$ such that $\tau \subseteq \sigma \in K \Rightarrow \tau \in K$. A *p-simplex* $\sigma \subseteq V$ is a set of $p+1$ vertices, the collection of which is denoted as K^p. An *oriented p-simplex* $[\sigma]$ is an ordered set $[\sigma] = (-1)^{|\pi|}\left[v_{\pi(1)}, v_{\pi(2)}, \ldots, v_{\pi(p+1)}\right]$, where π is a permutation on $[\,p+1\,] = \{\,1, 2, \ldots, p+1\,\}$ and $|\pi|$ the number of its inversions. The *p-boundary* $\partial_p[\sigma]$ of an oriented p-simplex $[\sigma] \in K$ is defined as the alternating sum of its oriented co-dimension 1 faces, which collectively for all $\sigma \in K^p$ define the p-th *boundary matrix* ∂_p of K:

$$\partial_p[i,j] \triangleq \begin{cases} (-1)^{s_{ij}} & \sigma_i \in \partial[\sigma_j] \\ 0 & \text{otherwise} \end{cases}, \qquad \partial_p[\sigma] \triangleq \sum_{i=1}^{p+1} (-1)^{i-1}[v_1, \ldots, v_{i-1}, v_{i+1}, \ldots v_{p+1}] \tag{2.1}$$

where $s_{ij} = \mathrm{sgn}([\sigma_i], \partial[\sigma_j])$ records the orientation. Extending (2.1) to all simplices in $\sigma \in K$ for all $p \leq \dim(K)$ yields the *full boundary matrix* ∂. With a small abuse in notation, we use ∂_p to denote both the boundary operator and its ordered matrix representative. When it is not clear from the context, we will clarify which representation is intended.

Generalizing beyond simplices, given a field $\mathbb{F}$, an *oriented p-chain* is a formal $\mathbb{F}$-linear combination of oriented p-simplices of K whose boundary $\partial_p[c]$ is defined linearly in terms of its constitutive simplices. The collection of p-chains under addition yields an $\mathbb{F}$-vector space $C_p(K)$ whose boundaries $c \in \partial_p[c']$ satisfying $\partial_p[c] = 0$ are called *cycles*. Together, the collection of p-boundaries and p-cycles forms the groups $B_p(K) = \operatorname{Im} \partial_{p+1}$ and $Z_p(K) = \operatorname{Ker} \partial_p$, respectively. The quotient space $H_p(K) = Z_p(K)/B_p(K)$ is called the *p-th homology group of K* with coefficients in $\mathbb{F}$ and its dimension β_p is the *p-th Betti number* of K.

A *filtration* is a pair (K, f) where $f : K \to I$ is a *filter function* over an index set I satisfying $f(\tau) \leq f(\sigma)$ whenever $\tau \subseteq \sigma$, for any $\tau, \sigma \in K$. For every pair $(a, b) \in I \times I$ satisfying $a \leq b$, the sequence of inclusions $K_a \subseteq \cdots \subseteq K_b$ induce linear transformations $h_p^{a,b} : H_p(K_a) \to H_p(K_b)$ at the level of homology. When $\mathbb{F}$ is a field, this sequence of homology groups uniquely decompose (K, f) into a pairing (σ_a, σ_b) demarcating the evolution of homology classes [37]: σ_a marks the creation of a homology class, σ_b marks its destruction, and the difference $|a - b|$ records the lifetime of the class, called its *persistence*. The persistent homology groups are the images of these maps and the persistent Betti numbers are their dimensions:

$$H_p^{a,b} = \begin{cases} H_p(K_a) & a = b \\ \operatorname{Im} h_p^{a,b} & a < b \end{cases}, \qquad \beta_p^{a,b} = \begin{cases} \beta_p(K_a) & a = b \\ \dim(H_p^{a,b}) & a < b \end{cases} \tag{2.2}$$

For a fixed $p \geq 0$, the collection of persistent pairs (a, b) together with unpaired simplices (c, ∞) form a summary representation $\mathrm{dgm}_p(K, f)$ called the *p-th persistence diagram of* (K, f). Conceptually, $\beta_p^{a,b}$ counts the number of persistent pairs lying inside the box $(-\infty, a\,] \times (\,b, \infty)$—the number of persistent homology groups born at or before a that died sometime after b. When a given quantity depends on fixed parameters that are irrelevant or unknown, we use an asterisk. Thus, $H_p^*(K)$ refers to any homology group of K.

We will at times need to generalize the notation given thus far to the *parameterized* setting. Towards this end, for some $\mathcal{A} \subseteq \mathbb{R}^d$, we define an *$\mathcal{A}$-parameterized filtration* as a pair (K, f_α) where K is a simplicial complex and $f : K \times \mathcal{A} \to \mathbb{R}$ an $\mathcal{A}$-parameterized filter function satisfying:

$$f_\alpha(\tau) \leq f_\alpha(\sigma) \ \forall\, \tau \subseteq \sigma \in K \quad \text{and} \quad f_\alpha(\sigma) \text{ is continuous in } \alpha \in \mathcal{A} \text{ for every } \sigma \in K \tag{2.3}$$

Intuitively, when $\mathcal{A} = \mathbb{R}$, one can think of α as a *time* parameter (see Figure 1) and each $f_\alpha(\sigma)$ as tracing a curve in $\mathbb{R}^2$ parameterized by α. Examples of parameterized filtrations include:

- (Constant filtration) For a filter $f : K \to \mathbb{R}$, let (K, f_α) denote the parameterized filtration obtained by declaring $f_\alpha(\sigma) = f(\sigma)$ for all $\alpha \in \mathcal{A}$ and all $\sigma \in K$. We refer to (K, f_α) as the *constant filtration.*
- (Dynamic Metric Spaces) For a finite set X, let $\gamma_X = (X, d_X(\cdot))$ denote a dynamic metric space [22], where $d_X(\cdot) : \mathbb{R} \times X \times X$ denotes a time-varying metric. For any fixed $K \subset \mathcal{P}(X)$, the pair (K, f_α) obtained by setting $f_\alpha(\sigma) = \max_{x,x' \in \sigma} d_X(\alpha)(x, x')$ recovers the notion of a *time-varying Rips filtration.*
- (Filter combinations) For $f, g : K \to \mathbb{R}$ filters over K, a natural family of filtrations (K, h_α) is obtained by $h_\alpha = (1-\alpha)f + \alpha g$ for all $\alpha \in [0, 1]$, i.e. *convex combinations* of f and g.
- (Multi-filtrations) More generally, a d-dimensional filtration on the category of simplicial complexes **Simp** is a functor $\mathcal{F} : \mathbb{R}^d \to \textbf{Simp}$ satisfying $\mathcal{F}(a, b) : \mathcal{F}_a \to \mathcal{F}_b$ an inclusion for all $a \leq b$ []. By fixing $K \in \textbf{Simp}$ and letting $\mathcal{A} = \mathbb{R}^d$, we recover the notion of a *multi-filtration.*

2.1 Technical background

The following results summarize some technical observations motivating this effort, which will be used in several proofs. Though these observations are background material, they contextualize our non-traditional computation of the rank invariant (Corollary 2) and serve as the motivation for this work.

Among the most widely known results for persistence is the structure theorem [37], which shows 1-parameter persistence modules decompose in an *essentially unique* way. Computationally, the corresponding Pairing Uniqueness Lemma [17] asserts that if $R = \partial V$ decomposes the boundary matrix $\partial \in \mathbb{F}^{N \times N}$ to a *reduced* matrix $R \in \mathbb{F}^{N \times N}$ using left-to-right column operations, then:

$$R[i, j] \neq 0 \ \Leftrightarrow \ \mathrm{rank}(R^{i,j}) - \mathrm{rank}(R^{i+1,j}) + \mathrm{rank}(R^{i+1,j\text{-}1}) - \mathrm{rank}(R^{i,j\text{-}1}) \neq 0 \tag{2.4}$$

where $R^{i,j}$ denotes the lower-left submatrix defined by the first j columns and the last $m - i + 1$ rows (rows i through m, inclusive). In other words, the existence of non-zero "pivot" entries in R may be inferred entirely from the ranks of certain submatrices of R. One non-obvious consequence of this fact is the following lemma:

Lemma 1. *Given filtration (K, f) of size $N = |K|$, let $R = \partial V$ denote the decomposition of the filtered boundary matrix $\partial \in \mathbb{F}^{N \times N}$. Then, for any pair (i, j) satisfying $1 \leq i < j \leq N$, we have:*

$$\mathrm{rank}(R^{i,j}) = \mathrm{rank}(\partial^{i,j}) \tag{2.5}$$

Equivalently, all lower-left submatrices of ∂ have the same rank as their corresponding submatrices in R.

An explicit proof of this can be found in [14], though it was also noted in passing by Edelsbrunner [17]. It can be shown by combining (2.4) with the fact that left-to-right column operations preserves the ranks of these "lower-left" submatrices. Though this observation is typically viewed as a minor fact needed to prove the correctness of the reduction algorithm, its implications are quite general, as recently noted by [3]:

Corollary 1 (Bauer et al. [3])**.** *Any persistence algorithm which preserves the ranks of the submatrices $\partial^{i,j}(K, f)$ for all $i, j \in [N]$ is a valid persistence algorithm.*

Indeed, though R is not unique, its non-zero pivots are, and these pivots *define* the persistence diagram. Moreover, due to (2.5), both β_p^* and μ_p^* may be written as a sum of ranks of submatrices of ∂_p and ∂_{p+1}:

Corollary 2 ([10, 14])**.** *Given a fixed $p \geq 0$, a filtration (K, f) with filtration values $\{ a_i \}_{i=1}^N$, and a rectangle $R = [a_i, a_j] \times [a_k, a_l] \subset \Delta_+$, the persistent Betti and multiplicity functions may be written as:*

$$\beta_p^{a_i,a_j}(K, f) = \mathrm{rank}(C_p(K_i)) - \mathrm{rank}(\partial_p^{1,i}) - \mathrm{rank}(\partial_{p+1}^{1,j}) + \mathrm{rank}(\partial_{p+1}^{i+1,j}) \tag{2.6}$$

$$\mu_p^R(K, f) = \mathrm{rank}(\partial_{p+1}^{j+1,k}) - \mathrm{rank}(\partial_{p+1}^{i+1,k}) - \mathrm{rank}(\partial_{p+1}^{j+1,l}) + \mathrm{rank}(\partial_{p+1}^{i+1,l}) \tag{2.7}$$

These rank-based expressions seem neither well known nor widely used—to the authors knowledge, the expression for (2.7) was first pointed out by Chen & Kerber [10], though a more recent and explicit derivation of both expressions is given by Dey & Wang [14]. For completeness, we give our own detailed proof of corollary 2 in the appendix.

Two important observations regarding the expressions from (2.6) and (2.7) are (1) they are comprised strictly of *rank* computations, and (2) all terms involve *unfactored* boundary matrices. The former suggests variational perspectives of the rank function may yield useful relaxations of (2.7) and (2.6); the latter suggests alternate computation strategies beyond reduction, such as e.g. iterative, *matrix-free* approximation schemes. Moreover, the invariance of the rank function under adjoint transformations with zero-characteristic fields coupled with measure-theoretic perspectives on persistence [9] suggest connections to other areas of applied mathematics, such as the rich theory of matrix functions [] or the tools developed as part of "The Laplacian Paradigm" []. The rest of the paper is dedicated to exploring these connections and their implications.

3 Spectral relaxation and its implications

In this section, we will introduce our proposed relaxation of the persistence quantities by successively relaxing and generalizing different aspects of (2.6). To motivate these relaxations, it is instructive to examine the how traditional expressions of the persistent rank invariants compare to those from Corollary 2. Given a filtration (K, f) of size $N = |K|$ with $f : K \to I$ defined over some index set I, its p-th persistent Betti number $\beta_p^{a,b}$ at index $(a, b) \in I \times I$, is defined as follows:

$$\begin{aligned}
\beta_p^{a,b} &= \dim\left(Z_p(K_a)/B_p(K_b)\right) \\
&= \dim\left(Z_p(K_a)/(Z_p(K_a) \cap B_p(K_b)\right) \\
&= \dim\left(Z_p(K_a)\right) - \dim\left(Z_p(K_a) \cap B_p(K_b)\right)
\end{aligned} \tag{3.1}$$

Computationally, observe that (3.1) reduces to one nullity computation and one subspace intersection computation. While the former is easy to re-cast as a spectral computation, computing the latter typically requires obtaining bases via matrix decomposition. Constructing these bases explicitly using conventional [4, 19] or persistence-based [25, 37] algorithms effectively[1] requires $\Omega(N^3)$ time and $\Omega(N^2)$ space. As the persistence algorithm also exhibits $O(N^3)$ time complexity and completely characterizes $\beta_p^{a,b}$ over *all* values $(a, b) \in I \times I$, there is little incentive to compute $\beta_p^{a,b}$ with such direct methods (and indeed, they are largely unused). Because of this, we will focus on expressions (2.6) and (2.7) throughout the rest of the paper.

