

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 how this PBN characterization admits certain computational advantages in both static and parameterized settings. Namely we show the p -th PBN of a filtered simplicial complex K_\bullet which 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 4.

2 Background & Notation

Diagrams are PBNs are Diagrams

Both the persistent homology (PH) groups and their corresponding persistent Betti numbers (PBNs) have long been studied from multiple, equivalent perspectives by several authors, see [1, 2, 4, 12] and references therein for an overview. From an algebraic perspective, Carlsson et al. [12] 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. They also give a cubic-time algorithm to compute these groups on spaces in arbitrary dimensions over any field. In [4], 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:

$$\text{dgm}_p(f) = \{(a_i, a_j) : \mu_p^{i,j} \neq 0\} \cup \Delta \quad (1)$$

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

$$\mu_p^{i,j} = (\beta_p^{i,j-1} - \beta_p^{i,j}) - (\beta_p^{i-1,j-1} - \beta_p^{i-1,j}) \quad \text{for } 0 < i < j \leq n+1 \quad (2)$$

For M a decomposable persistence module over \mathbb{R} , Chazal [2] generalize (2) by introducing several alternative notions of ‘tameness’, and show that whenever a persistence diagram is sought, it is enough to construct its corresponding *persistence measure*:

$$\mu_p(R; M) = \text{card} \left(\text{dgm}_p(M)|_R \right) \quad \text{for all rectangles } R \subset \mathbb{R}^2 \quad (3)$$

The measure-theoretic perspective from (3) re-interprets the multiplicity function μ_p^* as an integer-valued measure over rectangles in the plane. Since μ_p is also defined in terms of PBNs, this perspective gives an indirect way of interpreting PBNs in measure-theoretic terms. Indeed, Cerri et al. [1] 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:

$$x = (i, j) \in \text{dgm}_p(f) \iff \mu_p(x) > 0 \iff \min_{\epsilon > 0} (\beta_p^{i+\epsilon, j-\epsilon} - \beta_p^{i+\epsilon, j+\epsilon}) - (\beta_p^{i-\epsilon, j-\epsilon} - \beta_p^{i-\epsilon, j+\epsilon}) > 0 \quad (4)$$

One may compare (2) with (4). One of the primary contributions from [1] is a representation theorem expressing the persistent Betti number function as a sum of multiplicity functions. A consequence of this theorem is that any distance between persistence diagrams induces a distance between PBN functions $\beta_* : \Delta_+ \rightarrow \mathbb{N} \cup \{\infty\}$ —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 [1] 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, justifying their use and study in continuously parameterized settings.

Despite the stability of the PBNs in parameterized settings, a number of barriers prevent their application in real-world settings. For instance, the main stability theorem from [4] assumes that the underlying filtering function

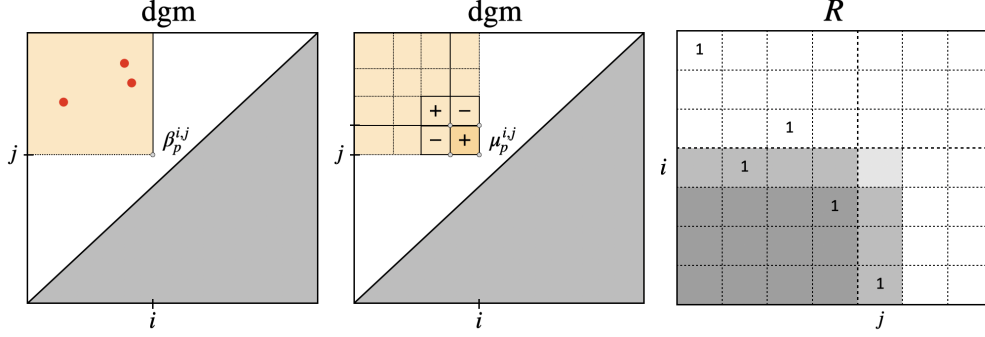


Figure 1: (Left) the persistent Betti number $\beta_p^{i,j}$ counts the number of points (3) in upper left-corner of $\text{dgm}_p(K_\bullet)$. (Middle) The additivity of PBNs can be used to express multiplicity $\mu_p^{i,j}$ of any given box. (Right) The computational interpretation of the Pairing Uniqueness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

