

1 Introduction

Motivation:

Organization: In what follows, we investigate how to formulate the persistent Betti number (PBN) computation on filtered simplicial complexes in parameterized settings. In particular, in section 3, we show how the PBN may be expressed as a sum of rank computations on unfactored boundary (sub)matrices. By representing the boundary operators implicitly and exploiting a variety of properties of the rank function, we demonstrate the rank-based PBN expression admits certain computational advantages in both static and parameterized settings. We show the p -th PBN of a filtered simplicial complex K_\bullet may be computed in essentially quadratic time and linear storage, as opposed to the cubic time and quadratic storage complexity required by persistence. Finally, we illustrate both the computational and practical advantages our expression has with a few applications in section 6.

2 Background & Notation

A *simplicial complex* $K \subseteq \mathcal{P}(V)$ over a vertex set $V = \{v_1, v_2, \dots, v_n\}$ is a collection of simplices $\{\sigma : \sigma \in \mathcal{P}(V)\}$ such that $\tau \subseteq \sigma \in K \implies \tau \in K$. We denote with $K^p = \{\sigma \in K : \dim(\sigma) = p\}$ the p -simplices of K and by $K^{(p)} = \{\sigma \in K : \dim(\sigma) \leq p\}$ the p -skeleton of K . A *filtration* $K_\bullet = \{K_i\}_{i \in I}$ of a simplicial complexes indexed by a totally ordered set I is a family of complexes such that $i < j \in I \implies K_i \subseteq K_j$. K_\bullet is called *simplexwise* if $K_j \setminus K_i = \{\sigma_j\}$ whenever j is the immediate successor of i in I and K_\bullet is called *essential* if $i \neq j$ implies $K_i \neq K_j$:

$$\emptyset = K_0 \subsetneq K_1 \subsetneq \dots \subsetneq K_m = K_\bullet, \quad K_i = K_{i-1} \cup \{\sigma_i\} \quad (1)$$

Filtrations may be equivalently defined via *filter functions* $f : K \rightarrow I$ satisfying $f(\tau) \leq f(\sigma)$ whenever $\tau \subseteq \sigma$. Here, we consider two index sets for I : \mathbb{R} and $[n] = \{1, \dots, n\}$. Any finite filtration may be trivially converted into an essential, simplexwise filtration via a set of *condensing*, *refining*, and *reindexing* maps [1]. For simplicity, but without loss of generality, we exclusively consider essential simplexwise filtrations and for brevity refer to them as filtrations.

For K a simplicial complex and \mathbb{F} a field, a p -chain is a formal \mathbb{F} -linear combination of p -simplices of K . The collection of p -chains under addition yields an \mathbb{F} -vector space denoted $C_p(K)$. 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:

$$\partial_p(\sigma) = \partial_p([v_0, v_1, \dots, v_p]) := \sum_{i=0}^p (-1)^i [v_0, \dots, v_{i-1}, v_{i+1}, \dots, v_p] \quad (2)$$

The p -boundary of a p -chain is defined linearly in terms of its constitutive simplices. A p -chain c with zero boundary $\partial_p c = 0$ is called a p -cycle. Together, the collection of p -boundaries and p -cycles forms the groups $B_p(K) = \text{Im } \partial_{p+1}$ and $Z_p(K) = \text{Ker } \partial_p$, respectively. Since $\partial_p \circ \partial_{p+1} = 0$ for all $p \geq 0$, the quotient space $H_p(K) = Z_p(K)/B_p(K)$ is well-defined, and $H_p(K)$ is called the p -th homology of K with coefficients in \mathbb{F} . The dimension of the p -th homology group $\beta_p(K) = \dim(H_p(K))$ of K is called the p -th *Betti number* of K .

Let $K_\bullet = \{K_i\}_{i \in [m]}$ denote a filtration of size $|K_\bullet| = m$, and let $\Delta_+^m = \{(i, j) : 0 \leq i \leq j \leq m\}$ denote the set of filtration index pairs. For every such pair $(i, j) \in \Delta_+^m$, the inclusions $K_i \subsetneq K_{i+1} \subsetneq \dots \subsetneq K_j$ induce linear transformations $h_p^{i,j}$ at the level of homology:

$$0 = H_p(K_0) \rightarrow \dots \rightarrow H_p(K_i) \xrightarrow{h_p^{i,j}} H_p(K_j) \rightarrow \dots \rightarrow H_p(K_m) = H_p(K_\bullet) \quad (3)$$

When \mathbb{F} is a field, this sequence of homology groups uniquely decomposes K_\bullet into a pairing of simplices (σ_i, σ_j) demarcating the evolution of homology classes [18]: σ_i marks the creation of a homology class, σ_j marks its destruction, and the difference $|i - j|$ records the lifetime of the class, called its *persistence*. The p -th persistent homology groups are the images of these transformations and the p -th persistent Betti numbers are their dimensions:

$$H_p^{i,j} = \begin{cases} H(K_i) & i = j \\ \text{Im } h_p^{i,j} & i < j \end{cases}, \quad \beta_p^{i,j} = \begin{cases} \beta_p(K_i) & i = j \\ \dim(H_p^{i,j}) & i < j \end{cases} \quad (4)$$

For a fixed $p \geq 0$, the collection of persistent pairs (i, j) together with unpaired simplices (l, ∞) form a summary representation $\text{dgm}_p(K_\bullet)$ called the p -th *persistence diagram* of K_\bullet . Conceptually, $\beta_p^{i,j}$ counts the number of persistent pairs lying inside the box $(-\infty, i] \times (j, \infty)$ (see Figure 1)—the number of persistent homology groups born at or before i that died sometime after j .

The duality between PBNs and Diagrams

The connection between the persistent homology (PH) groups and their corresponding persistent Betti numbers (PBNs) has long been studied from multiple perspectives by several authors [3, 4, 8, 18]. From an algebraic perspective, Carlsson et al. [18] observed that the PH groups over a filtration may be viewed as the standard homology groups of a particular graded module M over a polynomial ring. In [8], Cohen-Steiner et al. give a more discrete perspective on PH by defining the persistence diagram in terms of a *multiplicities*: given a tame function $f : \mathcal{X} \rightarrow \mathbb{R}$ over a topological space \mathcal{X} , its homological critical values $\{a_i\}_{i=1}^n$, and an interleaved sequence $\{b_i\}_{i=0}^n$ satisfying $b_{i-1} < a_i < b_i$ for all $1 \leq i \leq n$, the p -th persistence diagram over f is given as:

$$\text{dgm}_p(f) = \{(a_i, a_j) : \mu_p^{i,j} \neq 0\} \cup \Delta \quad (5)$$

where Δ denotes the diagonal, counted with infinite multiplicity, and $\mu_p^{i,j}$ is the *multiplicity function*, defined as:

$$\mu_p^{i,j} = (\beta_p^{i,j-1} - \beta_p^{i,j}) - (\beta_p^{i-1,j-1} - \beta_p^{i-1,j}) \quad \text{for } 0 \leq i < j \leq n+1 \quad (6)$$

Equation (6) illuminates an intrinsic connection between the multiplicity function and the persistent Betti numbers. Namely, the inclusion-exclusion property that (6) obeys suggests that diagrams completely characterize their PBNs. Indeed, the fundamental lemma of persistent homology [11] states that for every pair of indices $0 \leq k \leq l \leq n+1$:

$$\beta_p^{k,l} = \sum_{i \leq k} \sum_{j > l} \mu_p^{i,j} \quad (7)$$

The direct consequence of (7) is that if one is interested in computing any of the PBNs of some space \mathcal{X} , then it is sufficient to compute $\text{dgm}_p(\mathcal{X})$ and read them off directly. In this effort, as we will show, we will take the inverse mentality by recovering portions of the diagram via multiplicity evaluations.

