

Spectral relaxations of persistent rank invariants

With a focus on *parameterized* settings

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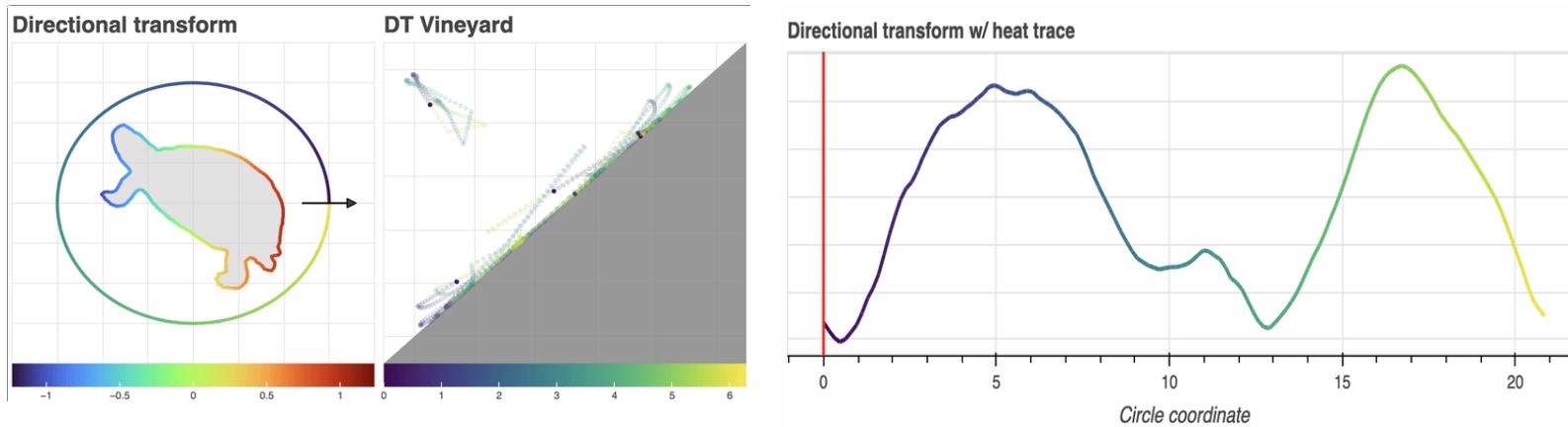
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This Talk

We introduce *spectral-relaxation* of the rank invariants β_p^* and μ_p^* that:

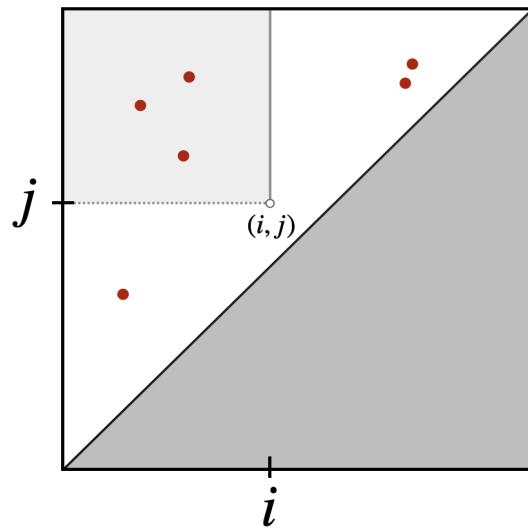
1. Smoothly interpolates¹ the *persistent rank* function
2. Admits $(1-\epsilon)$ approximation for any $\epsilon > 0$ in essentially $O(n^2)$ time
3. Is computable in a “matrix-free” fashion in $O(n)$ memory
4. Has variety of applications, e.g. featurization, optimization, metric learning



(1) The Schatten-1 norms of the operators driving the relaxation are differentiable over the positive semi-definite cone

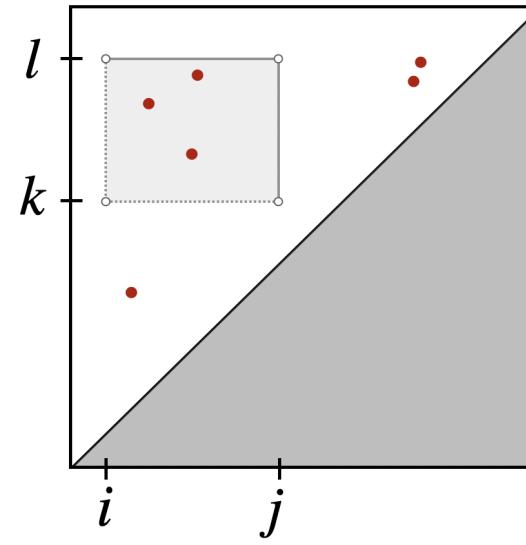
The rank invariants

dgm



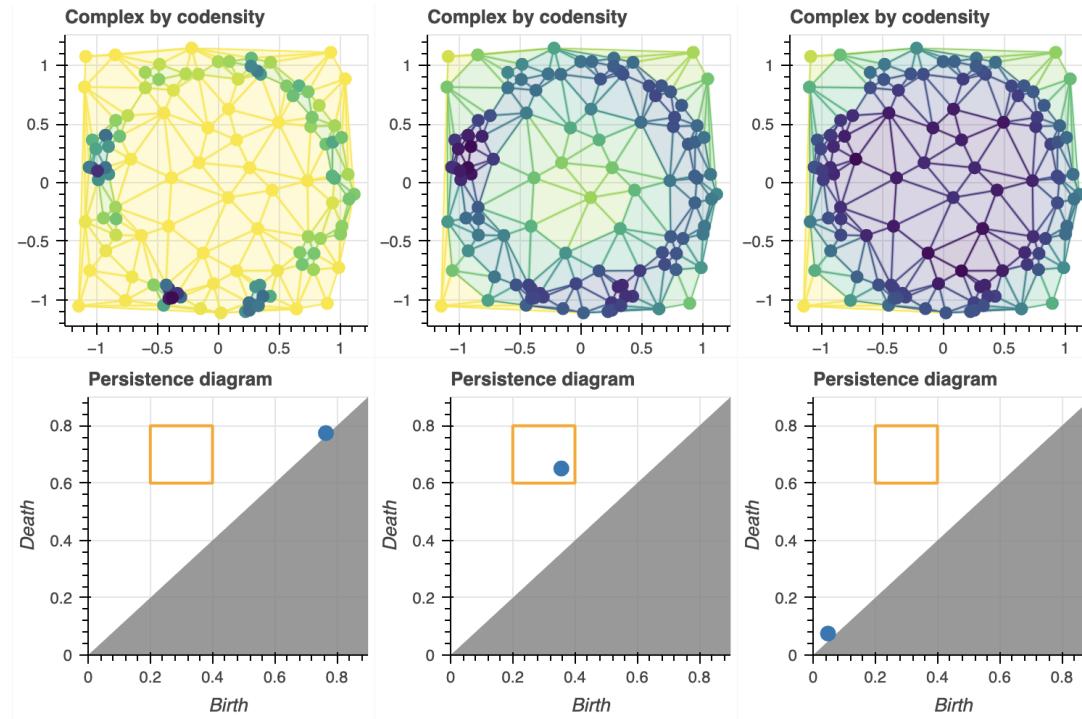
$$\beta_p^{i,j}(K)$$

dgm



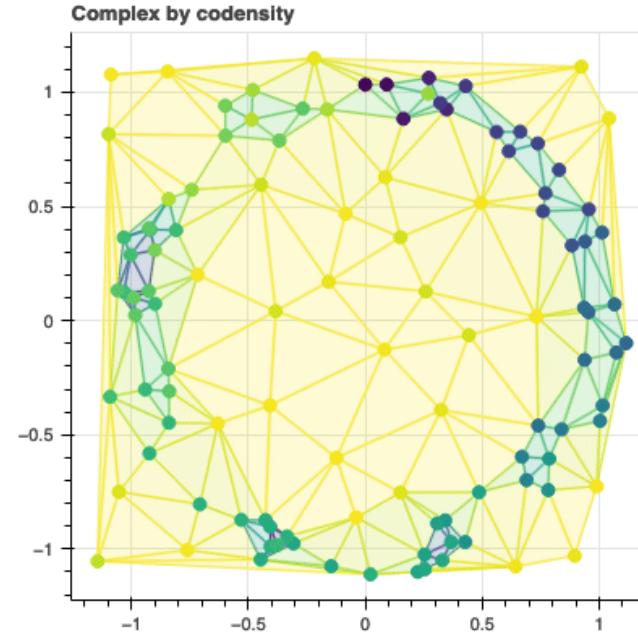
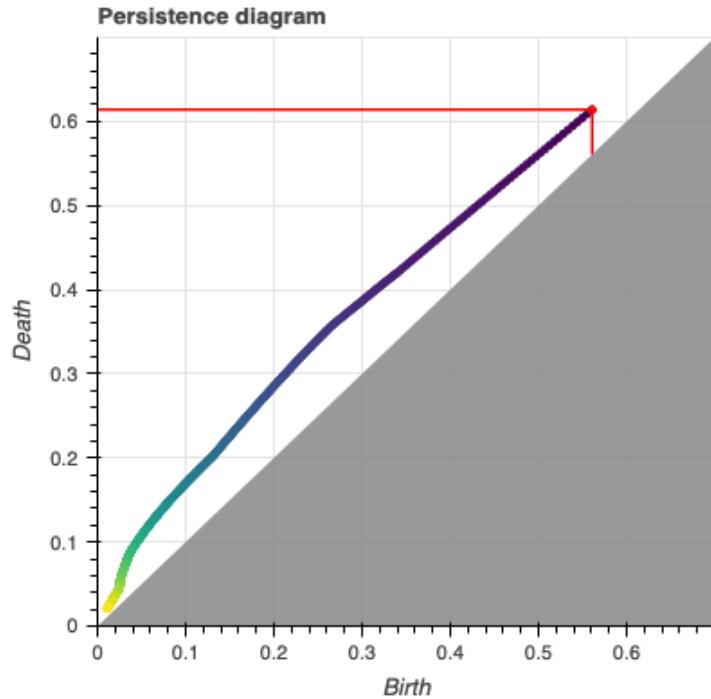
$$\mu_p^R(K)$$

