

# Persistent Betti Numbers *over time*

Theory, computation, and applications

## "Murmurations"



# Persistent Homology is an *intrinsic invariant*

Persistent Homology (PH) is a well-established tool in the sciences<sup>[1,2]</sup>

PH has many attractive properties beyond homology:

1. *General* : Persistence can be generalized *via rank functions*<sup>[5,6]</sup>
2. *Descriptive* :  $d_B(\text{dgm}_p(X), \text{dgm}_p(Y))$  lower-bounds  $d_{GH}(X, Y)$ <sup>[7]</sup>
3. *Geometric* : distributed dgm's interpolate local geometry  $\leftrightarrow$  global topology<sup>[4]</sup>
4. *Stable* :  $d_B(\text{dgm}(f), \text{dgm}(g)) \leq \|f - g\|_\infty$  between function  $f, g$ <sup>[3]</sup>

Collections of dgm's uniquely characterize simplicial complexes in  $\mathbb{R}^d$ <sup>[7]</sup>

PH is more than just a homology inference tool!

1. Wigner, Eugene P. "The unreasonable effectiveness of mathematics in the natural sciences." *Mathematics and Science*. 1990. 291-306.

2. Turkeš, Renata, Guido Montúfar, and Nina Otter. "On the effectiveness of persistent homology." *arXiv preprint arXiv:2206.10551* (2022).

3. Cohen-Steiner, David, Herbert Edelsbrunner, and John Harer. "Stability of persistence diagrams." *Discrete & computational geometry* 37.1 (2007): 103-120.

4. Solomon, Elchanan, Alexander Wagner, and Paul Bendich. "From geometry to topology: Inverse theorems for distributed persistence." *arXiv preprint arXiv:2101.12288* (2021).

5. Zomorodian, Afra, and Gunnar Carlsson. "Computing persistent homology." *Discrete & Computational Geometry* 33.2 (2005): 249-274.

6. Bergomi, Mattia G., and Pietro Vertechi. "Rank-based persistence." *arXiv preprint arXiv:1905.09151* (2019).

7. Turner, Katharine, Sayan Mukherjee, and Doug M. Boyer. "Persistent homology transform for modeling shapes and surfaces." *Information and Inference: A Journal of the IMA* 3.4 (2014): 310-344.



# Persistent Homology is a ~~intrinsic~~ difficult invariant

The persistence computation scales  $\sim O(m^3)$  over  $K$  with  $m = |K|$  simplices

Morozov gave an counter-example<sup>[1]</sup> showing this bound to be tight (i.e.  $\Omega(m^3)$ )

$\implies$  computing  $\text{dgm}_p(K) \sim \Theta(m^3) = \Theta(n^{3(p+2)})$  over an  $n$ -point set, for  $p \geq 1$

*Simple algorithm  $\neq$  simple implementation*

1. Computing  $R = \partial V$  is *memory intensive*:  $|V| \sim O(m^2)$
2.  $K$ 's structure affects complexity (e.g. 2-manifolds  $\sim O(n\alpha(n))$ <sup>[2]</sup>)
3. Theory is extensive: *clearing*<sup>[3]</sup>, *apparent pairs*<sup>[4]</sup>, *cohomology*<sup>[5]</sup>, ...
4.  $\mathbb{F}$  matters:  $\mathbb{Z}_2$  columns  $\leftrightarrow$  64-arity bit-trees + DeBruijn "magic" tables<sup>[6]</sup>

1. Morozov, Dmitriy. "Persistence algorithm takes cubic time in worst case." BioGeometry News, Dept. Comput. Sci., Duke Univ 2 (2005).

2. Dey, Tamal Krishna, and Yusu Wang. Computational topology for data analysis. Cambridge University Press, 2022.

3. Chen, Chao, and Michael Kerber. "Persistent homology computation with a twist." Proceedings 27th European workshop on computational geometry. Vol. 11. 2011.

4. Bauer, Ulrich. "Ripser: efficient computation of Vietoris–Rips persistence barcodes." Journal of Applied and Computational Topology 5.3 (2021): 391–423.

5. De Silva, Vin, Dmitriy Morozov, and Mikael Vejdemo-Johansson. "Dualities in persistent (co) homology." Inverse Problems 27.12 (2011): 124003.