3.1 Parameterized boundary operators

In typical dynamic persistence settings (e.g. [13]), a decomposition $R = \partial V$ of the boundary matrix ∂ must be permuted and modified frequently to maintain a total order with respect to f_α. In contrast, the rank function is permutation invariant, i.e. for any $X \in \mathbb{R}^{n\times n}$ and permutation P we have:

$$\mathrm{rank}(X) = \mathrm{rank}(P^T X P)$$

This suggests rank computations on boundary matrices need not maintain this ordering—as long as they have the same non-zero pattern as their filtered counterparts, their ranks will be identical. In this section, we exploit this fact by showing how the expressions from (2.6) and (2.7) may be made *permutation invariant.*

Let (K, f_α) denote parameterized family of filtrations of a simplicial complex of size $|K^p| = n$. Fix an arbitrary linear extension $(K, \preceq)$ of the face poset of K. Define the $\mathcal{A}$*-parameterized boundary operator* $\hat{\partial}_p(\alpha) \in \mathbb{R}^{n\times n}$ of (K, f_α) as the $n \times n$ matrix ordered by $\preceq$ for all $\alpha \in \mathcal{A}$ whose entries (k, l) satisfy:

$$\partial_p(\alpha)[k, l] = \begin{cases} s_{kl} \cdot f_\alpha(\sigma_k) \cdot f_\alpha(\sigma_l) & \text{if } \sigma_k \in \partial_p(\sigma_l) \\ 0 & \text{otherwise} \end{cases} \tag{3.2}$$

where $s_{kl} = \mathrm{sgn}([\sigma_k], \partial[\sigma_l])$ is the sign of the oriented face $[\sigma_k]$ in $\partial[\sigma_l]$. Observe that (1) the non-zero entries from (3.2) vary continuously in f_α and (2) $\partial_p(\alpha)$ decouples into a product of diagonal matrices $D_*(f_\alpha)$:

$$\partial_p(\alpha) \triangleq D_p(f_\alpha) \cdot \partial_p(K_\preceq) \cdot D_{p+1}(f_\alpha) \tag{3.3}$$

[1]Note about matrix multiplication constant

where $D_p(f_\alpha)$ and $D_{p+1}(f_\alpha)$ are diagonal matrices whose non-zero entries are ordered by restrictions of f_α to $K^p_\preceq$ and $K^{p+1}_\preceq$, respectively. Clearly, $\mathrm{rank}(\partial_p(\alpha)) = \mathrm{rank}(\partial_p(K_\preceq))$ when the diagonal entries of D_p and D_{p+1} are strictly positive. Moreover, observe we may restrict to those "lower left" matrices from Lemma 1 via post-composing step functions $\bar{S}_a(x) = \mathbb{1}_{x>a}(x)$ and $S_b(x) = \mathbb{1}_{x \leq b}(x)$ to D_p and D_{p+1}, respectively:

$$\hat{\partial}_p^{a,b}(\alpha) \triangleq D_p(\bar{S}_a \circ f_\alpha) \cdot \partial_p(K_\preceq) \cdot D_{p+1}(S_b \circ f_\alpha) \tag{3.4}$$

Though these step functions are discontinuous at their chosen thresholds a and b, we may retain the element-wise continuity of (3.3) by exchanging them with clamped *smoothstep* functions $\mathcal{S} : \mathbb{R} \to [0,1]$ that interpolate the discontinuous step portion of S along a fixed interval $(a, a+\omega)$, for some $\omega > 0$ (see Figure 2).

These observations motivate our first relaxation. Without loss in generality, assume the orientation of the simplices induced by $(K, \preceq)$ is inherited from the order on the vertex set V. To simplify the notation, we write $A^x = A^{*,x}$ to denote the submatrix including all rows of A and all columns of A up to x.

Proposition 1. *Given (K, f_α), any rectangle $R = [a,b] \times [c,d] \subset \Delta_+$, and $\delta > 0$ the number satisfying $a + \delta < b - \delta$ from (1.2) the $\mathcal{A}$-parameterized invariants $\beta_p^{a,b} : \mathcal{A} \times K \to \mathbb{N}$ and $\mu_p^R : \mathcal{A} \times K \to \mathbb{N}$ defined by:*

$$\beta_p^{a,b}(\alpha) \triangleq \mathrm{rank}\big(D_p(S_a \circ f_\alpha)\big) - \mathrm{rank}\big(\,\hat{\partial}_p^{a}(\alpha)\,\big) - \mathrm{rank}\big(\,\hat{\partial}_{p+1}^{b}(\alpha)\,\big) + \mathrm{rank}\big(\,\hat{\partial}_{p+1}^{a+\delta,b}(\alpha)\,\big) \tag{3.5}$$

$$\mu_p^R(\alpha) \triangleq \mathrm{rank}\big(\,\hat{\partial}_{p+1}^{b+\delta,c}(\alpha)\,\big) - \mathrm{rank}\big(\,\hat{\partial}_{p+1}^{a+\delta,c}(\alpha)\,\big) - \mathrm{rank}\big(\,\hat{\partial}_{p+1}^{b+\delta,d}(\alpha)\,\big) + \mathrm{rank}\big(\,\hat{\partial}_{p+1}^{a+\delta,d}(\alpha)\,\big) \tag{3.6}$$

yield the correct quantities $\mu_p^R(K, f_\alpha) = \mathrm{card}\left(\mathrm{dgm}_p(f_\alpha)\big|_R\right)$ and $\beta_p^{a,b} = \dim(H_p^{a,b}(K, f_\alpha))$ for all $\alpha \in \mathcal{A}$.

For completeness, a proof of Proposition 1 is given in the appendix. Note that in (3.4), we write $\partial_p(K_\preceq)$ (as opposed to $\partial_p(K, f)$) to emphasize $\partial_p(K_\preceq)$ is ordered according to a fixed linear ordering $(K, \preceq)$. The distinction is necessary as evaluating the boundary terms from corollary 2 would require ∂ to be explicitly filtered in the total ordering induced by f_α—which varies in $\mathcal{A}$—whereas the expressions obtained by replacing the constitutive terms in (2.6) and (2.7) with (3.5) and (3.6), respectively, require no such explicit filtering.

3.2 Parameterized Laplacians

For the sake of generality, it is important to make the class of expressions for β_p^* and μ_p^* as large as possible. Towards this, we exploit another identity of the rank function applicable to zero-characteristic fields $\mathbb{F}$:

$$\mathrm{rank}(X) = \mathrm{rank}(XX^T) = \mathrm{rank}(X^T X), \quad \text{for all } X \in \mathbb{F}^{n \times m}$$

In the context of boundary operators, note that $\partial_1 \partial_1^T$ is the well known *graph Laplacian* [11], indicating we may express $\beta_0^*(\alpha)$ and $\mu_0^*(\alpha)$ using the ranks of Laplacian[2] matrices. Indeed, a direct result of the singular value decomposition (SVD) is that the eigenvalues of XX^T (or $X^T X$) are given by the squares of the singular values of X; thus, we may study the singular values of boundary operators through the spectra of Laplacians. For any simplicial complex K, its *p-th combinatorial Laplacian* $\Delta_p(K)$ is given by:

$$\Delta_p(K) = \underbrace{\partial_{p+1} \circ \partial_{p+1}^T}_{L_p^{\mathrm{up}}} + \underbrace{\partial_p^T \circ \partial_p}_{L_p^{\mathrm{dn}}} \tag{3.7}$$

All three operators Δ_p, L_p^{up}, and L_p^{dn} are symmetric, positive semi-definite, and compact [25] and thus have non-negative eigenvalues—moreover, the multisets $\Lambda(L_p^{\mathrm{up}})$ and $\Lambda(L_{p+1}^{\mathrm{dn}})$ differ only in the multiplicities of zero, implying they must have identical ranks (see Theorem 2.2 and 3.1 of [21]). Thus, from a persistent rank-based perspective, it suffices to consider any one of these operators.

Let (K, f_α) denote a parameterized family of filtrations of a simplicial complex K equipped with a fixed but arbitrary linear extension $\preceq$ of its face poset and fixed orientations $s(\sigma)$ inherited from the total order on the vertex set $(V, \preceq)$. Without loss of generality, we define the weighted p up-Laplacian $\mathcal{L}_p \triangleq L_p^{\mathrm{up}}$.

$$\mathcal{L}_p^{a,b}(\alpha) \triangleq D_p(\bar{S}_a \circ f_\alpha) \cdot \partial_{p+1}(K_\preceq) \cdot D_{p+1}^2(S_b \circ f_\alpha) \cdot \partial_{p+1}^T(K_\preceq) \cdot D_p(\bar{S}_a \circ f_\alpha) \tag{3.8}$$

[2] By convention, we define $\partial_p = 0$ for all $p \leq 0$.

where $D_p(f)$ denotes a diagonal matrix whose entries represent the application of f to the p-simplices of K. As in (3.4), fixing step function S_a and $\bar{S}_b$ at values $a, b \in \mathbb{R}$ yields operators whose ranks correspond to the ranks of certain "lower-left" submatrices of the matrix decomposition of (K, f). In particular, if $R = \partial V$ is the decomposition of (K, f_α) for some fixed choice of $\alpha \in \mathcal{A}$, then for any pair $a, b \in \Delta_+$ there exists indices $i = \sum_{\sigma \in K}(S_a \circ f_\alpha)(\sigma)$ and $j = \sum_{\sigma \in K}(S_b \circ f_\alpha)(\sigma)$ such that:

$$\operatorname{rank}(R^{i,j}_{p+1}) = \operatorname{rank}(\partial^{i,j}_{p+1}) = \operatorname{rank}(\hat{\partial}^{a,b}_{p+1}) = \operatorname{rank}\left((\hat{\partial}^{a,b}_{p+1})(\hat{\partial}^{a,b}_{p})^T\right) = \operatorname{rank}(\mathcal{L}^{a,b}_p) \tag{3.9}$$

where the second last equality uses the identity $\operatorname{rank}(X) = \operatorname{rank}(X^T X)$. Thus, we may substitute any of the parameterized boundary operators used in Proposition 1 with weighted Laplacian operators $\partial^*_{p+1} \mapsto \mathcal{L}^*_p$ equipped with the appropriate down- and up-step functions S_* and $\bar{S}_*$, respectively.

Remark 1. In the context of inner products, One may interpret sending p-simplices to 0 as restricting to a sub-complex $L \subseteq K$, which suggests simplicial pairs (L, K) satisfying $L \hookrightarrow K$ as in [25]. However, our definition

3.3 Spectral rank relaxation

Under mild assumptions on f_α, the entries of the boundary operators from (3.4) are continuous functions of α. In contrast, as integer-valued invariants, the quantities from Proposition 1 are discontinuous functions. To understand how these discontinuities arise, we consider the spectral characterization of the rank function:

$$\operatorname{rank}(X) = \sum_{i=1}^{n} \operatorname{sgn}_+(\sigma_i(X)), \qquad \operatorname{sgn}_+(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases} \tag{3.10}$$

In the above, $\{\sigma_i\}_{i=1}^n$ are the singular values $\Sigma = \operatorname{diag}(\{\sigma_i\}_{i=1}^n)$ from the singular value decomposition (SVD) $X = U\Sigma V^T$ of $X \in \mathbb{R}^{n\times m}$, and $\operatorname{sgn}_+ : \mathbb{R} \to \{0, 1\}$ is the one-sided sign function. As the singular values vary continuously under perturbations in X [4], it is clear the discontinuity in (3.10) manifests from the one-sided sign function—thus, a natural approach to relaxing (3.10) is to first relax the sgn+ function.

Our approach follows the seminal work of Mangasarian et al. [24]. Let $p : \mathbb{R}_+ \to \mathbb{R}_+$ denote a continuous density function and $\nu : \mathbb{R}_+ \to \mathbb{R}_+$ is a continuous increasing function satisfying $\nu(0) = 0$. One way to approximate the sgn_+ function is to integrate τ-smoothed variations $\hat{\delta}$ of the Dirac delta measure δ:

$$(\forall\, z \geq 0, \tau > 0\,) \qquad \phi(x, \tau) \triangleq \int_{-\infty}^{x} \hat{\delta}(z, \tau)\, dz, \qquad \hat{\delta}(z, \tau) = \frac{1}{\nu(\tau)} \cdot p\left(\frac{z}{\nu(\tau)}\right) \tag{3.11}$$

In contrast to the sgn_+ function, if p is continuous on $\mathbb{R}_+$ then $\phi(\cdot, \tau)$ is continuously differentiable on $\mathbb{R}_+$, and if p is bounded above on $\mathbb{R}_+$, then $\phi(\cdot, \tau)$ is globally Lipshitz continuous on $\mathbb{R}_+$. Moreover, varying $\tau \in \mathbb{R}_+$ in (3.11) yields an τ-parameterized family of continuous sgn_+ relaxations $\phi : \mathbb{R}_+ \times \mathbb{R}_{++} \to \mathbb{R}_+$, where $\tau > 0$ controls the accuracy of the relaxation.

Many properties of the sign approximation from (3.11) extend naturally to the rank function when substituted appropriately via (3.10). In particular, pairing $X = U\Sigma V^T$ with a scalar-valued ϕ that is continuously differentiable at every entry σ of Σ yields a corresponding *Löwner operator* Φ_τ [5]:

Definition 1 (Spectral ϕ-approximation)**.** Given $X \in \mathbb{R}^{n\times m}$ with SVD $X = U\Sigma V^T$, a fixed $\tau > 0$, and any choice of $\phi : \mathbb{R}_+ \times \mathbb{R}_{++}$ satisfying (3.11), define the *spectral ϕ-approximation* $\Phi_\tau(X)$ of X as:

$$\Phi_\tau(X) \triangleq \sum_{i=1}^{n} \phi(\sigma_i, \tau) u_i v_i^T \tag{3.12}$$

where u_i and v_i are the ith columns of U and V, respectively.

At a high level, Definition (3.12) is closely related to that of a *matrix function* $f(A) \triangleq U f(\Lambda) U^T$ defined over square matrices [4]. By imposing additional restrictions via (3.11) on ϕ, the operator Φ_τ exhibits a variety of attractive properties related to rank-approximation, monotonicity, and differentiability.

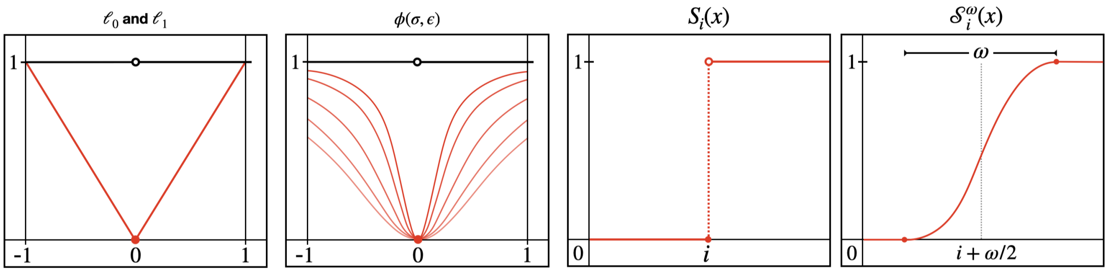


Figure 2: From left to right—the ℓ_1 norm (red) forms a convex envelope over the ℓ_0 (black) pseudo-norm on the interval $[-1,1]$; $\phi(\cdot,\tau)$ from (3.18) at various values of $\tau>0$ (red) and at $\tau=0$ (black); the step function $S_i(x)$ from (3.4); the smoothstep relaxation $\mathcal{S}_i^{\omega}$ from (**??**).