or persistence module is *tame* and are defined over triangulable spaces. When the number of corner points is finite, the corresponding distance between PBNs reduces to the bottleneck distance from [4]. By assuming the filtering functions are just continuous (as in equation (4)), instead of tame, we encounter two problems on the practical side: 1. the number of corner points is countably infinite, and 2. the matching distance between PBN functions $\beta_p(f)$, $\beta_p(g)$ requires as input knowledge of the diagrams $\text{dgm}_p(f)$, $\text{dgm}_p(g)$ themselves.

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 some index $(i, j) \in \Delta_+^m$ is defined as:

$$\begin{aligned} \beta_p^{i,j} &= \dim(H_p^{i,j}) \\ &= \dim(Z_p(K_i) / (Z_p(K_i) \cap B_p(K_j))) \\ &= \dim(Z_p(K_i)) - \dim(Z_p(K_i) \cap B_p(K_j)) \end{aligned} \quad (5)$$

While $Z_p(K_i) = \text{nullity}(\partial_p(K_i))$ and is thus easily obtained, efficient computation of the intersection term (the persistence part) is a bit more subtle. Zomorodian et al [12] give a procedure 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, making the PBN computation no more efficient than the full persistence computation.

In what follows, we outline a different approach to computing (5) that 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:

$$r_A(i, j) = \text{rank}(A^{i,j}) - \text{rank}(A^{i+1,j}) + \text{rank}(A^{i+1,j-1}) - \text{rank}(A^{i,j-1}) \quad (6)$$

The structure theorem from [12] 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 [5], 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 result 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 [6]). *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:*

$$\text{rank}(R^{i,j}) = \text{rank}(\partial^{i,j}) \quad (7)$$

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 [3] in their rank-based persistence algorithm—the first output-sensitive algorithm given for computing persistent homology of a filtered complex. In fact, Lemma 1 may be further generalized to arbitrary rectangles in Δ_+ via μ -queries [3]: box-parameterized rank-based queries that count the number of persistence pairs that intersect a fixed “box” placed in the upper half-plane. Our first result of this effort we show is that this Lemma allows us to write the persistent Betti number as a sum of rank functions.

Proposition 1. *For any fixed $p \geq 0$, let ∂_p denote the p -dimensional boundary matrices of filtration K_\bullet of size $n = |K^{(p)}|$, $m = |K^{(p+1)}|$. For any pair $(i, j) \in ([n], [m])$, the persistent Betti number $\beta_p^{i,j}$ at (i, j) is given by:*

$$\beta_p^{i,j} = \text{rank}(I_p^{1,i}) - \text{rank}(\partial_p^{1,i}) - \text{rank}(\partial_{p+1}^{1,j}) + \text{rank}(\partial_{p+1}^{i+1,j}) \quad (8)$$

where $I_p^{1,i}$ denotes the first i columns of the $n \times n$ identity matrix.

A detailed proof using Lemma 1 is given in the appendix. The main utility this proposition provides is that it enables the persistent Betti number as a combination of rank computations performed directly on the *unfactored* dimension p and $(p+1)$ boundary matrices. We dedicate the rest of the paper to exploring the consequences of this fact.

To get some intuition on what the structure and size of these matrices, we include a picture of each of the terms in Equation (8). Boundary matrices are sparse and highly structured: given K_\bullet with m simplices $\sigma_1, \sigma_2, \dots, \sigma_m$