Application: optimizing filtrations



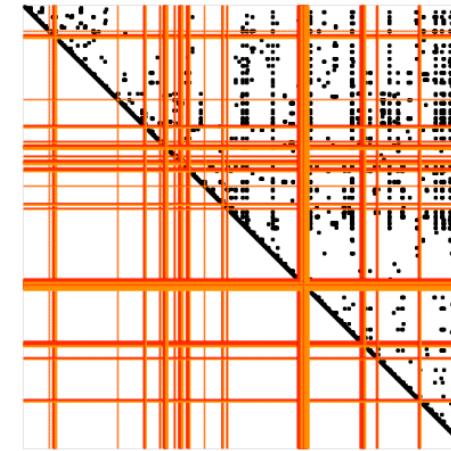
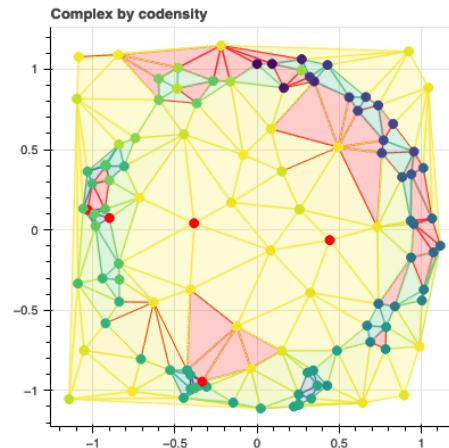
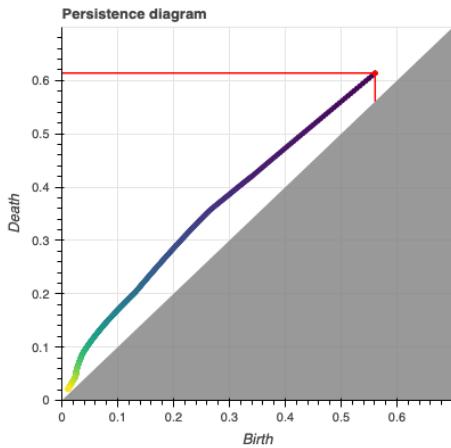
$$\alpha^* = \arg \max_{\alpha \in \mathbb{R}} \text{card}(\text{dgm}(K_\bullet, f_\alpha)|_R)$$

Why not just use diagrams?



Pro: Diagrams are stable, well-studied, and information rich.

Why not just use diagrams?



Con: Extending the $R = \partial V$ to parameterized settings is non-trivial

Maintaining the $R = \partial V$ decomposition “across time” \implies huge memory bottleneck

For details, see Piekenbrock and Perea (2021) or Bauer et al. (2022) (also Lesnick and Wright (2015))

Beyond dgm's: Revisiting the rank computation

$$\beta_p^{i,j} : \text{rank}(H_p(K_i) \rightarrow H_p(K_j))$$

$$\begin{aligned}\beta_p^{i,j} &= \dim(\text{Ker}(\partial_p(K_i)) / \text{Im}(\partial_{p+1}(K_j))) \\ &= \dim(\text{Ker}(\partial_p(K_i)) / (\text{Ker}(\partial_p(K_i)) \cap \text{Im}(\partial_{p+1}(K_j)))) \\ &= \text{dim}(\text{Ker}(\partial_p(K_i))) - \text{dim}(\text{Ker}(\partial_p(K_i)) \cap \text{Im}(\partial_{p+1}(K_j)))\end{aligned}$$

Rank-nullity yields the **left term**:

$$\dim(\text{Ker}(\partial_p(K_i))) = |C_p(K_i)| - \dim(\text{Im}(\partial_p(K_i)))$$

Computing the **right term** more nuanced:

- Pseudo-inverse¹, projectors², Neumann's inequality³, etc.
- PID algorithm⁴, Reduction algorithm⁵, Persistent Laplacian⁶

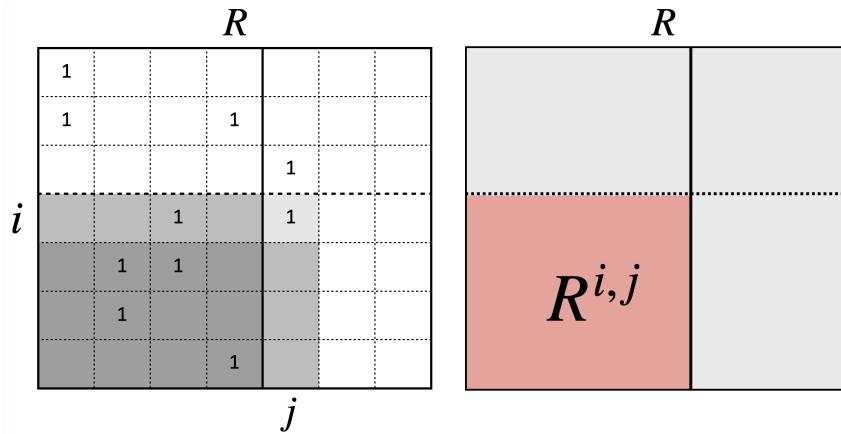
Anderson Jr and Duffin (1969), Ben Israel (1967), Ben-Israel (2015), Zomorodian and Carlsson (2004), Edelsbrunner, Letscher, and Zomorodian (2000), Mémoli, Wan, and Wang (2022)

Key technical observation

Structure theorem for persistence modules can be used to show:

$$(i, j) \in \text{dgm}(K_\bullet)$$

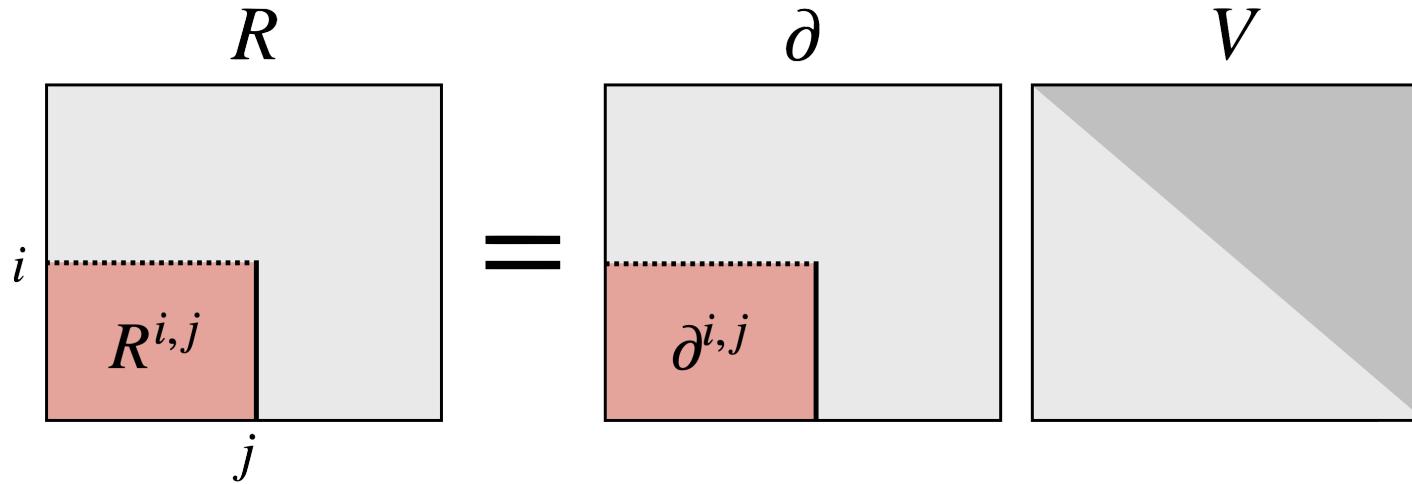
$$\Leftrightarrow \text{rank}(R^{i,j}) - \text{rank}(R^{i+1,j}) + \text{rank}(R^{i+1,j-1}) - \text{rank}(R^{i,j-1}) \neq 0$$



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

Key technical observation

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



Take-a-way: Can deduce the dgm from ranks of “lower-left” submatrices of $\partial_p(K_\bullet)$

Key technical observation

$$\text{rank}(R^{i,j}) = \text{rank}(\partial^{i,j}) \quad (1)$$

(1) often used to show correctness of reduction, but far more general, as it implies:

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

$$(1) \Rightarrow \beta_p^{i,j} = |C_p(K_i)| - \text{rank}(\partial_p^{1,i}) - \text{rank}(\partial_{p+1}^{1,j}) + \text{rank}(\partial_{p+1}^{i+1,j}) \quad (2)$$

$$(2) \Rightarrow \mu_p^R = \text{rank}(\partial_{p+1}^{j+1,k}) - \text{rank}(\partial_{p+1}^{i+1,k}) - \text{rank}(\partial_{p+1}^{j+1,l}) + \text{rank}(\partial_{p+1}^{i+1,l}) \quad (3)$$

Edelsbrunner, Letscher, and Zomorodian (2000) noted (1) in passing showing correctness of reduction; Tamal Krishna Dey and Wang (2022) explicitly prove (2); (3) was used by Chen and Kerber (2011). (2) & (3) are connected to relative homology.