Proposition 2 (Bi et al. [5])**.** *The operator* $\Phi_\tau : \mathbb{R}^{n\times m} \to \mathbb{R}^{n\times m}$ *defined by* (3.12) *satisfies:*

1. *For any* $\tau \geq 0$*, the Schatten-1 norm* $\|\Phi_\tau(X)\|_*$ *of* $\Phi_\tau(X)$ *is given by* $\sum_{i=1}^{n} \phi(\sigma_i,\tau)$
2. *For any* $\tau' \geq \tau$*,* $\|\Phi_{\tau'}(X)\|_* \leq \|\Phi_\tau(X)\|_*$ *for all* $X \in \mathbb{R}^{n\times m}$*.*
3. *For any given* $X \in \mathbb{R}^{n\times m}$ *with rank* $r = \operatorname{rank}(X)$ *and positive singular values* $\Lambda(X) = \{\sigma_1,\sigma_2,\ldots,\sigma_r\}$*:*

   $$0 \leq r - \|\Phi_\tau(X)\|_* \leq r\cdot(1-\phi(\sigma_r,\tau))$$

   Moreover, if τ *satisfies* $0<\tau\leq \sigma_r/r$*, then* $r-\|\Phi_\tau(X)\|_*$ *is bounded above by a constant* $c_\phi(r)\geq 0$*.*
4. $\|\Phi_\tau(X)\|_*$ *is globally Lipshitz continuous and semismooth*[3] *on* $\mathbb{R}^{n\times m}$*.*

Noting property (4), since the sum Lipshitz functions is also Lipshitz, it is easy to verify that replacing the rank function in all of the constitutive terms from Proposition 1 yields Lipshitz continuous functions whenever the filter function f_α is itself Lipshitz and the step functions from (3.4) are smoothed ($\omega>0$).

Remark 2. Though Φ_τ is a continuously differentiable operator[4] in $\mathbb{R}^{n\times m}$ for any $\tau>0$, its Schatten-1 norm $\|\Phi_\tau(X)\|_*$ is only directionally differentiable everywhere on $\mathbb{R}^{n\times m}$ in the Hadamard sense, due to Proposition 2.2(d-e) of [5]. However, $\|\Phi_\tau(X)\|_*$ is differentiable on the positive semi-definite cone $\mathbb{S}_+^n$.

Interpretation #1: In sparse inverse applications, it is commonplace to regularize an objective function to prevent the problem from being ill-posed. For example, the classical least-squares approach to solving the linear system $Ax=b$ is often augmented with the *Tikhonov regularization* (TR) for some $\tau>0$:

$$x_\tau^* = \underset{x\in\mathbb{R}^n}{\arg\min}\|Ax-b\|^2 + \tau\|x\|^2 = (A^TA+\tau I)^{-1}A^Tb \tag{3.13}$$

When $\tau=0$, one recovers the standard ℓ_2 minimization, whereas when $\tau>0$ solutions x_τ^* with small norm are favored. Similarly, by parameterizing ϕ by $\nu(\tau)=\sqrt{\tau}$ and $p(x)=2x(x^2+1)^{-2}$, one obtains via (3.11):

$$\phi(x,\tau) = \int_0^z \hat{\delta}(z,\tau)dz = \frac{2}{\tau}\int_0^z z\cdot\left((z/\sqrt{\tau})^2+1\right)^{-2}dz = \frac{x^2}{x^2+\tau} \tag{3.14}$$

By substituting $\operatorname{sgn}_+ \mapsto \phi$ and composing with the singular value function (3.12), the corresponding spectral rank approximation reduces[5] to the following *trace* formulation:

$$\|\Phi_\tau(A)\|_* = \sum_{i=1}^{n}\frac{\sigma_i(A)^2}{\sigma_i(A)^2+\tau} = \operatorname{Tr}\left[(A^TA+\tau I)^{-1}A^TA\right] \tag{3.15}$$

[3] Here, "semismooth" refers to the existence certain directional derivatives in the limit as $\tau\to 0^+$, see [4, 5].
[4] In fact, it may be shown to be twice continuously differentiable at X if ϕ is twice-differentiable at each $\sigma_i(X)$, see [15])
[5] See Theorem 2 of [36] for a proof of the second equality.

The relaxation parameter τ may be thought of as a bias term that preferences smaller singular values: larger values smooth out $\|\Phi_\tau(\cdot)\|_*$ by making the pseudo-inverse less sensitive to perturbations, whereas smaller values lead to a more faithful[6] approximations of the rank. In this sense, we interpret the quantities obtained by applying (3.12) to the terms from Proposition 1 as *Tikhonov regularized rank invariant approximations.*

Interpretation #2: In shape analysis applications, matrix functions are often used to simulate diffusion processes on meshes or graphs embedded in $\mathbb{R}^d$ to obtain information of about their geometry. For example, consider a weighted graph $G = (V, E)$ with $n = |V|$ vertices with graph Laplacian $L_G = \partial_1 \partial_1^T$. The *heat* of every vertex $v(t) \in \mathbb{R}^n$ as a function of time $t \geq 0$ is governed by L_G and the *heat equation* []:

$$v'(t) = -L_G v(0) \quad \iff \quad L_G \cdot u(x,t) = -\partial u(x,t)/\partial t \tag{3.16}$$

To simulate a diffusion process on G from an initial distribution of heat $v(0) \in \mathbb{R}^n$, it suffices to construct the *heat kernel* $H_t \triangleq \exp(-t \cdot L_G)$ via the spectral decomposition $L_G = U \Lambda U^T$ of L_G:

$$v(t) = H_t \, v(0), \text{ where } H_t = \sum_{i=1}^{n} e^{-t\lambda_i} \, u_i \, u_i^T \tag{3.17}$$

The heat kernel is invariant under isometric deformations, stable under perturbations, and is known to contain multiscale geometric information due to its close connection to geodesics []. As is clear from (3.17), it is also a matrix function. Now, consider (3.11) with $\nu(\tau) = \tau$ and $p(\lambda) = \exp(-\lambda_+)$ where $x_+ = \max(x, 0)$:

$$\phi(\lambda, \tau) = \int_0^z \hat{\delta}(z, \tau) dz = \frac{1}{\tau} \int_0^z \exp(-z/\tau) dz = 1 - \exp(-\lambda/\tau), \quad \text{for all } \lambda \geq 0 \tag{3.18}$$

In the context of diffusion, observe the parameter τ is inversely related diffusion time (i.e. $t = 1/\tau$) and that as $t \to 0$ (or $\tau \to \infty$) the expression $1 - \exp(-\lambda/\tau)$ approaches the sgn_+ function on the interval $[0, \infty)$. As above, substituting ϕ appropriately into Definition (3.12) again yields an equivalent trace expression:

$$\|\Phi_\tau(L_G)\|_* = \sum_{i=1}^{n} 1 - \exp(-t \cdot \sigma_i) = n - \mathrm{Tr}\left[H_t\right] \tag{3.19}$$

The heat kernel trace $\mathrm{Tr}(H_t)$ has been shown to informative at characterizing geometric signatures []. In this sense, we interpret the quantities obtained by applying ... as *geometrically sensitive rank invariant approximations.*

3.4 Properties & Interpretations

To better understand the implications of the relaxations discussed so far, we discuss some of its properties. In what follows, let $\mathcal{L}_p : C^p(K, \mathbb{R}) \to C^p(K, \mathbb{R})$ denote some choice of Laplacian operator and (Φ, ϕ) a τ-parameterized spectral pair satisfying the conditions in definition 3.12.

Proposition 3. *Given any pair (K, f), a rectangle $R = [a, b] \times [c, d] \subset \Delta_+$, and any τ-parameterized spectral function $\phi : \mathbb{R} \to \mathbb{R}$ from definition 3.12, the spectral rank invariants $\hat{\mu}_p^R(\tau)$ and $\hat{\beta}_p^{a,b}(\tau)$ satisfy:*

$$\lim_{\tau \to 0^+} \hat{\mu}_p^R(\tau) = \mu_p^R(K, f), \qquad \lim_{\tau \to 0^+} \hat{\beta}_p^{a,b}(\tau) = \beta_p^{a,b}(K, f)$$

Moreover, for any $\tau \geq 0$, the following inclusion-exclusion relationship always holds:

$$\hat{\mu}_p^R(\tau) = \hat{\beta}_p^{b,c}(\tau) - \hat{\beta}_p^{a,c}(\tau) - \hat{\beta}_p^{b,d}(\tau) + \hat{\beta}_p^{a,d}(\tau)$$

Proof. For limit, use monotonicity + corollary that shows $\phi \to \mathrm{sgn}_+$ in the limit. For the inclusion exclusion, use additivity/ cancellation property / maybe norm properties of Φ from Chazal. □

[6] This can be seen directly by (3.13) as well, wherein increasing τ lowers the condition number of $A^T A + \tau I$ monotonically, signaling a tradeoff in stability at the expense of accuracy.

As an immediate corollary of this, we may generalize the multiplicity function $\hat{\mu}_p^*$ to any arbitrary rectilinear $\mathcal{R} \subset \Delta_+$. This follows from the general theory developed by Chazal et al. [9] on *persistence measures.*

Corollary 3. *The spectral-relaxed* persistence measure *of any simple and connected rectilinear sieve* $\mathcal{R} \subset \Delta_+$ *with* h *corner points* $\partial\mathcal{R} = \{ (a_1, b_1), (a_2, b_2), \ldots, (a_h, b_h) \}$ *given by:*

$$\hat{\mu}_p^{\mathcal{R}} = \sum_{(a,b) \in \partial \mathcal{R}} s_{ab} \cdot \|\Phi(\hat{\mathcal{L}}_p^{a,b})\|_*$$

can be computed using at most $O(h)$ *spectral rank computations, where the sign* $s_{ij} \in \{-1, 1\}$ *is determined by the inclusion-exclusion relationship given by Proposition 3.*

Proof. By the additivity of the multiplicity function, we can vertically or horizontally partition any rectangular into two disjoint rectangles and add their total multiplicity to recover the multiplicity of the whole []. Moreover, if $\mathcal{R}$ is simple and hole-free with h corner points, then it is known that it can be decomposed into a minimal set of $h/2 - g - 1 \sim O(h)$ disjoint rectangles (of which several algorithms are known), where g is the number of axis-parallel line segments connecting concave vertices of $\mathcal{R}$ []. □

Though the inclusion-exclusion relationship between the relaxations $\hat{\mu}_p^*(\tau)$ and $\hat{\beta}_p^*(\tau)$ holds for any $\tau \geq 0$, certain monotonicity properties of $\hat{\beta}_p^*(\tau)$ lose their exactness when $\tau > 0$. As the rank invariant is fundamentally a combinatorial invariant, this is in some sense necessary.

Fortunately, we may bound the degree to $\hat{\beta}_p^*$ remains "Betti-like" in the sense of being cumulative.

Proposition 4 (ϕ-monotone)**.** *For all* $a < b$ *and all* $c < d$*, there exists a positive constant* $c_\phi(\tau) \in \mathbb{R}_+$ *such that* $\hat{\beta}_p^*$ *satisfies the following monotonicity properties:*

$$\hat{\beta}_p^{a,c} \leq \hat{\beta}_p^{b,c} + c_\phi(|a - b|), \qquad \hat{\beta}_p^{a,c} \geq \hat{\beta}_p^{a,d} - c_\phi(|c - d|) \tag{3.20}$$

When $\phi = \mathrm{sgn}_+$*,* c_ϕ *is identically zero, recovering the monotonicity of the PBN (see section 2.1 of [7]).*

Proof. Use Proposition above part (b) with a specific ϕ, then use PBN property. □

In fact, under mild conditions, its been shown that the Tikhonov relaxation ϕ_τ is actually a *uniform* approximation of the rank function []. This is important in rank minimization contexts, wherein it is

4 Computational Implications

Matrix-free computation

Our approach to computing the spectral quantities $\hat{\mu}_p^*$ and $\hat{\beta}_p^*$ is to employ the *Lanczos method* [23], which estimates the eigenvalues of any symmetric linear operator A via projection onto successive Krylov subspaces. Given a symmetric A with eigenvalues $\lambda_1 \geq \lambda_2 > \cdots \geq \lambda_r > 0$ and a vector $v \neq 0$, the order-j Krylov subspaces of the pair (A, v) are the spaces (matrices, resp.) spanned by:

$$\mathcal{K}_j(A, v) \triangleq \mathrm{span}\{v, Av, A^2v, \ldots, A^{j-1}v\}, \quad K_j(A, v) \triangleq [v \mid Av \mid A^2v \mid \cdots \mid A^{j-1}v] \tag{4.1}$$

TODO:

The Lanczos iteration and related subspace methods [] are often called "matrix free" spectral methods due to their singular dependence on a matrix-vector product operator $v \mapsto Av$—this implies A need not necessarily be explicitly represented in memory. Indeed, due to the *three-term recurrence* (A.20), the Lanczos method requires just three $O(n)$-sized vectors and a few $O(n)$ vector operations, motivating the following result:

Lemma 2 ([28, 34])**.** *Given a symmetric rank-*r *matrix* $A \in \mathbb{R}^{n \times n}$ *whose matrix-vector operator* $A \mapsto Ax$ *requires* $O(\eta)$ *time and* $O(\nu)$ *space, the Lanczos iteration computes* $\Lambda(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_r\}$ *in* $O(\max\{\eta, n\} \cdot r)$ *time and* $O(\max\{\nu, n\})$ *space, when computation is done in exact arithmetic.*

For sparse symmetric matrices $A \in \mathbb{R}^{n \times n}$ with an average of ν nonzeros per row, Lanczos requires $O(n\nu r)$ operations per iteration [19]. Thus, the efficiency of the Lanczos method depends on the availability of a fast `matvec` operator, which arises typically in either very sparse or very structured operators. For example, when A is a graph Laplacian $L = \partial_1 \partial_1^T$, the complexity of the $x \mapsto Lx$ operation is linear in $|E|$ due to its graph structure. It is not immediately clear whether a similar result generalizes to combinatorial Laplacian operators derived from simplicial complexes—our next result affirms this.

Lemma 3. *For any $p \geq 0$ and simplicial complex K with $n = |K^p|$ and $m = |K^{p+1}|$, if there exists a hash function $h : K^p \to [n]$ with $O(1)$ access time and $O(c)$ storage, then there exists a two-phase algorithm for computing the inner product $x \mapsto \langle L_p, x \rangle$ in $O(m(p+1))$ time and $O(\max(c, m))$ storage.*

The algorithm and proof are given in appendix section A.1. From a practical perspective, many hash table implementations achieve expected $O(1)$ access time using only a linear amount of storage, and as $p \geq 0$ is typically quite small—typically no greater than two—the operation $x \mapsto Lx$ in practice exhibits $\approx O(m)$ time and space complexities. We delegate more practical issues regarding the computation to appendix C. Combining Lemmas 2 and 3 yields the following result.