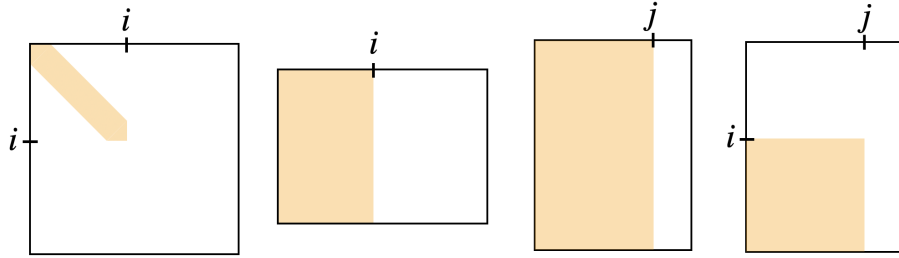


Figure 2: The four matrices whose ranks yield $\beta_p^{i,j}$ in the same order as given in (8). Each solid portion represents (sparse) blocks of non-zero entries, while each white portion is zero. Observe $\partial_{p+1}^{i+1,j} \subseteq \partial_{p+1}^{1,j}$ can be obtained by intersecting the non-zero entries of $\partial_{p+1}^{1,j}$ with the non-zero entries in the complement of $\partial_p^{1,i}$.

constructed from a p -dimensional complex K , its full boundary matrix ∂ is upper-triangular and has a storage complexity of:

$$\text{nnz}(\partial) \sim O(m \log m) \quad (9)$$

To see this, note that since a p -simplex has $2^{p+1} - 1$ faces, $p \leq \log(m+1) - 1$. Moreover, since each column of ∂_p^* contains exactly $p+1$ non-zero entries, $\text{nnz}(\partial) \sim O((p+1)m)$. Indeed, the relation $\partial_{p+1}^{i+1,j} \subseteq \partial_{p+1}^{1,j}$ implies the largest number of non-zeros in any matrix in (8) is $O(\max\{pi, (p+1)j\})$. As a result, we have the following corollary:

Corollary 1. *Given a filtration K_\bullet of size $n = |K_i^{(p)}|$ and $m = |K_j^{(p+1)}|$ and two indices $i \in [n]$, $j \in [m]$, computing $\beta_p^{i,j}$ can be done in time and storage complexity $O(\max\{R_\partial(n, i, p), R_\partial(m, j, p+1)\})$ where $R_\partial(a, b, c)$ is the complexity of computing the rank of a c -dimensional $a \times b$ boundary matrix with $b \cdot (c+1)$ non-zero \mathbb{F} entries.*

In the next section, we show how extend these complexity statements to parameterized settings. We address the storage and time complexity of $R_\partial(\cdot, \cdot)$ in section 2.

A Parameterized Boundary Matrix Relaxation: One advantage of expressing the PBN via equation (8) is that certain properties of rank function may be exploited in *parameterized* settings, i.e. settings where the scalar-valued filter function and corresponding filtration belong to a parametric family. One simple such property of the rank function is permutation invariance: given any square matrix $A \in \mathbb{R}^{n \times n}$, $\text{rank}(A) = \text{rank}(P^T A P)$ for any

permutation matrix P . Observe the boundary matrices ∂_p in (8) need not be in filtration order induced by (K_\bullet, f) to be evaluated—one may permute the matrices in (8) and obtain the same Betti number, so long as the matrices have the same essential non-zero pattern. Notice this lies in stark contrast to e.g. the vineyards algorithm [5]—which requires a $\approx O(m^2)$ maintenance procedure¹ to simulate persistence across a homotopy, the canonical continuous parameterized setting. PBNs need no such procedure even in parameterized settings. We elaborate in the following section.

Recall that the boundary operator ∂_p for a filtration pair (K_\bullet, f) with $m = |C_p(K_\bullet)|$ and $n = |C_{p-1}(K_\bullet)|$ can be represented by an ordered $(n \times m)$ boundary matrix ∂_p whose columns and rows correspond to p -simplices and $(p-1)$ -simplices. After orienting K in an arbitrary but consistent way, the entries of ∂_p have the form:

$$\partial_p[k, l] = \begin{cases} c(\sigma_j) & \text{if } \sigma_l \in \partial_p(\sigma_k) \\ 0 & \text{otherwise} \end{cases} \quad (10)$$

where $c(\sigma_*) \in \mathbb{F}$ is an arbitrary constant satisfying $c(\sigma) = -c(\sigma')$ if σ and σ' are opposite orientations of the same simplex, typically set to ± 1 . In what follows, we assume a fixed orientation is given on K , and write $\pm c(\sigma)$ to indicate the sign of $c(\sigma)$ depends on the orientation of σ . Note the ordering of ∂_p must respect the facet poset of K_\bullet : if $\tau, \sigma \in K_\bullet^{(p)}$ and $f(\tau) \leq f(\sigma)$, then the chain $\partial_p(\tau)$ must appear before $\partial_p(\sigma)$.