Overview

- Introduction
 - Rank duality
 - Bypassing diagrams
 - Technical observations
- Spectral rank relaxation
 - Parameterizing $C(K, \mathbb{R})$
 - Spectral functions
 - Variational interpretations + examples
- Computation
 - Lanczos Iteration
 - Stochastic trace estimation
 - Scalability

The Implications

From now on, we work strictly with field coefficients in \mathbb{R}

$$\mu_p^R = \text{rank} \begin{bmatrix} \partial_{p+1}^{j+1,k} & 0 \\ 0 & \partial_{p+1}^{i+1,l} \end{bmatrix} - \text{rank} \begin{bmatrix} \partial_{p+1}^{i+1,k} & 0 \\ 0 & \partial_{p+1}^{j+1,l} \end{bmatrix}$$

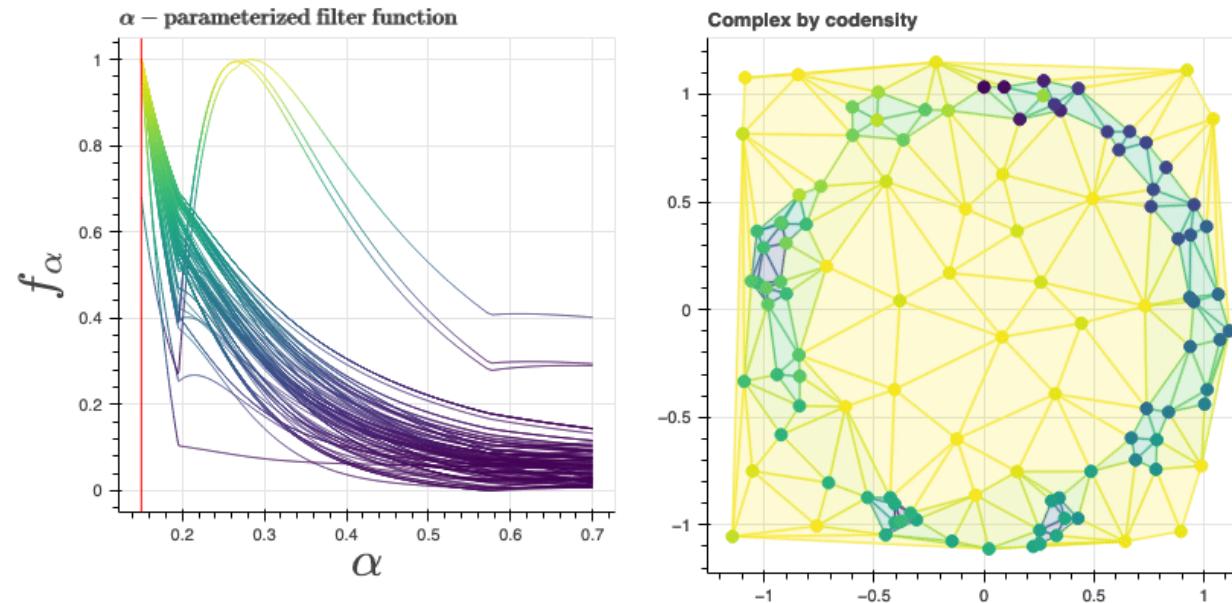
There are advantages to preferring *this* expression for μ_p^R

1. Inner terms are *unfactored*
2. Variational perspectives on **rank function** well-studied (\mathbb{R})
3. Theory of **persistent measures*** readily applicable

Parameterized filtrations

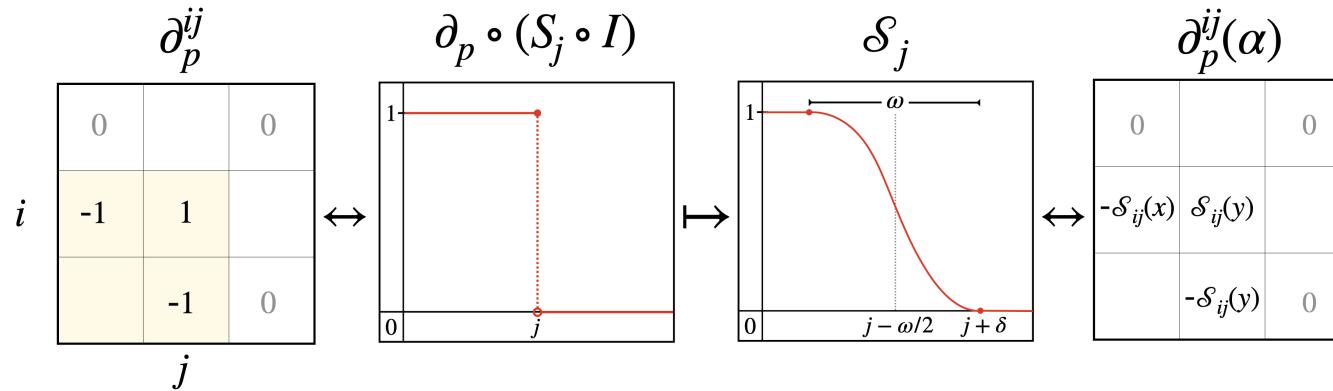
Suppose we have an α -parameterized filtration (K, f_α) where $f_\alpha : K \rightarrow \mathbb{R}_+$ satisfies:

$$f_\alpha(\tau) \leq f_\alpha(\sigma) \quad \text{if } \tau \subseteq \sigma \quad \forall \tau, \sigma \in K \text{ and } \alpha \in \mathbb{R}$$



Relax #1: Parameterized *boundary matrices*

Parameterize $C_p(K; \mathbb{R})$ with $\mathcal{S} \circ f_\alpha : K \rightarrow \mathbb{R}_+$ where $\mathcal{S} : \mathbb{R} \rightarrow [0, 1]$



$$\boxed{\partial_p^{i,j}(\alpha) = D_p(\mathcal{S}_i \circ f_\alpha) \circ \partial_p(K_{\preceq}) \circ D_{p+1}(\mathcal{S}_j \circ f_\alpha)}$$

Note: $P^T \partial_p^{i,j}(\alpha) P$ has rank = rank($R_p^{i,j}(\alpha)$) for all $\alpha \in \mathbb{R}$.

Replacing $S \mapsto \mathcal{S}$ ensures continuity of $\partial_p^{i,j}(\alpha)$

Spectral functions

Relaxation #2: Approximate rank with *spectral functions* (Bhatia 2013)

$$\text{rank}(X) = \sum \text{sgn}_+(\sigma_i) \approx \sum \phi(\sigma_i, \tau), \quad \phi(x, \tau) \triangleq \int_{-\infty}^x \hat{\delta}(z, \tau) dz$$

$$\text{where } \hat{\delta}(x, \tau) = \frac{1}{\nu(\tau)} p\left(\frac{x}{\nu(\tau)}\right), \quad \tau > 0, \quad \nu \text{ inc.}$$

$\Phi_\tau(X)$ is a Löwner operator when ϕ is operator monotone (Jiang and Sendov 2018)

$$A \succeq B \implies \phi_\tau(A) \succeq \phi_\tau(B)$$

Closed-form proximal operators exist when ϕ_τ convex + minor conditions¹

(1) See Beck (2017) and Bauschke, Combettes, et al. (2011) for existence and optimality conditions.

Löwner Operators

For any smoothed Dirac measure¹ $\hat{\delta}$ and differentiable operator monotone function $\phi : \mathbb{R}_+ \times \mathbb{R}_{++} \rightarrow \mathbb{R}_+$, (Bi, Han, and Pan 2013) show that:

(τ -approximate) $0 \leq \text{rank}(X) - \|\Phi_\tau(X)\|_* \leq c(\hat{\delta})$

(Monotone) $\|\Phi_\tau(X)\|_* \geq \|\Phi_{\tau'}(X)\|_*$ for any $\tau \leq \tau'$

(Smooth) Semismooth² on $\mathbb{R}^{n \times m}$, differentiable on \mathbf{S}_+^m

(Explicit) Differential $\partial \|\Phi_\tau(\cdot)\|_*$ has closed-form soln.

Function/operator pairs (Φ_τ, Φ_τ) particular specializations of *matrix functions*:

$$\Phi_\tau(X) = U\Phi_\tau(\Sigma)V^T$$

Commonly used in many application areas, e.g. compressed sensing ([Li 2014](#))

1. Any $\hat{\delta}$ of the form $\nu(1/\tau)p(z \cdot \nu(1/\tau))$ where p is a density function and ν positive and increasing is sufficient.

2. Here semismooth refers to the existence of directional derivatives.

Interpretation: Regularization

Ill-posed linear systems $Ax = b$ are often solved by “regularized” least-squares:

$$x_{\tau}^{*} = \arg \min_{x \in \mathbb{R}^n} \|Ax - b\|^2 + \tau \|x\|_1$$

The minimizer is given in closed-form by the regularized pseudo-inverse:

$$x_{\tau}^{*} = (A^T A + \tau I)^{-1} A^T b$$

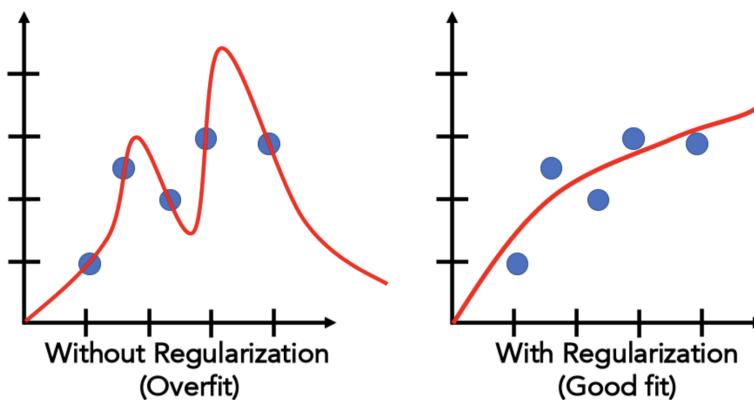


Image from: <https://thaddeus-segura.com/lasso-ridge/>

Interpretation: Regularization

Under the appropriate parameters¹ for ν and p , ϕ takes the form:

$$\phi(x, \tau) = \frac{2}{\tau} \int_0^z z \cdot ((z/\sqrt{\tau})^2 + 1)^{-2} dz = \frac{x^2}{x^2 + \tau}$$