6. See PHAT's source: [https://github.com/blazs/phant/blob/master/include/phant/representations/bit\\_tree\\_pivot\\_column.h](https://github.com/blazs/phant/blob/master/include/phant/representations/bit_tree_pivot_column.h)

# This Talk: Persistent Betti numbers over *time*

The persistence dgm of function  $f$  is *defined* by persistent Betti numbers (PBNs)

$$\text{dgm}_p(f) \subset \overline{\mathbb{R}}^2 \Leftrightarrow (i, j) \text{ such that } \mu_p^{i,j} \neq 0$$

where  $\mu_p^{i,j}$  is called the *multiplicity function*, defined as:

$$\mu_p^{i,j} = (\beta_p^{i,j-1} - \beta_p^{i,j}) - (\beta_p^{i-1,j-1} - \beta_p^{i-1,j})$$

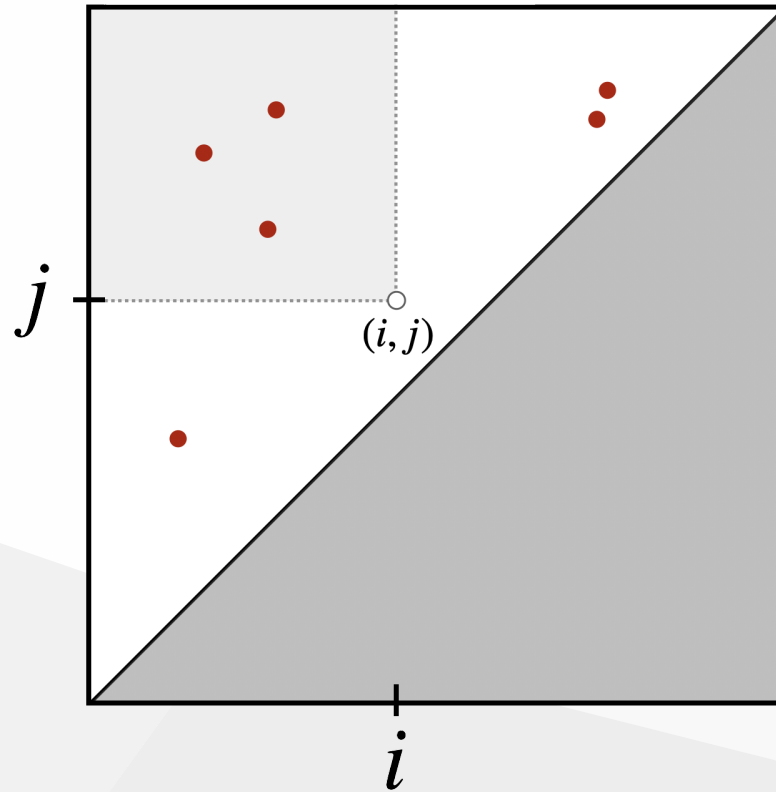
$$\beta_p : K_{\bullet} \times \mathbb{R} \rightarrow \mathbb{Z}_+ \implies \text{Betti curve over filtration}$$

$$\beta_p : \mathcal{P}(X) \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{Z}_+ \implies \text{Betti curves over 1-parameter family}$$

$$\beta_p^{i,j} : \mathcal{P}(X) \times \mathbb{R} \rightarrow \mathbb{Z}_+ \implies \text{Persistent Betti curves for fixed } i, j \in I$$