The duality between diagrams and PBNs derived from persistence modules indexed over the real line was further studied by Chazal [4] in a measure-theoretic setting. By reinterpreting the multiplicity function μ_p^* as a certain kind of integer-valued measure over rectangles in the plane, a generalization of (6) was shown by demonstrating that one may recover the diagram of a persistence module M over \mathbb{R} by constructing its corresponding *persistence measure*:

$$\mu_p(R; M) = \text{card} \left(\text{dgm}_p(M) \big|_R \right) \quad \text{for all rectangles } R \subset \mathbb{R}^2 \quad (8)$$

Cerri et al. [3] incorporate this interpretation in their work studying the stability of PBNs in multidimensional persistence by showing that *proper cornerpoints* in the persistence diagram are points $x = (i, j) \in \Delta_+$ satisfying:

$$x = (i, j) \in \text{dgm}_p(f) \iff \mu_p(x) > 0 \iff \min_{\epsilon > 0} (\beta_p^{i+\epsilon, j-\epsilon} - \beta_p^{i+\epsilon, j+\epsilon}) - (\beta_p^{i-\epsilon, j-\epsilon} - \beta_p^{i-\epsilon, j+\epsilon}) > 0 \quad (9)$$

One may compare (6) with (9). One of the primary contributions from [3] is a representation theorem akin to (7) (Theorem 3.11) expressing the persistent Betti number function $\beta_* : \Delta_+ \rightarrow \mathbb{N} \cup \{\infty\}$ as a sum of multiplicity functions. A consequence of this theorem is that distances between diagrams induces a distance between PBN functions—if X is a triangulable space and $f, g : X \rightarrow \mathbb{R}$ are two continuous functions, then $d(\beta_f, \beta_g) \leq \max_{x \in X} |f(x) - g(x)|$, where:

$$d(\beta_f, \beta_g) = \inf_{\phi} \sup_{p \in \text{dgm}(f)} \|p - \phi(p)\|_{\infty}$$

is the (extended) matching distance between PBN functions (β_f, β_g) , ϕ ranges over all multi-bijections between $\text{dgm}(f)$ and $\text{dgm}(g)$, and $\|\cdot\|_{\infty}$ measures the pseudo-distance [3] between points. Thus, PBN functions are stable functions: small changes in continuous scalar-valued filtering functions imply small changes in the corresponding persistent Betti numbers functions.

Like persistence diagrams, the stability of PBN functions justifies their use and study in continuously parameterized settings. Despite this, much of persistence-related research has concentrated on exploiting properties of the diagram itself [], as opposed to the PBNs ([3, 5] are notable exceptions). Nonetheless, as we shall show, there are certain advantages the PBN computation has over the “standard” reduction algorithm from [11]. Indeed, (6) implies one may in theory recover the diagram through [a finite number of] PBN computations alone via a divide-and-conquer like approach [5], suggesting an alternative computational paradigm—distinct from the reduction family of algorithms—with which to approach the persistence computation.

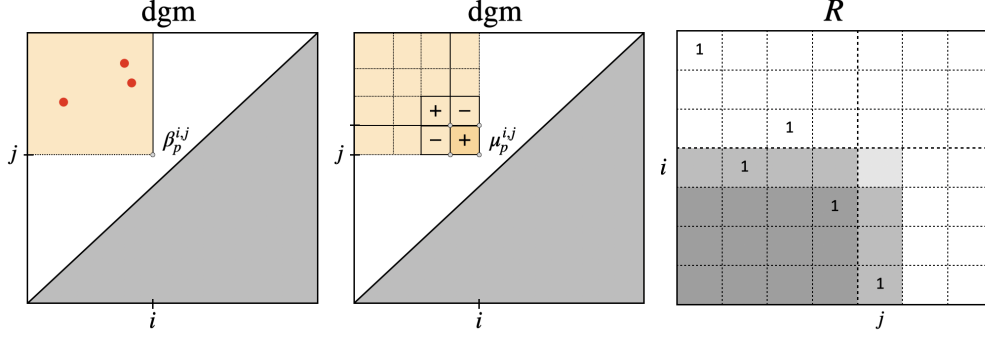


Figure 1: (Left) the persistent Betti number $\beta_p^{i,j}$ counts the number of points (3) in upper left-corner of $\text{dgm}_p(K_\bullet)$. (Middle) The additivity of PBNs can be used to express multiplicity $\mu_p^{i,j}$ of any given box. (Right) The computational interpretation of the Pairing Uniqueness Lemma; in this case $r_R(i, j) = 3 - 2 + 1 - 2 = 0$ yields whether the entry $R[i, j]$ is non-zero.

3 Motivating Derivation

Let $B_p(K_\bullet) \subseteq Z_p(K_\bullet) \subseteq C_p(K_\bullet)$ denote the p -th boundary, cycle, and chain groups of a given filtration K_\bullet , respectively. Additionally, let $\partial_p : C_p(K_\bullet) \rightarrow C_p(K_\bullet)$ denote the boundary operator sending p -chains to their respective boundaries. With a slight abuse of notation, we also use ∂_p to also denote the filtration boundary matrix with respect to an ordered basis $(\sigma_i)_{1 \leq i \leq m_p}$. The p -th persistent Betti number $\beta_p^{i,j}$ at index $(i, j) \in \Delta_+^m$, where $\Delta_+^m := \{(i, j) \in [m] \times [m] : i < j\}$, is defined as:

$$\begin{aligned} \beta_p^{i,j} &= \dim(H_p^{i,j}) = \dim(Z_p(K_i)/B_p(K_j)) \\ &= \dim(Z_p(K_i)/(Z_p(K_i) \cap B_p(K_j))) \\ &= \dim(Z_p(K_i)) - \dim(Z_p(K_i) \cap B_p(K_j)) \end{aligned} \quad (10)$$

While $Z_p(K_i) = \text{nullity}(\partial_p(K_i))$ and thus reduces to a matrix rank computation, the intersection term (the persistence part) is more subtle. Zomorodian et al. [18] outline an algorithm to compute a basis for $Z_p(K_i) \cap B_p(K_j)$ via a sequence of boundary matrix reductions; the subsequent Theorem (5.1) reduces the complexity of computing PH groups with coefficients in any PID to that of computing homology groups. However, the standard homology computations require $O(m^2)$ space and $O(m^3)$ time to compute, implying either of these approaches to computing the PBN computation exhibits same complexity as the full persistence computation.

