Some statistical challenges of topological inference in the 1D case

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Setup

Consider one-dimensional signal $f : [0, 1] \to \mathbb{R}$ with k modes.
Suppose f is observed by a finite number of measurements:

$$Y_i = f(t_i) + \epsilon_i, \quad 0 = t_0 < t_1 < \cdots < t_n = 1 \ .$$

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Noise (ϵ_i) independently distributed with mean zero s.t. for some $\kappa > 0$, $v > 0$ and all $m \geq 2$:

$$\mathbb{E}\,|\epsilon_i|^m \leq v m! \kappa^{m-2}/2 \ \text{ for all } i = 1, \ldots, n.$$

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- Not on our agenda: *First regularize (filter) data, then perform topological inference* (Bubenik, Carlsson, Chazal, Cohen-Steiner, Guibas, Kim, Mémoli, Mérigot, Oudot, Sheehy, ...).

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- Hard to analyze effect of filtering from statistical perspective *without* a priori assumptions on data or oracles.
- Goal: Statistical bounds on number of modes of f inferred from data Y only, *without* reconstructing f along the way.

Persistent homology [Edelsbrunner et al., 2002]

Investigate change of homology for sublevel sets

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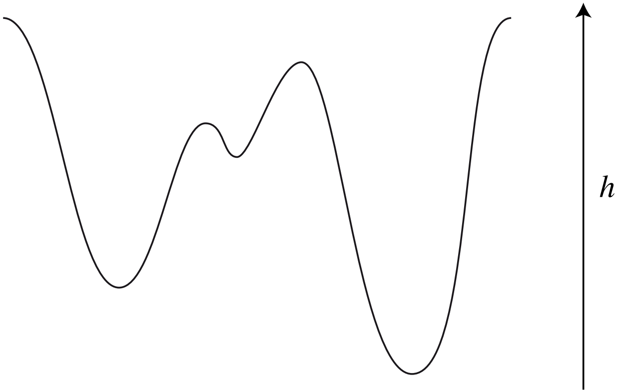
Example: connected components in 1D



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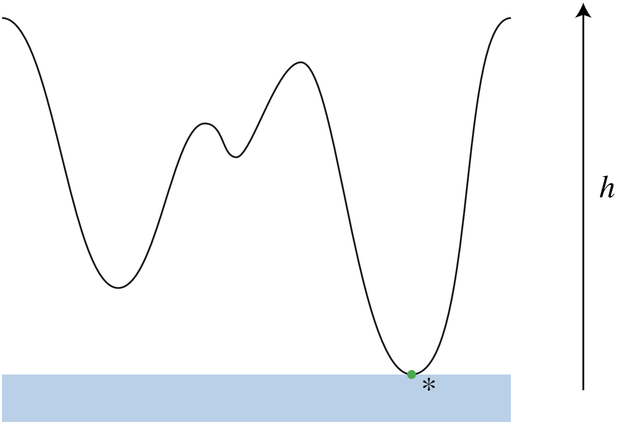

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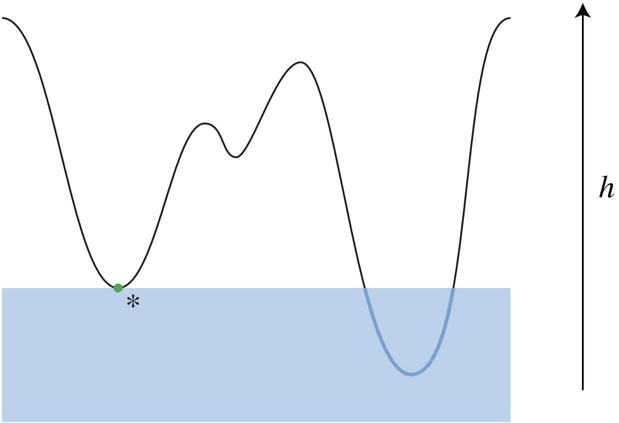

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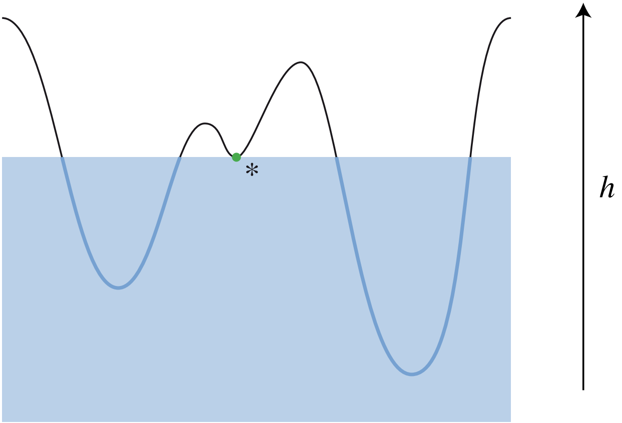