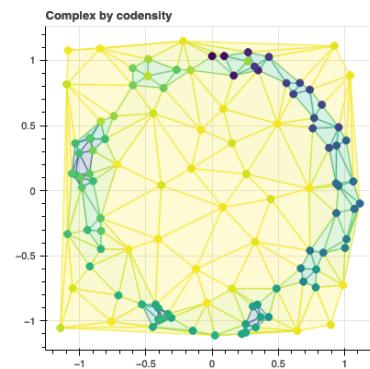
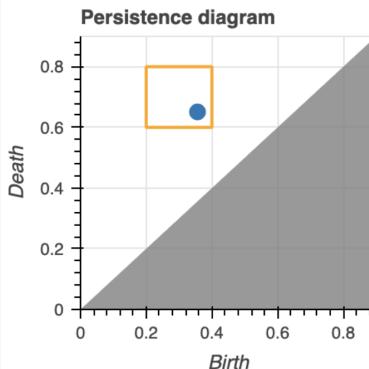
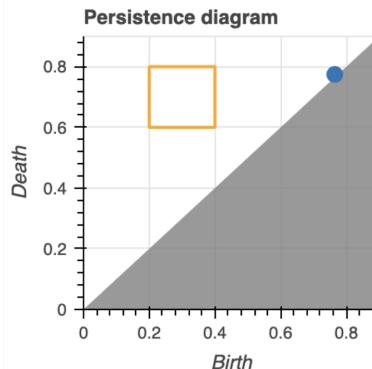
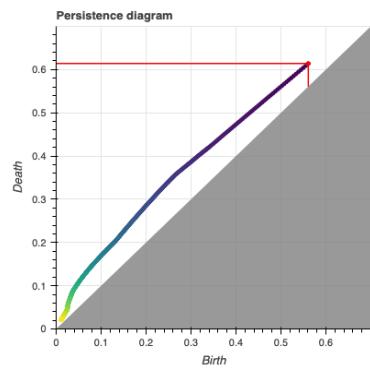
The corresponding Löwner operator and its Schatten 1-norm is given² by:

$$\Phi_\tau(X) = (X^T X + \tau I_n)^{-1} X^T X, \quad \|\Phi_\tau(X)\|_* = \sum_{i=1}^n \frac{\sigma_i(X)^2}{\sigma_i(X)^2 + \tau}$$

This the *Tikhonov regularization* in standard form used in ℓ_1 -regression (LASSO)

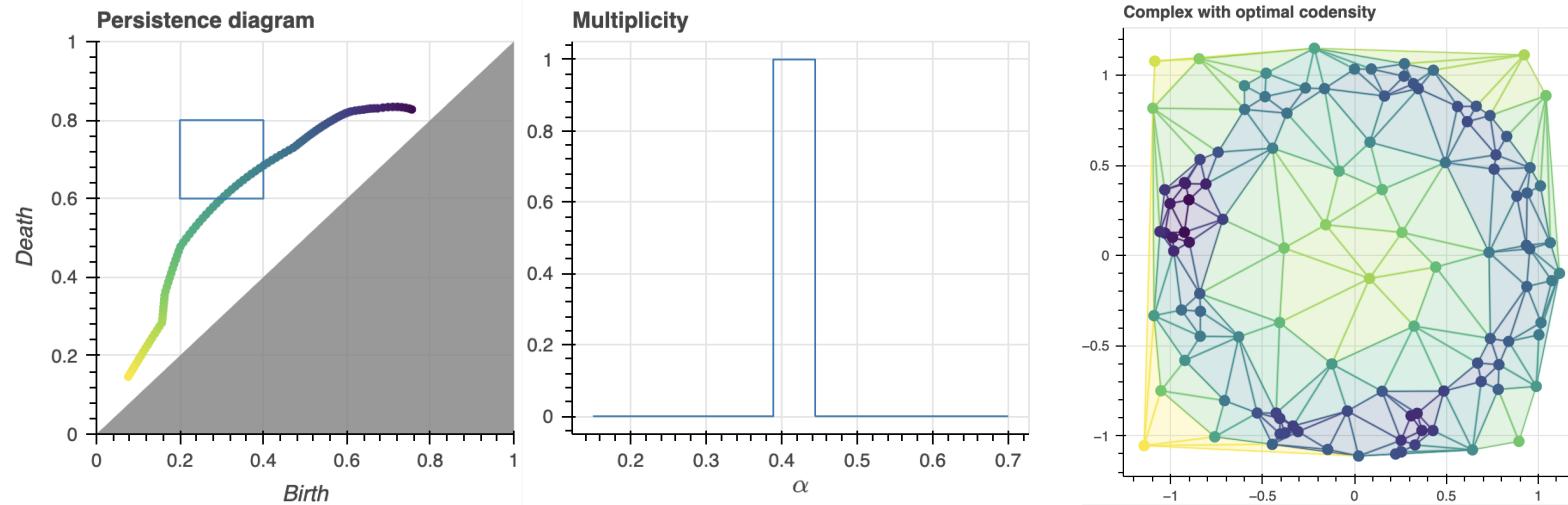
(1) This ϕ corresponds to setting $\nu(\tau) = \sqrt{\tau}$ and $p(x) = 2x(x^2 + 1)^{-2}$; (2) See Theorem 2 in Zhao (2012).

Application #1: Filtration optimization



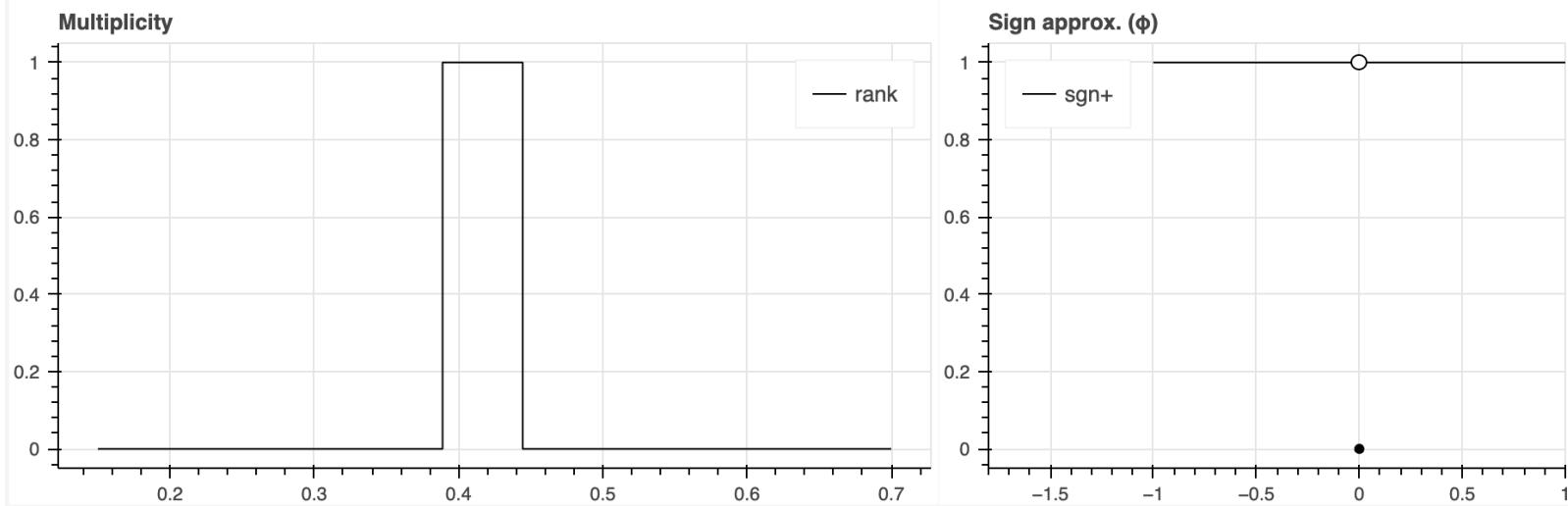
$$\alpha^* = \arg \max_{\alpha \in \mathbb{R}} \text{card}(\text{dgm}(K_\bullet, f_\alpha)|_R)$$

Application #1: Filtration optimization



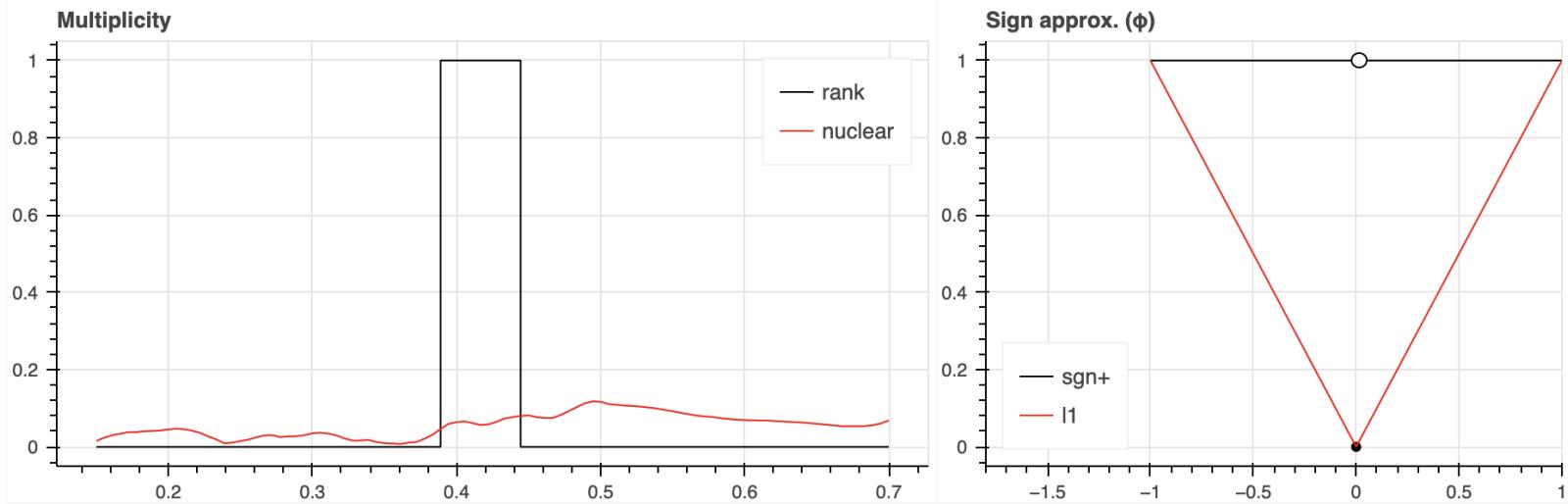
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Application #1: Filtration optimization