Proposition 5. *For any constant $p \geq 0$, the spectra $\Lambda(L_p)$ of a rank-r combinatorial Laplacian operator $L_p : \mathbb{R}^n \to \mathbb{R}^n$ derived from a simplicial complex K with $n = |K^p|$ and $m = |K^{p+1}|$ can be computed in $O(mr)$ time and $O(m)$ storage via the Lanczos iteration, when carried out in exact arithmetic.*

Remark 3. The standard reduction-family of algorithms computes the p-th persistent homology of a filtration K of size $N = |K|$ in $O(N^3)$ time and $O(N^2)$ space, respectively (these bounds are actually tight $\Theta(N^3)$, see []). Interestingly, Chen and Kerber [10] have shown that since the persistence diagram contains at most $N/2 = O(N)$ points, it may be constructed using at most $2N - 1$ "μ-queries" (evaluations of μ_p^R) via a divide-and-conquer scheme on the index-persistence plane—thus, by Theorem 5, we can match the same $O(N^3)$ complexity in constructing the full diagram using only rank computations.

As in [28], the assumption of exact arithmetic simplifies both the presentation of the theory and the corresponding complexity statements. In practice, finite-precision arithmetic introduces both rounding and cancellation errors into the computation, which primarily manifests as loss of orthogonality between the Lanczos vectors. These errors not only affect the methods convergence rate towards an invariant subspace, but in fact they muddle the termination condition entirely.

Randomized approximation

Recently, it's been discovered that

Subspace acceleration

As in [28], the assumption of exact arithmetic simplifies both the presentation of the theory and the corresponding complexity statements. Although this assumption is unrealistic in practical settings, it yields a grounded expectation of what is possible to achieve in the *finite-precision* regime: any implementation computing the largest j eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_j\}$ using the Lanczos iteration in finite-precision arithmetic requires at least $\Omega(\max\{\eta, n\} \cdot j)$ time and $\Omega(\max\{\nu, n\})$ space to complete.

In practice, finite-precision arithmetic introduces both rounding and cancellation errors into the computation, which manifests as loss of orthogonality between the Lanczos vectors. These errors not only affect the methods convergence rate towards an invariant subspace, but in fact they muddle the termination condition entirely. One option to ameliorate this issue is to orthogonalize q_{j+1} against $k > 3$ Lanczos vectors to retain the simplicity of the iteration. Another option is to continue the expansion of the Krylov subspace. For a Laplacian operator $\mathcal{L}$ of size $|n|$, it is not uncommon for a naive Lanczos implementation to require upwards of $\approx O(n)$ (or worse) `matvec`'s to converge towards small or locally clustered eigenvalues. Fortunately, several decades of research have been dedicated to developing orthogonality-enforcement schemes that retain the simplicity of the Lanczos iteration without increasing either the time or space complexities by non-trivial factors.

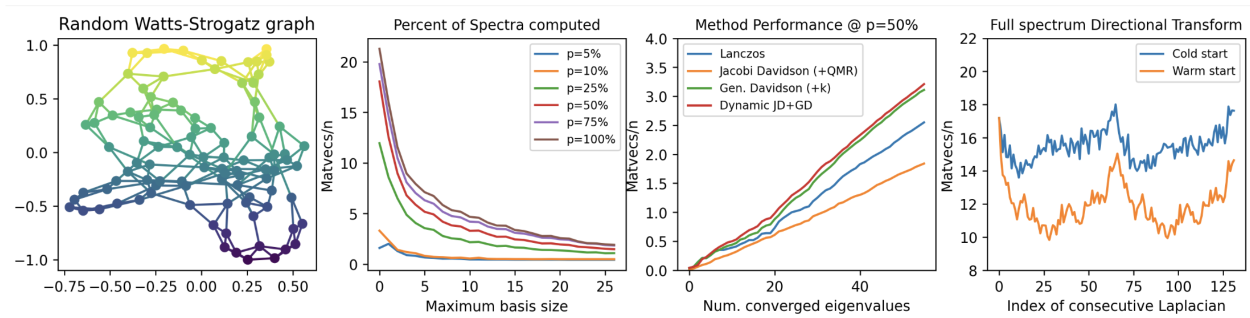
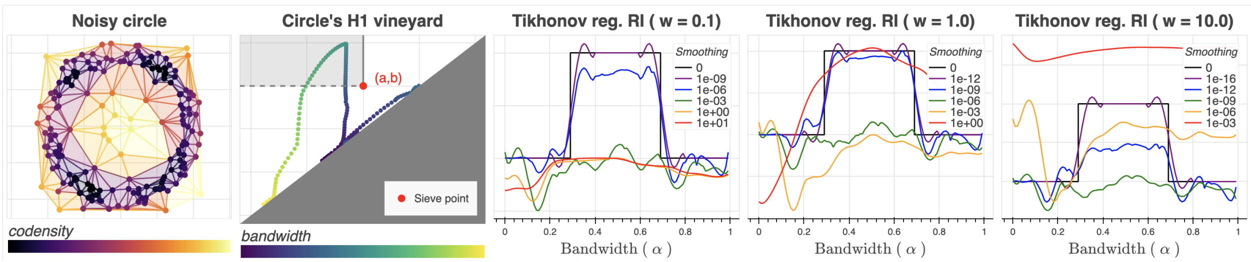


Figure 3: Random Watts-Strogatz "Small world" graph example

4.1 Empirical experiments

The first and most general application of the work presented here is the matrix-free computation of persistent rank invariants in effectively $O(n^2)$ time and $O(m)$ storage, where $n = |K^p|$ and $m = |K^{p+1}|$. To demonstrate this empirically, we sampled 30 random graphs according to the Watts-Strogatz [] rules with parameters $n = 500, k = 10, p = 0.15$. These graphs tend to exhibit 'small world' characteristics inherited by many real-world networks, such as social networks, gene networks, and transportation networks. For our purposes, since the graph distance between pairs of nodes scale logarithmically with the size of the graph, we ensure the sampled random graphs to be uniformly sparse. The corresponding incidence matrix $\partial_1 \in \mathbb{R}^{n \times m}$ and up-Laplacians $L_0^{\mathrm{up}} \in \mathbb{R}^{n \times n}$ would have $\approx 5,000$ and $\approx 5,500$ non-zero entries, were they to be formed explicitly, which are weighted according randomly by embedding the graph in the plane and filtering graph via its sublevel sets in a random direction. To test the scability of the laplacian operator studied here, we computed various percentages of the spectra of these 30 graphs via iterative methods discussed in section **??** and reported various of their time- and storage- related statistics in figure 3. All statistics reported are the average statistics collected from all 30 random graphs, which were collected using various iterative methods implemented the PRIMME software []. On the far left of figure 3, we display a random metric embedding of a small Watts-Strogatz graph to convey the structure of the type of graphs we consider. On the left side of figure 3 next to the example network model, we record the ratio of `matvec` operations (relative to n) needed to compute $p\%$ of the spectrum as a function of the maximum number basis vectors kept in-memory for reorthogonalization purposes. The ideal Lanczos method needs just 3 such vectors in exact arithmetic due to the three-term recurrence, justifying the space complexity record in 2; in contrast, with finite-precision arithmetic, one needs additional basis vector to ensure the orthonormality of the eigenvectors to machine precision. Each additional basis vector simultaneously increases both the cost of performing a Lanczos step and the accuracy of the orthogonalization, which subsequently decreases the number of total `matvec` operations needed. As one can see from the plot, having $\approx 20 - 25$ basis vectors is more than enough to ensure the ratio of `matvec` operations is kept to a small constant (in this case, less than 5) when approximating any portion of the spectra. This justifies our claim that combinatorial Laplacian operators, for many real-world data sets, requires just $O(m)$ memory complexity to compute eigenvalues (and thus, the persistent rank invariants). The remaining two figures on the right side of figure 3 show the same ratio of `matvecs`$/n$—effectively the constant associated with quadratic time complexity statement in 2



5 Applications & Experiments

Filtration optimization

It is common in TDA for the filter function $f : K \to \mathbb{R}$ to itself be parameterized by some hyper-parameters. For example, consider the removal of noisy outliers from a point set $X \subset \mathbb{R}^d$ prior to studying X through the lens of persistence. Though persistence is stable under the Hausdorff noise model [], diagrams are notably unstable with respect to *strong outliers*—these outliers can obscure the detection of non-trivial topological space. Even a single point can suppress presence of an otherwise strongly persistent pair.

To illustrate an exemplary use-case of our spectral relaxation, we re-cast the problem of identifying strong outliers as a *filtration optimization* problem. Consider a fixed Delaunay complex K realized from a set of points $X \subset \mathbb{R}^2$ sampled around S^1, shown in figure **??**. Observe the point set contains both points affected by Hausdorff noise and strong outliers. To detect both these strong outliers and the presence of S^1, we first filter K by the sublevel sets $\hat{f}_h^{-1}((-\infty, t]) \subseteq X$ of a kernel density estimate $\hat{f}_h : X \to \mathbb{R}_+$ [], which itself depends on bandwidth parameter $h > 0$ and the choice of a smooth kernel function $\mathcal{K}_h : \mathbb{R} \to \mathbb{R}_+$. Subsequently, for some fixed $(i, j) \in \Delta_+$, we seek a bandwidth h^* maximizing the persistent Betti number $\beta_p^{i,j}$ of (K, f_h):

$$h^* = \underset{h \in \mathbb{R}}{\arg\max}\ \beta_p^{i,j}(K, \hat{f}_h), \qquad \text{where } \hat{f}_h(x) = \frac{1}{nh} \sum_i \mathcal{K}_h(x_i - x) \tag{5.1}$$

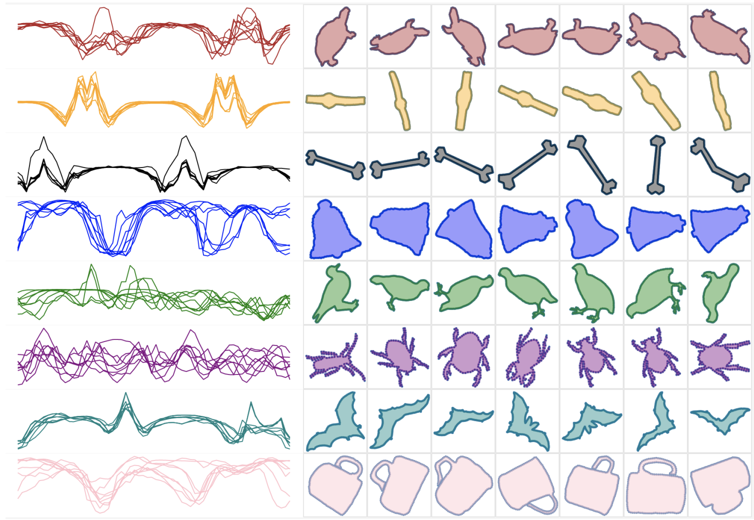
Assuming the pair (i, j) is chosen well enough such that the objective $\beta_p^{i,j}$ is not trivially zero for all $h > 0$, observe the objective function $\beta_p^{i,j}$ is discontinuous, and non-differentiable. To obviate this difficulty, we substitute the objective $\beta_p^{i,j} \mapsto \hat{\beta}_p^{i,j}$ with a spectral relaxation $\hat{\beta}_p^{i,j}(h; \phi_\tau)$ for some matrix function ϕ_τ that depends on a smoothness parameter $\tau \geq 0$. When $h > 0$, the objective is differentiable, thus first-order optimization techniques may be used.

Shape comparison

In general, both combinatorial and topological aspects of a given topological space are encoded in the spectra of Laplacian operators. Through their null-space, combinatorial Laplacians encode a complexes basic topology via its homology groups—this is identical for most of the Laplace operators, whether they are normalized, weighted, signless, and so on []. In contrast, these operators differ in the nonzero part of the spectrum, which encode specific geometric information in addition to topological properties.

6 Conclusion & Future Work

Interestingly, our results also imply the existence of an efficient output-sensitive algorithm for computing Γ-persistence pairs with at least $(\Gamma > 0)$-persistence (via [10]) that requires the operator $x \mapsto \partial x$ as its only input, which we consider to be of independent interest.



A Appendix

Expanded Intro

Though homology is primarily studied as a topological invariant, the fact that persistent homology encodes both topological and geometric information in its diagram has motivated its use not only as a shape descriptor but also as a metric invariant. Metric invariants, or "signatures," are commonly used in metric learning to ascertain whether two comparable data sets X, Y represent the same object—typically up to a some notion of invariance. One mathematically attractive model for measuring the dissimilarity between shapes/datasets is the Gromov-Hausdorff (GH) distance $d_{\mathrm{GH}}((X, d_X), (Y, d_Y)$ between compact metric spaces $(\mathcal{X}, d_X), (\mathcal{Y}, d_Y)$: by altering the choice of metric (d_X, d_Y), the corresponding metric-distance d_{GH} can be adapted to a chosen notion of invariance [] or to increase its discriminating power []. Though it is NP-hard to compute [], the GH distance defines a metric on the set of isomorphism classes of compact metric spaces endowed with continuous real-valued functions, justifying its study as a mathematical model for shape matching and metric learning. Moreover, it is known that the GH distance is tightly lower-bounded by the bottleneck distance between persistence diagrams constructed over Rips filtrations $R(X, d_X), R(Y, d_Y)$ [], which can be computed in polynomial time. Indeed, Solomon et al [] showed distributed persistence invariants characterize the quasi-isometry type of the underlying space, allowing one to provably interpolate between geometric and topological structure.

Though theoretically well-founded and information dense, persistence diagrams come with their own host of practical issues: they are sensitive to strong outliers, far from injective, and their de-facto standard computation exhibits high algorithmic complexity. Moreover, the space of persistence diagrams $\mathcal{D}$ is a Banach space, preventing one from doing even basic statistical operations, such as averaging []. As a result, many researchers have focused on extending, enhancing, or otherwise supplementing persistence diagrams with additional information. Turner et al [] proposed associating a collection a shape descriptors with a PL embedded $X \subset \mathbb{R}^d$—one descriptor for each point on S^{d-1}—which they called a *transform*. More exactly, suppose both the data X and its geometric realization K are PL embedded in $\mathbb{R}^d$ and has centered and scaled appropriately. The main theorem in [] is that associating a persistence diagram, or even a simpler descriptor such as the Euler characteristic, for every point on S^{d-1} is actually sufficient information to theoretically reconstruct K.