This talk will focus on relaxing  $\beta_p^{i,j}$  for *time-varying settings*

dgm



$$\beta_p^{i,j} = \dim(H_p(K_i) \rightarrow H_p(K_j))$$

# Outline

→ Background ←

Simplicial Complexes

Cycle, Boundary, and Chain Groups

Filtrations and Persistent Homology

The Main Result

$\beta_p^{i,j}$ 's definition + computation

A clever observation + trick

Re-thinking chains and ranks w/ coefficients in  $\mathbb{R}$

Relaxation: definition and properties

Applications

A  $(1 - \epsilon)$ -approximation of  $\beta_p^{i,j}$

Signatures of time-varying systems

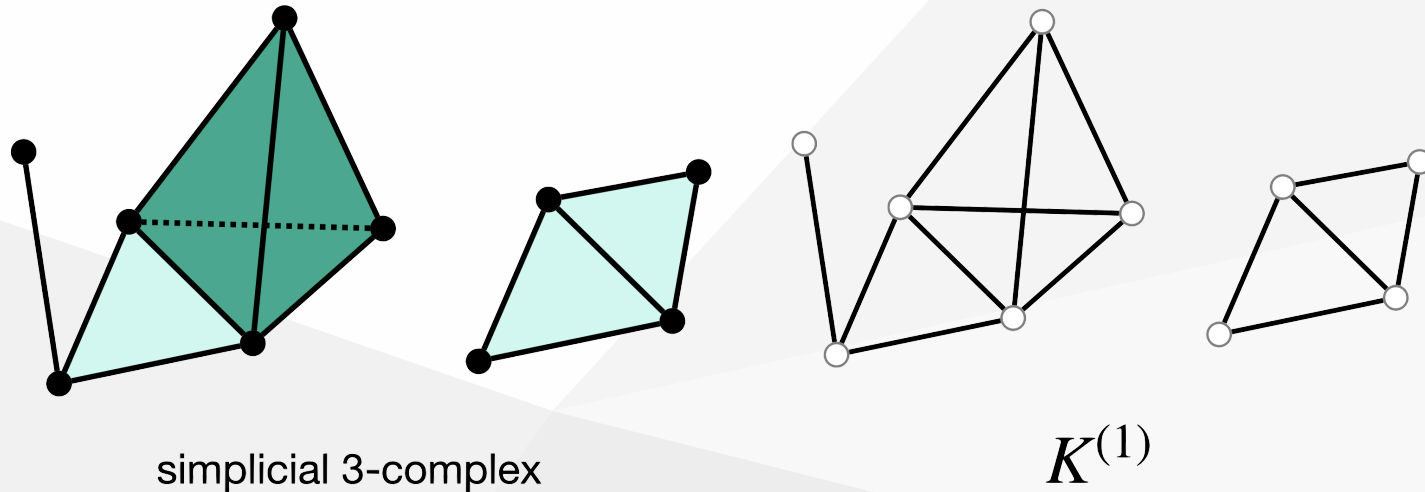
Leveraging PHT theory

## Background: Simplicial Complexes

A simplicial complex  $K = \{\sigma : \sigma \in \mathcal{P}(V)\}$  over set  $V = \{v_1, \dots, v_n\}$  satisfies:

(vertex)  $v \in V \implies \{v\} \in K$

(face)  $\tau \subseteq \sigma \in K \implies \tau \in K$



All computations here will be with *finite simplicial complexes*

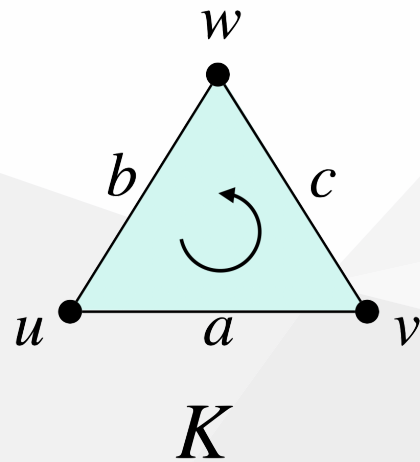


## Background: Boundaries

Given an *oriented*  $p$ -simplex  $\sigma \in K$ , define its  $p$ -boundary as the alternating sum:

$$\partial_p(\sigma) = \partial_p([v_0, v_1, \dots, v_p]) = \sum_{i=0}^p (-1)^i [v_0, \dots, \hat{v}_i, \dots, v_p]$$

We will make heavy use of *oriented boundary matrices*



	$a$	$b$	$c$
$u$	1		1
$v$	-1	1	
$w$		-1	-1

$\partial_p$

By default, we will work generically with the simplex-wise lexicographical order

## Background: The Groups

Given a pair  $(K, \mathbb{F})$ , a  $p$ -chain is a formal  $\mathbb{F}$ -linear combination of  $p$ -simplices of  $K$

The operator  $\partial_p$  extends linearly to  $p$ -chains via their constitutive simplices

$$c = \sum_{i=1}^{m_p} \alpha_i \sigma_i, \quad c + c' = \sum_{i=1}^{m_p} (\alpha_i + \alpha'_i) \sigma_i$$

Given  $\mathbb{F}$  a field and  $K$  a simplicial complex, the following groups are defined<sup>[1]</sup>

$$C_p(K) = (K, +, \times, \mathbb{F}) \iff \text{vector space of } p\text{-chains}$$

$$B_p(K) = (\text{Im} \circ \partial_{p+1})(K) \iff \text{boundary group}$$

$$Z_p(K) = (\text{Ker} \circ \partial_p)(K) \iff \text{cycle group}$$

$$H_p(K) = Z_p(K) / B_p(K) \iff \text{homology group}$$

## Background: Filtrations

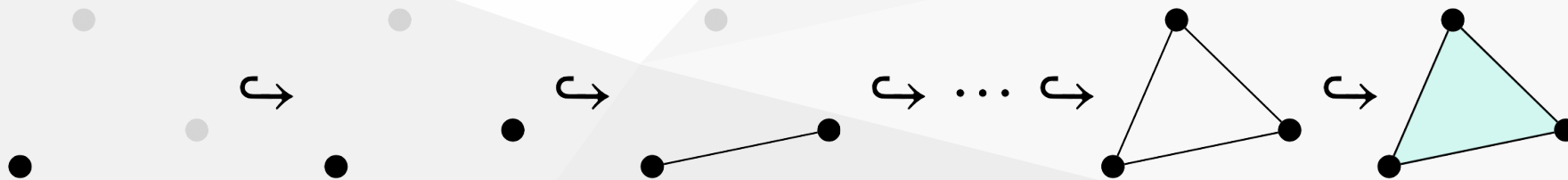
A *filtration*  $K_\bullet$  is a family  $\{K_i\}_{i \in I}$  indexed over a totally ordered index set  $I$ :

$$\text{Filtered} \iff K_0 \subsetneq K_1 \subsetneq \cdots \subsetneq K_m = K_\bullet$$

$$\text{Essential} \iff i \neq j \text{ implies } K_i \neq K_j$$

$$\text{Simplexwise} \iff K_j \setminus K_i = \{\sigma_j\} \text{ when } j = \text{succ}(i)$$