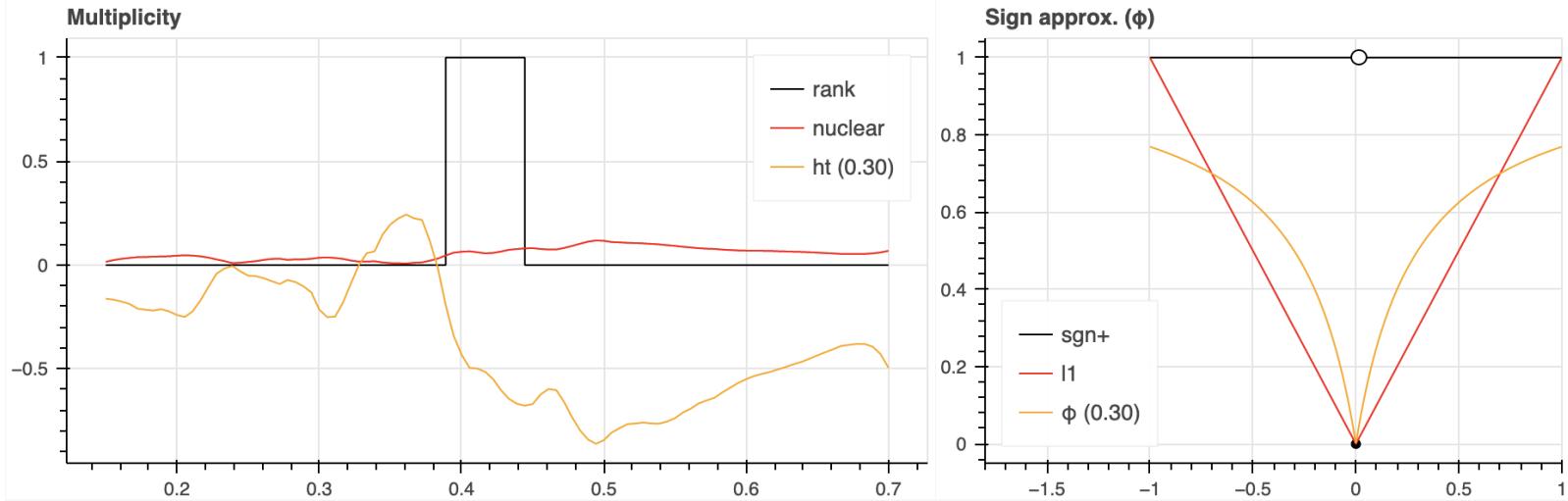
$$\mu_p^R = \text{rank} \begin{bmatrix} \partial_{p+1}^{j+1,k} & 0 \\ 0 & \partial_{p+1}^{i+1,l} \end{bmatrix} - \text{rank} \begin{bmatrix} \partial_{p+1}^{i+1,k} & 0 \\ 0 & \partial_{p+1}^{j+1,l} \end{bmatrix}$$

Application #1: Filtration optimization



$$\mu_p^R = \text{tr} \begin{bmatrix} \|\partial_{p+1}^{j+1,k}\|_* & 0 \\ 0 & \|\partial_{p+1}^{i+1,l}\|_* \end{bmatrix} - \text{tr} \begin{bmatrix} \|\partial_{p+1}^{i+1,k}\|_* & 0 \\ 0 & \|\partial_{p+1}^{j+1,l}\|_* \end{bmatrix}$$

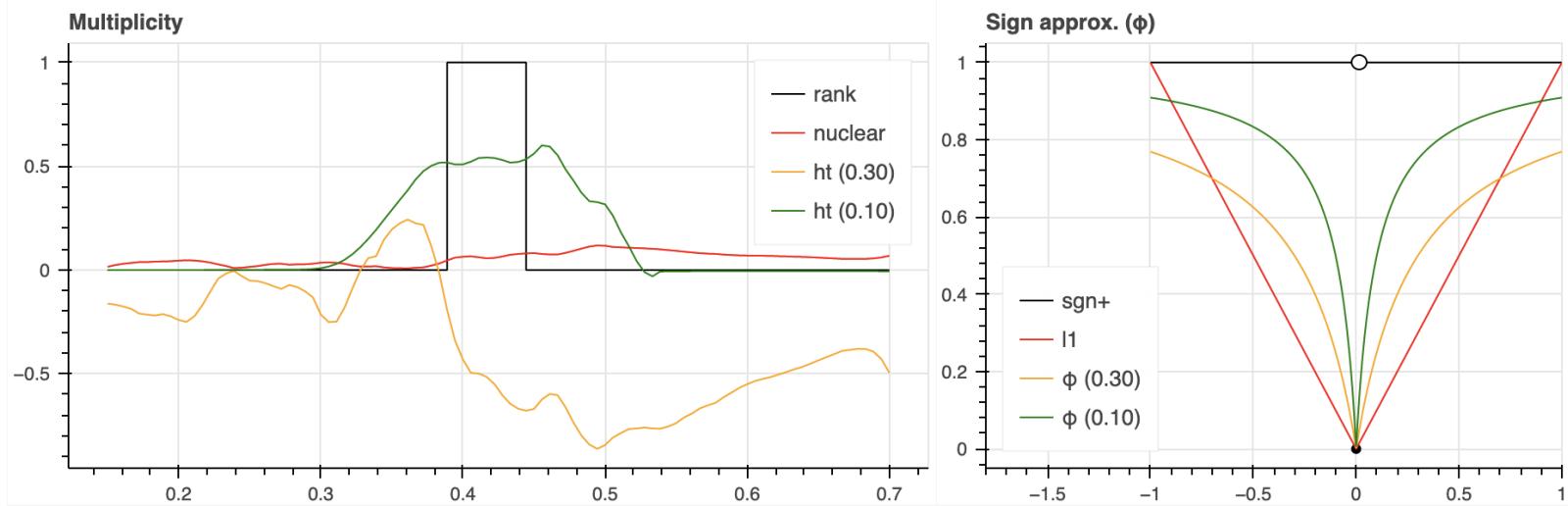
Application #1: Filtration optimization



$$\hat{\mu}_p^R = \text{tr} \begin{bmatrix} \Phi_\tau(\partial_{p+1}^{j+1,k}) & 0 \\ 0 & \Phi_\tau(\partial_{p+1}^{i+1,l}) \end{bmatrix} - \text{tr} \begin{bmatrix} \Phi_\tau(\partial_{p+1}^{i+1,k}) & 0 \\ 0 & \Phi_\tau(\partial_{p+1}^{j+1,l}) \end{bmatrix}$$

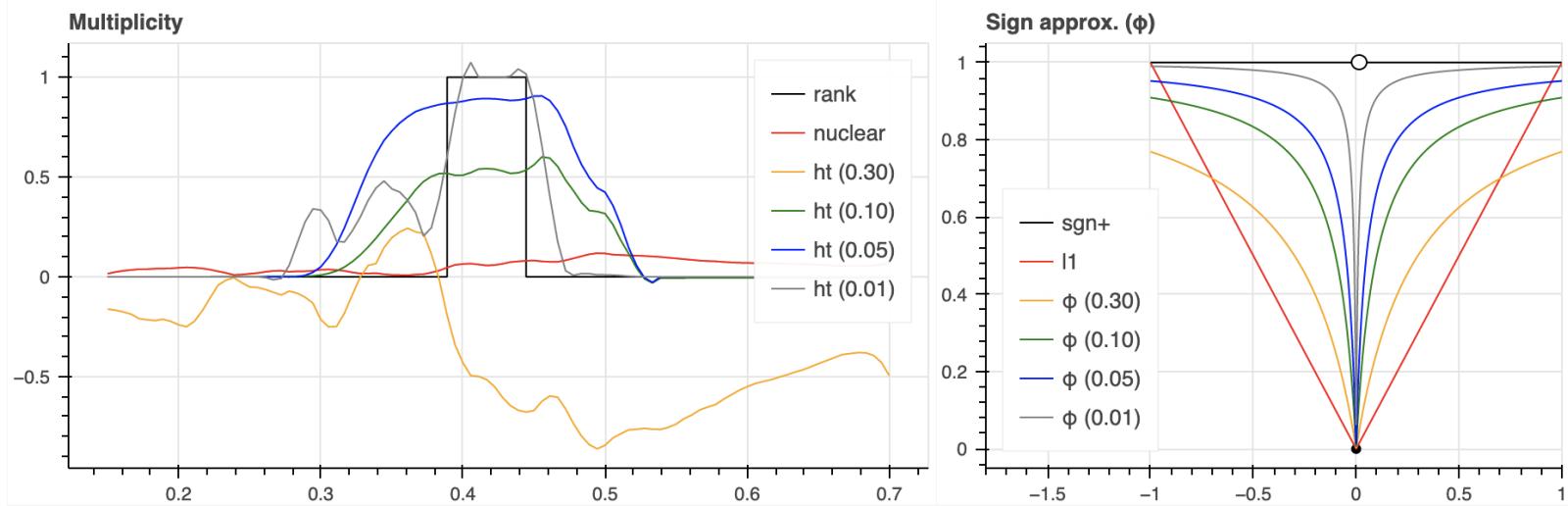
There exists a positive $\tau^* > 0$ such that $\mu_p^R = \lceil \hat{\mu}_p^R \rceil$ for all $\tau \in (0, \tau^*]$

Application #1: Filtration optimization



$$\mu_p^R = \text{tr} \begin{bmatrix} \Phi_\tau(\partial_{p+1}^{j+1,k}) & 0 \\ 0 & \Phi_\tau(\partial_{p+1}^{i+1,l}) \end{bmatrix} - \text{tr} \begin{bmatrix} \Phi_\tau(\partial_{p+1}^{i+1,k}) & 0 \\ 0 & \Phi_\tau(\partial_{p+1}^{j+1,l}) \end{bmatrix}$$