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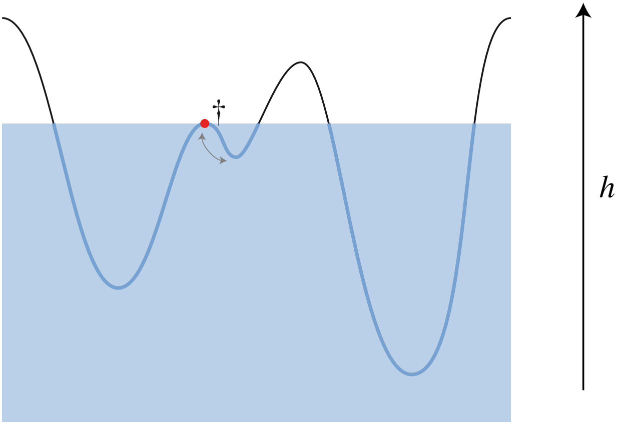

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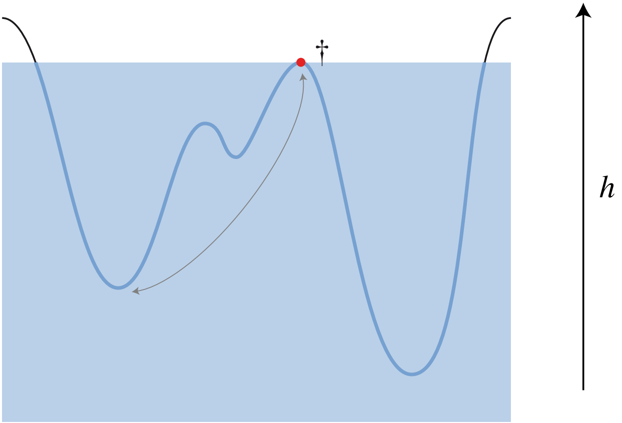

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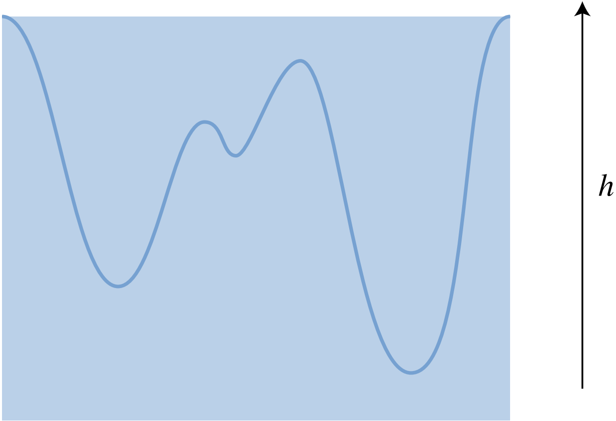

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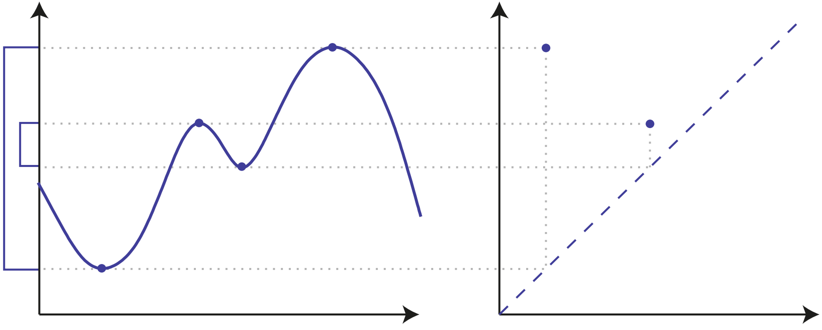

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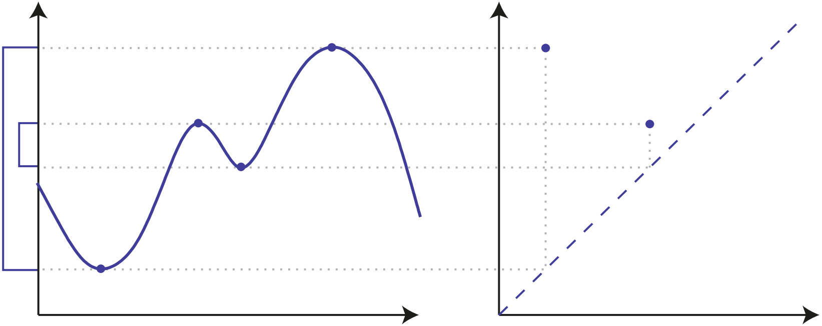

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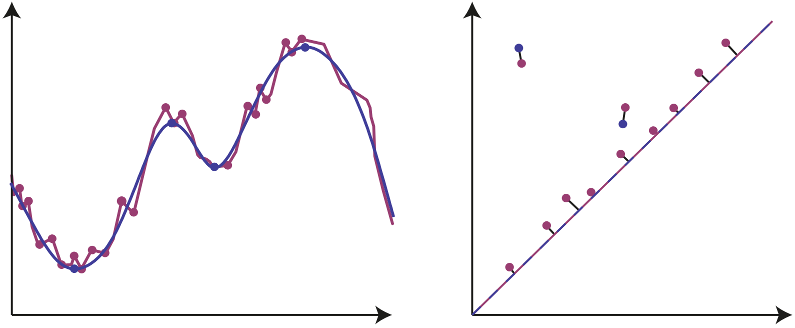

