Multiparameter Persistence and Nonlinear Hierarchical Clustering

Oliver Gäfvert

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Contour Learning

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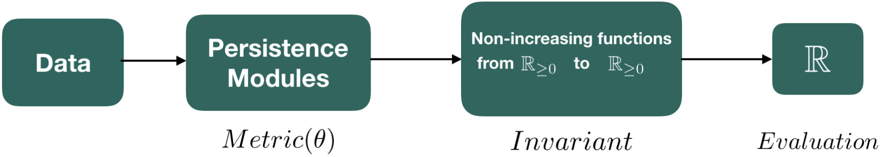

Preliminaries

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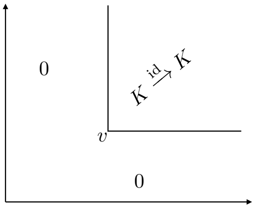

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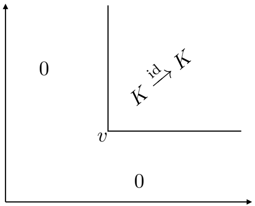

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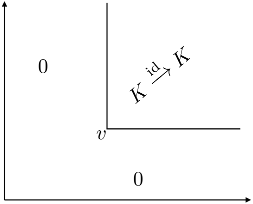

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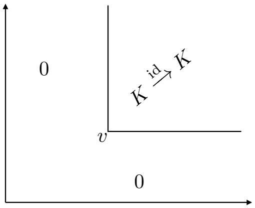

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- F is *finitely presented* if it is f.g and the kernel of ϕ is also f.g.

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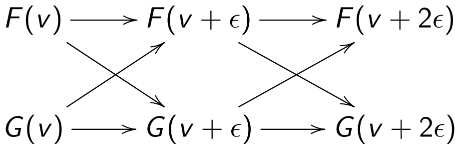

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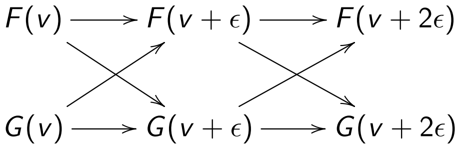

$$d_{\bowtie} = \inf\{\epsilon \mid F \text{ and } G \text{ are } \epsilon\text{-interleaved}\}$$

Multiparameter Persistent Homology

The categories of:

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Slogan

We can identify a finitely presented persistence module with an n-graded $K[x_1, \ldots, x_n]$-module by restricting to a small enough grid $\mathbb{N}^n \subset \mathbb{R}^n$.

Invariants

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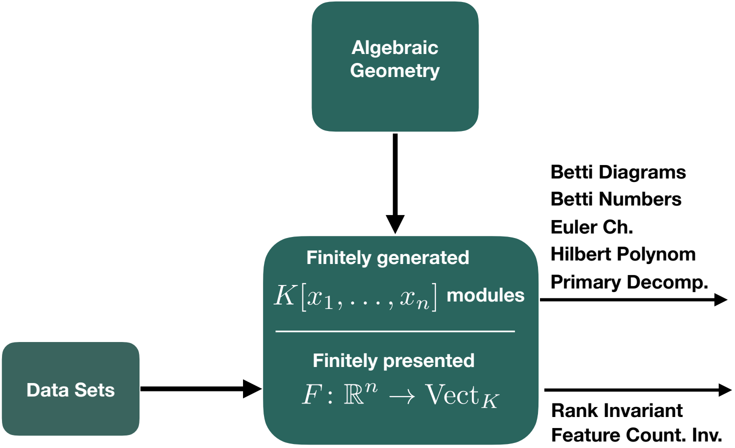
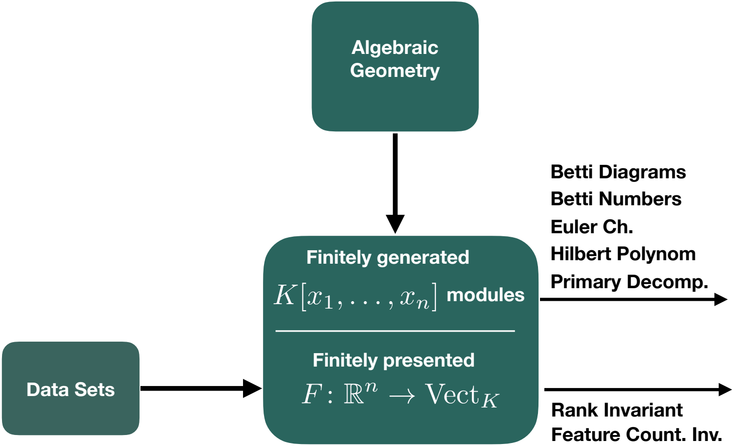