Any  $K_\bullet \mapsto$  essential & simplexwise via *condensing + refining + reindexing maps* <sup>[1]</sup>



Note here that  $I$  may be  $\mathbb{R}_+$  or  $[m] = \{1, 2, \dots, m\}$ , depending on the context!

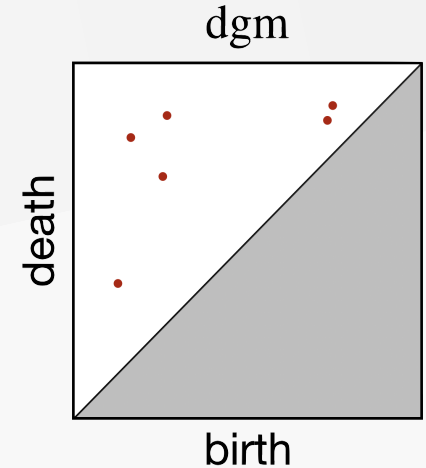
## Background: Persistent Homology

Inclusions  $K_i \hookrightarrow K_j$  induce linear transformations  $h_p^{i,j}$  between homology groups

$$H_p(K_0) \rightarrow \cdots \rightarrow H_p(K_i) \underbrace{\rightarrow \cdots \rightarrow}_{h_p^{i,j}} H_p(K_j) \rightarrow \cdots \rightarrow H_p(K_m) = H_p(K_\bullet)$$

Properties of persistent homology groups:

1.  $H_p(K_\bullet)$  admits a *pair decomposition*  $\text{dgm}(K) \subseteq \bar{\mathbb{R}}^2$
2.  $\text{dgm}(K)$  is *unique* iff  $\mathbb{F}$  is a field
3.  $\beta_p^{i,j}$  can be read-off directly for any  $i, j$  from  $\text{dgm}_p(K)$
4. Computed via matrix decomposition  $R = \partial V$



For simplicity, we will use  $\partial_p^i = \partial_p(K_i)$ ,  $Z_p^i = Z_p(K^i)$ ,  $B_p^i = B_p(K^i)$ , etc.

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→ The Main Result ←

$\beta_p^{i,j}$ 's definition + computation

A clever observation + trick

Re-thinking chains and ranks w/ coefficients in  $\mathbb{R}$

Relaxation: definition and properties

## Applications

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Signatures of time-varying systems

Leveraging PHT theory

## $\beta_p^{i,j}$ : starting with the definition

Before extending  $\beta_p^{i,j}$  to the time-varying setting, first consider its definition:

$$\begin{aligned}\beta_p^{i,j} &= \dim(H_p(K_i) \rightarrow H_p(K_j)) \\ &= \dim(Z_p(K_i) / B_p(K_j)) \\ &= \dim(Z_p(K_i) / (Z_p(K_i) \cap B_p(K_j))) \\ &= \dim(Z_p(K_i)) - \dim(Z_p(K_i) \cap B_p(K_j)) \\ &= \dim(C_p(K_i)) - \dim(B_{p-1}(K_i)) - \dim(Z_p(K_i) \cap B_p(K_j))\end{aligned}$$

Replacing the groups above with appropriate matrices / constants, we have:

$$\beta_p^{i,j} = |K_i^{(p)}| - \text{rank}(\partial_p^i) - \text{rank}(\partial_p^{i,j})$$

where  $\partial_p^{i,j}$  is **some matrix** whose columns span  $Z_p(K_i) \cap B_p(K_j)$ ...



# Computing the *persistent* Betti number $\beta_p^{i,j}$

$$\beta_p^{i,j} = \underbrace{\dim(C_p(K_i))}_{(1)} - \underbrace{\dim(B_{p-1}(K_i))}_{(2)} - \underbrace{\dim(Z_p(K_i) \cap B_p(K_j))}_{(3)}$$

Both (1) and (2) are easy to obtain. Computing (3) is more subtle:

$$\text{PH / reduction algorithm} \implies \sum_{k=1}^j \mathbf{1}(\text{low}_{R_{p+1}}[k] \leq i)$$

$$\text{Gaussian elimination}^{[1]} \implies (\text{ see Zomorodian \& Carlsson [1] })$$

$$\text{Anderson-Duffin formula}^{[2]} \implies P_{\mathbf{Z} \cap \mathbf{B}} = 2P_{\mathbf{Z}}(P_{\mathbf{Z}} + P_{\mathbf{B}})^{\dagger} P_{\mathbf{B}}$$

$$\text{Alternative: } \beta_p^{i,j} = \text{null}(\Delta_p^{i,j}) \text{ where } \Delta_p^{i,j} \text{ is the } \textit{persistent Laplacian}^{[4]}$$

*All of these rely on explicit reductions or expensive projectors. Not great!*

1. Zomorodian, Afra, and Gunnar Carlsson. "Computing persistent homology." Discrete & Computational Geometry 33.2 (2005): 249-274.