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 you wanted to compute $\beta_p^{i,j}$ over \mathcal{H} . We give several application settings where this kind of formulation occurs naturally in section 4. To simplify this process, we introduce the notion of a *parameterized boundary matrix*.

Definition 1 (Parameterized boundary matrix). *Let X denote a data set of interest of size $|X| = n$, equipped with parameterized filtering function $f : \mathcal{P}(X) \times \mathcal{H} \rightarrow \mathbb{R}$. Define $(\mathcal{P}(X), \preceq^*)$ be a fixed linear extension of the face poset of the standard $(n-1)$ -simplex. For fixed $i, j \in \mathbb{F}$, define the \mathcal{H} -parameterized p -th boundary matrix $\hat{\partial}_p^{i,j}(h)$ at scale (i, j) to be the $\binom{n}{p} \times \binom{n}{p+1}$ matrix ordered by \preceq^* for all $h \in \mathcal{H}$, and whose entries (k, l) satisfy:*

$$\hat{\partial}_p^{i,j}(h)[k, l] = \begin{cases} \pm S_{i,j}(\sigma_k, \sigma_l) & \text{if } \sigma_k \in \partial_p(\sigma_l) \\ 0 & \text{otherwise} \end{cases} \quad (11)$$

where $S_{i,j} : \mathcal{P}(X) \times \mathcal{P}(X) \rightarrow \{0, 1\}$ is a step function that accepts a face/coface pair (σ_k, σ_l) and returns a 1 if $f(\sigma_k) \geq i$ and $f(\sigma_l) \leq j$, and 0 otherwise.

The result of definition 1 is that, in parameterized settings, the PBN can be written in essentially the same form as (8). To simplify the notation, we write $A^x = A^{1,x}$ for the setting where only columns up to x of A are being selected, and let $q = p + 1$. We also write $r(A) = \text{rank}(A)$.

$$\begin{aligned} \hat{\beta}_p^{i,j} : \mathcal{H} &\rightarrow \mathbb{N} \\ h &\mapsto |K_i^{(p)}(h)| - (r \circ \hat{\partial}_p^i)(h) - (r \circ \hat{\partial}_q^j)(h) + (r \circ \hat{\partial}_q^{i+1,j})(h) \end{aligned} \quad (12)$$

One remark is in order: note that although definition 1 specifies $\hat{\partial}_p^{i,j}$ as a full $\binom{n}{p} \times \binom{n}{q}$ matrix, implying a memory complexity of $O((p+1)n^{p+1})$ for all $h \in \mathcal{H}$, we remark that there is no need to fully allocate this much memory as the rows/columns corresponding to the set of p/q face/coface pairs (σ_k, σ_l) with $f(\sigma_l) < i$ or $f(\sigma_k) > j$ are entirely 0. As we will show below, it is enough to have access to the simplices $K_j^{(q)}(h)$.

Laplacian Connection: Due to its connection as the discrete analogue of the Laplace differential operator, the graph Laplacian and its spectrum have been studied in many areas of mathematical research as they often have particular geometric interpretations in physical chemistry, and financial mathematics []. Since the investigation of the question “can you hear the shape of a drum?” by [] investigates, the question of what geometric properties of a manifold are determined by its Laplace operator has been of pertinent interest.