In what follows, we outline a different approach to computing (10) that we argue is both simpler and computationally more attractive. To illustrate our approach, we require more notation. If A is a $m \times n$ matrix, let $A^{i,j}$ denote the lower-left submatrix defined by last $m - i + 1$ rows (rows i through m , inclusive) and the first j columns. For any $1 \leq i < j \leq m$, define the quantity $r_A(i, j)$ as follows:

$$r_A(i, j) = \text{rank}(A^{i,j}) - \text{rank}(A^{i+1,j}) + \text{rank}(A^{i+1,j-1}) - \text{rank}(A^{i,j-1}) \quad (11)$$

The structure theorem from [18] shows that 1-parameter persistence modules can be decomposed in an *essentially unique* way into indecomposables. Computationally, a consequence of this phenomenon is the Pairing Uniqueness Lemma [9], which asserts that if $R = \partial V$ is the decomposition of the boundary matrix, then:

$$r_R(i, j) \neq 0 \Leftrightarrow R[i, j] \neq 0$$

Since the persistence diagram is derived completely from R , this suggests that information about a diagram can be obtained through rank computations alone. For a more geometric description of this idea, see the third picture in Figure 1. We record a non-trivial fact that follows from this observation:

Lemma 1 (Dey & Wang [10]). *Let $R = \partial V$ denote the matrix decomposition of a given filtered boundary matrix ∂ derived from the associated filtration K_\bullet . For any pair (i, j) satisfying $1 \leq i < j \leq m$, we have:*

$$\text{rank}(R^{i,j}) = \text{rank}(\partial^{i,j}) \quad (12)$$

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

Lemma 1 was the essential motivating step used by Chen et al [5] in their rank-based persistence algorithm—the first output-sensitive algorithm given for computing persistent homology of a filtered complex. Though (12) is defined over the full boundary matrix ∂ , there is no loss in generality in extending this lemma to p -dimensional homology, for any fixed choice $p \geq 0$. To see this, note that since the reduction algorithm only adds p -chains to p -chains, we may simply ignore all q -chains for $q \neq p$. That is, if the p -chain of a p -simplex σ_j corresponds to column j in ∂ , the only columns that may be added to j must correspond to simplices of dimension p . Hence, if we set all columns corresponding to simplices of dimension $q \neq p$ to 0 in the $m \times m$ boundary matrix ∂ , then ∂ represents the p -th boundary operator $\partial_p : C_p(K_\bullet) \rightarrow C_{p-1}(K_\bullet)$.

In what follows, we will use ∂_p and R_p to refer to matrices of ∂ and R whose q -chains are set to 0, for $q \neq p$. The first fact we prove is that Lemma 1 may be used to write the persistent Betti number as a sum of rank functions.

Proposition 1. *Given a fixed $p \geq 0$, a filtration K_\bullet of size $m = |K_\bullet|$, and any pair $(i, j) \in \Delta_+^m$, the persistent Betti number $\beta_p^{i,j}(K_\bullet)$ at (i, j) is given by:*

$$\beta_p^{i,j}(K_\bullet) = i - \text{rank}(\partial_p^{1,i}) - \text{rank}(\partial_{p+1}^{1,j}) + \text{rank}(\partial_{p+1}^{i+1,j}) \quad (13)$$

A detailed proof of Proposition 1 is given in the appendix. It turns out Lemma 1 can also be used to generalize (13) to arbitrary rectangles in Δ_+ via μ -queries: box-parameterized rank queries which count the number of persistence pairs that intersect a fixed “box” placed in the upper half-plane [5]. As a result, the p -th multiplicity function can also be defined in a rank-based formulation akin to (13).

Proposition 2 (Chen & Kerber [5]). *Given a fixed $p \geq 0$, a filtration K_\bullet of size $m = |K|$, and a $R = [i, j] \times [k, l]$ whose indices (i, j, k, l) satisfy $0 \leq i < j \leq k < l \leq m$, the p -th multiplicity μ_p^R of K_\bullet is given by:*

$$\mu_p^R(K_\bullet) = \text{rank}(\partial_{p+1}^{j+1,k}) - \text{rank}(\partial_{p+1}^{i+1,k}) - \text{rank}(\partial_{p+1}^{j+1,l}) + \text{rank}(\partial_{p+1}^{i+1,l}) \quad (14)$$

Computationally, the complexity of computing the PBN reduces the complexity of computing the rank of a set of boundary matrices. We summarize this with the following corollary:

Corollary 1. *Given a filtration K_\bullet of size $m = |K_\bullet|$ and indices $i, j \in \Delta_+^m$, computing $\beta_p^{i,j}$ using expression (13) requires $O(R_p(j))$ time, where $R_p(k)$ denotes the complexity of computing the rank of square $k \times k$ matrix with $O((p+2)k)$ non-zero \mathbb{F} entries.*

Observe the relation $\partial_{p+1}^{i+1,j} \subseteq \partial_{p+1}^{1,j}$ implies the dominant cost of computing (13) lies in computing either $\text{rank}(\partial_p^{1,i})$ or $\text{rank}(\partial_{p+1}^{1,j})$. As a result, we get a more localized bound for computing μ_p^R .

Corollary 2. *Given a filtration K_\bullet of size $m = |K_\bullet|$ and a rectangle $R = [i, j] \times [k, l]$ with indices $0 \leq i < j \leq k < l \leq m$, computing μ_p^R using expression (14) requires $O(R_p(l-i))$ time, where $R_p(k)$ denotes the complexity of computing the rank of square $k \times k$ matrix with $O((p+1)k)$ non-zero \mathbb{F} entries.*

Compared to other classical methods of obtaining $\beta_p^*(K_\bullet)$ and $\mu_p^*(K_\bullet)$, such as those in [11, 18], the primary advantage the rank-based expressions from (13)-(14) have is that their computations are performed directly on *unfactored* boundary matrices. Exploiting this, we show how to compute both topological invariants in essentially $O(m)$ memory, while also accelerating their re-computation in parameterized settings. Moreover, we achieve these computations all without performing any reductions to ∂ as used in the standard algorithm [11], without using any $O(m^2)$ combinatorial preprocessing procedure as in [9], and without reducing the computation matrix multiplication time $O(n^\omega)$ with Strassen-like reductions [14]. Indeed, our formulation need not even have ∂ in memory explicitly. We dedicate the rest of the paper to exploring the consequences of this fact.

A Parameterized Boundary Matrix Relaxation: Expressing the PBN via (13) enables us to exploit properties of the rank function which are advantageous in *parameterized* settings, i.e. settings where the input data is thought to be generated from a parameterized family. One such property is permutation invariance: given any $A \in \mathbb{R}^{n \times n}$, it is well known that $\text{rank}(A) = \text{rank}(P^T A P)$ for any permutation matrix P . Though the boundary matrices ∂_p in (13) are given in filtration order to elucidate their structure, the permutation invariance of the rank function suggests they need not be in such an order to be evaluated—so long as the constitutive terms have the same non-zero pattern as their filtration-ordered counterparts, their ranks and thus their PBNs will be identical. In what follows, we re-define the boundary matrix to exploit this permutation invariance.

All of the notation given thus far, such as the definitions of the PH groups (3) and the the PBN (10), have used integer indices $(i, j) \in \Delta_+^m$ to describe the PH groups over a filtration pair (K_\bullet, f) of size $|K| = m$. Equivalently, we

have thus far implicitly assumed the range of the filter function $f : K \rightarrow I$ to be the typical index set $I = [m]$. In practice, the filter function f is often derived from geometrical settings wherein it is more informative to interpret the persistence of a persistent-pair $(\sigma_i, \sigma_j) \in \text{dgm}(K_\bullet)$ as $f(\sigma_j) - f(\sigma_i)$, rather than as $j - i$, as the filter function $f : K \rightarrow \mathbb{R}$ is quite often real-valued. In what follows, in the spirit of (9), we alter our notation by re-defining $\beta_p^{i,j}$ using pairs $(i, j) \in \Delta_+$ from the upper-half plane $\Delta_+ = \{(x, y) \in \mathbb{R}^2 : y > x\}$.