Algebraic Geometry
Betti Diagrams
Betti Numbers
Euler Ch.
Hilbert Polynom
Primary Decomp.
Finitely generated
$K[x_1, \ldots, x_n]$ modules
Finitely presented
$F\colon \mathbb{R}^n \to \mathrm{Vect}_K$
Data Sets
Rank Invariant
Feature Count. Inv.

Invariants



Need for stable invariants!

Feature Counting Invariant

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Using *persistence contours*, we can show:

Theorem (G. and Chachólski, 2017, [2])

For $n \geq 2$, computing $\widehat{\beta}_0(F)$ is NP-hard.

Persistence Contours

(Metrics on persistence modules)

Persistence Contours

A *persistence contour* is a functor $C\colon \mathbb{R}^n_\infty \times \mathbb{R} \to \mathbb{R}^n_\infty$ s.t, for any $v \in \mathbb{R}^n_\infty$ and any $\epsilon, \tau \in \mathbb{R}$:

1. $v \leq C(v, \epsilon)$,
2. $C(C(v, \epsilon), \tau) \leq C(v, \epsilon + \tau)$.

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- The *ϵ-shift*,

  $$F[\epsilon] = \langle \{F(v_i \leq C(v_i, \epsilon))(g_i) \in F(C(v_i, \epsilon))\} \rangle$$

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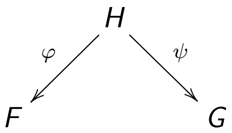
- 

  F and G are *ϵ-close* if $\ker \varphi[a] = \operatorname{coker} \varphi[b] = \ker \psi[c] =$
  $= \operatorname{coker} \psi[d] = 0$ and $a + b + c + d \leq \epsilon$.

Persistence Contours

Given a choice of persistence contour:

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Example

Let $C(v, \epsilon) = v + \epsilon\mathbf{1}$. This is called the *standard persistence contour*.

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Theorem

For the standard persistence contour:

$$\frac{1}{6} d(F, G) \leq d_{\bowtie}(F, G) \leq d(F, G)$$

Constructing Persistence Contours

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We define $C_\theta \colon \mathbb{R}_\infty \times \mathbb{R} \to \mathbb{R}_\infty$ as the solution to the following equation:

$$t = \int_{v}^{C_\theta(v,t)} \rho_\theta(\alpha) d\alpha$$

where $\rho_\theta(\alpha)$ is some positive real-valued function, parametrized by $\theta \in \mathbb{R}^m$.

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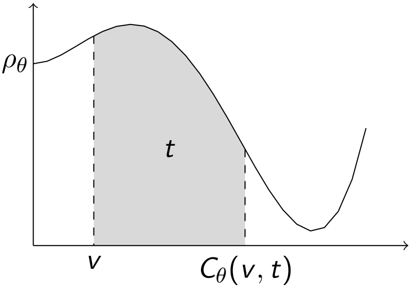