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

$$L = D - A = \partial_1 \partial_1^T \quad (13)$$

¹The bound $O(m^2)$ assumes the homotopy changes each filtration value monotonically throughout the homotopy. Otherwise the number of order changes is clearly unbounded.

where D is a diagonal matrix whose entries $d_{ii} = \{\deg(v_i)\}$ are the degrees $\deg(v_i) = \sum_{j \neq i} A[i, j]$ of the vertices $v \in V$. The graph Laplacian and its many variants [] are well studied. Structurally, they admit a number of attractive features: L is symmetric and thus its eigenvalues are real-valued; L is positive semi-definite ($L \succeq 0$) and thus satisfies $x^T L x \geq 0$ for all $x \neq 0$; $\text{rank}(L)$ is given by $n - \text{cc}(G)$, where $\text{cc}(G)$ is the number of connected components of G (and thus, $0 \in \Lambda(L)$ with multiplicity $\omega(G)$). For a list of additional properties, see []. In particular, the quadratic form that L admits has the particular graph interpretation:

$$x^T L x = \sum_{i \sim j} (x_i - x_j)^2, \quad x \in \mathbb{R}^n \quad (14)$$

where we use the notation $i \sim j$ to indicate vertices $i, j \in V$ are path-connected in G . The graph Laplacian is generally known to capture the connectivity structure of G . To make this more concrete, we adapt an example from [9]. Suppose the vertices of G are ordered and labeled from 1 to n arbitrarily such that we may define column vector $x = (x_i)$ whose components $x_i = 1$ indicate $i \in X$ and $x_i = 0$ otherwise. Consider any subset $X \subseteq V$, and let $X' = V \setminus X$ denote the complement set and $c_v(X) = \{(v, w) \in E \mid v \in X \text{ and } w \in V \setminus X\}$ denote the *cutset* of G restricted to v , i.e. the set of edges having as one endpoint $v \in X$ and another endpoint outside of X . Given $y = Lx$, we have:

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

In other words, L captures exactly how X is connected to the rest of G . Notice that if $X = V$, then $y = 0$ and thus 0 must be an eigenvalue of L . This example can be generalized to powers of L , wherein just as entries in A^k model paths, entries in L^k are seen to model boundaries, see [9].

To understand the connection to the Laplacian, we focus on another property of the rank function that we may exploit is -invariance: $\text{rank}(A) = \text{rank}(AA^T) = \text{rank}(A^T A)$.

$$\begin{aligned} \hat{\beta}_p^{i,j} &= |K_i^{(p)}| - \text{rank}(\partial_p^i) - \text{rank}(\partial_q^j) + \text{rank}(\partial_q^{i+1,j}) \\ &= |K_i^{(p)}| - \text{rank}((\partial_p^i)(\partial_p^i)^T) - \text{rank}((\partial_q^j)(\partial_q^j)^T) + \text{rank}((\partial_q^{i+1,j})(\partial_q^{i+1,j})^T) \\ &= |K_i^{(p)}| - \text{rank}(L_p^i) - \text{rank}(L_q^j) + \text{rank}(L_q^{i+1,j}) \end{aligned} \quad (15)$$

Complexity of Persistence:

Rank Computation: In this section we discuss a few iterative methods for finding the eigenvalues of a Hermitian matrices. In particular, we focus on the Lanczos iteration, and related adaptations to positive semi-definite, diagonally dominant (DD) and strictly diagonally dominant (SDD) cases. We also show, where applicable, how these methods made be adapted to efficiently compute (12).

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 are the spaces spanned by:

$$\mathcal{K}_j(A, v) := \text{span}\{v, Av, A^2v, \dots, A^{j-1}v\} = \text{range}(K_j(A, v)) \quad (16)$$

where $K_j(A, v) = [v \mid Av \mid A^2v \mid \dots \mid A^{j-1}v]$ are the corresponding Krylov matrices. To generate an orthonormal basis for $\mathcal{K}_j(A, v)$, the Lanczos method proceeds by constructing a reduced QR factorizations of $K_j(A, v) = Q_j R_j$, for all $j = 1, 2, \dots, n$. Due to orthogonality of Q_j , when A is symmetric and real, we have $q_k^T A q_l = q_l^T A^T q_k = 0$ for $k > l + 1$, implying the corresponding projections $T_j = Q_j^T A Q_j$ have a tridiagonal structure:

$$T_j = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_{j-1} \\ & & & \beta_{j-1} & \alpha_j \end{bmatrix}, \beta_j > 0, j = 1, 2, \dots, n \quad (17)$$