Suppose that instead of being given a fixed pair (K_\bullet, f) , the filter function was parameterized $f : \mathcal{H} \times K \rightarrow \mathbb{R}$ and one was interested in computing $\beta_p^{i,j}$ over \mathcal{H} . We give several application contexts where this kind of formulation occurs naturally in section 6. As a first step to simplifying the PBN computation in this setting, we introduce the notion of a *parameterized boundary matrix*.

Definition 1 (Parameterized boundary matrix). *Let K denote an abstract simplicial complex of size $|K| = m$, equipped with parameterized filtering function $f : K \times \mathcal{H} \rightarrow \mathbb{R}$. Assume K is ordered along a fixed but arbitrary linear extension (K, \preceq^*) of the face poset of K . For fixed $(i, j) \in \Delta_+$, define the \mathcal{H} -parameterized p -th boundary matrix $\hat{\partial}_p^{i,j}(h)$ at scale (i, j) to be the $m \times m$ matrix ordered by \preceq^* for all $h \in \mathcal{H}$, and whose entries (k, l) satisfy:*

$$\hat{\partial}_p^{i,j}(h)[k, l] = \begin{cases} \pm (S_i \circ f_h)(\sigma_k) \cdot (\tilde{S}_j \circ f_h)(\sigma_l) & \text{if } \sigma_k \in \partial_p(\sigma_l) \\ 0 & \text{otherwise} \end{cases} \quad (15)$$

where $S_i : \mathbb{R} \rightarrow \{0, 1\}$ is a step function satisfying $S_i(x) = 0$ if $x \leq i$ and 1 otherwise, $\tilde{S}_i = 1 - S_i$, and $f_h(\sigma) = f(\sigma, h)$.

We now show definition 1 simplifies the expression of the PBN in parameterized settings. To simplify the notation, we write $A^x = A^{*,x}$ for the setting where only columns up to x of A are being selected, and let $q = p + 1$. Let $V = \{v_1, v_2, \dots, v_n\}$ denote a fixed vertex set. The parameterized PBN can be written as:

$$\begin{aligned} \beta_p^{i,j} : \mathcal{H} \times \mathcal{P}(V) &\rightarrow \mathbb{N} \\ h, K &\mapsto |K_i^{(p)}(h)| - \text{rank}(\hat{\partial}_p^i(h)) - \text{rank}(\hat{\partial}_q^j(h)) + \text{rank}(\hat{\partial}_q^{i+\epsilon,j}(h)) \end{aligned} \quad (16)$$

where $\epsilon > 0$ is an arbitrarily small positive number. Observe (16) is essentially the same form as (13). By Proposition 2, we also have a parameterized multiplicity function for any rectangle $R = [i, j] \times [k, l]$ in the upper half-plane Δ_+ satisfying $i < j \leq k < l$:

$$\begin{aligned} \mu_p^R : \mathcal{H} \times \mathcal{P}(V) &\rightarrow \mathbb{N} \\ h, K &\mapsto \text{rank}(\hat{\partial}_q^{j+\epsilon,k}(h)) - \text{rank}(\hat{\partial}_q^{i+\epsilon,k}(h)) - \text{rank}(\hat{\partial}_q^{j+\epsilon,l}(h)) + \text{rank}(\hat{\partial}_q^{i+\epsilon,l}(h)) \end{aligned} \quad (17)$$

Complexity of Persistence: TODO

An quadratic-time rank computation

In this section we discuss the computational details involved in evaluating the rank function on the boundary matrices whose columns take the form (2). Given a matrix $X \in \mathbb{R}^{n \times m}$ satisfying $n < m$ and its singular value decomposition (SVD) $X = U\Sigma V^T$, define the *rank* of X as the composition:

$$\text{rank}(X) = \sum_{i=1}^n \text{sgn}_+(\sigma_i(X)), \quad \text{sgn}_+(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases} \quad (18)$$

where $\Sigma = \text{diag}(\{\sigma_1, \sigma_2, \dots, \sigma_n\})$ are the singular values and $\text{sgn}_+ : \mathbb{R} \rightarrow \{0, 1\}$ is the one-sided sign function. As (18) is defined completely in terms of the singular values of X , and the singular values of X are given by the square roots of eigenvalues of XX^T (or X^TX), we focus on iterative methods for finding the eigenvalues of Hermitian matrices. In particular, we focus on the Lanczos iteration applied to positive semi-definite matrices, diagonally dominant (DD) and strictly diagonally dominant (SDD) matrices, and combinatorial Laplacians. We also show how these methods made be adapted to efficiently compute (16) and (17).

The Lanczos iteration: For a real, square matrix A of order n , the quadratic form $x^T A x$ defines a continuous real-valued function of $x \in \mathbb{R}^n$. When A is symmetric positive definite, the implicit equation $x^T A x = 1$ defines an n -dimensional ellipsoid $y^T \Lambda y = 1$ whose n principle axes are eigenvectors $\{v_i\}_{i=1}^n$ and whose lengths are the squares of eigenvalues $\Lambda(A)$ of A . Each eigen-pair (λ, v) satisfies $Av = \lambda v$, and when A is symmetric, every λ is real-valued

and every pair of eigenvectors $v, u \in \mathbb{R}^n$ whose corresponding eigenvalues $\lambda \neq \lambda'$ are orthogonal. Thus we may reveal the spectrum $\Lambda(A)$ of A —effectively the lengths of the aforementioned ellipsoid—via orthogonal diagonalization:

$$A = V\Lambda V^T = \sum_{i=1}^n \lambda_i v_i v_i^T \quad (19)$$

Factorizing A as in (19) is known as the *symmetric eigenvalue problem*. Computing the eigen decompositions of symmetric matrices generally consists of two phases: (1) reduction to tridiagonal form $Q^T A Q = T$ via orthogonal similarity transformations $Q = Q_1 Q_2 \dots Q_{n-2}$, and (2) diagonalization of the tridiagonal form $T = Y \Theta Y^T$. Note the latter may be performed in $O(n \log n)$ time [13], whereas the former is effectively bounded below by $\Omega(n^3)$ for dense full rank matrices using non-Strassen-like operations, and thus this reduction to tridiagonal form dominates the computation. Lanczos [14] 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 $\lambda_1 \geq \lambda_2 > \dots \geq \lambda_r > 0$ and a vector $v \neq 0$, the order- j Krylov subspaces of the pair (A, v) are the spaces spanned by:

$$\mathcal{K}_j(A, v) := \text{span}\{v, Av, A^2v, \dots, A^{j-1}v\} = \text{range}(K_j(A, v)) \quad (20)$$

where $K_j(A, v) = [v \mid Av \mid A^2v \mid \dots \mid A^{j-1}v]$ 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 subspace¹ 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 $j = 1, 2, \dots, n$. Due to A 's symmetry and the orthogonality of Q_j , we have $q_k^T A q_l = q_l^T A^T q_k = 0$ for $k > l + 1$, implying the corresponding $T_j = Q_j^T A Q_j$ have a tridiagonal structure:

$$T_j = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_{j-1} \\ & & & \beta_{j-1} & \alpha_j \end{bmatrix}, \quad \beta_j > 0, \quad j = 1, 2, \dots, n \quad (21)$$

