An output-sensitive algorithm for persistence

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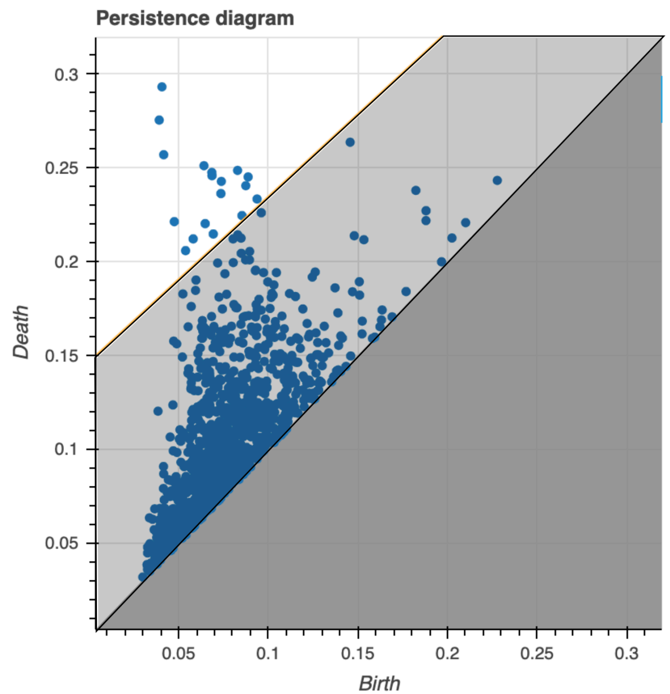
CompPers24 - Austria

Overview

(Chen and Kerber 2011) introduced a *rank-based* algorithm for computing persistence

The algorithms main attractions are:

- It can be used to compute only homology classes with persistence at least Γ



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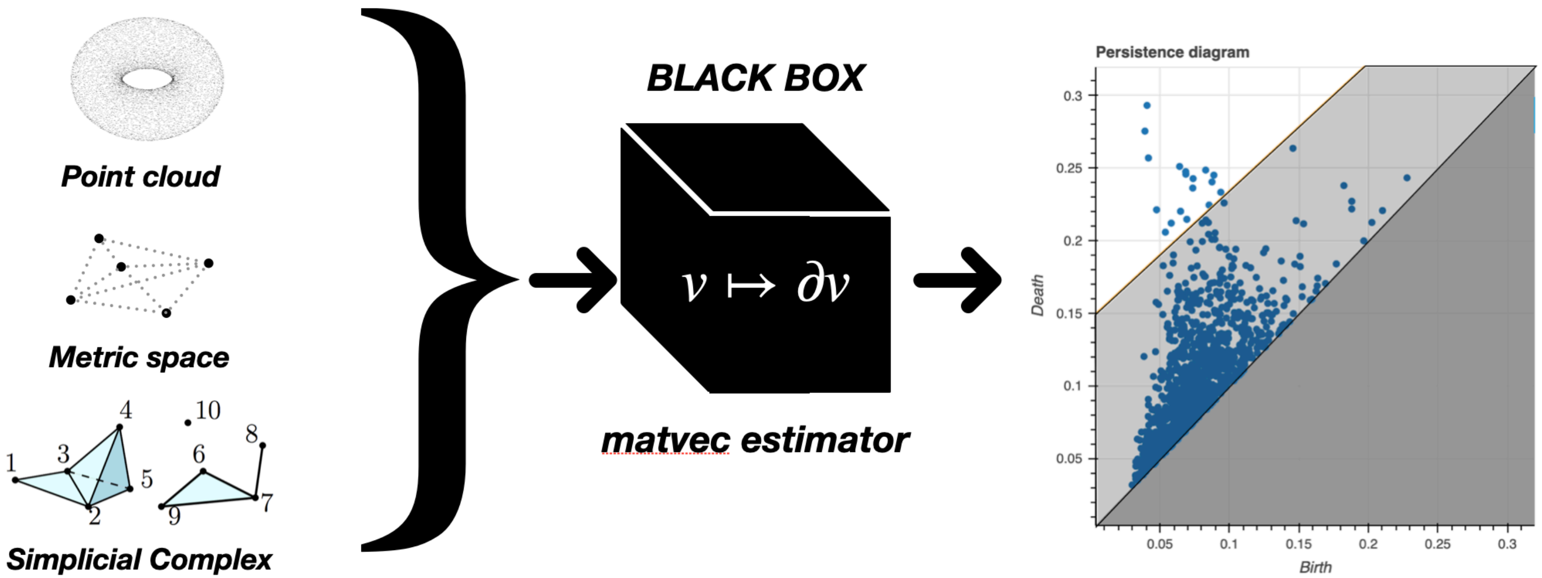

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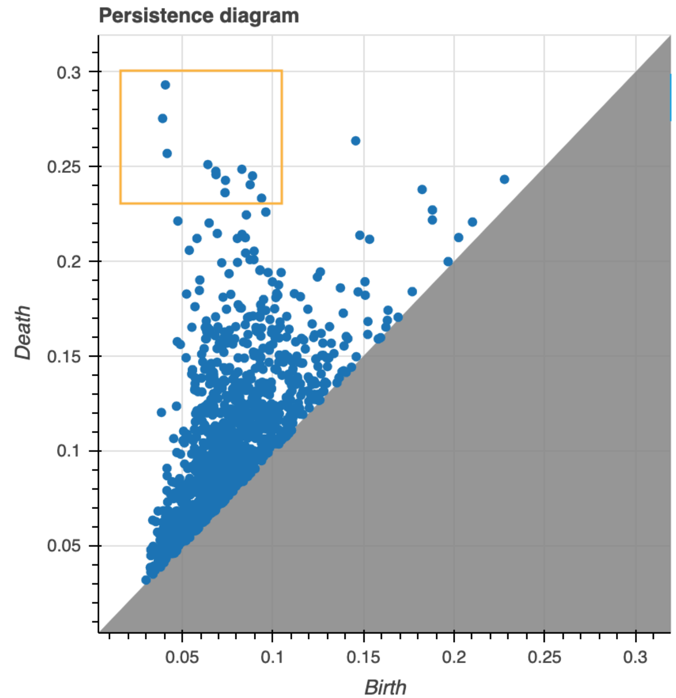
- It is comprised entirely of 'black-boxed' rank / matvec computations
- Its runtime is sensitive to the size of the output[1] (# of persistent pairs)



1 The running time of an *output sensitive* algorithm depends on the size of the output instead of, of in addition to, the input (wiki)