Unlike the spectral decomposition $A = U\Lambda U^T$, 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 . Instead, the Lanczos method exploits a particular connection between the iterates $K_j(A, v)$ (for any $j < n$) 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 $Q Q^T = I_n$, then:

$$K_n(A, q_1) = Q Q^T K_n(A, q_1) = Q [e_1 \mid T e_1 \mid T^2 e_1 \mid \cdots \mid T^{n-1} e_1] \quad (18)$$

is the QR factorization of $K_n(A, q_1)$ —that is, Q may be generated completely by tridiagonalizing A with respect to an orthogonal matrix Q whose first column vector is q_1 . More explicitly, the Implicit Q Theorem [7] 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) . Thus, given an initial pair (A, q_1) , we may restrict and project A to its j -th Krylov subspace T_j via:

$$A Q_j = Q_j T_j + \beta_j q_{j+1} e_j^T \quad (19)$$

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} , e_j is the standard j identity vector, and $\beta_j > 0$. Equating the j -th columns on each side of (19) yields the three-term recurrence:

$$A q_j = \beta_{j-1} q_{j-1} + \alpha_j q_j + \beta_j q_{j+1} \quad (20)$$

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 $q_{j+1} = r_j / \beta_j$. Observe that if q_{j-1}, β_j and q_j are known, then α_j, β_{j+1} and q_{j+1} are completely determined and (20) may be used to obtain T_j —this sequential process is called the *Lanczos iteration*. Note that if we encounter $\beta_j = 0$ for some $j < n$, then $\text{range}(Q_j) = \mathcal{K}_j(A, q_1)$ is A -invariant subspace, the iteration stops, and we have $j = \text{rank}(A)$ and $\Lambda(T_j) = \Lambda(A)$.

The Lanczos iteration is computationally attractive due to the fact that each step consists of a matrix-vector multiplication, and inner product, and a few vector operations. If one can efficiently compute $v \mapsto Av$ because A is sparse and/or has special structure, then the Lanczos method may require significantly less than the $O(n^3)$ operations needed by the more direct methods. Indeed, the three-term recurrence from (20) implies the Lanczos iteration of A may be carried out with just three $O(n)$ -sized vectors. 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 [7]. In general, the reduction to tridiagonal form is the more difficult part of the two-phase computation: once T_j has been obtained for sufficient $j > 0$, the corresponding spectrum $\Lambda(T_j)$ may be obtained in $O(n \log n)$ time [8].

The sparsity pattern ∂_p inherits from the simplicial structure of K confers a few computational advantages compared to more general linear operators. Observe each column of ∂_p corresponds to a p -chain of the form (10), which is a constant up to difference in sign. Thus, evaluating $y = \partial_p^T v$ reduces to computing the locations $(k_1, k_2, \dots, k_{p+1})$:

$$y_i = y_i \pm S_{i,j}(\sigma_k, \sigma_l) \quad (21)$$

In particular, the operator ∂_p need not be represented explicitly in memory. To make this more precise, we start with a useful lemma:

Lemma 2. *For any fixed $p \geq 0$, given simplicial complex K with m (n , respectively) simplices of dimension p ($p-1$, respectively) and an arbitrary vector v of size $|v| = n$, the operation $v \mapsto \partial_p \partial_p^T v$ can be evaluated $O(\max\{m, n\})$ time and $O(\max\{m, n\})$ memory.*

From this lemma, we have the following result:

Proposition 2 ([10, 11]). *Given a simplicial complex K with $m = |K^{(p+1)}|$ and $n = |K^{(p)}|$. Without loss of generality, assume $n < m$, and that $\text{rank}(\partial_p) = r$. Moreover, assume we may carry out the computation $v \mapsto \partial_p \partial_p^T v$ with coefficients in $\mathbb{F} = \mathbb{R}$ in exact arithmetic in $O(m)$ time. Then the Lanczos iteration from [] yields the quantity:*

$$\dim(B_{p-1}(K; \mathbb{R})) = \text{rank}(\partial_p(K)) \quad (22)$$

in $O(mr)$ time and $O(m)$ storage complexity.

A proof of this proposition is given in the appendix.