Unfortunately, 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 $Q = [q_1 \mid q_2 \mid \dots \mid q_n]$ is an $n \times n$ orthogonal matrix $Q Q^T = I_n = [e_1, e_2, \dots, e_n]$, then:

$$K_n(A, q_1) = Q Q^T K_n(A, q_1) = Q [e_1 \mid T e_1 \mid T^2 e_1 \mid \dots \mid T^{n-1} e_1] \quad (22)$$

is the QR factorization of $K_n(A, q_1)$. Thus, tridiagonalizing A with respect to a unit-norm q_1 completely characterizes Q . Indeed, the Implicit Q Theorem [12] asserts that if an upper Hessenberg 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:

$$A Q_j = Q_j T_j + \beta_j q_{j+1} e_j^T \quad (\beta_j > 0) \quad (23)$$

where $Q_j = [q_1 \mid q_2 \mid \dots \mid q_j]$ is an orthonormal set of vectors mutually orthogonal to q_{j+1} . Equating the j -th columns on each side of (23) and rearranging the terms yields the *three-term recurrence*:

$$\beta_j q_{j+1} = A q_j - \alpha_j q_j - \beta_{j-1} q_{j-1} \quad (24)$$

where $\alpha_j = q_j^T A q_j$, $\beta_j = \|r_j\|_2$, $r_j = (A - \alpha_j I)q_j - \beta_{j-1} q_{j-1}$, and $q_{j+1} = r_j / \beta_j$. Equation (24) is a variable-coefficient second-order linear difference equation, and it is a known fact that such equations have unique solutions: if (q_{j-1}, β_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 by

¹Recall 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 $x \in S$.

exploiting the recurrence from (24) is called the *Lanczos iteration*. Note that if A is singular and we encounter $\beta_j = 0$ for some $j < n$, then $\text{range}(Q_j) = \mathcal{K}_j(A, q_1)$ is an A -invariant subspace, the iteration stops, and we have solved the symmetric eigenvalue problem (19): $\Lambda(T_j) = \Lambda(A)$, $j = \text{rank}(A)$, and T_j is orthogonally similar to A .

The Lanczos iteration and its many variants are part of a family of so-called “matrix free” methods—obtaining an eigen-decomposition of a symmetric real matrix A requires only a matrix-vector $v \mapsto Av$ operator. Additionally, since A is not modified at all during the computation, the entire iteration may be carried out without explicitly storing A in memory. In fact, the three-term recurrence from (24) implies the Lanczos iteration may be carried out with just three $O(n)$ -sized vectors and $O(1)$ additional storage. We summarize these benefits with a Lemma.

Lemma 2 ([16, 17]). *Given a symmetric rank- r matrix $A \in \mathbb{R}^{n \times n}$ whose matrix-vector operator $A \mapsto Ax$ has complexity $O(\mathcal{M}(n))$ time, the Lanczos iteration computes $\Lambda(A) = \{\lambda_1, \lambda_2, \dots, \lambda_r\}$ in $O(\mathcal{M}(n) \cdot r)$ time and $O(n)$ storage complexity, when computation is done in exact arithmetic.*

As in [16], the assumption exact arithmetic simplifies both the presentation of the theory and the corresponding complexity statements. In practice, this is unrealistic, and we must use finite-precision arithmetic. Nonetheless, the assumption of exact arithmetic gives use the a useful corollary.

Corollary 3. *Given the same inputs as Lemma 2, any implementation that computes $\Lambda(A) = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$ using the Lanczos iteration in finite-precision arithmetic requires $\Omega(\mathcal{M}(n) \cdot r)$ time and $\Omega(n)$ storage complexity.*

Extending the Lanczos to retain similar complexity guarantees using finite-precision arithmetic is a complex and multifaceted topic; we defer its discussion to section 3.5. As Lemma 2 makes clear, the usefulness of the Lanczos iteration hinges on the availability of a fast matrix-vector product. For any symmetric $A \in \mathbb{R}^{n \times n}$ rank- r matrix with an average of ν nonzeros per row, approximately $(2\nu + 8)n$ flops are needed for a single Lanczos step, implying a $O(n\nu r)$ time complexity for a single iteration [12]. In the next section, we demonstrate how to reduce this complexity using the structure of the boundary operator.

Laplacian: In principle, the Lanczos method may only be effectively applied to sparse, symmetric matrices. Though the boundary matrix ∂ is not symmetric, it is well known that the spectrum of $\partial_p \partial_p^T$ contains the same information as the singular values of ∂_p , since the latter are by definition the nonnegative square roots of former and thus $\text{rank}(A) = \text{rank}(AA^T) = \text{rank}(A^T A)$. Moreover, the matrix $\partial_1 \partial_1^T$ is the well studied *graph Laplacian*. Thus, we can consider the study of spectra of combinatorial Laplacians as the study of singular values of boundary operators. For simplicity, we focus on the case where $p = 0$, and defer higher dimensions for later.

Given a graph $G = (V, E)$ with edge set $E \subseteq V \times V$, let $A \in \mathbb{R}^{n \times n}$ denote its *adjacency matrix* with non-zero entries $A[i, j] = 1$ for every $(i, j) \in E$, and 0 otherwise. The *graph Laplacian* L is defined as:

$$L = D - A = \partial_1 \partial_1^T \quad (25)$$

where D is a diagonal matrix whose entries $d_{ii} = \{\deg(v_i)\}$ are the vertex degrees $\deg(v_i) = \sum_{j \neq i} A[i, j]$. The graph Laplacian is heavily structured matrix that is known to capture the connectivity structure of G . In particular, the structure of the graph Laplacian imply linear and quadratic forms which have particular graph interpretations:

$$(\forall x \in \mathbb{R}^n) \quad (Lx)_i = \deg(v_i) \cdot x_i - \sum_{i \sim j} x_j, \quad x^T Lx = \sum_{i \sim j} (x_i - x_j)^2 \quad (26)$$

where we use the notation $i \sim j$ to indicate vertices $i, j \in V$ are path-connected in G . Moreover, L is symmetric, positive semi-definite, and the connection between L and ∂_1 via (25) suggests the elementary chain modifications from (15) can be adapted to the linear and quadratic forms from (35). The entries in ?? are parameterized using functions which defined over face and coface pairs, and thus to extend the structure of the graph Laplacian to our setting we require three Laplacian variants: Laplacians whose p -chains are parameterized by their $(p - 1)$ faces, Laplacians whose p -chains are parameterized by their p -faces, and the hadamard product between the two. Consider boundary matrices ∂_1^E and ∂_1^V whose chain entries are parameterized by edge and vertex functions, $f_E : V \times V \rightarrow \mathbb{R}$ and $f_v : V \rightarrow \mathbb{R}$:

$$\partial_1^E[k, l] = \begin{cases} \pm f_E(\sigma_l) & \text{if } \sigma_k \in \partial_p(\sigma_l) \\ 0 & \text{otherwise} \end{cases}, \quad \partial_1^V[k, l] = \begin{cases} \pm f_V(\sigma_k) & \text{if } \sigma_k \in \partial_p(\sigma_l) \\ 0 & \text{otherwise} \end{cases} \quad (27)$$

Both parameterizations generate two kinds of weighted graph Laplacians via (25). In the edge-weighted case, the Laplacian matrix-vector form is given by:

$$((\partial_1^E)(\partial_1^E)^T x)_i = (L^E x)_i = x_i \cdot d_f(v_i) - \sum_{i \sim j} x_j \cdot f_E(v_i, v_j)^2 \quad (28)$$

where $d_f(v_i) = \sum_{j \sim i} f_E(v_i, v_j)^2$. In the vertex-weighted case, it is given by:

$$((\partial_1^V)(\partial_1^V)^T x)_i = (L^V x)_i = x_i \cdot d(v_i) \cdot f_V(v_i)^2 - \sum_{i \sim j} x_j \cdot f_V(v_i) \cdot f_V(v_j) \quad (29)$$