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- It can be used to compute only homology classes with persistence at least Γ
- It is comprised entirely of 'black-boxed' rank / matvec computations
- Its runtime is sensitive to the size of the output
- Its space complexity is $\approx$ linear in the size of the complex

If $X \subset \mathbb{R}^{n \times d}$, computing $\mathrm{dgm}_p(K)$ takes[1]

$$O\left(\binom{n}{p+2}^3\right) \text{ time } + O\left(\binom{n}{p+2}^2\right) \text{ s}$$

when $p > 0$. The improvement in space:

$$O\left(\binom{n}{p+2}\right) \text{ space}$$

1. See (Gómez and Mémoli 2024)

Overview - The Algorithm

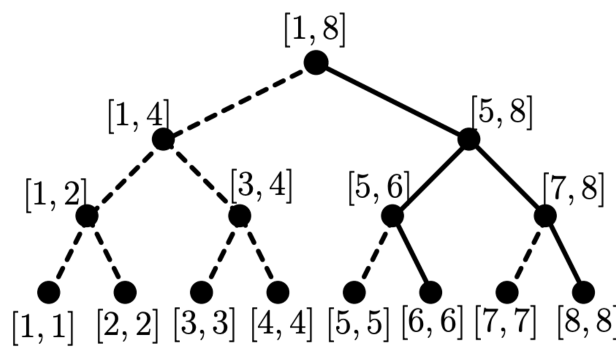
1. Characterize μ_p as a rank computation on boundary (sub)matrices

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

2. Express pivot condition as a recurrence relation

$$\mathrm{low}_R(j) = i \;\Leftrightarrow\; \exists n_{[i,i]} \in \mathcal{T}_m^{[k,l]} \text{ w/ } \mu(n_{[i,i]}) = 1$$

3. Divide-and-conquer (in the index persistence plane)



Notation

Computing persistence requires a family $\{K_i\}_{i \in I}$ of simplicial complexes indexed by a *totally ordered* set I, such that:

- (filtered) for any $i, j \in I$, we have $i < j \implies K_i \subseteq K_j$
- (simplexwise) $K_j \setminus K_i = \{\sigma_j\}$ if $j = \mathrm{succ}(i)$

Any filtration $\to$ *simplexwise* via *condensing*, *refining*, and *reindexing* maps (Bauer 2021)

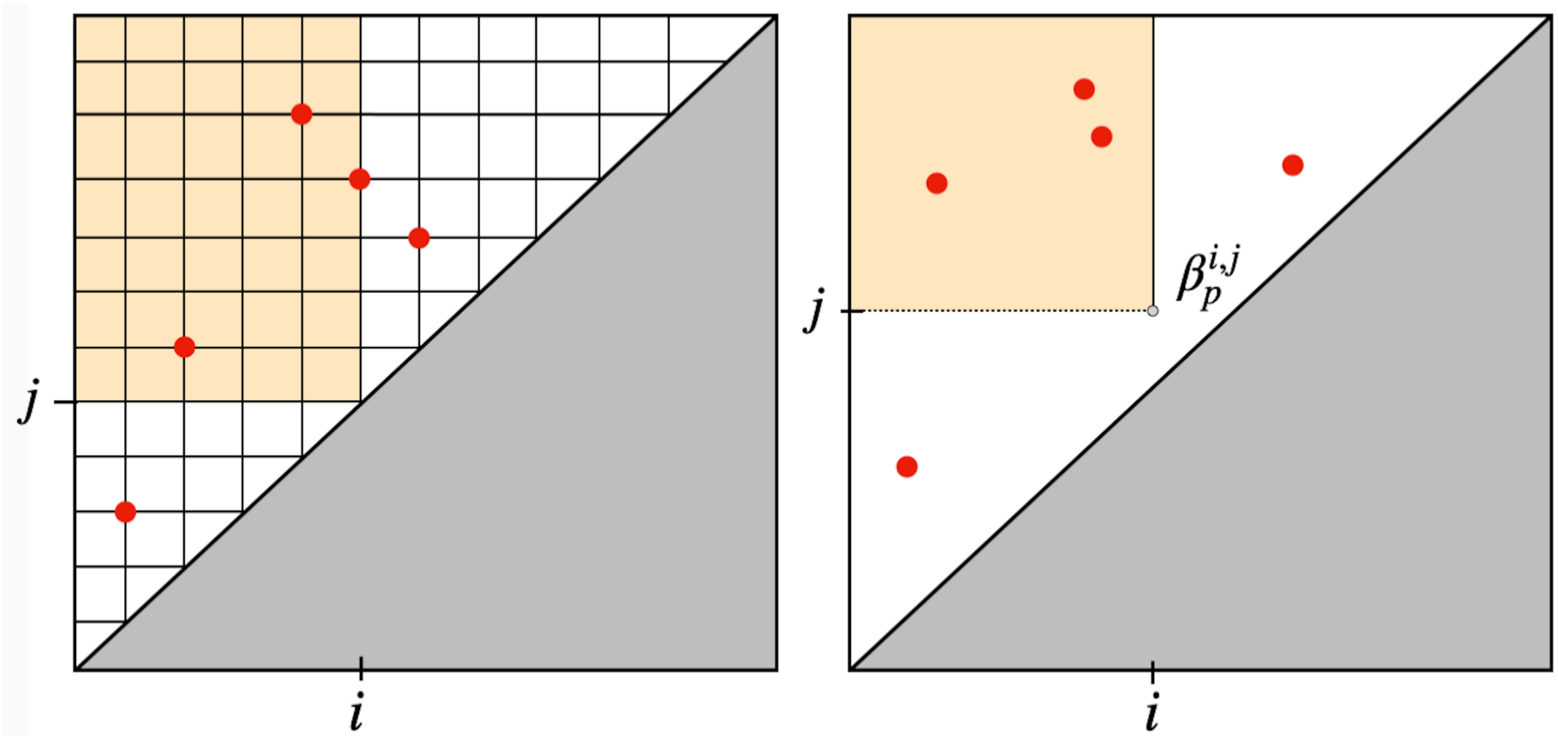
Example: Define (K, f) where $f : K \to I$ satisfies $f(\tau) \leq f(\sigma)$ whenever $\tau \subseteq \sigma$. Then, for any pair $\sigma, \sigma' \in K$ with $\sigma \neq \sigma'$, order I by:

1. $f(\sigma) \leq f(\sigma')$
2. $\dim(\sigma) \leq \dim(\sigma')$
3. $N(\sigma) < N(\sigma')$, where $N : K_p \to [\binom{n}{p+1}]$ is a fixed bijection

Common choices for N includes various bijections to the *combinatorial number system*, e.g. induces by the lexicographical ordering of vertices. However, other choices can be made as well, such as *gray codes*.