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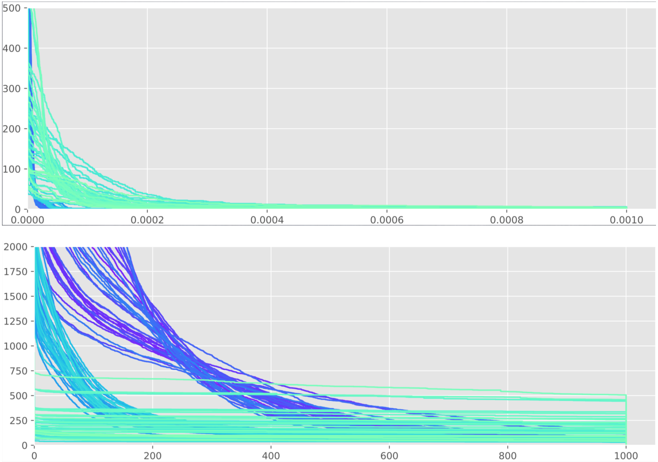
We consider persistence contours parametrized by $\theta \in \mathbb{R}^m$, with the property:

$$C_\theta(v, t) = (C_\theta^1(v_1, t), \ldots, C_\theta^n(v_n, t))$$

where $v = (v_1, \ldots, v_n)$.

Tree Contour Example

Forest tree data from Henri Riihimäki:



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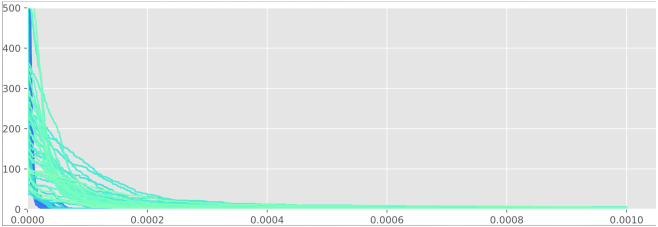

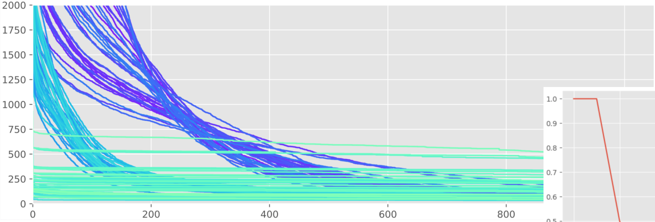

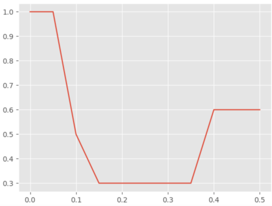

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Solution

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Solution

Define a distance d_θ, using persistence contours, and solve the following metric learning problem:

$$\begin{aligned} \min_\theta \sum_{F, F' \in \phi^{-1}(0)} d_\theta(F, F') + \sum_{F, F' \in \phi^{-1}(1)} d_\theta(F, F') \\ \text{s.t} \sum_{\substack{F \in \phi^{-1}(0) \\ F' \in \phi^{-1}(1)}} d_\theta(F, F') \geq 1 \end{aligned} \tag{1}$$

One-parameter contour learning

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- If $H \supset F[\tau]$, then $\text{rank}(H) \geq \text{rank}(F[\tau])$.

□

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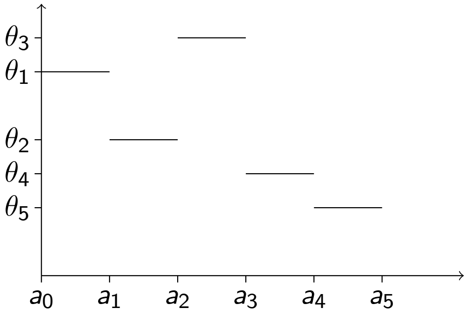

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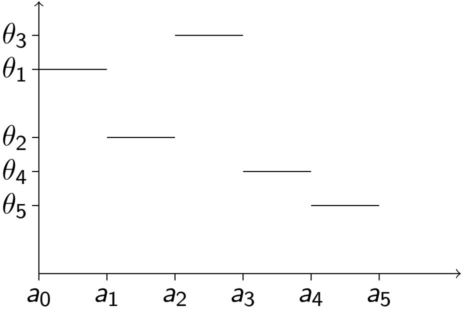

we will adjust the step heights θ_i to solve the metric learning problem (1).