Ignoring sign cancellations, the (i, j) -th entry of the Laplacian matrix L^{VE} formed by combining (25) with the hadamard product $\partial_1^{VE} = \partial_1^V \circ \partial_1^E$ has the following form:

$$L^{VE}[i, j] = ((\partial_1^{VE})(\partial_1^{VE})^T)[i, j] = \begin{cases} d_f(v_i) \cdot f_V(v_i)^2 & i = j \\ -(f_E(v_i, v_j)^2 \cdot f_V(v_i) \cdot f_V(v_j)) & i \sim j \\ 0 & i \not\sim j \end{cases} \quad (30)$$

In all cases, if $L = \partial_1 \partial_1^T$ where $\partial_1 \in \mathbb{R}^{n \times m}$ and $n < m$, then one may observe that the corresponding matrix-vector product for equations (28)-(30) can all be evaluated in $O(m)$ time. We end this section with a proposition, which essentially follows by combining the above observations with Lemma 2.

Proposition 3. *Given a filtration (K, f) of maximum dimension 1 with n vertices and m edges, the Lanczos iteration on the graph Laplacian $L = \partial_1 \partial_1^T$ computes:*

$$\dim(B_0(K; \mathbb{R})) = \text{rank}(L) = \text{rank}(\partial_1(K)) \quad (31)$$

in $O(mr)$ time and $O(m)$ storage complexity, when computation is done in exact arithmetic.

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 [16] 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 [12]—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.

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 $\{(\theta_1^{(j)}, y_1^{(j)}), \dots, (\theta_j^{(j)}, y_j^{(j)})\}$ 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 :

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

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 $\Lambda(A) = \{(\lambda_1, v_1), \dots, (\lambda_j, v_j)\}$, 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:

$$\|Av_i^{(j)} - v_i^{(j)}\theta_i^{(j)}\| = \beta_i^{(j)} = \beta_{j+1} \cdot |\langle e_j, y_i^{(j)} \rangle| \quad (32)$$

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 $\{\theta_1^{(1)}, \theta_1^{(2)}, \dots, \theta_1^{(j)}\}$ of T_j satisfy:

$$|\lambda - \theta_i^{(j)}| \leq (\beta_i^{(j)})^2 / (\min_{\mu} |\mu - \theta_i^{(j)}|) \quad (33)$$

Thus, these

4 Continuous PBN Relaxation

One disadvantage in working with counting-type functions restricted to portions of real-plane is that they are integer-valued and thus not smooth. Namely, if (K, f_h) is an \mathcal{H} -parameterized filtration where K is a fixed simplicial complex and $f_h : K \rightarrow \mathbb{R}$ is a filter function that is perturbed by some small $\epsilon > 0$, for the multiplicity function μ_p^R to be considered stable we would need to show there exists a non-negative constant C such that $\|\mu_h^R - \mu_{h+\epsilon}^R\| \leq \epsilon \cdot C$, where $\mu_h^R = \mu_p^R(K, h)$. However, it is easy to construct counter examples where $\|\mu_h^R - \mu_{h+\epsilon}^R\| \sim O(|K_p|)$ for any arbitrarily small ϵ ; intuitively, it's always possible to encounter such situations where small changes in the input affect the corresponding invariant in a non-Lipshitz way.

Like the PBN, the discontinuous nature of the rank function is due to its inherently combinatorial properties. In particular, the discontinuity in (18) manifests due to the one-sided sign function. Several other authors [1], have confronted this discontinuity by relaxing $\text{rank}(X)$ with the nuclear norm $\|X\|_*$. To see the motivation for this, let $X \in \mathbb{R}^{n \times m}$ denote a given real matrix with SVD $X = U\Sigma V^T$, and let $\vec{\sigma} = (\sigma_1, \dots, \sigma_n)$ denote a vector containing the singular values of X .

$$\text{rank}(X) = \|\vec{\sigma}\|_0 \approx \|\vec{\sigma}\|_1 = \|X\|_* \quad (34)$$

In the context of the Rank Minimization Problem (RMP), the nuclear norm is often used as a surrogate for the rank function due to the fact that it forms a convex envelope of the rank function in the space of all $n \times n$ matrices on the unit-ball in the operator norm [1]. Paired with the observation that the rank function can be equivalently expressed as composing the singular value function with the ℓ_0 pseudo-norm (as in (34)), replacing rank optimization problems with nuclear norm minimization problems has become an active area of research which has lead to many fruitful results in the areas of compressed sensing and matrix completion.

We consider a family of continuous sgn approximation functions $\phi : \mathbb{R}_+ \times \mathbb{R}_{++} \rightarrow \mathbb{R}_+$, each of which when composed with the singular value function yield a continuous function that approximates the rank function to any pre-prescribed accuracy. Given a positive $\epsilon > 0$, the basic qualities we want out of ϕ are:

$$(\forall x > 0) \quad \text{rank}(X) \approx \sum_{i=1}^n \phi(\sigma_i(X), \epsilon), \quad \lim_{\epsilon \rightarrow 0^+} \phi(x, \epsilon) = \text{sgn}_+(x) \quad (35)$$

Following the seminal work done by Chen et al. [6] on parameterizing smooth approximations of the one-sided sign function sgn_+ , Bi et al. [2] give a framework for constructing such functions via integration of smoothed versions $\hat{\delta}$ of the Dirac delta function δ :

$$\phi(x, \epsilon) := \int_{-\infty}^x \hat{\delta}(z, \epsilon) dz, \quad \forall z \geq 0, \epsilon > 0 \quad (36)$$

where $\hat{\delta}(z, \epsilon) = \nu(\epsilon)^{-1} p(z\nu \cdot (\epsilon)^{-1})$ for some continuous density function $p : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ and some choice of continuous increasing $\nu : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ satisfying $\nu(0) = 0$ and $\nu(\epsilon) > 0$. In contrast to the rank function, if p is continuous on \mathbb{R}_+ , then $\phi(\cdot, \epsilon)$ is continuously differentiable in \mathbb{R}_+ , and if p is bounded above on \mathbb{R}_+ , then $\phi(\cdot, \epsilon)$ is globally Lipshitz continuous on \mathbb{R}_+ . Moreover, consider the operator Φ_ϵ defined as:

$$\begin{aligned} \Phi_\epsilon : \quad \mathbb{R}^{n \times m} &\rightarrow \mathbb{R}^{n \times m} \\ X &\mapsto U \text{diag}(\tilde{\phi}(\sigma_1, \epsilon), \tilde{\phi}(\sigma_2, \epsilon), \dots, \tilde{\phi}(\sigma_n, \epsilon)) V^T \end{aligned} \quad (37)$$

where $\tilde{\phi}(x, \epsilon) = \phi(|x|, \epsilon)$ and $\epsilon > 0$ is fixed. Since $\phi(0, 0) = 0$, Φ_ϵ is a continuously differentiable operator in $\mathbb{R}^{n \times m}$ and one can verify that the nuclear norm of the operator is given by composing $\phi(\cdot, \epsilon)$ with the singular value function. We summarize this with a definition:

Definition 2 (Continuous Rank Approximation). *Given $X \in \mathbb{R}^{n \times m}$, a fixed approximation parameter $\epsilon > 0$, and a choice of $\phi : \mathbb{R}_+ \times \mathbb{R}_{++}$ satisfying (36), define the continuous rank approximation $\|\Phi_\epsilon(X)\|_*$ of X as:*

$$\|\Phi_\epsilon(X)\|_* = \sum_{i=1}^n \phi(\sigma_i, \epsilon) \quad (38)$$

Compared to the rank function, this operator turns out to have a variety of attractive properties related to monotonicity and differentiability. Moreover, as desired, it serves as a smooth approximation of the rank function. We summarize a few properties below.