Example

Common choices for I include $[m] = \{1, \ldots, m\}$ and $\mathbb{R}$



When $\mathrm{dgm}(K, \mathbb{F})$ is defined over $[m]$, we call it *index persistence*

Background: Reduction

Decomposition Invariants (Edelsbrunner and Harer 2008)

- $R = \partial V$ where ∂ is the filtered boundary matrix of (K, f)
- V is full-rank upper-triangular
- R is *reduced*: if $\mathrm{col}_i(R) \neq 0$ and $\mathrm{col}_j(R) \neq 0$, then $\mathrm{low}_R(i) \neq \mathrm{low}_R(j)$

$$
\begin{array}{c}\partial_1 \\ \\ u \\ v \\ w\end{array}
\begin{array}{c} a \; b \; c \\ \left[\begin{array}{ccc} 1 & & 1 \\ & 1 & 1 \\ 1 & \underline{1} & \end{array}\right]\end{array},
\begin{array}{c}I_1 \\ \\ a \\ b \\ c\end{array}
\begin{array}{c} a \; b \; c \\ \left[\begin{array}{ccc} 1 & & \\ & 1 & \\ & & 1 \end{array}\right]\end{array}
\rightarrow
\begin{array}{c} \\ \\ u \\ v \\ w\end{array}
\begin{array}{c} a \; b \; c \\ \left[\begin{array}{ccc} 1 & 1 & 1 \\ & 1 & \underline{1} \\ 1 & & \end{array}\right]\end{array},
\begin{array}{c} \\ \\ a \\ b \\ c\end{array}
\begin{array}{c} a \; b \; c \\ \left[\begin{array}{ccc} 1 & 1 & \\ & 1 & \\ & & 1 \end{array}\right]\end{array}
\rightarrow
\begin{array}{c}R_1 \\ \\ u \\ v \\ w\end{array}
\begin{array}{c} a \; b \; c \\ \left[\begin{array}{ccc} 1 & 1 & \\ & 1 & \\ 1 & & \end{array}\right]\end{array},
\begin{array}{c}V_1 \\ \\ a \\ b \\ c\end{array}
\begin{array}{c} a \; b \; c \\ \left[\begin{array}{ccc} 1 & 1 & 1 \\ & 1 & 1 \\ & & 1 \end{array}\right]\end{array}
$$

Persistence Diagrams

Persistence diagrams are often defined in terms of their Betti numbers:

$$\mathrm{dgm}_p(K, f) \triangleq \{ (i, j) \in \Delta_+ : \mu_p^{i,j} \neq 0 \} \cup \Delta$$

$$\mu_p^{i,j} = \left(\beta_p^{i,j-1} - \beta_p^{i,j}\right) - \left(\beta_p^{i-1,j-1} - \beta_p^{i-1,j}\right), \quad \beta_p^{k,l} = \sum_{i \leq k} \sum_{j > l} \mu_p^{i,j}$$

Theorem(Dey and Wang 2022): Let $\partial \in \mathbb{F}^{m \times m}$ be a boundary matrix for simplexwise filtration (K, f) with decomposition $R = \partial V$. Then the simplices $\sigma_i, \sigma_j \in K$ forms a **persistent pair** $(f(\sigma_i), f(\sigma_j))$ *if and only if* $\mathrm{low}_R(j) = i$

- Unpaired simplices $\sigma_i \in K$ form *essential pairs* $(f(\sigma_i), \infty)$
- Though the pairing is unique, the decomposition $R = \partial V$ is a not
- In the index persistence case, $f : K \to [m]$, thus $f(\sigma_i) = i$

Here, we define $\Delta_+ = \{(x, y) \in I \times (I \cup \{+\infty\}) : x \leq y\}$ and the diagonal $\Delta = \{(x, x)\}$ is counted with infinite multiplicity.

Pairing Uniqueness Lemma

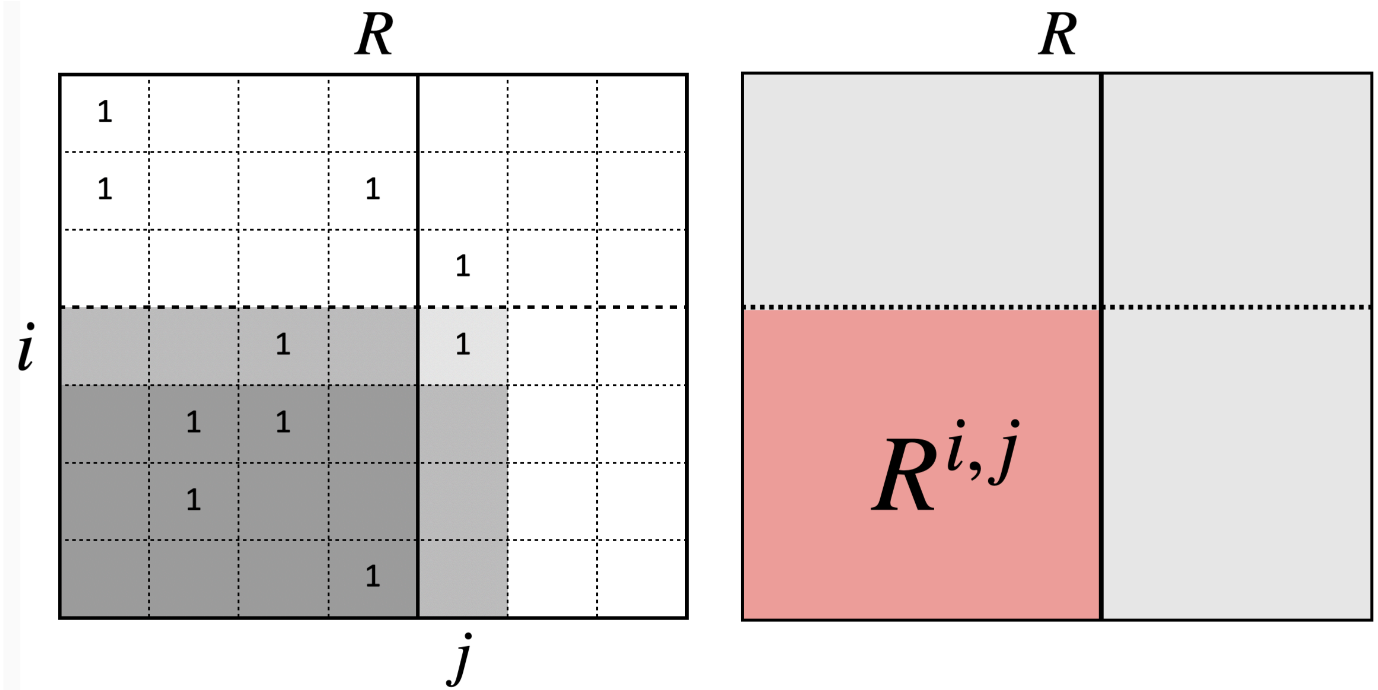
Proposition (Cohen-Steiner, Edelsbrunner, and Morozov 2006): For any simplexwise filtration (K, f), if $R = \partial V$ is a decomposition of its boundary matrix $\partial \in \mathbb{F}^{m \times m}$ obtained using left-to-right column operations, then:

$$\mathrm{low}_R(j) = i \;\Leftrightarrow\; \mathrm{rk}(\partial^{i,j}) - \mathrm{rk}(\partial^{i+1,j}) + \mathrm{rk}(\partial^{i+1,j-1}) - \mathrm{rk}(\partial^{i,j-1}) \neq 0$$

where $\partial^{i,j} \equiv$ "lower-left" submatrix given by rows $[i, m]$ and columns $[1, j]$.

Pairing Uniqueness (single)

If $(\sigma_i, \sigma_j) \in \mathrm{dgm}(K, \mathbb{F})$, then $\mathrm{low}_R(j) = i$ ($R[i,j] \neq 0$)



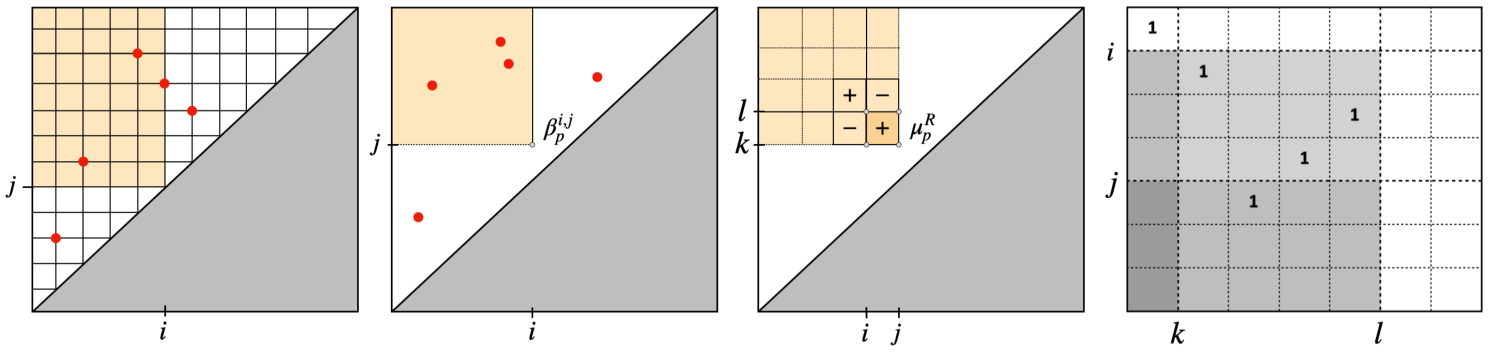
$$R[i,j] \neq 0 \;\leftrightarrow\; \mathrm{rk}(\partial^{i,j}) - \mathrm{rk}(\partial^{i+1,j}) + \mathrm{rk}(\partial^{i+1,j-1}) - \mathrm{rk}(\partial^{i,j-1}) \neq 0$$

Pairing Uniqueness (general)

For any box $R = [i, j] \times [k, l] \subset \Delta_+$ in the index upper-left halfplane Δ_+:

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

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



$*$:The expression for β_p^R in terms in boundary operators is given by (Dey and Wang 2022).

Pairing Uniqueness (interpretation)

R

1						
1			1			
				1		
		1		1		
	1	1				
	1					
			1			

S

1						
				1		
		1				
	1					
			1			

Chen's and Kerbers idea: Let $S_{ij} = 1$ if $\mathrm{low}_R(j) = i$ and 0 otherwise.

Then $\#S^{i,j} = \mathrm{rank}(R^{i,j})$ for all $i < j$, and μ_p^R is like "counting" non-zeros in S

The Key Lemma

Lemma (Dey and Wang 2022): Given a filtration (K, f) of size $m = |K|$ and decomposition $R = \partial V$, for any pair $1 \leq i \leq j \leq m$ we have:

$$\mathrm{rk}(R^{i,j}) = \mathrm{rk}(\partial^{i,j})$$

where $(*)^{i,j} \equiv$ "lower-left" submatrix given by columns $[1, j]$ and rows $[i, m]$.

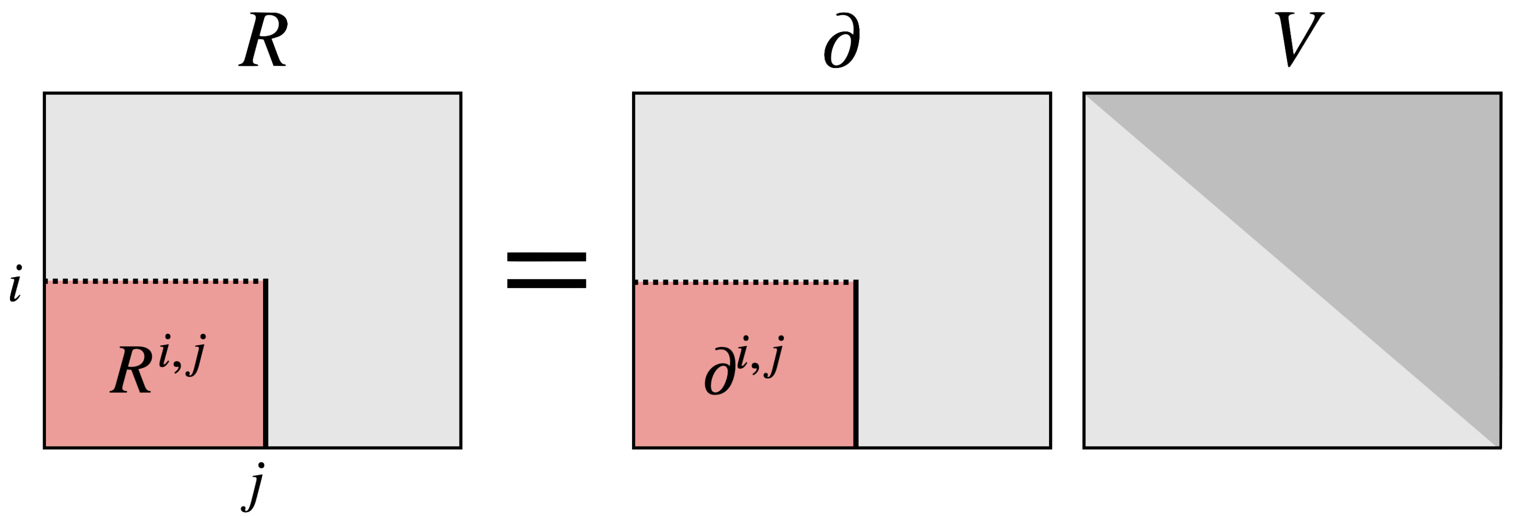
- This also holds for restrictions $R_p^{i,j}$ and $\partial_p^{i,j}$
- Constructing R requires $O(m^3)$ time via reduction
- Constructing $\partial^{i,j}$ requires $O(j - i)$ time for constant $p \geq 0$, and satisfies:

$$\mathrm{nnz}(\partial) = O(m \log m)^* \qquad \text{(sparsity of } \partial\text{)}$$

In fact, if K is d-dimensional, any $k \times k$ submatrix of ∂ has $O(dk)$ non-zero entries. Since a d-simplex has $2^{d+1} - 1$ faces, $d \leq \log(m+1) - 1$, which shows the above sparsity argument. See (Chen and Kerber 2011) for details.

The Key Lemma

Pairing uniqueness lemma[1] $\implies \operatorname{rank}(R^{i,j}) = \operatorname{rank}(\partial^{i,j})$



Corollary (Bauer et al. 2022): Any algorithm that preserves the ranks of the submatrices $\partial^{i,j}$ for all $i, j \in \{1, \ldots, n\}$ is a valid barcode algorithm.

Towards a new algorithm

Corollary(Chen and Kerber 2011): If $\mathcal{R}_d(n)$ denotes the cost of computing the rank of an $n \times n$ square matrix with $O(dn)$ non-zero $\mathbb{F}$-entries, then $\mu_p^R = O(\mathcal{R}_{p+2}(l-i))$

Proof: For any box $R = [i, j] \times [k, l] \subset \Delta_+$, consider the multiplicity expression:

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

Since $R \subset \Delta_+$, we have $i < j \leq k < l$ and thus the inclusions:

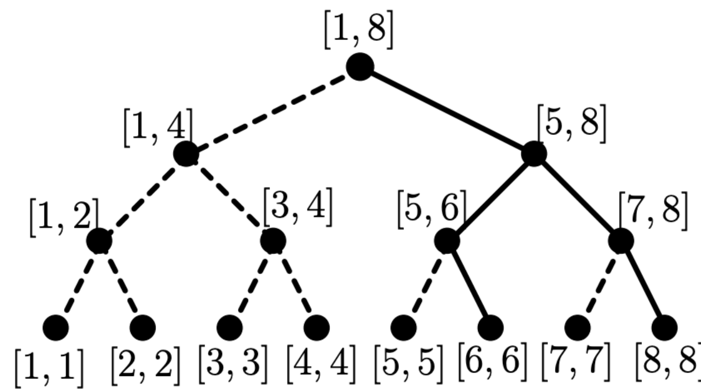
$$\partial_{p+1}^{j+1,k} \subset \partial_{p+1}^{i+1,k}, \quad \partial_{p+1}^{j+1,l} \subset \partial_{p+1}^{i+1,l}, \quad \partial_{p+1}^{i+1,k} \subset \partial_{p+1}^{i+1,l}$$

Thus the complexity is dominated by $\partial_{p+1}^{i+1,l}$. Though this matrix has l columns and $m - i + 1$ rows, there exists a submatrix of size $(l-i)$ rows / columns containing at most $(p+2)$ non-zero $\mathbb{F}$ entries per column. The above corollary follows. ■

Chen and Kerbers Algorithm

For filtration (K, f) indexed by $I = [m]$ and a *fixed* interval $[k, l]$, define $\mathcal{T}_m^{[k,l]}$ as a binary tree[1] with nodes $n_{[a,b]}$ representing subintervals $[a, b] \subseteq [1, m]$ and satisfying:

- Root node is given by $n_{[1,m]}$
- If $n_{[a,b]}$ and $k = \lfloor \frac{a+b}{2} \rfloor$, then:
  - $\mathrm{left}(n_{[a,b]}) = n_{[a,k]}$
  - $\mathrm{right}(n_{[a,b]}) = n_{[k+1,b]}$
- Leaves cover singletons, i.e. $n_{[i,i]}$



Assign every node $n \in \mathcal{T}_m$ a μ-value as follows:

$$\mu(n_{[a,b]}) = \mu_p^{a,b}(K, f), \text{ where } R = [a, b] \times [k, l]$$

1. Chen and Kerber call $\mathcal{T}_m$ a *bisection tree*. In data structures, this is analogous to a *segment tree*.

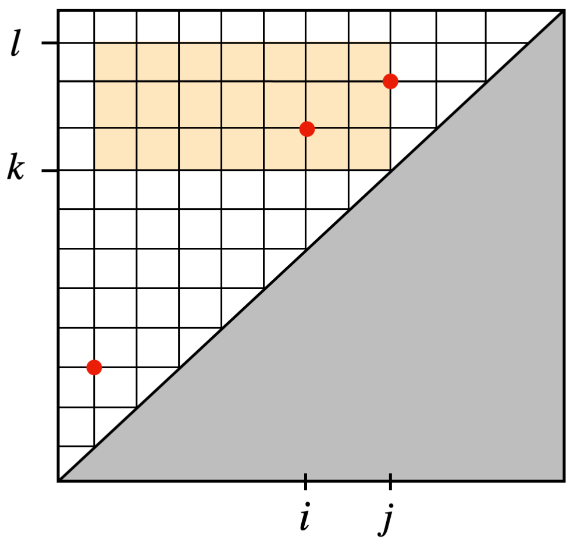
Bisection Tree properties

Prop: Let $\mathcal{T}_m^{[k,l]}$ be a binary tree for some interval $[k,l] \subseteq [1,m]$ whose nodes satisfy:

$$\mu(n_{[a,b]}) = \mu_p^R(K,f), \text{ where } R = [a,b] \times [k,l]$$

$\forall\ (\sigma_i, \sigma_j) \in \mathrm{dgm}_p(K,f)$ with $j \in [k,l]$, there $\exists$ a node $n_{[i,i]} \in \mathcal{T}_m^{[k,l]}$ w/ $\mu(n_{[i,i]}) = 1$