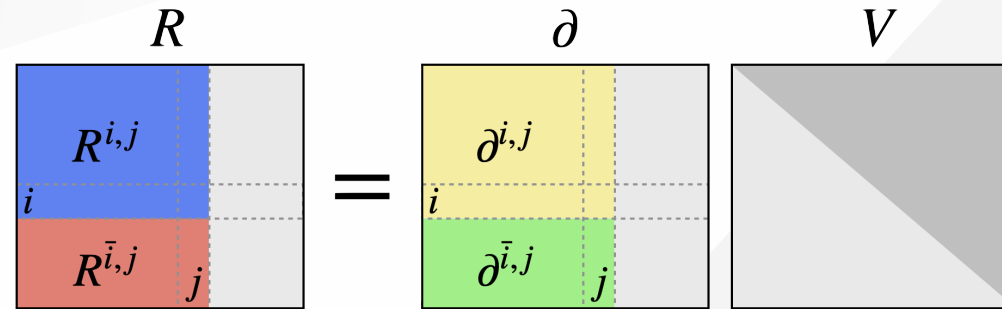
2. Ben-Israel, A., and A. Charnes. "On the intersections of cones and subspaces." Bulletin of the American Mathematical Society 74.3 (1968): 541-544.

3. Neumann, J. Von. "Functional Operators, Vol. II. The Geometry of Orthogonal Spaces. Annals of Math." Studies Nr. 22 Princeton Univ. Press (1950).

4. Mémoli, Facundo, Zhengchao Wan, and Yusu Wang. "Persistent Laplacians: Properties, algorithms and implications." SIAM Journal on Mathematics of Data Science 4.2 (2022): 858-884.

## A clever observation

Let  $R = \partial V$ . Define the submatrices  $R^{i,j}$ ,  $R^{\bar{i},j}$ ,  $\partial^{i,j}$ ,  $\partial^{\bar{i},j}$  as follows:



The Pairing Uniqueness Lemma<sup>[2]</sup> can be used to show:

$$\text{low}_R[j] = i \iff r_R(i, j) \neq 0 \iff r_{\partial}(i, j) \neq 0 \iff \text{rank}(R^{\bar{i},j}) = \text{rank}(\partial^{\bar{i},j})$$

$$\text{where } r_A(i, j) := \text{rank}(A^{\overline{i-1},j}) - \text{rank}(A^{\bar{i},j}) + \text{rank}(A^{\bar{i},j-1}) - \text{rank}(A^{\overline{i-1},j-1})$$

Take-a-way:  $\text{rank}(R^{\bar{i},j})$  can be deduced from  $\text{rank}(\partial^{\bar{i},j})$ , for any  $1 \leq i < j < m$

This was the motivating exploit in first output-sensitive persistence algorithm<sup>[1,2]</sup>

## A clever trick

Pairing uniqueness<sup>[1]</sup>  $\implies \text{rank}(R^{\bar{i},j}) = \text{rank}(\partial^{\bar{i},j})$ , for any  $1 \leq i < j < m$

Dey & Wang show<sup>[2]</sup> have shown the following:

$$\begin{aligned}\dim(Z_p^i \cap B_p^j) &= \dim(B_p^j) - \#(\text{col}_{R_{p+1}}[k] \neq 0 \mid k \in [j], \text{low}_{R_{p+1}}[k] > i) \\ &= \text{rank}(R_{p+1}^{j,j}) - \text{rank}(R_{p+1}^{\bar{i},j}) \\ &= \text{rank}(\partial_{p+1}^{j,j}) - \text{rank}(\partial_{p+1}^{\bar{i},j})\end{aligned}$$