Proposition 4 ([2]). *The operator $\Phi_\epsilon : \mathbb{R}^{n \times m} \rightarrow \mathbb{R}^{n \times m}$ defined by (37) satisfies:*

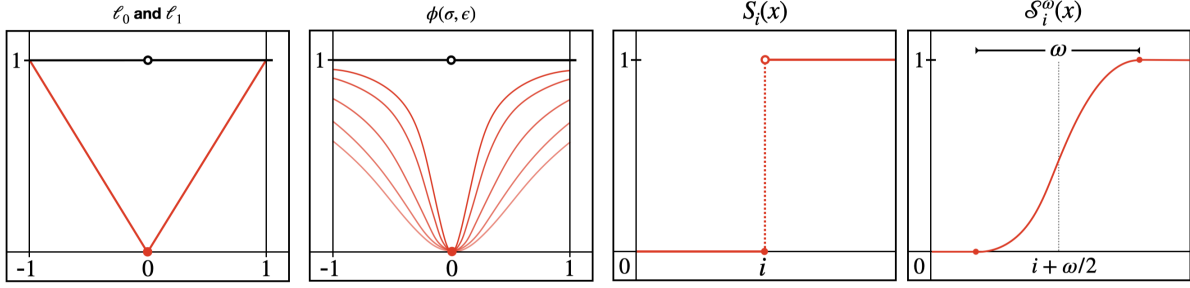


Figure 2: From left to right: the ℓ_1 norm (red) forms a convex envelope over the ℓ_0 (black) pseudo-norm on the interval $[-1, 1]$; $\tilde{\phi}(\cdot, \epsilon)$ at various values of ϵ , with $p(x) = 2x(x^2 + 1)^{-2}$ and $\nu(\epsilon) = \sqrt{\epsilon}$ (red) and at $\epsilon = 0$ (black); the step function $S_i(x)$ from definition 1; the smoothstep relaxation S_i^ω from (39).

1. For any $\epsilon \leq \epsilon'$, $\|\Phi_\epsilon(X)\|_* \geq \|\Phi_{\epsilon'}(X)\|_*$ for all $X \in \mathbb{R}^{n \times m}$.
2. For any given $X \in \mathbb{R}^{n \times m}$ with rank $r = \text{rank}(X)$, if ϵ satisfies $0 < \epsilon \leq \sigma_r/r$, then:

$$0 \leq r - \|\Phi_\epsilon(X)\|_* \leq c(r)$$

where $c(r)$ is a positive constant that depends only on r .

3. The function $\|\Phi_\epsilon(X)\|_*$ is globally Lipschitz continuous and semismooth on $\mathbb{R}^{n \times m}$.

It's worth noting that $\|\Phi_\epsilon(X)\|_*$ is not necessarily differentiable on $\mathbb{R}^{n \times m}$, but it is differentiable on the positive semi-definite cone \mathbb{S}_+^n , and that the notion of semismoothness here refers to the existence certain directional derivatives in the limit as $\epsilon \rightarrow 0^+$, see [] for more details.

Smoothstep: To adapt these relaxations to the counting functions defined in equations (7) and (14), we need to modify the expression of the boundary chains (2) to vary continuously in \mathcal{H} . Fortunately, this requires a simple augmentation to the step function from (??), similar to this change in the sign function. In particular, we swap out the step functions $S : \mathbb{R} \rightarrow \{0, 1\}$ in (15) with continuous *smoothstep* functions $\mathcal{S} : \mathbb{R} \rightarrow [0, 1]$. These are clamped sigmoid-like functions which interpolate between a prescribed lower and upper bounds $(a, a + \omega)$ via an ‘‘S-curve’’:

$$\mathcal{S}_a^\omega(x) = \begin{cases} 0 & x \leq a \\ S_n(\omega^{-1}((a + \omega) - x)) & a < x < a + \omega \\ 1 & a + \omega \leq x \end{cases} \quad (39)$$

where $S_n : [0, 1] \rightarrow [0, 1]$ is a generic n -th order polynomial whose coefficients are fixed such that $S_n(0) = 0$ and $S_n(1) = 1$. These polynomials have found applications computer graphics and machine learning applications []. Our motivation to use them here is based on the observations shown in Figure 2: by substituting \mathcal{S}_n^ω for the step functions in (15), we have a version of the parameterized boundary matrix whose entries varies continuously in \mathcal{H} but which retain the same rank as their discontinuous counterparts. By composing with (30) and substituting $\text{rank}(\cdot)$ with $\Phi(\cdot, \epsilon)$ for some appropriately chosen $\epsilon > 0$, we have ϵ -approximate, continuously-varying multiplicity function.

Definition 3.

$$\hat{\mu}_{p,\epsilon}^R(h) = \|\Phi_\epsilon^h(\tilde{\partial}_q^{j+\epsilon,k})\|_* - \|\Phi_\epsilon^h(\tilde{\partial}_q^{j+\epsilon,k})\|_* - \|\Phi_\epsilon^h(\tilde{\partial}_q^{j+\epsilon,k})\|_* + \|\Phi_\epsilon^h(\tilde{\partial}_q^{j+\epsilon,k})\|_* \quad (40)$$

The formulation of the PBN relaxation is synonymous.

Since the sum of two Lipschitz functions f and g results in another Lipschitz function $f + g$, by the continuity of \mathcal{S}_*^ω and the global Lipschitz continuity of (38), it is clear that $\hat{\mu}_p^R$ is Lipschitz continuous.

(1- ϵ) Approximations: Note that when $\nu(\epsilon) = \sqrt{\epsilon}$ and $p(x) = 2x(x^2 + 1)^{-2}$, Equation (38) reduces to:

$$\|\Phi_\epsilon(X)\|_* = \sum_{i=1}^n \frac{\sigma_i(X)^2}{\sigma_i(X)^2 + \epsilon} = \text{Tr} [X^T (X X^T + \epsilon I_n) X]$$

which is the generic rank approximation studied by [1]. Moreover, by the cyclic property of the trace operator, since $X = \partial_1$ here and $L = \partial_1 \partial_1^T = [l_1, l_2, \dots, l_n]$ we have:

$$\|\Phi_\epsilon(X)\|_* = \text{Tr}[(L + \epsilon I_n)^{-1} L] = \sum_{i=1}^n (L_\epsilon^{-1} l_i)_i$$

Thus we may solve this problem by solving n sparse linear systems of that take the form $Ax = b$, where here A is a Laplacian matrix with an $\epsilon \cdot I_n$ addition to it's diagonal. 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, [2] 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.

5 Parameterized setting & Perturbation theory

For f a real-valued filter function that varies 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 [3].