Missing from the above work is the are two important directions: how do you configure such transforms to retain the important topological/geometric information and discard irrelevant information, and (2) how may we efficiently compute them? The former question is synonymous with choosing the invariance model in the GH framework, which seems to be highly domain specific. In the latter case, though we know the number of directions is bounded [], the bound is simply too high to be of any practical use. While there are efficient algorithms for both the ECC and persistence computations in static settings, the state of the art in parameterized settings is non-trivial and ongoing research area.

Expanded Background

Laplacian Energy: Ever since Kirchoff's matrix tree theorem, which relates any cofactor of the graph Laplacian to the number of spanning trees of a graph.... functions summarizing the spectra of Laplacian operators with a scalar value have found many applications, from quantifying hierarchical image complexities, to summarizing electrical resistance between vertices in a circuit network, to indicating the melting or boiling point of certain polycyclic aromatic hydrocarbons in chemical applications []. More generally, the sum of the largest k eigenvalues of L is related to the clique number of the graph, as a measure of complexity. is often termed the *Laplacian energy*, has used

Letters

As topological invariants, Betti numbers are invariant under homeomorphisms: any pair of filtrations (K, f) and (K', f') that are homotopy equivalent have identical homology classes and thus isomorphic persistence diagrams. This invariance can be a useful thing at the level of homology, as non-homeomorphic spaces can sometimes be differentiated by inspecting differences between their corresponding homology classes. However, invariance under homeomorphisms can at times discard geometric information that may be useful for differentiating objects. For example, consider creating a classifier for the alphabet of English characters in the font shown below:

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

If one were to triangulate images of each of the letters shown above and compute their Betti numbers, one would find just three homology classes: one class for those letters that have two holes (B), one class of letters that have one hole (A, D, O, P, Q, and R), and one class for the rest of the letters, which collapse to points. Thus, if one were concerned with differentiating letters of the alphabet, one may conclude that homology is not simply not strong enough of an invariant to do so.

It would be beneficial to have an invariant that was sensitive to the geometries between shapes, but also stable in some sense.

A.1 Combinatorial Laplacians

The natural extension of the graph Laplacian L to simplicial complexes is the *p-th combinatorial Laplacian* Δ_p, whose explicit matrix representation is given by:

$$\Delta_p(K) = \underbrace{\partial_{p+1} \circ \partial_{p+1}^T}_{L_p^{\text{up}}} + \underbrace{\partial_p^T \circ \partial_p}_{L_p^{\text{dn}}} \tag{A.1}$$

Indeed, when $p = 0$, $\Delta_0(K) = \partial_1 \partial_1^T = L$ recovers the graph Laplacian. As with boundary operators, $\Delta_p(K)$ encodes simplicial homology groups in its nullspace, a result known as the discrete Hodge Theorem []:

$$\tilde{H}_p(K; \mathbb{R}) \cong \ker(\Delta_p(K)), \quad \beta_p = \text{nullity}(\Delta_p(K)) \tag{A.2}$$

The fact that the Betti numbers of K may be recovered via the nullity of $\Delta_p(K)$ has been well studied (see e.g. Proposition 2.2 of []). In fact, as pointed out by [], one need not only consider Δ_p as the spectra of Δ_p, L_p^{up}, and L_p^{dn} are intrinsically related by the identities:

$$\Lambda(\Delta_p(K)) \doteq \Lambda(L_p^{\text{up}}) \,\dot{\cup}\, \Lambda(L_p^{\text{dn}}), \qquad \Lambda(L_p^{\text{up}}) \doteq \Lambda(L_{p+1}^{\text{dn}}) \tag{A.3}$$

where $A \doteq B$ and $A \,\dot{\cup}\, B$ denotes equivalence and union between the *non-zero* elements of the multisets A and B, respectively. Moreover, all three operators Δ_p, L_p^{up}, and L_p^{dn} are symmetric, positive semidefinite, and compact—thus, for the purpose of estimating β_p, it suffices to consider only one family of operators.

To translate the continuity results from definition **??** to any of the Laplacian operators above, we must consider weighted versions. Here, a *weight function* is a non-negative real-valued function defined over the set of all faces of K:

$$w : K \to \mathbb{R}_+ \tag{A.4}$$

The set of weight functions and the choice of scalar product on $C^p(K, \mathbb{R})$ wherein elementary cochains are orthogonal are in one-to-one correspondence [] (see Appendix A.1). In this way, we say that the weight function *induces* an inner product on $C^p(K, \mathbb{R})$:

$$\langle\, f, g \,\rangle_w = \sum_{\sigma \in K^p} w(\sigma) f([\sigma]) g([\sigma]) \tag{A.5}$$

Moreover, Laplacian operators are uniquely determined by the choice of weight function. This correspondence permits us to write the matrix representation of Δ_p explicitly:

$$\Delta_p(K, w) \triangleq W_p^+ \partial_{p+1} W_{p+1} \partial_{p+1}^T \; + \; \partial_p^T W_p^+ \partial_p W_{p+1} \tag{A.6}$$

where $W_p = \text{diag}(\{\, w(\sigma_i) \,\}_{i=1}^n)$ represents a non-negative diagonal matrices restricted $\sigma \in K^p$ and W^+ denotes the pseudoinverse. Note that (A.6) recovers (A.1) in the case where w is the constant map $w(\sigma) = 1$, which we call the *unweighted* case.

Unfortunately, various difficulties arise with weighting combinatorial Laplacians with non-constant weight functions, such as asymmetry, scale-dependence, and spectral instability. Indeed, observe that in general neither terms in (A.6) are symmetric unless $W_p = I_n$ (for L_p^{up}) or $W_{p+1} = I_m$ (for L_p^{dn}). However, as noted in [25], L_p^{up} may be written as follows:

$$L_p^{\text{up}} = W_p^+ \partial_{p+1} W_{p+1} \partial_{p+1}^T = W_p^{+/2} \big(W_p^{+/2} \partial_{p+1} W_{p+1} \partial_{p+1}^T W_p^{+/2} \big) W_p^{1/2} \tag{A.7}$$

Since (A.7) is of the form $W^+ P W$ where $P \in S_n^+$ and W is a non-negative diagonal matrix, this rectifies the symmetry problem. Towards bounding the spectra of L_p^{up}, Horek and Jost [] propose *normalizing* Δ_p by augmenting w's restriction to K^p:

$$w(\tau) = \sum_{\tau \in \partial(\sigma)} w(\sigma) \quad \forall\, \tau \in K^p,\, \sigma \in K^{p+1} \tag{A.8}$$

Substituting the weights of the p-simplices in this way is equivalent to mapping $W_p \mapsto \mathcal{D}_p$ where $\mathcal{D}_p$ is the *diagonal degree matrix*. The corresponding substitution in (A.7) yields the *weighted combinatorial normalized Laplacian* (up-)operator:

$$\mathcal{L}_p^{\mathrm{up}} = (\mathcal{D}_p)^{+/2} \partial_p W_{p+1} \partial_p^T (\mathcal{D}_p)^{+/2} = \mathcal{I}_n - \mathcal{A}_p^{\mathrm{up}} \tag{A.9}$$

where $\mathcal{A}_p^{\mathrm{up}}$ is a weighted adjacency matrix, and $\mathcal{I}_n$ is the identity matrix with $\mathcal{I}(\tau) = \mathrm{sign}(w(\tau))$ (see Section **??**). The primary benefit of this normalization is that it guarantees $\Lambda(\mathcal{L}_p^{\mathrm{up}}) \subseteq [0, p+2]$ for any choice of weight function, from which one obtains several useful implications, such as tight bounds on the spectral norm []. The same results holds for up-, down-, and combinatorial Laplacians. Moreover, as we will show in a subsequent section, one obtains stability properties with degree-normalization not shared otherwise.

Remark 4. Compared to (A.7), is it worth remarking that one important quality lost in preferring $\mathcal{L}_p^{\mathrm{up}}$ over L_p^{up} is diagonal dominance.

Inner Products

Though the general Laplacian operator carries with it an interpretation of its eigensets as representing information about the intersection pattern of the underlying complex, a more precise interpretation of the eigensets depends both the operator and weighting scheme in question. Many early results followed Kirchhoff's observations about the properties of L reflecting certain physical laws of electrical flows in circuit networks, wherein eigenvectors have certain interpretations useful for graph sparsification and graph partitioning [11]. More recently, Nadler observed the *normalized* graph Laplacian given by:

$$\mathcal{L} = D^{-1/2}(D - A)D^{-1/2} \tag{A.10}$$

connects the process of diffusion (over a probability density) to the eigensets to $\mathcal{L}$. Yet another choice of normalization relates the eigenfunctions of $\mathcal{L}$ to the discrete Laplace–Beltrami operator on manifolds [], which carries a certain "heat" interpretation with it. Ultimately, just as persistence diagrams encode geometric interpretations through their domain-specific filter functions, the geometry contained in the spectra of combinatorial Laplacians is reflected by the choice of a domain-specific weight function.

Weight functions may be interpreted through their action on the coboundary vector space $C^p(K, \mathbb{R}) := \mathrm{Hom}(K, \mathbb{R})$. As with $C_p(K, \mathbb{R})$, a basis for $C^p(K, \mathbb{R})$ is given by the set of its *elementary cochains*:

$$\{ \ \chi([\sigma]) \mid [\sigma] \in B_p(K, \mathbb{R}) \ \}, \text{ where } \chi([\sigma']) = \begin{cases} 1 & \text{if } [\sigma'] = [\sigma] \\ 0 & \text{otherwise} \end{cases} \tag{A.11}$$

It can be shown that for any choice of inner product on $C^p(K, \mathbb{R})$, there exists a positive weight function $f : K \to \mathbb{R}_+ \setminus \{0\}$ satisfying:

$$\langle \, g, h \, \rangle_f = \sum_{\sigma \in K^p} f(\sigma) g([\sigma]) h([\sigma]) \tag{A.12}$$

Furthermore, the set of weight functions and scalar product on $C^p(K, \mathbb{R})$ wherein elementary cochains are orthogonal are in one-to-one correspondence []. Indeed, if $f : (\mathbb{R}^n, H_n) \to (\mathbb{R}^m, H_m)$ be a linear map between inner product matrices $H_n \in \mathbb{R}^{n \times n}$ and $H_m \in \mathbb{R}^{m \times m}$, then by Proposition [] for any $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$, we have the following equivalence of inner products:

$$\langle fx, y \rangle_{\mathbb{R}^m} = \langle x, f^* y \rangle_{\mathbb{R}^n} = x^T F^T H_m y = x^T H_n F^* y$$

where $F \in \mathbb{R}^{m \times n}$ denotes the matrix representative of f and $F^* = H_n^{-1} F^T H_m$ a representative of the adjoint $f^* : (\mathbb{R}^m, H_m) \to (\mathbb{R}^n, H_n)$ of f. In this way, we say that the choice of weight function *induces* an inner product on $C^p(K, \mathbb{R})$[7]. In this way, we reduce the study of geometry to the study "weight functions" of laplacian operators.

[7] Nullspace comment

Laplacian matvec

We first recall the characteristics of the graph Laplacians $x \mapsto Lx$ operation. Given a simple undirected graph $G = (V, E)$, let $A \in \{0,1\}^{n \times n}$ denote its binary adjacency matrix satisfying $A[i,j] = 1 \Leftrightarrow i \sim j$ if the vertices $v_i, v_j \in V$ are adjacent in G, and let $D = \mathrm{diag}(\{\, \deg(v_i) \,\})$ denote the diagonal *degree* matrix, where $\deg(v_i) = \sum_{j \neq i} A[i,j]$. The *graph Laplacian*'s adjacency, incidence, and element-wise definitions are:

$$L = D - A = \partial_1 \circ \partial_1^T \,, \qquad L\,[i,j] = \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \sim j \\ 0 & \text{if } i \nsim j \end{cases} \tag{A.13}$$

Furthermore, by using the adjacency relation $i \sim j$ as in [11], the linear and quadratic forms of L may be succinctly expressed as:

$$(\,\forall\, x \in \mathbb{R}^n\,) \qquad (Lx)_i = \deg(v_i) \cdot x_i - \sum_{i \sim j} x_j \,, \qquad x^T L x = \sum_{i \sim j} (x_i - x_j)^2 \tag{A.14}$$

If G has m edges and n vertices taking labels in the set $[n]$, computing the product from (A.14) requires just $O(m)$ time and $O(n)$ storage via two edge traversals: one to accumulate vertex degrees and one to remove components from incident edges. By precomputing the degrees, the operation reduces further to a single $O(n)$ product and $O(m)$ edge pass, which is useful when repeated evaluations for varying values of x are necessary.

To extend the two-pass algorithm outlined above when $p > 0$, we first require a generalization of the connected relation from (A.14). Denote with $\mathrm{co}(\tau) = \{\, \sigma \in K^{p+1} \mid \tau \subset \sigma \,\}$ the set of proper cofaces of $\tau \in K^p$, or *cofacets*, and the (weighted) *degree* of $\tau \in K^p$ with:

$$\deg_w(\tau) = \sum_{\sigma \in \mathrm{co}(\tau)} w(\sigma)$$

Note setting $w(\sigma) = 1$ for all $\sigma \in K$ recovers the integral notion of degree representing the number of cofacets a given p-simplex has. Now, since K is a simplicial complex, if the faces τ, τ' share a common cofacet $\sigma \in K^{p+1}$, this cofacet $\{\sigma\} = \mathrm{co}(\tau) \cap \mathrm{co}(\tau')$ is in fact *unique* [18]. Thus, we may use a relation $\tau \overset{\sigma}{\sim} \tau'$ to rewrite the operator from (A.7) element-wise:

$$L_p^{\mathrm{up}}(\tau, \tau') = \begin{cases} \deg_w(\tau) \cdot w^{+}(\tau) & \text{if } \tau = \tau' \\ s_{\tau,\tau'} \cdot w^{+/2}(\tau) \cdot w(\sigma) \cdot w^{+/2}(\tau') & \text{if } \tau \overset{\sigma}{\sim} \tau' \\ 0 & \text{otherwise} \end{cases} \tag{A.15}$$

where $s_{\tau,\tau'} = \mathrm{sgn}([\tau], \partial[\sigma]) \cdot \mathrm{sgn}([\tau], \partial[\sigma])$. Ordering the p-faces $\tau \in K^p$ along a total order and choosing an indexing function $h : K^p \to [n]$ enables explicit computation of the corresponding matrix-vector product:

$$(L_p^{\mathrm{up}}\, x)_i = \deg_w(\tau_i) \cdot w^{+}(\tau_i) \cdot x_i + w^{+/2}(\tau_i) \sum_{\tau_j \overset{\sigma}{\sim} \tau_i} s_{\tau_i,\tau_j} \cdot x_j \cdot w(\sigma) \cdot w^{+/2}(\tau_j) \tag{A.16}$$

Observe (A.16) can be evaluated now via a very similar two-pass algorithm as described for the graph Laplacian if the simplices of K^{p+1} can be quickly enumerated and the indexing function h can be efficiently evaluated.