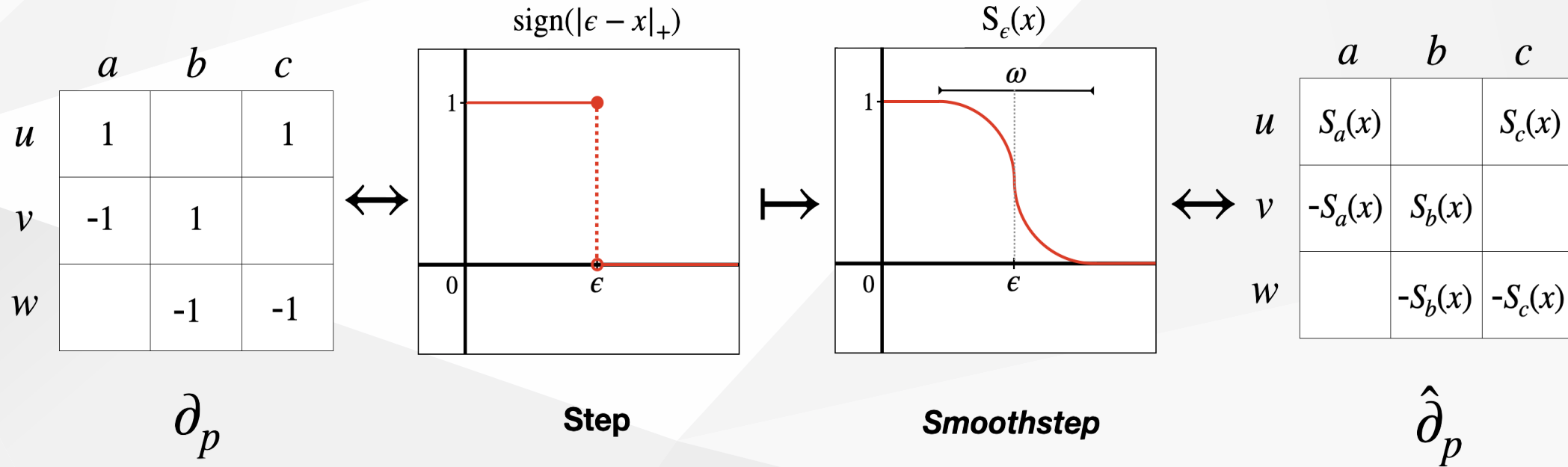
Let  $I_p^i$  be the diagonal matrix with whose first  $i$  entries are 1. We can now write:

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

Thus, we may write  $\beta_p^{i,j}$  completely in terms of *unfactored matrices*

# Parameterizing elementary $p$ -chains

Suppose we fix  $\mathbb{F} = \mathbb{R}$  and replace chain values with *smoothstep* functions  $S_\epsilon(x)$



$$\hat{\partial}_p[i, j] = \pm(S_{\epsilon_j} \circ f)(\sigma_j) \quad \text{if } \sigma_i \in \partial(\sigma_j), \quad \text{where } \epsilon_j = f(\sigma_j)$$

Advantage: If  $f$  varies continuous one-parameter family,  $\hat{\partial}_p$  also varies continuously

## A generic approximation of rank

Moreover, replace  $\text{rank}(A)$  with  $\Phi_\epsilon(A)$ , defined for some fixed  $\epsilon > 0$  as:

$$\Phi_\epsilon(A) = \text{tr} [A^T (AA^T + \epsilon I)^{-1} A] = \sum_i^n \frac{\sigma_i^2}{\sigma_i^2 + \epsilon}, \quad \text{where } \sigma_i^2 := \lambda_i(AA^T)$$

Observe  $\Phi_\epsilon(A) \leq \text{rank}(A)$ , with equality when  $\epsilon = 0$ , yielding the final relaxation:

$$\hat{\beta}_p^{i,j} = \Phi_\epsilon(\mathbf{I}_p^i) - \Phi_\epsilon(\hat{\partial}_p^{i,i}) - \Phi_\epsilon(\hat{\partial}_{p+1}^{j,j}) + \Phi_\epsilon(\hat{\partial}_{p+1}^{\bar{i},j})$$

We use the spectrum of  $\hat{\partial}_p^*$  is used to encode geometric information from  $f$

**Ex:** Let  $\delta_X = (X, d_X(\cdot))$ ,  $d_X : X \times X \times \mathbb{R}$  be a *dynamic metric space*, and let:

$$\hat{\beta}_p^{i,j}(t) = (\text{dim} \circ \mathbf{H}_p^{i,j} \circ \text{Rips} \circ \delta_X)(t)$$

Observe that  $\hat{\beta}_p^{i,j}(t) \in \mathbb{R}$  varies *continuously* with  $t$ —a time-varying relaxation!