$R = [1,8] \times [8,11]$



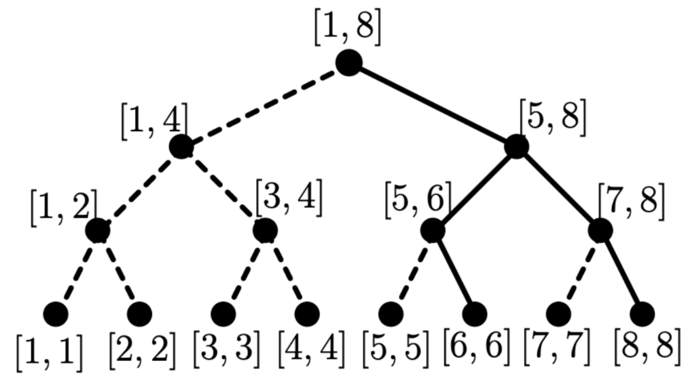
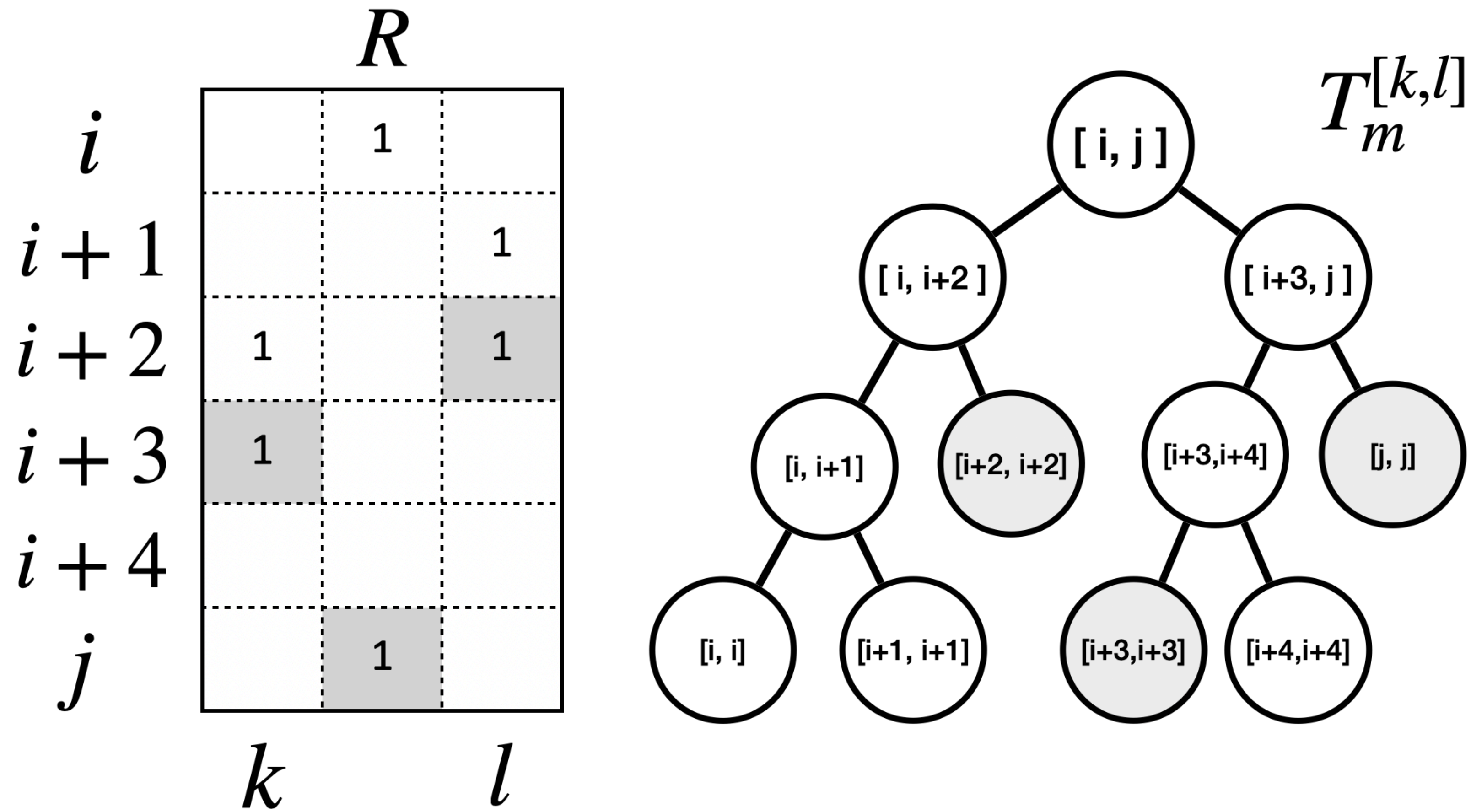


Figure 2: An illustration of the bisection tree of an interval $[i_1, i_2] = [1,8]$, which contains two creators, σ_6 and σ_8. Only the nodes on the two solid paths (and their siblings) are explored by the algorithm.

Bisection Tree Example



Querying creators

Lemma (Chen and Kerber 2011): For any box $R = [i, j] \times [k, l] \subset \Delta_+$, define:

$$P_R = \{\, (\sigma_a, \sigma_b) \in \mathrm{dgm}(K, f) : a \in [i, j], b \in [k, l] \,\}$$

If $\mu_p^R = \mathrm{card}(P_R)$, then computing the creators of P_R has time complexity:

$$O((1 + \mu_p^R \log(j - i))\mathcal{R}_d(l - i))$$

Proof: There are at most μ_p^R non-zero leaf-to-root paths, each of which has length $O(\log(j - i))$. Since $\mu(n_{[a,b]}) = \mu(\mathrm{left}(n_{[a,b]})) + \mu(\mathrm{right}(n_{[a,b]}))$, we only need query one of these children to descend each path. Since we need to perform one query at the root and since the complexity of any given query is $\mathcal{R}_d(l - i)$, the stated complexity follows.