Lanczos background

Computing eigen-decompositions $A = V \Lambda V^T$ of symmetric matrices $A \in S_n$ generally consists of two phases: (1) reduction to tridiagonal form $Q^T A Q = T$ via orthogonal similarity transformations Q, and (2) diagonalization of the tridiagonal form $T = Y \Theta Y^T$. While the latter may be performed in $O(n \log n)$ time [20], the former is effectively bounded below by $\Omega(n^3)$ for dense full-rank matrices using traditional (i.e. non-Strassen) matrix operations, and thus it is the reduction to tridiagonal form that dominates the computation. Lanczos [23] proposed the *method of minimized iterations*—now known as the *Lanczos method*—as an attractive alternative for reducing A into a tridiagonal form and thus revealing its spectrum.

The means by which the Lanczos method estimates eigenvalues is by projecting onto successive Krylov subspaces. Given a large, sparse, symmetric $n \times n$ matrix A with eigenvalues $\lambda_1 \geq \lambda_2 > \cdots \geq \lambda_r > 0$ and a vector $v \neq 0$, the order-j Krylov subspaces of the pair (A, v) are the spaces spanned by:

$$\mathcal{K}_j(A, v) := \operatorname{span}\{v, Av, A^2v, \ldots, A^{j-1}v\} = \operatorname{range}(K_j(A, v)) \tag{A.17}$$

where $K_j(A, v) = [v \mid Av \mid A^2v \mid \cdots \mid A^{j-1}v]$ are their corresponding Krylov matrices. Krylov subspaces arise naturally from using the minimal polynomial of A to express A^{-1} in terms of powers of A. In particular, if A is nonsingular and its minimal polynomial has degree m, then $A^{-1}v \in K_m(A, v)$ and $K_m(A, v)$ is an invariant subspace[8] of A. Since A is symmetric, the spectral theorem implies that A is orthogonally diagonalizable and that we may obtain $\Lambda(A)$ by generating an orthonormal basis for $\mathcal{K}_n(A, v)$. To do this, the Lanczos method constructs successive QR factorizations of $K_j(A, v) = Q_j R_j$ for each $j = 1, 2, \ldots, n$. Due to A's symmetry and the orthogonality of Q_j, the identity $q_k^T A q_l = q_l^T A^T q_k = 0$ is satisfied for all $k > l + 1$, giving the corresponding $T_j = Q_j^T A Q_j$ a tridiagonal structure:

$$T_j = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_{j-1} \\ & & & \beta_{j-1} & \alpha_j \end{bmatrix}, \ \beta_j > 0, \ j = 1, 2, \ldots, n \tag{A.18}$$

Unlike the spectral decomposition $A = V\Lambda V^T$—which identifies a diagonalizable A with its spectrum $\Lambda(A)$ up to a change of basis $A \mapsto M^{-1}AM$—there is no canonical choice of T_j due to the arbitrary choice of v. However, there is a connection between the iterates $K_j(A, v)$ and the full tridiagonalization of A: if $Q^T A Q = T$ is tridiagonal and $Q = [\, q_1 \mid q_2 \mid \cdots \mid q_n \,]$ is an $n \times n$ orthogonal matrix $QQ^T = I_n = [e_1, e_2, \ldots, e_n]$, then:

$$K_n(A, q_1) = QQ^T K_n(A, q_1) = Q[\, e_1 \mid Te_1 \mid T^2 e_1 \mid \cdots \mid T^{n-1} e_1 \,] \tag{A.19}$$

is the QR factorization of $K_n(A, q_1)$—that is, tridiagonalizing A with respect to a unit-norm q_1 determines Q. Indeed, the Implicit Q Theorem [19] asserts that if an upper Hessenburg matrix $T \in \mathbb{R}^{n \times n}$ has only positive elements on its first subdiagonal and there exists an orthogonal matrix Q such that $Q^T A Q = T$, then Q and T are *uniquely* determined by (A, q_1). As a result, given an initial pair (A, q_1) satisfying $\|q_1\| = 1$, we may restrict and project A to its j-th Krylov subspace T_j via:

$$AQ_j = Q_j T_j + \beta_j q_{j+1} e_j^T \qquad (\beta_j > 0) \tag{A.20}$$

where $Q_j = [\, q_1 \mid q_2 \mid \cdots \mid q_j \,]$ is an orthonormal set of vectors mutually orthogonal to q_{j+1}. Equating the j-th columns on each side of (A.20) and rearranging the terms yields the *three-term recurrence*:

$$\beta_j \, q_{j+1} = Aq_j - \alpha_j \, q_j - \beta_{j\text{-}1} \, q_{j\text{-}1} \tag{A.21}$$

where $\alpha_j = q_j^T A q_j$, $\beta_j = \|r_j\|_2$, $r_j = (A - \alpha_j I)q_j - \beta_{j\text{-}1} q_j$, and $q_{j+1} = r_j / \beta_j$. Equation (A.21) is a variable-coefficient second-order linear difference equation, and it is a known fact that such equations have unique solutions: if $(q_{j\text{-}1}, \beta_j, q_j)$ are known, then $(\alpha_j, \beta_{j+1}, q_{j+1})$ are completely determined. The sequential process that iteratively builds T_j via the recurrence from (A.21) is called the *Lanczos iteration*. Note that if A is singular and we encounter $\beta_j = 0$ for some $j < n$, then $\operatorname{range}(Q_j) = \mathcal{K}_j(A, q_1)$ is an A-invariant subspace, the iteration stops, and we have solved the symmetric eigenvalue problem: $\Lambda(T_j) = \Lambda(A)$, $j = \operatorname{rank}(A)$, and T_j is orthogonally similar to A.

Directional Transform

The canonical interpretation of the information displayed by a persistence diagram is that is summarizes the persistence of the sublevel sets of filtered space. Given a filtration pair $(\, K, f \,)$ where K is a finite simplicial

[8] Recall that if $S \subseteq \mathbb{R}^n$, then S is called an *invariant subspace* of A or A-*invariant* iff $x \in A \implies Ax \in S$ for all $x \in S$.

complex and $f : K \to \mathbb{R}$ is a real-valued function, the sublevel sets $|K|_i = f^{-1}(-\infty, i]$ deformation retract to... If K is embedded in $\mathbb{R}^d$, then geometrically f takes on the interpretation of a 'height' function whose range yields the 'height' of every simplex in K.

Let $X \subset \mathbb{R}^d$ denote a data set which can be written as a finite simplicial complex K whose simplices are PL-embedded in $\mathbb{R}^d$. Given this setting, define the *directional transform* (DT) of K as follows:

$$\begin{aligned} \mathrm{DT}(K) : S^{d-1} &\to K \times C(K, \mathbb{R}) \\ v &\mapsto (K_\bullet, f_v) \end{aligned}$$

where we write $(K_\bullet, f)$ to indicate the filtration on K induced by f_v for all $\alpha \in \mathbb{R}$, i.e.:

$$K_\bullet = K(v)_\alpha = \{ \, x \in X \mid \langle x, v \rangle \leq \alpha \, \} \tag{A.22}$$

Conceptually, we think of DT as an S^{d-1}-parameterized family of filtrations.

The Persistent Homology Transform (PHT) is a shape statistic that establishes a fundamental connection between the topological information summarized by K's PH groups and the geometry of its associated embedding. Given a complex K built from X, it is defined as:

$$\begin{aligned} \mathrm{PHT}(K) : S^{d-1} &\to \mathcal{D}^d \\ v &\mapsto \big(\, \mathrm{dgm}_0(K, v), \mathrm{dgm}_1(K, v), \ldots, \mathrm{dgm}_{d-1}(K, v) \, \big) \end{aligned} \tag{A.23}$$

where $\mathcal{D}$ denotes the space of p-dimensional persistence diagrams, for all $p = 0, \ldots, d-1$ and S^{d-1} the unit $d-1$ sphere. The stability of persistence diagrams ensures that the map $v \mapsto \mathrm{dgm}_p(K, v)$ is Lipschitz with respect to the bottleneck distance metric $d_B(\cdot, \cdot)$ whenever K is a finite simplicial complex. Thus, the PHT may be thought of as an element in $C(S^{d-1}, \mathcal{D}^d)$: .

The primary result of [] is that the PHT is injective on the space of subsets of R^d that can be written as finite simplicial complexes[9], which we denote as $\mathcal{K}_d$. Equivalently, $\mathcal{K}_d$ decomposes space of all pairs (K, f) under the equivalence $(K, f) \sim (K, f')$ when $f(K) = f'(K)$.

A.2 Complexity of Persistence & Related work

We briefly recount the main complexity results of the persistence computation. With a few key exceptions, the majority of persistent homology implementations and extensions is based on the *reduction algorithm* introduced by Edelsbrunner and Zomorodian [17]. This algorithm factorizes the filtered boundary into a decomposition $R = \partial V$, where V is full rank upper-triangular and R is said to be in reduced form: if its i-th and j-th columns are nonzero, then $\mathrm{low}_R(i) \neq \mathrm{low}_R(j)$, where $\mathrm{low}_R(i)$ denotes the row index of the lowest non-zero in column i. We refer to [17, 2, 14] for details.

Given a filtration (K, f) of size $m = |K|$ with filter $f : K \to [m]$, the reduction algorithm in form given in [17] computes $\mathrm{dgm}_p(K; \mathbb{Z}/2) = \{ \, (\tau_1, \sigma_1), (\tau_2, \sigma_2), \ldots, (\tau_k, \sigma_k) \, \}$ runs in time proportional to the sum of the squared (index) persistences $\sum_{i=1}^k (f(\sigma_i) - f(\tau_i))^2$. As k is at most $m/2$, this implies a $O(m^3)$ upper bound on the complexity of the general persistence computation, which incidentally Morozov showed was a tight $\Theta(m^3)$ under the assumption that each column reduction takes $O(m)$ time. By exploiting the matrix-multiplication results, a similar result can be shown to reduce to $O(m^\omega)$, where ω is the matrix-multiplication constant, which is ≈ 2.37 as of this time of writing. It worth remarking that the complexity statements above are all given in terms of the number of *simplices* m: if $n = |K^0|$ is the size of the vertex set, the above implies a worst-case bound of $O(n^{\omega(p+2)})$ on the general persistence computation. For example, if we use non-Strassen-based matrix multiplication ($\omega = 3$) and we are concerned with $p = 1$ homology computation, the complexity of the reduction algorithm scales $O(n^9)$ in the number of vertices of the complex, which is essentially intractable for most real world application settings.

Despite the seemingly immense intractability of the persistence computation, decades of advancements have been made in reducing the complexity or achieving approximate results in reasonable time and space complexities. The complexity of the reduction algorithm is complicated by the fact that it depends heavily

[9] Implicit in the injectivity statement of the PHT is that, given a subset $X \subset \mathbb{R}^d$ which may be written as finite simplicial complex K, the restriction $f : X \to \mathbb{R}$ to any simplex in K must is linear.

on the structure of the associated filtration K, the homology dimension p, the field of coefficients $\mathbb{F}$, and the assumptions about the space K manifests from. In [], Sheehy presented an algorithm for producing a sparsified version $(\tilde{K}, \tilde{f})$ of a given Vietoris-Rips filtration (K, f) constructed from an n-point metric space (X, d_X) whose total number of p-simplices is bounded above by $n \cdot (\epsilon^{-1})^{O(pd)}$, where d is the doubling dimension of X. It was shown that $\mathrm{dgm}_p(\tilde{K})$ is guaranteed to be a multiplicative c-approximation to the $\mathrm{dgm}_p(K)$, where $c = (1 - 2\epsilon)^{-1}$ and $\epsilon \leq 1/3$ is a positive approximation parameter. When $p = 0$ and the filtration function $f : K \to \mathbb{R}$ is PL, the reduction algorithm can be bypassed entirely in favor of simple $O(n \log n + \alpha(n)m) \approx O(m)$ algorithm (see Algorithm 5 in [14]), where $n = |K^0|$ and $m = |K^1|$ and $\alpha(n)$ is the extremely slow-growing inverse Ackermann function. Moreover, the $d-1$ persistence pairs can be computed in $O(n\alpha(n))$ time algorithm for filtrations of simplicial d-manifolds essentially reducing the problem to computing persistence on a dual graph [14]. For clique complexes, the apparent pairs optimization—which preemptively removes zero-persistence pairs from the computation prior to the reduction—has been empirically observed to reduce the number of columns needing reduced for clique complexes by $\approx 98-99\%$ [2]. Numerous other optimizations, including e.g. the *clearing optimization*, the use of *cohomology*, the *implicit reduction* technique, have further reduced both the non-asymptotic constant factors of the reduction algorithm significantly, see [2] and references therein for a full overview.

Despite the dramatic reductions in time and space needed for the persistence algorithm to complete, to the author knowledge relatively little has been done in improving the complexity and effective runtime of the reduction in parameterized settings. Although both of these algorithms have shown significant constant-factor reductions in the (re)-reduction of the associated sparse matrices, all of the techniques require $O(m^2)$ storage to execute as the R and V matrices must be maintained throughout the computation. Moreover, all three of the above methods intrinsically work within the reduction framework, wherein simulating persistence in dynamic contexts effectively reduces to the combinatorial problem of maintaining a valid $R = \partial V$ decomposition.