For expository purposes, the preceding sections assumed exact arithmetic.

In principle, if the Lanczos iteration doesn't break down due to rounding errors (T_k is full rank), then the characteristic polynomial of T_k is the unique polynomial $p^k \in P^k$ that achieves []:

$$\|p^k(A)b\| = \text{minimum} \quad (23)$$

In fact, there is more we can say: if $S = \mathcal{K}_k(A, q_1)$, then applying the Lanczos iteration yield the *Ritz pairs* (θ, y) of A , which are the pairs satisfying $w^T(Ay - \theta y) = 0$ for all $w \in S$. The essential result from [1] is that the eigenvalues $\Lambda(T_k) = \{\theta_1, \theta_2, \dots, \theta_k\}$ are ‘optimal’ in the sense that $T_k = B$ is the matrix that minimizes $\|AQ_k - QkB\|_2$ over the space of all $k \times k$ matrices. Thus, if $\text{rank}(A) = r$, the eigenvalues of T_k for some $k < r$ tend to converge quickly to the largest eigenvalues of A .

The iteration typically converges geometrically and can be stopped as soon as the desired accuracy is reached.

4 Applications

Consider an $n \times m$ boundary matrix ∂_p representing the boundary operator $C_p(K) \rightarrow C_{p-1}(K)$. Our goal is to have the ability to compute the ranks of submatrices of ∂_p as efficiently as possible, possibly in a parameterized stream.

In general, the complexity of computing the rank of a $n \times m$ matrix A depends heavily on both the structure of A (e.g. its sparsity) as well as the choice of coefficients \mathbb{F} . Typical persistence computations are carried out using coefficients in $\mathbb{Z}/2\mathbb{Z}$ as the computation is greatly simplified in this setting. Indeed, the persistence computation is not invariant to the choice of field \mathbb{F} .

Here, we consider the complexity of computing $\beta_p^{i,j}$ with real-valued coefficients. Since real numbers may not be representable explicitly in finite precision, we will consider the *numerical rank*.

Definition 2 (Numerical Rank). *Let $A \in \mathbb{R}^{m \times n}$ have singular values $\sigma_1(A) \geq \sigma_2(A) \geq \dots \geq \sigma_r(A) > 0$. For some $0 < \epsilon < 1$, the ϵ -rank of A , denoted by $\text{rank}_\epsilon(A)$, is the smallest integer k such that:*

$$\text{rank}_\epsilon(A) = \min_{k \geq 0} \{ k : \sigma_{k+1}(A) \leq \epsilon \cdot \|A\|_2 \} \quad (24)$$

The most direct way to compute (24) is compute the singular values of a matrix up to working precision, however this requires $O(mn^2)$ complexity in general \square .

It is instructive to consider Observe that computation of β_p^* involves rank computations on subsets of the $p, p+1$ boundary matrices. When $p = 0$, we have:

$$\begin{aligned} \beta_0^{i,j} &= \text{rank}(I_p^{1,i}) - \text{rank}(\partial_p^{1,i}) - \text{rank}(\partial_{p+1}^{1,j}) + \text{rank}(\partial_{p+1}^{i+1,j}) \\ &= |C_0(K_i)| - \text{rank}_\epsilon((\partial_1^{1,j})(\partial_1^{1,j})^T) + \text{rank}_\epsilon((\partial_1^{i+1,j})(\partial_1^{i+1,j})^T) \\ &= |C_0(K_i)| - \text{rank}_\epsilon(L_1^j) + \text{rank}_\epsilon((\partial_1^{i+1,j})(\partial_1^{i+1,j})^T) \end{aligned}$$

Where L_1^j is a graph Laplacian the subgraph of K consisting of only edges $e \in K_1$ with $f(e) \leq j$.