Application #1: Filtration optimization



$$\mu_p^R = \text{tr} \begin{bmatrix} \Phi_\tau(\partial_{p+1}^{j+1,k}) & 0 \\ 0 & \Phi_\tau(\partial_{p+1}^{i+1,l}) \end{bmatrix} - \text{tr} \begin{bmatrix} \Phi_\tau(\partial_{p+1}^{i+1,k}) & 0 \\ 0 & \Phi_\tau(\partial_{p+1}^{j+1,l}) \end{bmatrix}$$

Similar to the Iterative Soft-Thresholding Algorithm (ISTA) ([Beck 2017](#))

Combinatorial Laplacian

Relax #3: Replace $\partial \mapsto L$ with *combinatorial Laplacians* (Horak and Jost 2013):

$$\Delta_p = \underbrace{\partial_{p+1} \partial_{p+1}^T}_{L_p^{\text{up}}} + \underbrace{\partial_p^T \partial_p}_{L_p^{\text{dn}}}$$

f_α is 1-to-1 correspondence with inner products on cochain groups $C^p(K, \mathbb{R})$

$$L_p^{i,j}(\alpha) \Leftrightarrow \langle f, g \rangle_\alpha \text{ on } C^{p+1}(K, \mathbb{R})$$

Benefits: Symmetric, positive semi-definite, have “nice” linear and quadratic forms:

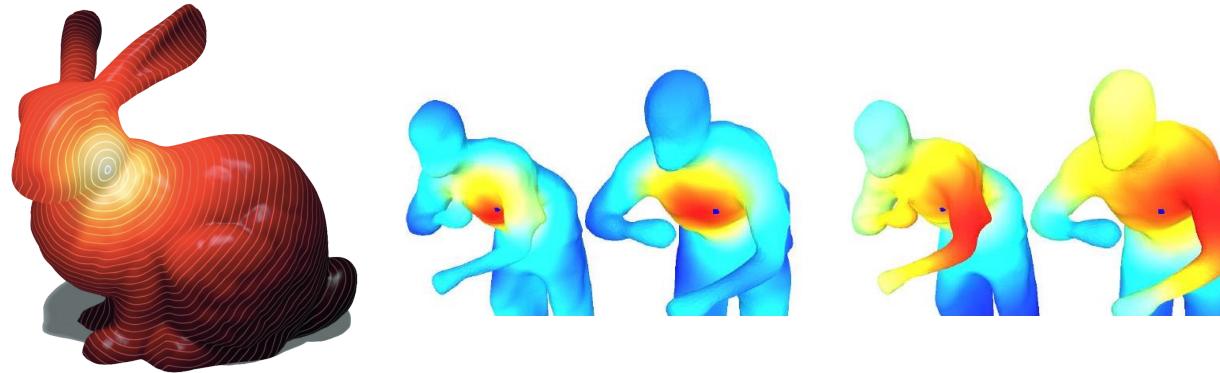
$$L_p^{\text{up}}(\tau, \tau') = \begin{cases} \deg_f(\tau) \cdot f^{+/2}(\tau) & \text{if } \tau = \tau' \\ s_{\tau, \tau'} \cdot f^{+/2}(\tau) \cdot f(\sigma) \cdot f^{+/2}(\tau') & \text{if } \tau \stackrel{\sigma}{\sim} \tau' \\ 0 & \text{otherwise} \end{cases}$$

⇒ can represent operator in “matrix-free” fashion

Interpretation: Diffusion

Diffusion processes on graphs often modeled as time-varying $v^{(t)} \in \mathbb{R}^n$ via:

$$v'^{(t)} = -Lv^{(t)} \quad \Leftrightarrow \quad L \cdot u(x, t) = -\frac{\partial u(x, t)}{\partial t}$$



Value of $v(t)$ at time t given by the *Laplacian exponential diffusion kernel*:

$$v^{(t)} = \exp(-tL)v^{(0)}$$

Images from Crane, Weischedel, and Wardetzky (2017) and Sharma et al. (2011)

Interpretation: Diffusion

Under the appropriate parameters for ν and ρ^1 , ϕ takes the form:

$$\phi(x, \tau) = 1 - \exp(-x/\tau)$$

The corresponding Löwner operator and its Schatten 1-norm is given by (for $t = \tau^{-1}$):

$$\Phi_\tau(X) \simeq U \exp(-t\Lambda) U^T, \quad \|\Phi_\tau(X)\|_* \simeq \sum_{i=1}^n \exp(-t \cdot \lambda_i)$$

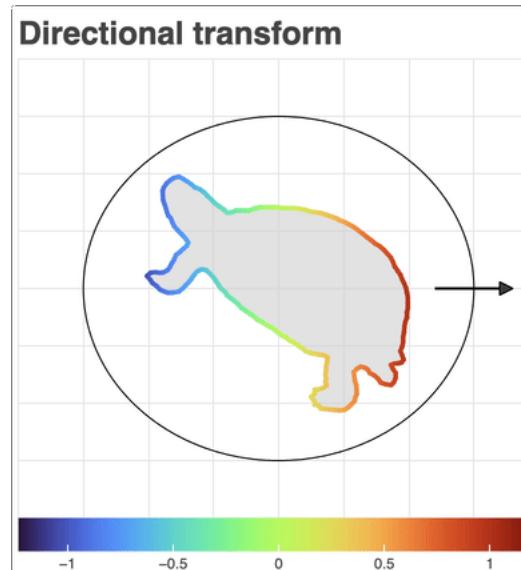
This is the *Heat kernel* and its Schatten-1 norm is the *heat kernel trace*

¹ This ϕ corresponds to setting $\nu(\tau) = \tau$ and $\rho(x) = \exp(-x)$ for $x > 0$ and $\rho(x) = 0$ otherwise

Application #2: Directional Transform

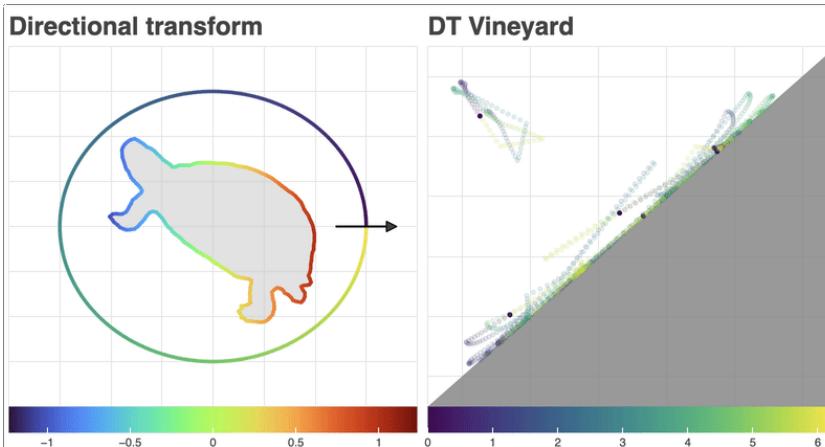
Consider filtering a fixed K embedded in R^d by a 1-parameter directions in S^{d-1}

$$K_{\bullet} = K(v)_i = \{ x \in X \mid \langle x, v \rangle \leq i \}$$



Application #2: Directional Transform

$$K_{\bullet} = K(v)_i = \{ x \in X \mid \langle x, v \rangle \leq i \}$$



$$\{ \text{dgm}(v) : v \in S^{d-1} \} \Leftrightarrow \text{Persistent Homology Transform (PHT)}$$

Turner et al.¹ show PHT(X) is injective, sparking an inverse theory for persistence!

(1): Turner, Mukherjee, and Boyer (2014)

Application #2: Directional Transform

Injectivity of the PHT \implies can impose metric \mathcal{D} over *shape space* by integrating d_B :

$$\mathcal{D}(X, Y) \triangleq \sum_{p=0}^d \int_{S^{d-1}} d_B (\text{dgm}_p(X, v), (\text{dgm}_p(Y, v)) dv$$

To make $\mathcal{D}(\cdot, \cdot)$ blind to rotations, Turner¹ minimize \mathcal{D} over rotations $\{R_i\}_{i=1}^m$:

$$d_{\text{PHT}}(X, Y) = \inf_{i=1, \dots, m} \mathcal{D}(X, R_i(Y))$$

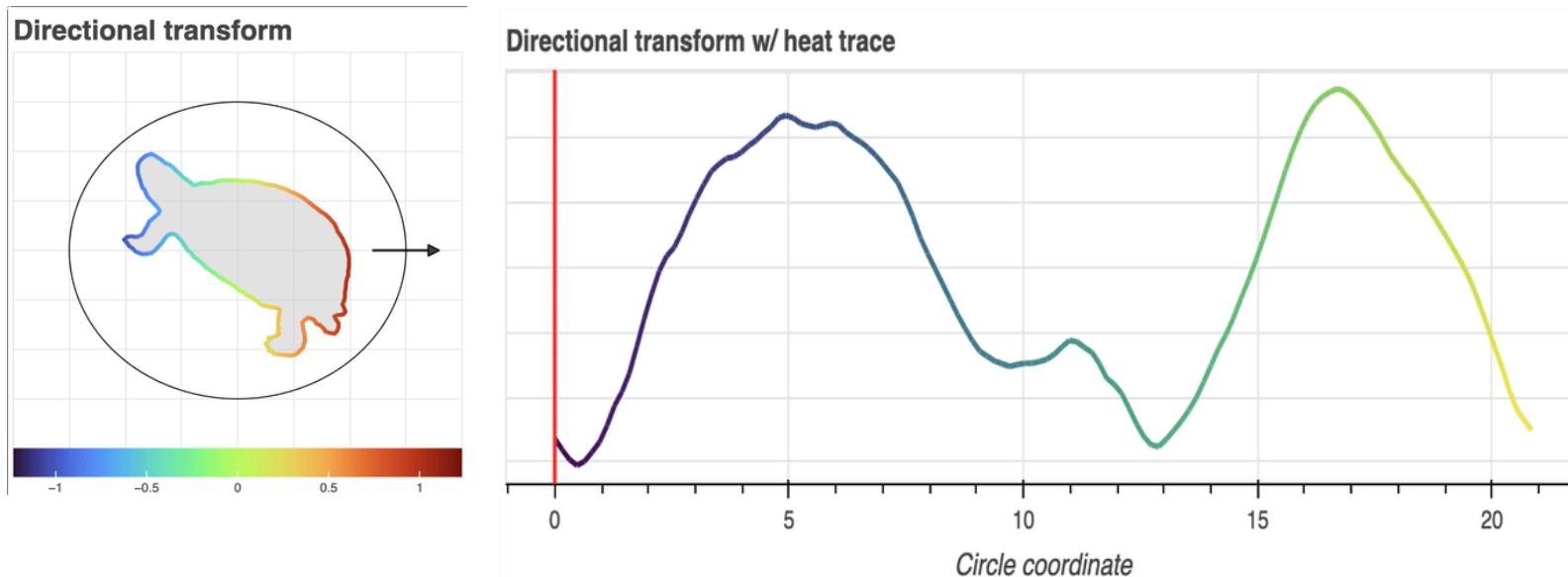
When $m = |V|$, computing $d_{\text{PHT}}(X, Y)$ requires:

1. Computing $\text{dgm}_p(\cdot, v)$ for $\{X, Y\}$ over sufficiently dense $\mathcal{V} \subset S^{d-1}$ ($O(m \cdot N^3)$)
2. Minimizing \mathcal{D} over all m rotations ($\approx O(m^2 \cdot N^{1.5} \log N)$)¹

(1) Assumes $d_B \sim O(n^{1.5} \log n)$, following (Kerber, Morozov, and Nigmetov 2017).