As noted in [14], the reduction algorithm is essentially a variant of Gaussian elimination. Indeed, the persistence of a given filtration can be computed by the PLU factorization of a matrix. The explicit decompositional approach of factorizing a large matrix into constitutive parts is known historically in numerical linear algebra as a *direct method*—methods would yield the exact solution within a finite number of steps. In contrast, iterative methods start with approximate solution and progressively update the solution up to arbitrary accuracy. The iterative methods well-known to the numerical linear algebra community, such as Krylov methods, are typically often attractive not only due to the reduction in computational work over direct approaches but also of the limited amount of memory that is required. Despite the success of iterative methods in efficiently solving linear systems manifesting from diagonally dominant sparse matrices is [], such advancements have not yet been extended to the persistence setting.

Output sensitive multiplicity and Betti

We record this fact formally with two corollaries. Let $\mathrm{R}_p(k)$ denotes the complexity of computing the rank of square $k \times k$ matrix with at most $O((p+1)k)$ non-zero $\mathbb{F}$ entries. Then we have:

Corollary 4. *Given a filtration $K_\bullet$ of size $N = |K_\bullet|$ and indices $(i, j) \in \Delta_+^N$, computing $\beta_p^{i,j}$ using expression* (2.6) *requires $O\big(\max\{\mathrm{R}_p(n_i), \mathrm{R}_{p+1}(m_j)\}\big)$ time, where $n_i = |K_i^p|$ and $m_j = |K_j^{p+1}|$.*

Observe the relation $\partial_{p+1}^{i+1,j} \subseteq \partial_{p+1}^{1,j}$ implies the dominant cost of computing (2.6) lies in computing either $\mathrm{rank}(\partial_p^{1,i})$ or $\mathrm{rank}(\partial_{p+1}^{1,j})$, which depends on the relative sizes of $|K^p|$ and $|K^{p+1}|$. In contrast, μ_p^R is localized to the pair (K_i, K_l) and depends only on the $(p+1)$-simplices in the interval $[i, l]$, yielding the following corollary.

Corollary 5. *Given a filtration $K_\bullet$ of size $N = |K_\bullet|$ and a rectangle $R = [i, j] \times [k, l]$ with indices $0 \leq i < j \leq k < l \leq N$, computing μ_p^R using expression* (2.7) *requires $O(\mathrm{R}_{p+1}(m_{il}))$ time $m_{il} = |K_l^{p+1}| - |K_i^{p+1}|$.*

A.3 Finite-precision arithmetic

It is well established in the literature that the Lanczos iteration, as given in its original form, it effectively useless in practice due to significant rounding and cancellation errors. Such errors manifest as loss of orthogonality between the computed Lanczos vectors, which drastically affects the convergence of the method. At first glance, this seems to be a simple numerical issue, however the analysis from Parlett [28] showed, loss of orthogonality is not merely the result of gradual accumulation of roundoff error—it is in fact is intricately connected to the convergence behavior of Lanczos iteration. One obvious remedy to this is to reorthogonalize the current Lanczos vectors $\{q_{j-1}, q_j, q_{j+1}\}$ against all previous vectors using Householder matrices [19]—a the *complete reorthogonalization* scheme. This process guarantees orthogonality to working precision, but incurs a cost of $O(jn)$ for each Lanczos step, effectively placing the iteration back into the cubic time and quadratic memory regimes the direct methods exhibit. A variety of orthogonality enforcement schemes have been introduced over years, including implicit restart schemes, selective reorthogonalization, thick restarts, block methods, and so on; see [] for an overview.

A.4 Laplacian Interpretation

In what follows we make a connection between boundary matrices and the graph Laplacian to illustrate how the Laplacian captures the "connectivity" aspects of the underlying simplicial complex.

Example A.1 (Adapted from [26])**.** Suppose the ordered vertices of G are labeled from 1 to n such that, given any subset $X \subseteq V$, we may define column vector $x = (\, x_i \,)$ whose components $x_i = 1$ indicate $i \in X$ and $x_i = 0$ otherwise. Then, given $X \subseteq V$ and its complement set $X' = V \setminus X$, we have:

$$\begin{aligned}
(Lx)_i > 0 &\iff i \in X \text{ and } |c_i(X)| = (Lx)_i \\
(Lx)_i < 0 &\iff i \in X' \text{ and } |c_i(X')| = |(Lx)_i| \\
(Lx)_i = 0 &\iff i \in X \cup X' \text{ and } c_i(X) = \emptyset
\end{aligned}$$

where $c_v(X) = \{(v, w) \in E \mid v \in X \text{ and } w \in V \setminus X\}$ denotes the *cutset* of X restricted to v, i.e. the set of edges having as one endpoint $v \in X$ and another endpoint outside of X.

In other words, example A.1 demonstrates that L captures exactly how X is connected to the rest of G. Notice that if $X = V$, then $Lx = 0$ and thus 0 must be an eigenvalue of L with an eigenvector pair $\mathbf{1}$. Like the adjacency matrix, the interpretation of the matrix-vector product has a natural extension to powers of L, wherein just as entries in A^k model paths, entries in L^k are seen to model boundaries [26].

Parameterizing Settings

We include a few examples of potential application areas of work. Namely, we show a few promising examples of "parameterized settings" that may naturally benefit from our efforts here.

Dynamic Metric Spaces: Consider an $\mathbb{R}$-parameterized metric space $\delta_X = (X, d_X(\cdot))$ where X is a finite set and $d_X(\cdot) : \mathbb{R} \times X \times X \to \mathbb{R}_+$, satisfying:

1. For every $t \in \mathbb{R}, \delta_X(t) = (X, d_X(t))$ is a pseudo-metric space[10]
2. For fixed $x, x' \in X$, $d_X(\cdot)(x, x') : \mathbb{R} \to \mathbb{R}_+$ is continuous.

When the parameter $t \in \mathbb{R}$ is interpreted as *time*, the above yields a natural characterization of a "time-varying" metric space. More generally, we refer to an $\mathbb{R}^h$-parameterized metric space as *dynamic metric space*(DMS). Such space have been studied more in-depth [] and have been shown...

Rayleigh Ritz values Though the Lanczos iterations may be used to obtain the full tridiagonalization $A = QTQ^T$, intermediate spectral information is readily available in T_j, for $j < \text{rank}(A)$. Diagonalizing $T_j = Y\Theta Y^T$ yields value/vector pairs $\{(\theta_1^{(j)}, y_1^{(j)}), \ldots, (\theta_j^{(j)}, y_j^{(j)})\}$ satisfying $w^T(Ay - \theta y) = 0$ for all $w \in \mathcal{K}_j(A, q_1)$, called *Ritz pairs.* The values θ are called *Ritz values* and their associated vectors $v = Qy$ in the range of Q are called *Ritz vectors.* From the Ritz perspective, the Lanczos iteration implicitly maintains two orthonormal basis for $K_j(A, q_1)$—a Lanczos basis Q and the Ritz basis Y:

$$A = QTQ^T = QY\Theta Y^T Q^T \iff AQY = QY\Theta$$

[10] This is required so that if one can distinguish the two distinct points $x, x' \in X$ incase $d_X(t)(x, x') = 0$ at some $t \in \mathbb{R}$.

In principle, the Lanczos basis $\{q_i\}_{i=1}^{j}$ changes each iteration, while the Ritz basis $\{Qy_i^{(j)}\}_{i=1}^{j}$ changes after each subspace projection. The way in which the Ritz values approach the spectrum of A is well-studied [], as they are known to be Rayleigh-Ritz approximations of A's eigenpairs $\Lambda(A) = \{(\lambda_1, v_1), \ldots, (\lambda_j, v_j)\}$, and they are collectively known to be optimal in the sense that $T_k = B$ is the matrix that minimizes $\|AQ_k - Q_k B\|_2$ over the space of all $k \times k$ matrices. Moreover, Ritz values contain intrinsic information of the distance between $\Lambda(T_j)$ and $\Lambda(A)$. To see this, note that:

$$\|Av_i^{(j)} - v_i^{(j)}\theta_i^{(j)}\| = \beta_i^{(j)} = \beta_{j+1} \cdot |\langle e_j, y_i^{(j)} \rangle| \tag{A.24}$$

Thus, we need not necessarily keep the Lanczos vectors Q in memory to monitor how close the spectra of the T_j's approximate $\Lambda(A)$. In fact, it is known that the Ritz values $\{\theta_1^{(1)}, \theta_1^{(2)}, \ldots, \theta_1^{(j)}\}$ of T_j satisfy:

$$|\lambda - \theta_i^{(j)}| \leq \big(\beta_i^{(j)}\big)^2 / \big(\min_{\mu} |\mu - \theta_i^{(j)}|\big) \tag{A.25}$$

The full convergence of the Ritz values to the eigenvalues of A is known to converge at a rate that depends on the ratio between λ_1/λ_n. A full analysis is done in terms of Chebychev Polyonomials in [19]. In practice, it has been observed that the Lanczos iteration converges super-linearly towards the extremal eigenvalues of the spectrum, whereas for interior eigenvalues one typically must apply a shifting scheme.

Convergence Rate

The ability of the Krylov subspace iteration to capture the extremal portions of the spectrum remains unparalleled, and by using $O(n)$ memory, the Lanczos iteration uses optimal memory. As mentioned in section **??**, when the computation is carried out in finite-precision arithmetic, one may observe loss of orthogonality in the Lanczos vectors. Fortunately, the connection between the Lanczos method and the Rayleigh quotient ensures *eventual* termination of the procedure under by restarting the Lanczos method, and continue with the iteration until the spectrum has been approximated to some prescribed accuracy. Unfortunately, if the number of iterations k is e.g. larger than n^2, then the method may approach to $O(r \max(\mathcal{M}(n), n), n) \approx O(n^3)$ complexity one starts with. If the supplied matrix-vector product operation is fast, the number of iterations k needed for convergence of the Lanczos method becomes the main bottleneck estimating the spectrum of A.

Loss of orthogonality can be mitigated by re-orthogonalizaing against all previous Lanczos vectors, but this increases the Lanczos complexity to $\approx O(n^2)$ per iteration. Thus, the goal is strike a balance: find a way to keep all n Lanczos numerically orthonormal, so as to ensure super-linear convergence of the Ritz values θ, but do so using $c \cdot n$ memory, where c is a relatively small constant.

Since rates of convergence α increases the number of correct digits by an expoentnial rate with factor $alpha$, any super-linear convergent ($\alpha > 1$) method needs at most c terms to approximate an eigen-pair up to numerical precision. In the context of the Lanczos method, achieving even quadratic convergence would imply the number of iterations needed to obtain machine-precision is bounded by $T(c \cdot \mathcal{M}(n) \cdot r)$, where c is a small constant. We say that a method which achieves *superlinear* convergence has complexity *essentially* $O(c \cdot n) \approx O(n)$.

Among the more powerful methods for achieving super linear convergence towards a given eigenvalue λ is the Jacobi-Davidson method. This method seeks to correct:

Solving for t results in the *correction equation*

$$(I - uu^T)(A - \sigma I)(I - uu^T)t = \theta u - Au \tag{A.26}$$

where, since u is unit-norm, $I - uu^T$ is a projector onto the complement of span(u). It's been shown that solving exactly for this correction term essentially constructs an cubically-convergent sequence towards some $\theta \mapsto \lambda$ in the vicinity of σ. Solving for the correction equation exactly is too expensive, sparking efforts to approximate it. It turns out that, just as the Lanczos method in exact arithmetic is highly related to the conjugate gradient method for solving linear systems, solving for the correction equation exactly is in some ways conceptually similar to making an Newton step in the famous Newtons method from nonlinear optimization. Since (**??**) is approximated, the JD method is often called in the literature akin to making an "inexact newton step" [].

The JD method with inexact Newton steps yields an individual eigenvalue estimate with quadratic convergence—*essentially* $O(m)$ time after some constant number matrix-vector products and $O(n)$ memory. The Lanczos method, in contrast, estimates all eigenvalues in essentially quadratic time if the convergence rate is superlinear. Pairing these two methods is a non-trivial endeavor. In a sequence of papers, Stathopoulos et al [] investigated various strategies for approximately solving the correction equation. In , they give both theoretical and empricial evidence to suggest that by employing generalized Davidson and Jacobi-Davidson like solvers within an overarching Lanczos paradigm, they achieve nearly optimal methods for estimating large portions of the spectrum using $O(1)$ number of basis vectors. By approximating the inner iterations with the symmetric Quasi-Minimal Residual (QMR) method, they argue that JD cannot converge more than three times slower than the optimal method, and empirically they find the constant factor to be less than 2.

A common way of quantifying the sensitivity of the spectrum of a given linear operator M is through its condition number. For $M = XX^T$ a given positive definite matrix, its *condition number* $\kappa(M)$ is defined as:

$$\kappa(M) = \|M^{-1}\|\|M\| = |\lambda_1(M)| \;/\; |\lambda_n(M)| \tag{A.27}$$

The condition number $\kappa(M)$ directly measures of how sensitive the spectrum of M is too perturbations in its entries. In particular, if $E \in \mathbb{R}^{n\times n}$ represents a small perturbation of $M \in \mathbb{R}^{n\times n}$, then:

$$\frac{\|(M+E)^{-1} - M^{-1}\|}{\|M^{-1}\|} \leq \kappa(M)\frac{\|E\|}{\|M\|} \tag{A.28}$$

Thus, the effect of adding ϵI_n to a given matrix can be interpreted as a means of reducing κ arbitrarily—at the expense of accuracy—to stabilize the pseudo-inverse. For operators $\Phi_\epsilon(\cdot)$ in the form above, we can quantify this stabilization using perturbation analysis.

A.5 Proofs

Proof of rank equivalence

In general, it is not true that $\mathrm{rank}(A) = \mathrm{rank}(\mathrm{sgn}(A))$. However, it is true that $\mathrm{rank}(\partial_p) = \mathrm{rank}(\mathrm{sgn}(\partial_p))$.