6 Applications

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

Directional Transform: The canonical interpretation of the information displayed by a persistence diagram is that it summarizes the persistence of the sublevel sets of filtered space. Given a filtration pair (K, f) where K is a finite simplicial complex and $f : K \rightarrow \mathbb{R}$ 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:

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

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

$$K_\bullet = K(v)_\alpha = \{x \in X \mid \langle x, v \rangle \leq \alpha\} \quad (41)$$

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:

$$\begin{aligned} \text{PHT}(K) : S^{d-1} &\rightarrow \mathcal{D}^d \\ v &\mapsto (\text{dgm}_0(K, v), \text{dgm}_1(K, v), \dots, \text{dgm}_{d-1}(K, v)) \end{aligned} \quad (42)$$

where \mathcal{D} denotes the space of p -dimensional persistence diagrams, for all $p = 0, \dots, d-1$ and S^{d-1} the unit $d-1$ sphere. The stability of persistence diagrams ensures that the map $v \mapsto \text{dgm}_p(K, v)$ 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 [1] is that the PHT is injective on the space of subsets of \mathbb{R}^d that can be written as finite simplicial complexes², 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 Appendix

Laplacian Interpretation: We adapt an example from [15] to better convey the information carried by the Laplacian form of the boundary matrices.

Example A.1 (Adapted from [15]). Suppose the vertices of G are ordered and labeled from 1 to n arbitrarily 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. Given such a set $X \subseteq V$, let $X' = V \setminus X$ denote its complement set. By L ’s definition, 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 [15].

Proofs:

²Implicit 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 $f : X \rightarrow \mathbb{R}$ to any simplex in K must be linear.

Proof of Lemma 1

Proof. The Pairing Uniqueness Lemma [10] 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 $\text{low}_R[j] = i$ if and only if $r_{\partial}(i, j) = 1$. As a result, for $1 \leq i < j \leq m$, we have:

$$\text{low}_R[j] = i \iff r_R(i, j) \neq 0 \iff r_{\partial}(i, j) \neq 0 \quad (43)$$

Extending this result to equation (12) 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. \square

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 (10) as:

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

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:

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

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. $\{\text{col}_{R_{p+1}[k]} \neq 0 \mid k \in [j]\} \in \text{Im}(\partial_{p+1}^{1,j})$. Now, since the low entries of the non-zero columns of R_{p+1} are unique, we have:

$$\dim(Z_p(K_i) \cap B_p(K_j)) = |\Gamma_p^{i,j}| \quad (44)$$

where $\Gamma_p^{i,j} = \{\text{col}_{R_{p+1}[k]} \neq 0 \mid k \in [j], 1 \leq \text{low}_{R_{p+1}}[k] \leq i\}$. 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 $\text{low}_{R_{p+1}}[k] > i$. Combining rank-nullity with the observation above, we have:

$$|\bar{\Gamma}_p^{i,j}| = \dim(B_p(K_j)) - |\Gamma_p^{i,j}| = \text{rank}(R_{p+1}^{i+1,j}) \quad (45)$$

Combining equations (44) and (45) yields:

$$\dim(Z_p(K_i) \cap B_p(K_j)) = |\Gamma_p^{i,j}| = \dim(B_p(K_j)) - |\bar{\Gamma}_p^{i,j}| = \text{rank}(R_{p+1}^{1,j}) - \text{rank}(R_{p+1}^{i+1,j}) \quad (46)$$

Observing the final matrices in (46) are *lower-left* submatrices of R_{p+1} , the final expression (13) follows by applying Lemma 1 repeatedly. \square

Proof of boundary matrix properties

Proof. First, consider property (1). For any $t \in T$, applying the boundary operator ∂_p to $K_t = \text{Rips}_{\epsilon}(\delta_{\mathcal{X}}(t))$ with non-zero entries satisfying (??) by definition yields a matrix ∂_p satisfying $\text{rank}(\partial_p) = \dim(B_{p-1}(K_t))$. In contrast, definition (1) always produces p -boundary matrices of Δ_n ; however, notice that the only entries which are non-zero are precisely those whose simplices σ that satisfy $\text{diam}(\sigma) < \epsilon$. Thus, $\text{rank}(\partial_p^t) = \dim(B_{p-1}(K_t))$ 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 $t \in T$. \square

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

1. For every $t \in \mathbb{R}$, $\delta_X(t) = (X, d_X(t))$ is a pseudo-metric space³
2. For fixed $x, x' \in X$, $d_X(\cdot)(x, x') : \mathbb{R} \rightarrow \mathbb{R}_+$ 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...

³This 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 $t \in \mathbb{R}$.

Application: Time-varying : Let $\delta_{\mathcal{X}}$ denote an T-parameterized metric space $\delta_{\mathcal{X}}(\cdot) = (X, d_{\mathcal{X}}(\cdot))$, where $d_{\mathcal{X}} : T \times X \times X \rightarrow \mathbb{R}_+$ is called a *time-varying metric* and X is a finite set with fixed cardinality $|X| = n$. $\delta_{\mathcal{X}}$ as called a *dynamic metric space* (DMS) iff $d_{\mathcal{X}}(\cdot)(x, x')$ is continuous for every pair $x, x' \in X$ and $\delta_{\mathcal{X}}(t) = (X, d_{\mathcal{X}}(t))$ is a pseudo-metric space for every $t \in T$. For a fixed $t \in T$, the Rips complex at scale $\epsilon \in \mathbb{R}$ is the abstract simplicial complex given by

$$\text{Rips}_{\epsilon}(\delta_{\mathcal{X}}(t)) := \{\sigma \subset X : d_{\mathcal{X}}(t)(x, x') \leq \epsilon \text{ for all } x, x' \in \sigma\} \quad (47)$$

As before, the family of Rips complexes for varying $\epsilon > 0$ yields a filtration whose inclusion maps induce linear maps at the level of homology. The time-varying counterpart is analogous. In this context, we write the p -th persistent Betti number with respect to fixed values $i, j \in I$ as a function of $t \in T$:

$$\beta_p^{i,j}(t) = (\dim \circ H_p^{i,j} \circ \text{Rips} \circ \delta_{\mathcal{X}})(t) \quad (48)$$

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A Boundary matrix factorization

Definition 4 (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 $\text{low}_R[i] \neq \text{low}_R[j]$ iff its i -th and j -th columns are nonzero

where $\text{low}_R(i)$ 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, \square 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:

$$\mathcal{L}(G) = D^{-1/2} L D^{-1/2} \quad (49)$$

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 $f : V \rightarrow \mathbb{R}$ on G , when viewed as a column vector, \mathcal{L} satisfies:

$$\frac{\langle f, \mathcal{L}f \rangle}{\langle f, f \rangle} = \frac{\sum_{i \sim j} (g(v_i) - g(v_j))^2}{\sum_i g(v_i)^2 \cdot \deg(v_i)} \quad (50)$$

where $f = D^{1/2}g$ and $\langle f, g \rangle$ denotes the standard inner product in \mathbb{R}^n . Equation (50) may be used to show that the spectrum $\Lambda(\mathcal{L})$ is bounded in the interval $[0, 2]$. In particular, it is known that:

$$\lambda_i \leq \sup_f \frac{\langle f, \mathcal{L}f \rangle}{\langle f, f \rangle} \leq 2 \quad (51)$$

Recall that, when G is connected, 0 is an eigenvalue of both L and $\mathcal{L}(G)$, with multiplicity $\text{cc}(G)$. 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 [7] and references within.