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Smoothed version of the interleaving distance for non-increasing functions from $\mathbb{R}_{\geq 0}$ to $\mathbb{R}_{\geq 0}$:

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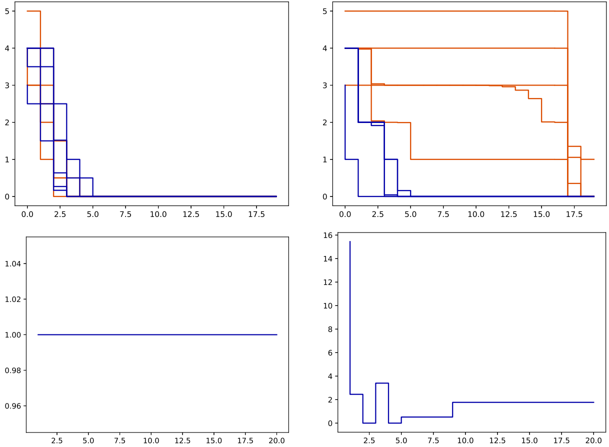
Then,

$$d_\theta(F, F') := d_{\bowtie}(\mathfrak{r}_\theta(F), \mathfrak{r}_\theta(F'))$$

Example

- B consists of ten barcodes, with five in each class.
- Choose $\rho_\theta(\alpha) := \theta_i$ if $i \leq \alpha < i+1$ and we let $\theta_i = \theta_{i+1}$ if $i \geq 19$. Consequently, $\theta \in \mathbb{R}^{20}$.



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It can be decomposed into rectangular blocks of the same hight,

$$HF = \cup_i h_i I_{(a_{i1},\ldots,a_{in}),(b_{i1},\ldots,b_{in})}$$

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This happens for multiparameter clustering.
Use the Hilbert function, $HF(v) := \dim F(v)$, to construct a smoothed feature counting function.
It can be decomposed into rectangular blocks of the same hight,

$$HF = \cup_i h_i I_{(a_{i1},\ldots,a_{in}),(b_{i1},\ldots,b_{in})}$$

and thus

$$\mathfrak{r}_\theta(F)(\tau) = \sum_i h_i \prod_{k=1}^{n} \frac{1}{1 + e^{k(a_{ik} - C^i_\theta(0,\tau))}} \frac{1}{1 + e^{k(C^i_\theta(0,\tau) - b_{ik})}}$$

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- Produces a nonlinear hierarchical clustering of the data by restricting the module to the curve outlined by $C(0, \tau)$.

Approximating the Feature Counting Invariant

Approximations

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$\{g_i \in F(v_i)\}$
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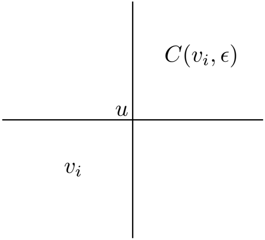
For ϵ large enough, there is u s.t:



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Can be phrased as the following *matrix rank minimization problem with an affine constraint set*:

Input Vectors $x_1, \ldots, x_m \in \mathbb{R}^n$ and subspaces $L_1, \ldots, L_m \subseteq \mathbb{R}^n$
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This is NP-hard, by reduction from a graph colouring problem [2].

Example

Calculating $\widehat{\beta}_0(F)(2)$ for the following functor requires you to solve such a rank minimization problem:

5	0	0	0	0	0	0
4	K	K^2	K^3/L_2	0	0	0
3	K	K^2	K^3	K^3/L_1	0	0
2	K	K^2	K^3	K^3	K^3/L_0	0
1	0	K	K^2	K^2	K^2	0
0	0	0	K	K	K	0
	0	1	2	3	4	5

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Case $F = H_0(X(-); K)$: The F is a functor $F\colon \mathbb{R}^n \to \text{Sets}$ and the matrix rank minimization turns into a vertex covering problem (which can be approximated).

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- Incorporating contour learning into common macine learning methods (logistic regression, SVM, etc).

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