Querying pairs

Lemma (Chen and Kerber 2011): For any box $R = [i,j] \times [k,l] \subset \Delta_+$, define:

$$P_R = \{\, (\sigma_a, \sigma_b) \in \mathrm{dgm}(K,f) : a \in [i,j], b \in [k,l] \,\})$$

If $\mu_p^R = \mathrm{card}(P_R)$, then computing all of the pairs P_R has time complexity:

$$O((1 + \mu_p^R \log(l-i))\mathcal{R}_d(l-i))$$

Proof: Fix a creator simplex σ_i that has been previously found in the tree $\mathcal{T}_m^{[k,l]}$. By definition, $\mu(n_{[i,i]}) = 1$, and its destroyer is the unique integer $j \in [k,l]$ with:

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

which can be found via binary search on $[k,l]$ in $O(\log(l-k)\mathcal{R}_d(l-i))$ time. Repeating for all creators yields the complexity in the theorem.

Querying Γ-pairs

Lemma (Chen and Kerber 2011): For any box $R = [i,j] \times [k,l] \subset \Delta_+$, define:

$$P(\Gamma)_R = \{\, (\sigma_a, \sigma_b) \in \mathrm{dgm}(K, f) : a \in [i,j], b \in [k,l], f(\sigma_b) - f(\sigma_a) \geq \Gamma \,\}$$

If $\mu_p^R(\Gamma) = \mathrm{card}(P_R(\Gamma))$, then computing all Γ-pairs $P_R(\Gamma)$ has time complexity:

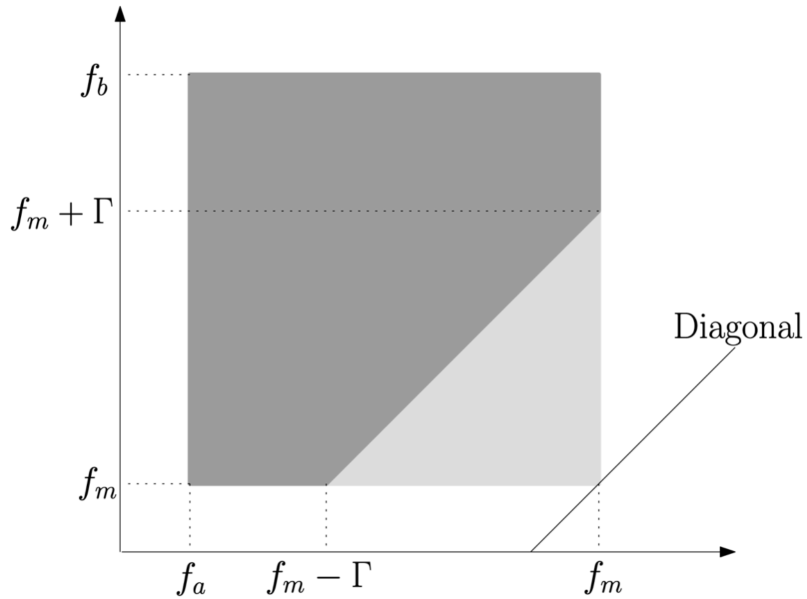
$$O\left(\left(\frac{1}{\delta} + C_{(1-\delta)\Gamma} \log n\right) \mathcal{R}_d(m)\right)$$

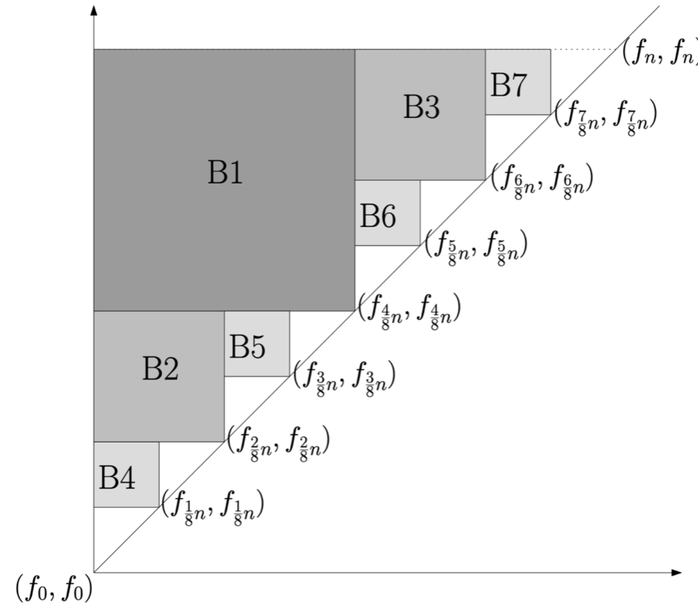
where $\delta \in (0,1)$ is an arbitrary constant and $C_{(1-\delta)\Gamma}$ is a constant given by:

$$C_{(1-\delta)\Gamma} = \mu_p^B((1-\delta)\Gamma), \quad B = [1,k] \times [k,m], \quad k = \lfloor m/2 \rfloor$$

Note: $C_{(1-\delta)\Gamma}$ counts the number of pairs with persistence at least Γ.