¹ Turner, Mukherjee, and Royer (2014)

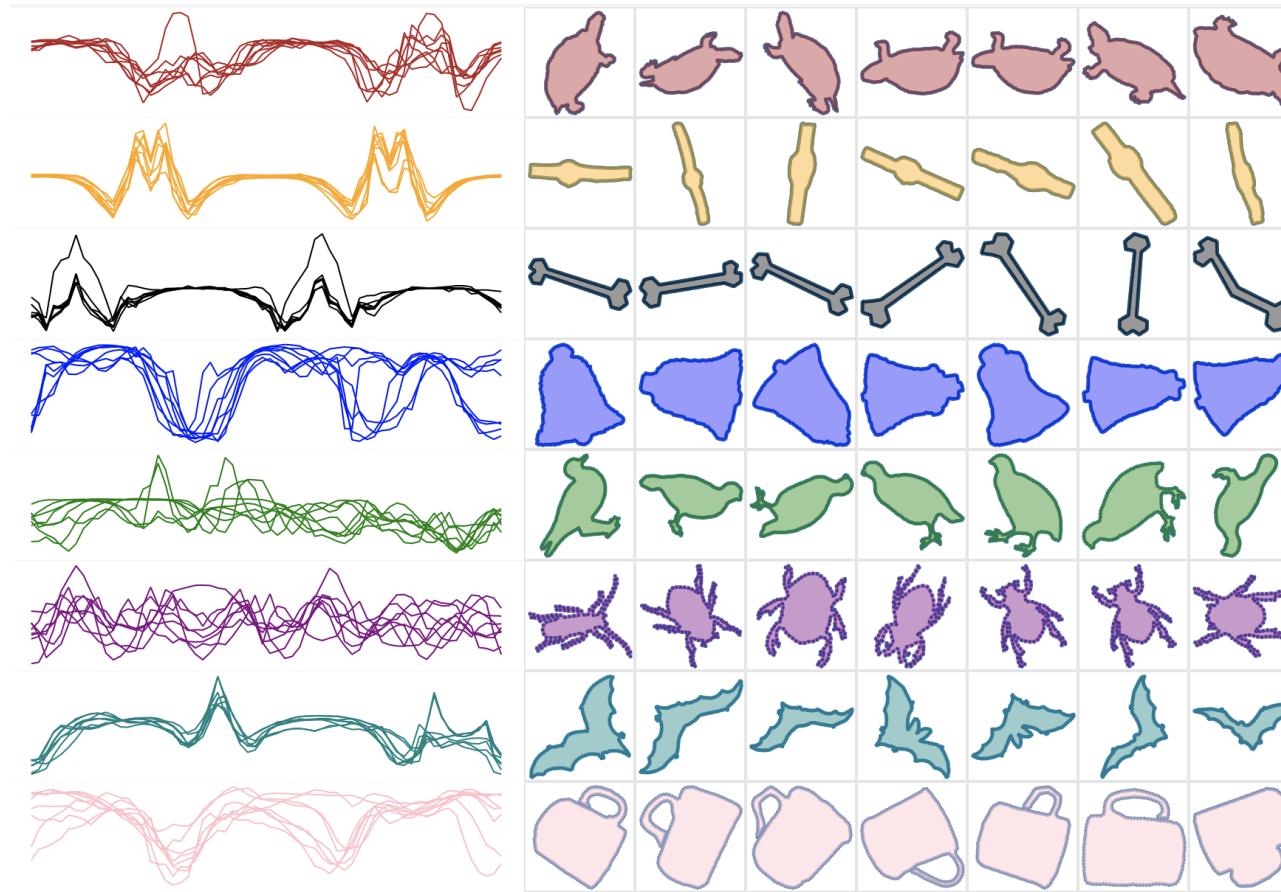
Application #2: Directional Transform



When $m = |V|$, computing $d_{\text{DT}}(X, Y)$ requires:

1. Computing $\text{tr}(\phi_\tau(\cdot))$ for $\{X, Y\}$ over sufficiently dense $\mathcal{V} \subset S^{d-1}$ ($\approx O(m \cdot N^2)$)
2. Phase-aligning two *periodic* signals via FFT ($O(m \log m)$)

Application #2: Directional Transform



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Computation in quadratic time

Computing $A = U\Lambda U^T$ for any $A \in \mathbf{S}_+^n$ bounded by $\Theta(n^3)$ time and $\Theta(n^2)$ space¹

However, if $v \mapsto Av \approx O(n)$, then $\Lambda(A)$ obtainable in $O(n^2)$ time and $O(n)$ space!

Idea: For some random $v \in \mathbb{R}^n$, expand successive powers of A :

$$K_j = [v \mid Av \mid A^2v \mid \cdots \mid A^{j-1}v] \quad (4)$$

$$Q_j = [q_1, q_2, \dots, q_j] \leftarrow \text{qr}(K_j) \quad (5)$$

$$T_j = Q_j^T A Q_j \quad (6)$$

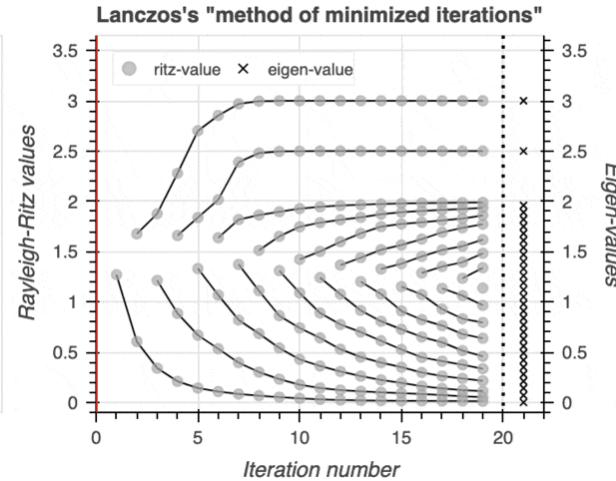
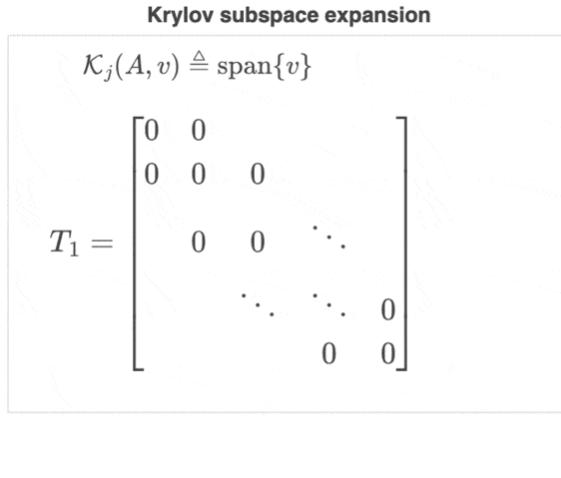
It turns out that every $A \in \mathbf{S}$ expanded this way admits a *three-term recurrence*

$$Aq_j = \beta_{j-1}q_{j-1} + \alpha_j q_j + \beta_j q_{j+1}$$

This is the renowned **Lanczos method** for Krylov subspace expansion

¹ Assumes the standard matrix multiplication model for simplicity (i.e., excludes the Strassen family)

Lanczos iteration



Theorem (Simon 1984): Given a symmetric rank- r matrix $A \in \mathbb{R}^{n \times n}$ whose matrix-vector operator $A \mapsto Ax$ requires $O(\eta)$ time and $O(\nu)$ space, the Lanczos iteration computes $\Lambda(A) = \{\lambda_1, \lambda_2, \dots, \lambda_r\}$ in $O(\max\{\eta, n\} \cdot r)$ time and $O(\max\{\nu, n\})$ space when executed in exact arithmetic.