## Basic properties of $\hat{\beta}_p^{i,j}$

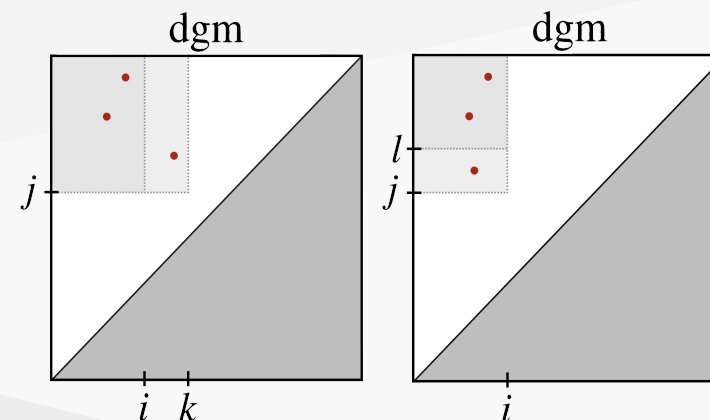
Observe  $\Phi_\epsilon(A) = \sum_{i=1}^n \sigma_i^2 / (\sigma_i^2 + \epsilon) \leq \text{rank}(A)$ , with equality obtained when  $\epsilon = 0$

1.  $\hat{\beta}_p^{i,j} \rightarrow \beta_p^{i,j}$  as  $\epsilon \rightarrow 0, \omega \rightarrow 0$
2. There  $\exists$  an  $\epsilon^* > 0$  such that  $\lceil \hat{\beta}_p^{i,j} \rceil = \beta_p^{i,j}$  for all  $\epsilon \in (0, \epsilon^*]$

$\hat{\beta}_p^{i,j}$  respects several of  $\beta_p^{i,j}$  monotonicity properties *approximately*

$$\forall i < k, \beta_p^{i,j} \leq \beta_p^{k,j} \implies \hat{\beta}_p^{i,j} + \delta_\epsilon(k - i) \leq \hat{\beta}_p^{k,j}$$

$$\forall j < l, \beta_p^{i,j} \geq \beta_p^{i,l} \implies \hat{\beta}_p^{i,j} + \delta_\epsilon(l - j) \leq \hat{\beta}_p^{i,l}$$



$\hat{\beta}_p^{i,j}$  also satisfies an  $\epsilon$ -approximate version of *jump monotonicity*<sup>[1]</sup>

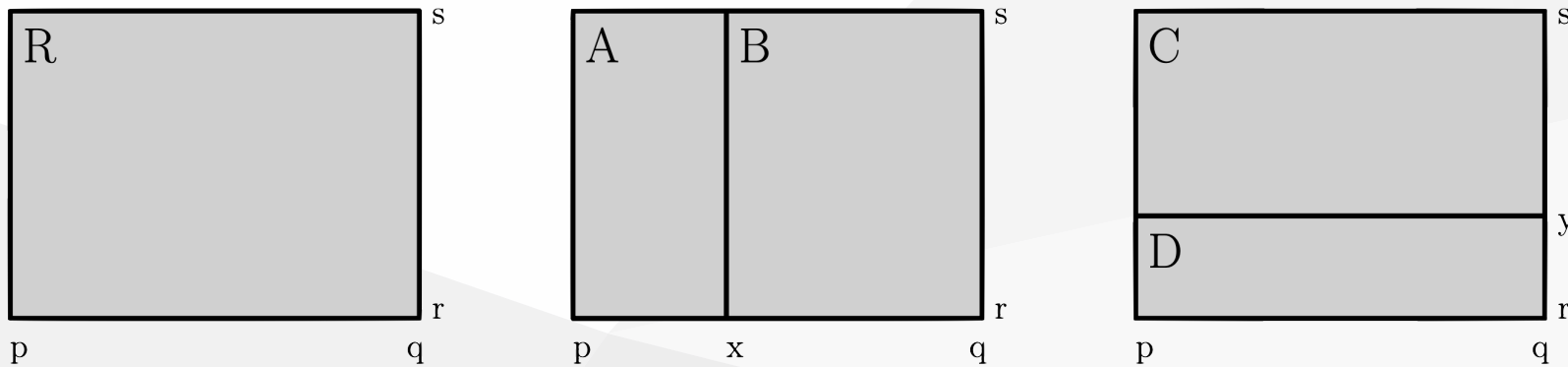


## Persistence measures

Pairs  $(i, j)$  in dgm's can also be defined as limiting points w/ non-zero multiplicity

$$\mu_p^{i,j} = \min_{\epsilon > 0} \{ \beta_p^{i+\epsilon, j-\epsilon} - \beta_p^{i-\epsilon, j-\epsilon} - \beta_p^{i+\epsilon, j+\epsilon} + \beta_p^{i-\epsilon, j+\epsilon} \}$$

PBN's also yield "counting measures" in  $\overline{\mathbb{R}}^2$ , due to their additivity under splitting:



$$\mu(R) = \mu(A) + \mu(B) = \mu(C) + \mu(D)$$

$\hat{\mu}_\epsilon$  also obeys inclusion/exclusion—can be interpreted as a persistence measure

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- Cycle, Boundary, and Chain Groups