Proof of Lemma 1

Proof. The Pairing Uniqueness Lemma [14] asserts that if $R = \partial V$ is a decomposition of the total $m \times m$ boundary matrix ∂, then for any $1 \leq i < j \leq m$ we have $\mathrm{low}_R[j] = i$ if and only if $r_\partial(i,j) = 1$. As a result, for $1 \leq i < j \leq m$, we have:

$$\mathrm{low}_R[j] = i \iff r_R(i,j) \neq 0 \iff r_\partial(i,j) \neq 0 \tag{A.29}$$

Extending this result to equation (2.5) can be seen by observing that in the decomposition, $R = \partial V$, the matrix V is full-rank and obtained from the identity matrix I via a sequence of rank-preserving (elementary) left-to-right column additions. □

Proof of Proposition 1

Proof. We first need to show that $\beta_p^{i,j}$ can be expressed as a sum of rank functions. Note that by the rank-nullity theorem, so we may rewrite (3.1) as:

$$\beta_p^{i,j} = \dim\left(C_p(K_i)\right) - \dim\left(B_{p-1}(K_i)\right) - \dim\left(Z_p(K_i) \cap B_p(K_j)\right)$$

The dimensions of groups $C_p(K_i)$ and $B_p(K_i)$ are given directly by the ranks of diagonal and boundary matrices, yielding:

$$\beta_p^{i,j} = \mathrm{rank}(I_p^{1,i}) - \mathrm{rank}(\partial_p^{1,i}) - \dim\left(Z_p(K_i) \cap B_p(K_j)\right)$$

To express the intersection term, note that we need to find a way to express the number of p-cycles born at or before index i that became boundaries before index j. Observe that the non-zero columns of R_{p+1} with index at most j span $B_p(K_j)$, i.e $\{ \mathrm{col}_{R_{p+1}[k]} \neq 0 \mid k \in [j] \} \in \mathrm{Im}(\partial_{p+1}^{1,j})$. Now, since the low entries of the non-zero columns of R_{p+1} are unique, we have:

$$\dim(Z_p(K_i) \cap B_p(K_i)) = |\Gamma_p^{i,j}| \tag{A.30}$$

where $\Gamma_p^{i,j} = \{ \mathrm{col}_{R_{p+1}[k]} \neq 0 \mid k \in [j], 1 \leq \mathrm{low}_{R_{p+1}}[k] \leq i \}$. Consider the complementary matrix $\bar{\Gamma}_p^{i,j}$, given by the non-zero columns of R_{p+1} with index at most j that are not in $\Gamma_p^{i,j}$, i.e. the columns satisfying $\mathrm{low}_{R_{p+1}}[k] > i$. Combining rank-nullity with the observation above, we have:

$$|\bar{\Gamma}_p^{i,j}| = \dim(B_p(K_j)) - |\Gamma_p^{i,j}| = \mathrm{rank}(R_{p+1}^{i+1,j}) \tag{A.31}$$

Combining equations (A.30) and (A.31) yields:

$$\dim(Z_p(K_i) \cap B_p(K_j)) = |\Gamma_p^{i,j}| = \dim(B_p(K_j)) - |\bar{\Gamma}_p^{i,j}| = \mathrm{rank}(R_{p+1}^{1,j}) - \mathrm{rank}(R_{p+1}^{i+1,j}) \tag{A.32}$$

Observing the final matrices in (A.32) are *lower-left* submatrices of R_{p+1}, the final expression (2.6) follows by applying Lemma 1 repeatedly. □

Proof of boundary matrix properties

Proof. First, consider property (1). For any $t \in T$, applying the boundary operator ∂_p to $K_t = \mathrm{Rips}_\epsilon(\delta_{\mathcal{X}}(t))$ with non-zero entries satisfying (**??**) by definition yields a matrix ∂_p satisfying $\mathrm{rank}(\partial_p) = \dim(\mathrm{B}_{p-1}(K_t))$. In contrast, operators of the from (3.4) always produce p-boundary matrices of Δ_n; however, notice that the only entries which are non-zero are precisely those whose simplices σ that satisfy $\mathrm{diam}(\sigma) < \epsilon$. Thus, $\mathrm{rank}(\partial_p^t) = \dim(\mathrm{B}_{p-1}(K_t))$ for all $t \in T$. < (show proof of (2))> Property (3) follows from the construction of ∂_p and from the inequality $\|A\|_2 \leq \sqrt{m}\|A\|_1$ for an $n \times m$ matrix A, as $\|\partial_p^t\|_1 \leq (p+1)\,\epsilon$ for all $t \in T$.

□

A.6 Proofs of basic properties

Proof. The above result immediately follows by applying the fact that $\lim_{\tau \to 0^+} \|\Phi_\tau(X)\|_* = \mathrm{rank}(X)$ to each of the constitutive terms of $\hat{\mu}_{p,\tau}^R$ and $\hat{\beta}_{p,\tau}^{i,j}$. □

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A Boundary matrix factorization

Definition 2 (Boundary matrix decomposition)**.** Given a filtration $K_\bullet$ with m simplices, let ∂ denote its $m \times m$ filtered boundary matrix. We call the factorization $R = \partial V$ the *boundary matrix decomposition* of ∂ if:

I1. V is full-rank upper-triangular

I2. R satisfies $\mathrm{low}_R[i] \neq \mathrm{low}_R[j]$ iff its i-th and j-th columns are nonzero

where $\mathrm{low}_R(i)$ denotes the row index of lowest non-zero entry of column i in R or null if it doesn't exist. Any matrix R satisfying property (I2) is said to be *reduced*; that is, no two columns share the same low-row indices.

B Laplacian facts

In general, the spectrum of the graph Laplacian L is unbounded, [] and instead many prefer to work within the "normalized" setting where eigenvalues are bounded. The *normalized Laplacian* $\mathcal{L}$ of a graph G is typically given as:

$$\mathcal{L}(G) = D^{-1/2} L D^{-1/2} \tag{B.1}$$

with the convention that $D^{-1}(v_i, v_i) = 0$ for $\deg(v_i) = 0$. The variational characterization of eigenvalues in terms of the Rayleigh quotient of $\mathcal{L}$ convey a particular form. Specifically, for any real-valued function $f : V \to \mathbb{R}$ on G, when viewed as a column vector, $\mathcal{L}$ satisfies:

$$\frac{\langle f, \mathcal{L} f\rangle}{\langle f, f\rangle} = \frac{\sum\limits_{i \sim j} (g(v_i) - g(v_j))^2}{\sum\limits_{i} g(v_i)^2 \cdot \deg(v_i)} \tag{B.2}$$

where $f = D^{1/2}g$ and $\langle f, g\rangle$ denotes the standard inner product in $\mathbb{R}^n$. Equation (B.2) may be used to show that the spectrum $\Lambda(\mathcal{L})$ is bounded in the interval $[0, 2]$. In particular, it is known that:

$$\lambda_i \leq \sup_f \frac{\langle f, \mathcal{L}f\rangle}{\langle f, f\rangle} \leq 2 \tag{B.3}$$

Recall that, when G is connected, 0 is an eigenvalue of both L and $\mathcal{L}(G)$, with multiplicity $\mathrm{cc}(G)$. Moreover, if G is the union of disjoint graphs $G_1, G_2, \dots, G_k$, then it has as its spectrum the union of the spectra $\Lambda(G_1), \Lambda(G_2), \dots, \Lambda(G_k)$. Certain parts of the spectrum of $\mathcal{L}$ can be deduced explicitly for very structured types of G, such as complete graphs, complete bipartite graphs, star graphs, path graphs, and cycle graphs, and n-cubes. For a list of additional properties the graph and normalized Laplacians satisfy, including bounds on eigenvalues, relation to random walks and rapidly-mixing Markov chains, identities tied to isoperimetric properties of graphs, and explicit connections to spectral Riemannian geometry, see [11] and references within.

C Laplacian `matvec` products

Below is pseudocode outlining how to evaluate a weighted (up) Laplacian matrix-vector multiplication built from a simplicial complex K with $m = |K^{p+1}|$ and $n = |K^p|$ in essentially $O(m)$ time when $m > n$ and p is considered a small constant. Key to the runtime of the operation being essentially linear is the constant-time determination of orientation between p-faces ($s_{\tau,\tau'}$)—which can be inlined during the computation—and the use of a deterministic $O(1)$ hash table $h : K^p \to [n]$ for efficiently determining the appropriate input/output offsets to modify (i and j). Note the degree computation occurs only once.

Algorithm 1 `matvec` for weighted p up-Laplacians in $O(m(p+1)) \approx O(m)$ time ($p \geq 0$)

Require: Fixed oriented complex K of size $N = |K|$
Optional: Weight functions $w_{p+1} : K^{p+1} \to \mathbb{R}_+$ and $w_p^l, w_p^r : K^p \to \mathbb{R}_+$
Output: $y = \langle\, L_p^{\mathrm{up}}, x \,\rangle = (W_p \circ \partial_{p+1} \circ W_{p+1} \circ \partial_{p+1}^T \circ W_p)x$

1: // Precompute weighted degrees $\deg_w$
2: Define $h : K^p \to [\,n\,]$
3: $\deg_w \leftarrow \mathbf{0}$
4: **for** $\sigma \in K^{p+1}$ **do**:
5:     **for** $\tau \in \partial[\sigma]$ **do**:
6:         $\deg_w[h(\tau)] \leftarrow \deg_w[h(\tau)] + w_p^l(\tau) \cdot w_{p+1}(\sigma) \cdot w_p^r(\tau)$
7:
8: **function** UpLaplacianMatvec($x \in \mathbb{R}^n$)
9:     $y \leftarrow \deg_w \odot x$ (element-wise product)
10:     **for** $\sigma \in K^{p+1}$ **do**:
11:         **for** $\tau,\ \tau' \in \partial[\sigma] \times \partial[\sigma]$ **where** $\tau \neq \tau'$ **do**:
12:             $s_{\tau,\tau'} \leftarrow \mathrm{sgn}([\tau], \partial[\sigma]) \cdot \mathrm{sgn}([\tau'], \partial[\sigma])$
13:             $i,\ j \leftarrow\ h(\tau),\ h(\tau')$
14:             $y_i \leftarrow y_i + s_{\tau,\tau'} \cdot x_j \cdot w_p^l(\tau) \cdot w_{p+1}(\sigma) \cdot w_p^r(\tau')$
15:     **return** y

In general, the signs of the coefficients $\mathrm{sgn}([\tau], \partial[\sigma])$ and $\mathrm{sgn}([\tau'], \partial[\sigma])$ depend on the position of τ, τ' as summands in $\partial[\sigma]$ (2.1), which itself depends on the orientation of $[\sigma]$ (**??**). Thus, evaluation of these sign terms takes $O(p)$ time to determine for a given $\tau \in \partial[\sigma]$ with $\dim(\sigma) = p$, which if done naively via line (12) in the pseudocode C increases the complexity of the algorithm. However, observe that the sign of their product is in fact invariant in the orientation of $[\sigma]$ (see Remark 3.2.1 of [18])—thus, if we fix the orientation of the simplices of K^p, the sign pattern $s_{\tau,\tau'}$ for every $\tau \overset{\sigma}{\sim} \tau'$ can be precomputed and stored ahead of time, reducing the evaluation $s_{\tau,\tau'}$ to $O(1)$ time and $O(m)$ storage. Alternatively, if the labels of the $p+1$ simplices $\sigma \in K^{p+1}$ are given an orientation induced from the total order on V, then we can remove the storage requirement entirely and simply fix the sign pattern during the computation.

A subtle but important aspect of algorithmically evaluating (A.16) is the choice of indexing function $h : K^p \to [n]$. This map is necessary to deduce the contributions of the components x_* during the operation (line (13)). While this task may seem trivial as one may use any standard associative array to generate this map, typical implementations that rely on collision-resolution schemes such as open addressing or chaining only have $O(1)$ lookup time in expectation. Moreover, empirical testing suggests that line (13) in C can easily bottleneck the entire computation due to the scattered memory access such collision-resolution schemes may involve. One solution avoiding these collision resolution schemes that exploits the fact that K is fixed is to build an order-preserving *perfect minimal hash function* (PMHF) $h : K^p \to [n]$. It is known how to build PMHF's over fixed input sets of size n in $O(n)$ time and $O(n \log m)$ bits [], and such maps have deterministic $O(1)$ access time. Note that this process happens only once for a fixed simplicial complex K: once h has been constructed, it is fixed for every `matvec` operation.

D Parameterized setting & Perturbation theory

If f is a real-valued filter function that various smoothly in $\mathcal{H}$, one would expect the spectra of the constitutive terms in β_p^* and μ_p^* to also vary smoothly as functions of $\mathcal{H}$. Indeed, since Laplacian matrices are normal matrices, we expect their spectra to be quite stable under perturbations [].

Small condition numbers often improve the convergence of iterative solvers and improve stability of spectrum with respect to perturbations in the entries of the matrix. $\kappa(M^{-1}A)$

$$M^{-1}Ax = M^{-1}b$$

where M is symmetric positive definite.

$$\min_{x \perp \mathbf{1}} \frac{1}{2} x^T (L + \epsilon I_n) x - b^T x \tag{D.1}$$

Since this nonsingular, positive definite, strictly diagonally dominant matrix, thus we may apply the famous Conjugate Gradient (CG) algorithm to solve such a system. It's well known that CG converges to the solution of $Ax = b$ in exactly $O(n)$ iterations (and often much earlier), of which each iteration requires one $O(m)$ matrix-vector product, implying a runtime of $O(mn^2)$ (compare with...). Moreover, and since this is a Laplacian matrix, the wealth of tools developed for said matrices may also be used. In particular, [] showed that *low-stretch spanning trees* act as good preconditioners to accelerate Laplacian solvers, wherein it's been shown that the preconditioned Conjugate Gradient (PCG) requires as most $O(\sqrt{m} \log n)$ iterations, each of which requires one matrix-vector product using L_G and in $O(m^{1/3} \log n \ln 1/\epsilon)$ iterations. This was later improved by, who showed that one can solve Laplacian systems effectively in $O(m \log^{O(1)} n)$ time, giving a bound of $O(rm \log^{O(1)} n)$ time to obtain....

Of course, if one wants to compute either of the counting invariants in... exactly for $p = 0$, of course, the fastest algorithm is to reduce the problem to the well-known elder-rule problem, which takes $O(m \log m + m\alpha(n))$ time for a general filtration. It is unlikely that we may beat this bound, either in theory or in practice, for $p = 0$. However, the fastest known algorithm for computing the full persistence diagram for $p \geq 1$ is $O()$, which is quite a jump in complexity; there is no generalization of disjoint-set algorithm for the case where $p \geq 1$. Moreover, these direct methods tend to be memory bound operations, pushing researchers who want to compute these diagrams in practice to focus on ways of reducing the memory usage, such as using $\mathbb{Z}_2$ field coefficients. In contrast, the means by which we compute these invariants scales quite well with larger p, it produces a stronger invariant, and is far more reaching to other areas of mathematics.