Randomized trace approximation

Let $A = \mathbb{R}^{n \times n}$. If $v \in \mathbb{R}^n$ a r.v. with $\mathbb{E}[vv^T] = I$, then:

$$\text{tr}(A) = \text{tr}(A\mathbb{E}[vv^T]) \quad (\text{identity})$$

$$= \mathbb{E}[\text{tr}(Avv^T)] \quad (\text{linearity})$$

$$= \mathbb{E}[\text{tr}(v^T Av)] \quad (\text{cyclic})$$

$$= \mathbb{E}[v^T Av] \quad (\text{symmetry})$$

$$\implies \text{tr}(A) \approx \frac{1}{n_v} \sum_{i=1}^{n_v} v_i^\top A v_i, \quad \text{for } v_i \sim \mathcal{N}(\mu = 0, \sigma = 1)$$

Randomized trace approximation

Theorem (Ubaru, Chen, and Saad 2017): For any $A \in S_+^n$, if $n_v \geq (6/\epsilon^2) \log(2/\eta)$ unit-norm $v \in \mathbb{R}^n$ are drawn uniformly from $\{-1, +1\}^n$, then for any $\epsilon, \eta \in (0, 1)$:

$$\Pr \left(|\text{tr}_{n_v}(A) - \text{tr}(A)| \leq \epsilon \cdot \text{tr}(A) \right) \geq 1 - \eta$$

⇒ Generalizes to spectral functions $\Phi_\tau(X)$ via stochastic Lanczos quadrature¹

$$\text{tr}(\Phi_\tau(X)) \approx \frac{n}{n_v} \left(e_1^T \Phi_\tau(T) e_1 \right), \quad T = \text{Lanczos}(X)$$

$$\Rightarrow \hat{\mu}_p^R \sim O(n \cdot s l^2)^1 \text{ time and } O(n) \text{ space}$$

Where $n \sim |K^p|$, and both $l, s \sim O(1)$ are small constants²

(1) See Ubaru, Chen, and Saad (2017). (2) We found setting the lanczos polynomial degree $l \leq 20$ and number of Monte-carlo iterations $s \leq 200$ was sufficient for most applications.

Scalability: matvecs's are all you need

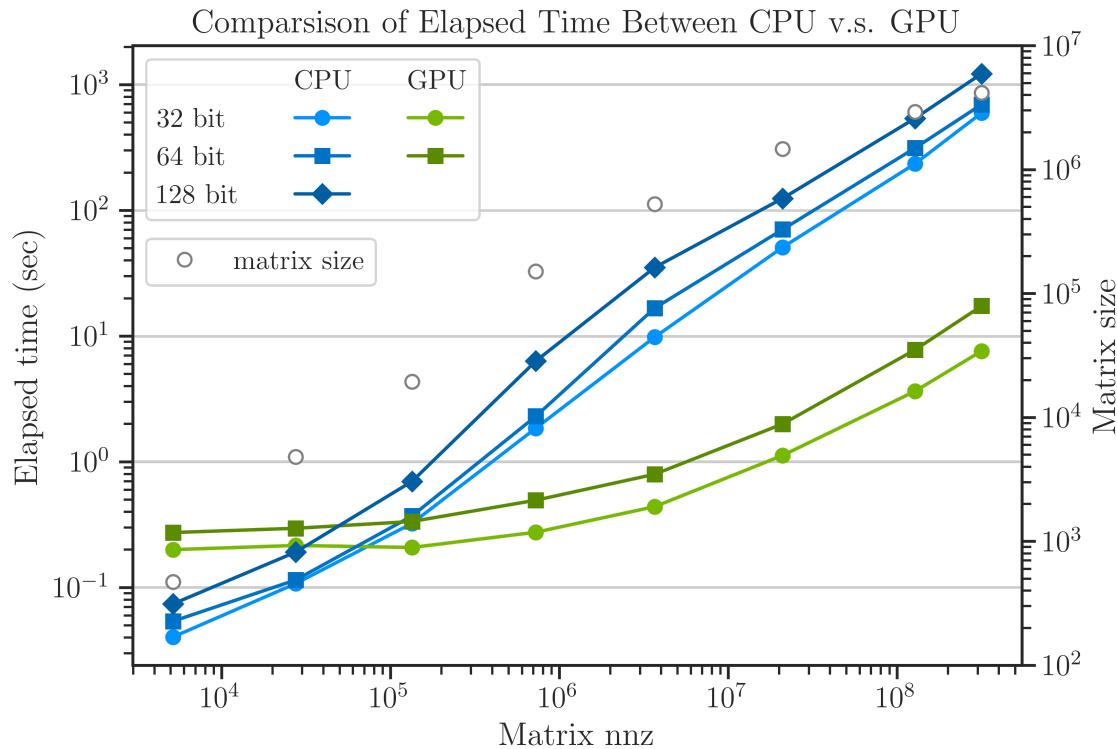


Figure taken from the new [imate](#) package documentation ([\[gh\]](#)/[ameli](#)/[imate](#))

Application #3: Computing dgm's

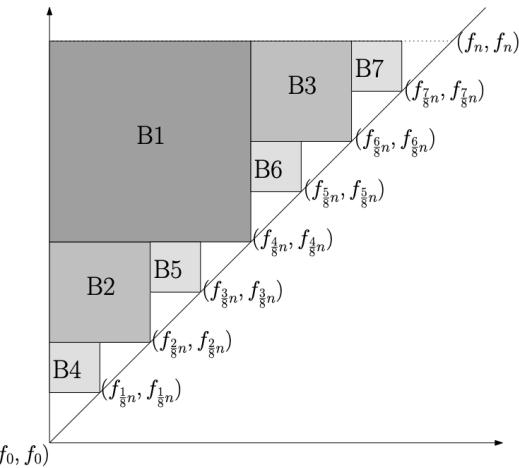


Figure 3: Compute persistence pairs in a divide and conquer fashion.

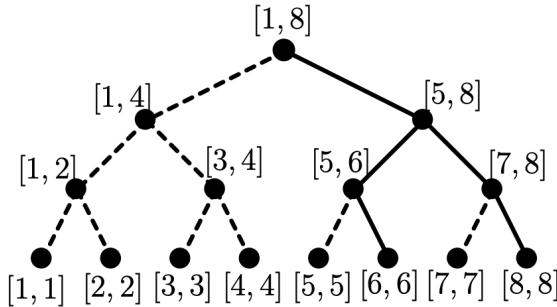
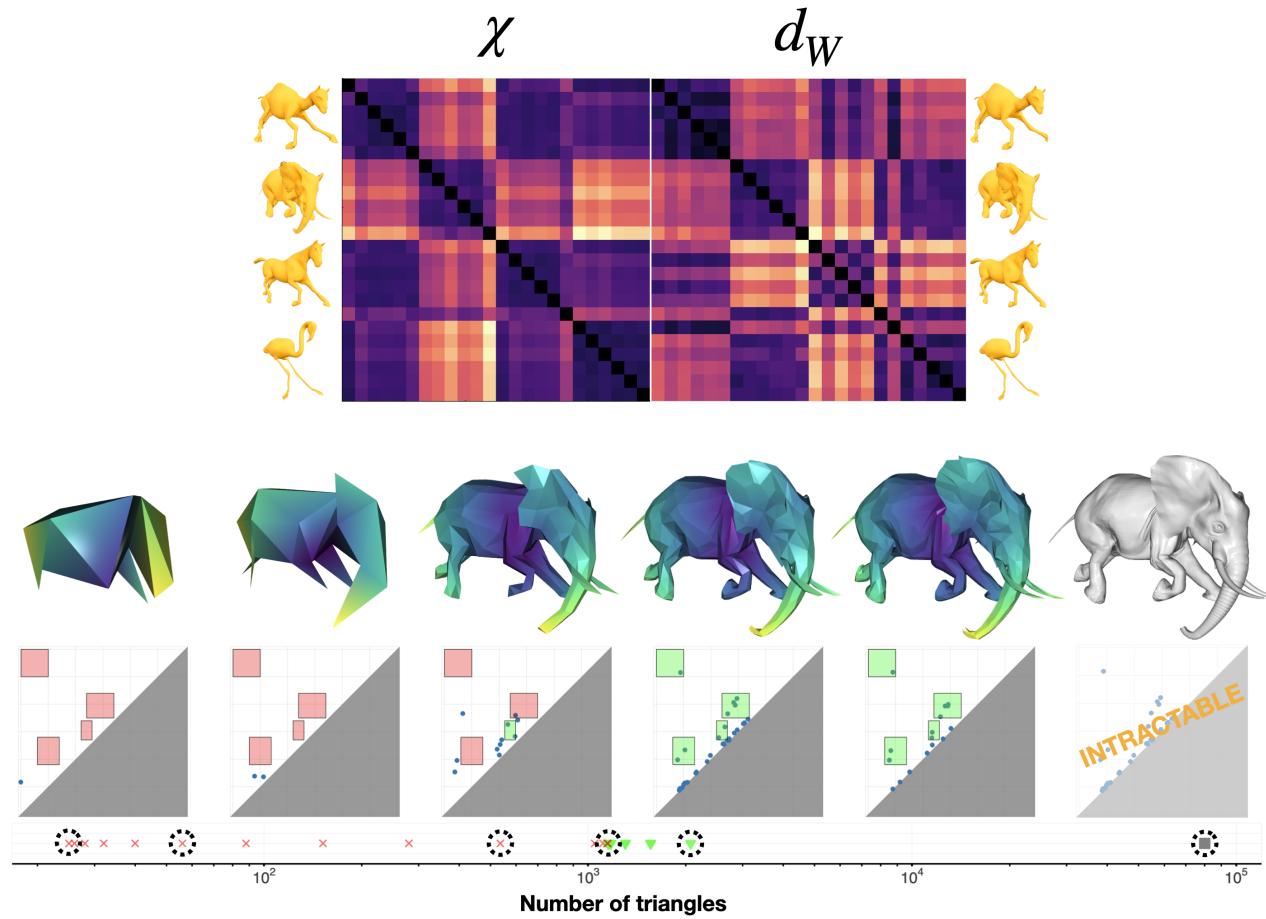


Figure 2: An illustration of the bisection tree of an interval $[i_1, i_2] = [1, 8]$, which contains two creators, σ_6 and σ_8 . Only the nodes on the two solid paths (and their siblings) are explored by the algorithm.

Theorem (Chen and Kerber 2011): For a simplicial complex K of size $|K| = n$, computing the Γ -persistent pairs requires $O(C_{(1-\delta)\Gamma} R(n) \log n)$ time and $O(n + R(n))$ space, where $R(n)$ ($R_S(n)$) is the time (space) complexity of computing the rank of a $n \times n$ boundary matrix.

Other applications (time permitting)



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 - SLQ due to Ubaru, Chen, and Saad ([2017](#)); code ported from [imate](#)
-

To see the code develop and track its progress, head to:

[\[gh\]/peekxc](#) or [mattpiekenbrock.com](#)

Thanks for listening!

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