A Appendix

Proofs:

Proof of Lemma 1

Proof. The Pairing Uniqueness Lemma [6] 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:

$$\text{low}_R[j] = i \iff r_R(i, j) \neq 0 \iff r_\partial(i, j) \neq 0 \quad (25)$$

Extending this result to equation (7) 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 (5) 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:

$$\dim(Z_p(K_i) \cap B_p(K_j)) = |\Gamma_p^{i,j}| \quad (26)$$

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:

$$|\bar{\Gamma}_p^{i,j}| = \dim(B_p(K_j)) - |\Gamma_p^{i,j}| = \text{rank}(R_{p+1}^{i+1,j}) \quad (27)$$

Combining equations (26) and (27) yields:

$$\dim(Z_p(K_i) \cap B_p(K_j)) = |\Gamma_p^{i,j}| = \dim(B_p(K_j)) - |\bar{\Gamma}_p^{i,j}| = \text{rank}(R_{p+1}^{1,j}) - \text{rank}(R_{p+1}^{i+1,j}) \quad (28)$$

Observing the final matrices in (28) are *lower-left* submatrices of R_{p+1} , the final expression (8) 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 $K_t = \text{Rips}_\epsilon(\delta_X(t))$ with non-zero entries satisfying (10) 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 space²
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...

Application: Time-varying : Let δ_X denote an T -parameterized metric space $\delta_X(\cdot) = (X, d_X(\cdot))$, where $d_X : T \times X \times X \rightarrow \mathbb{R}_+$ is called a *time-varying metric* and X is a finite set with fixed cardinality $|X| = n$. δ_X as called a *dynamic metric space* (DMS) iff $d_X(\cdot)(x, x')$ is continuous for every pair $x, x' \in X$ and $\delta_X(t) = (X, d_X(t))$ 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

$$\text{Rips}_\epsilon(\delta_X(t)) := \{ \sigma \subset X : d_X(t)(x, x') \leq \epsilon \text{ for all } x, x' \in \sigma \} \quad (29)$$

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 $t \in T$:

$$\beta_p^{i,j}(t) = (\dim \circ H_p^{i,j} \circ \text{Rips} \circ \delta_X)(t) \quad (30)$$

References

- [1] Andrea Cerri, Barbara Di Fabio, Massimo Ferri, Patrizio Frosini, and Claudia Landi. Betti numbers in multidimensional persistent homology are stable functions. *Mathematical Methods in the Applied Sciences*, 36(12):1543–1557, 2013.
- [2] Frédéric Chazal, Vin De Silva, Marc Glisse, and Steve Oudot. *The structure and stability of persistence modules*, volume 10. Springer, 2016.
- [3] Chao Chen and Michael Kerber. An output-sensitive algorithm for persistent homology. In *Proceedings of the twenty-seventh annual symposium on Computational geometry*, pages 207–216, 2011.

²This 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 $t \in \mathbb{R}$.

- [4] David Cohen-Steiner, Herbert Edelsbrunner, and John Harer. Stability of persistence diagrams. In *Proceedings of the twenty-first annual symposium on Computational geometry*, pages 263–271, 2005.
- [5] David Cohen-Steiner, Herbert Edelsbrunner, and Dmitriy Morozov. Vines and vineyards by updating persistence in linear time. In *Proceedings of the twenty-second annual symposium on Computational geometry*, pages 119–126, 2006.
- [6] Tamal Krishna Dey and Yusu Wang. *Computational topology for data analysis*. Cambridge University Press, 2022.
- [7] Gene H Golub and Charles F Van Loan. *Matrix computations*. JHU press, 2013.
- [8] Ming Gu and Stanley C Eisenstat. A divide-and-conquer algorithm for the symmetric tridiagonal eigenproblem. *SIAM Journal on Matrix Analysis and Applications*, 16(1):172–191, 1995.
- [9] Michael William Newman. The laplacian spectrum of graphs. Master’s thesis, 2001.
- [10] Beresford N Parlett. Do we fully understand the symmetric lanczos algorithm yet. *Brown et al*, 3:93–107, 1994.
- [11] Horst D Simon. Analysis of the symmetric lanczos algorithm with reorthogonalization methods. *Linear algebra and its applications*, 61:101–131, 1984.
- [12] Afra Zomorodian and Gunnar Carlsson. Computing persistent homology. In *Proceedings of the twentieth annual symposium on Computational geometry*, pages 347–356, 2004.

A Boundary matrix factorization

Definition 3 (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.