Querying Γ-pairs: proof 1

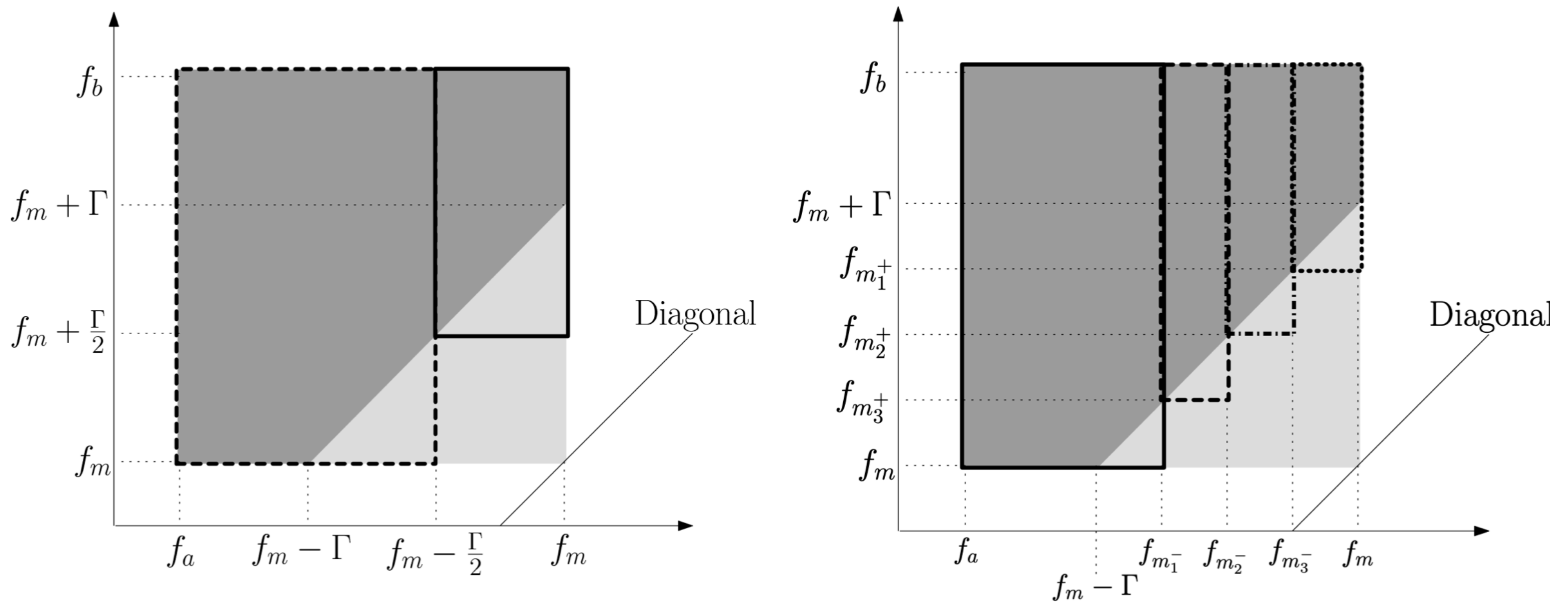




- (left) Dark gray polygon contains pairs in box $R \subset \Delta_+$ with persistence $\geq \Gamma$
- (right) Pairs computed via a divide-and-conquer

Proof Sketch 1: Excluding the $1/\delta$ term, the main complexity follows from writing the recurrence for $\mu_p^B(\Gamma)$ & applying the Master Theorem (Bentley, Haken, and Saxe 1980).

Querying Γ-pairs: proof 2



- (left) Two rectangles contain pairs with persistence Γ, plus extra $\Gamma/2$ pairs
- (right) Four rectangles contain pairs with persistence Γ, plus extra $\Gamma/4$ pairs

Proof Sketch 2: The $\delta \in (0, 1)$ term comes from defining any monotone increasing sequence of subdivision points $a_1, a_2, \ldots, a_{t-1}$ with $t = \lceil 1/\delta \rceil$ where $\Gamma \cdot (1 - \frac{i}{t})$

Instantiating Rank Algorithms

A variety of rank algorithms can be used for $\mathbb{Z}_2$ coefficients:

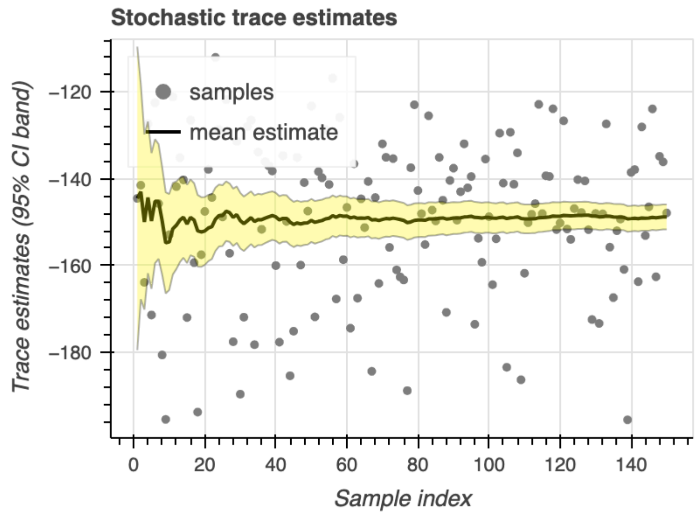
Method	**Rank Complexity**	**Persistence Computation**	**Type**
PLU	$O(n^\omega)$	$O(C_{(1-\delta)_\Gamma} n^{2.376} \log n)$	Deterministic
Las-Vegas	$\tilde{O}(n^{3-1/(\omega-1)})$	$O(C_{(1-\delta)\Gamma} n^{2.28})$	Deterministic
Monte-Carlo	$O(n^2 \log^2 n \log\log n)$	$O(C_{(1-\delta)\Gamma} n^2 \log^3 n \log\log n)$	Randomized

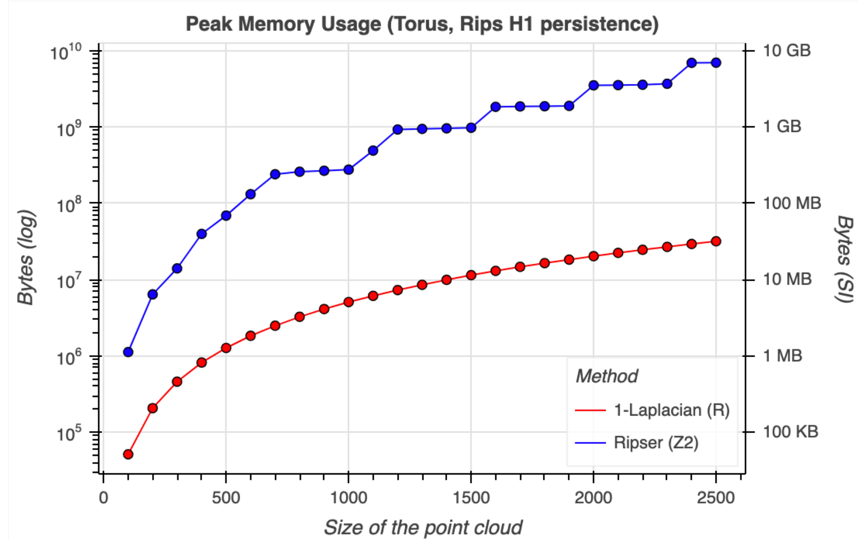
The algorithm can also be adapted to:

- Compute representative cycles (via solving a linear system)
- Work with generalized fields (via field extensions)
- Work with other complexes (e.g. cubical complexes)

Care must be taken to handle the randomized case

Some of my own work (Time permitting)





For $\mathbb{F} = \mathbb{R}$, this algorithm can be used to compute all persistence invariants (ranks, pairs, and repr.) in $O(m)$ space, though there are still many barriers that affect its practical use.

Certain use-cases *are* near to being practical with rank-based approach, such as persistence optimization and large scale homological inference

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