- Filtrations and Persistent Homology

## The Main Result

- $\beta_p^{i,j}$ 's definition + computation

- A clever observation + trick

- Re-thinking chains and ranks w/ coefficients in  $\mathbb{R}$

- Relaxation: definition and properties

## → Applications ←

- A  $(1 - \epsilon)$ -approximation of  $\beta_p^{i,j}$

- Signatures of time-varying systems

- Leveraging PHT theory

## $(1 - \delta)$ -approximation scheme for $\hat{\beta}_p^{i,j}$

The fixed parameters  $(\omega, \epsilon)$  completely determine the closeness of  $|\hat{\beta}_p^{i,j} - \beta_p^{i,j}|$

The *Lanczos* method<sup>[1,2]</sup> computes  $q$ -largest  $\sigma^2(A)$  of a sparse  $m \times m$  matrix  $A$  in:

$$O(m \cdot T_m(A) + q^2 \cdot m)$$

where  $T_m(A)$  is complexity of  $v \mapsto Av$ . Note  $\partial_*$  is highly structured, namely:

$$\text{nnz}(\partial_p) \leq (p+1)m_p \sim O(m_p \log(m_p))$$

$$v \mapsto \langle \partial_p, v \rangle \text{ takes } \sim O(\kappa_p) \text{ time where } \kappa_p = \sum \deg_p(\sigma_p)$$

$$\Delta_p = \text{tr}(\partial_p \partial_p^T) = \sum \sigma_i^2(\partial_p) \text{ can be determined in } O(m_p) \text{ time}$$

We deduce a  $(1 - \delta)$ -approximation by computing the  $q$ -largest  $\sigma_i^2$ 's such that:

$$\lceil \Delta_p^q / \Delta_p^{m_p} \rceil \geq (1 - \delta)$$

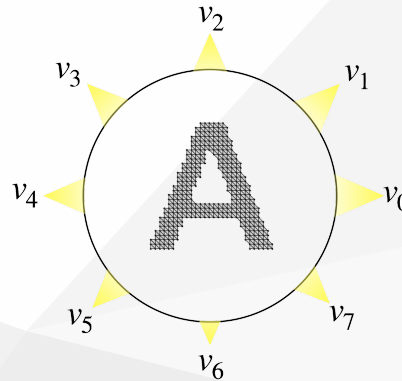
# The Persistent Homology Transform

The *PHT* characterizes the set of embeddeable s.c.'s in  $\mathbb{R}^d$  via a collection of dgm's

$$\text{PHT}(M) : \mathcal{S}^{d-1} \rightarrow \mathcal{D}^d$$

$$v \mapsto (X_0(M, v), X_1(M, v), \dots, X_{d-1}(M, v))$$

where  $\mathcal{D}^d$  is the space of  $\text{dgm}_p$ 's up to dimension  $p = d - 1$



The PHT is *injective*  $\implies$  dgm-distances (e.g. integrated  $d_B$ ) are *metrics*

The injectivity PHT theory allows for comparison of *non-diffeomorphic* shapes

## Applications: Leveraging PHT

**Pro:** PHT + it's associated distance metrics tend to do well at shape discrimination<sup>[1]</sup>

**Con:** Many dgm's +  $\int d_B(\dots)$  are highly non-trivial to compute



- (1) Choose a set rectangles  $\mathcal{R} = \{r_1, r_2, \dots, r_k\}$  in  $\mathbb{R}^2$  representing "features"
- (2) Compute multiplicities  $\mathbf{u}_p(X) = \{\hat{\mu}_p^\epsilon(r_1), \hat{\mu}_p^\epsilon(r_2), \dots, \hat{\mu}_p^\epsilon(r_k)\}$  for shapes  $X, Y$
- (3) Define  $\hat{d}_{\mathcal{R}}(X, Y) = \|\mathbf{u}_p(X) - \mathbf{u}_p(Y)\|$ , up to an optimal rotation<sup>[1]</sup>

We hope to do have more comparisons in the future

Thank you





## Properties of the rank function

The *rank* of a linear map  $\Phi$  is given as the dimension of its image:

$$r(\Phi) = \text{rank}(\Phi) = \dim(\text{Im}(\Phi))$$

When  $A, B \in \mathcal{M}_{(n \times n)}(\mathbb{R})$ , the *rank function* has many convenient properties:

$$\text{rank-nullity} \iff r(A) = |A| - \text{null}(A)$$

$$\text{subadditive} \iff r(A + B) \leq r(A) + r(B)$$

$$\text{transposition invariance} \iff r(A) = r(A^T) = r(A^T A) = r(AA^T)$$

$$\text{orthogonal invariance} \iff r(A) = r(QA) = r(AQ^T) \quad (Q := \text{orthogonal})$$

$$\text{permutation invariance} \iff r(A) = r(P^{-1}AP) \quad (P := \text{permutation matrix})$$

Let's see if we can apply some of these.