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Persistence signatures

Order persistence values from highest to lowest:

$$s_{0,\infty}(f) \geq s_{1,\infty}(f) \geq s_{2,\infty}(f) \geq \cdots \geq 0 \geq 0 \ldots$$

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Lemma (Bauer)

Let X denote the space of piecewise constant functions on (some) equipartition of $[0,1]$. Let $X_k \subset X$ denote the set of functions with at most k inner maxima (= modes). Then

$$s_{k,\infty}(f) = 2 \cdot \operatorname{dist}_\infty(f, X_k) \ .$$

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$$s_{k,\infty}(f) = 2 \cdot \mathrm{dist}_\infty(f, X_k) \; .$$

Note: Stability implies that $|s_{k,\infty}(f) - s_{k,\infty}(g)| \leq 2\|f - g\|_\infty \; \forall k$.
This gives *upper* bound $s_{k,\infty}(f) \leq 2 \cdot \mathrm{dist}_\infty(f, X_k)$.

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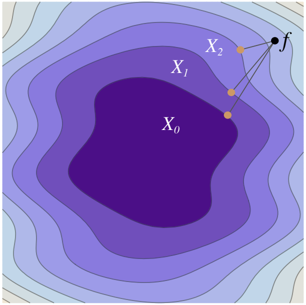
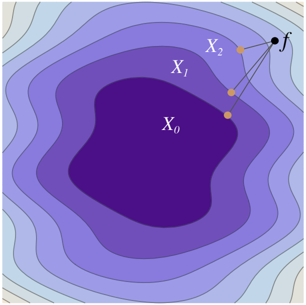


Interpret persistence signatures as distance to set of functions with at most k modes.

Different metrics – different signatures



Define *metric signature* $s_k(f) := \text{dist}(f, X_k)$ with respect to *some* metric d on X.

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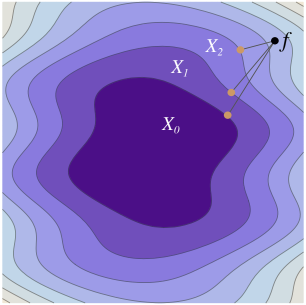

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Call d *descriptive* if for every f with at least $k + 1$ modes $s_k > 0$.

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For all metrics and all k: $|s_k(f) - s_k(g)| \leq d(f, g)$.

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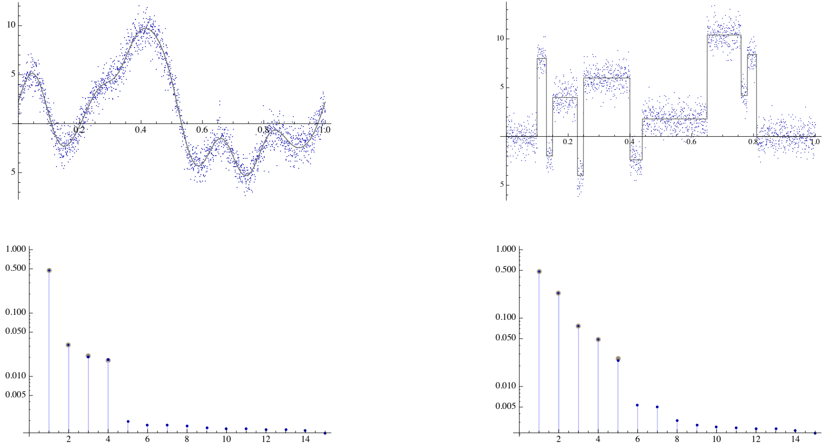
Consider the following descriptive metrics:

- Persistence signatures: $d_\infty(f, g) = sup_x|f(x) - g(x)|$.
- Kolmogorov signatures: $d_K(f, g) = sup_x|F(x) - G(x)|$ for antiderivatives F and G (with $F(0) = G(0) = 0$).

Thresholding metric signatures



Thresholding metric signatures

Empirical signatures: $s_0(Y) \geq s_1(Y) \geq s_2(Y) \geq \cdots$ Define:

$$k_q(Y) := \max \left\{ j : s_{j-1}(Y) \geq q \right\}$$

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Example 1:

$$f(x) = \begin{cases} 1 \text{ if } x \in [1/3, 2/3)\,, \\ 0 \text{ else}\,. \end{cases}$$

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Extreme value theory for i.i.d. normal noise: Largest value on $[1/3, 2/3)$ approaches $1 + \sqrt{2\log(n)}$, lowest value on complement approaches $-\sqrt{2\log(n)}$ with $\mathbb{P} \to 1$.

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Observation: Thresholding persistence signatures at $q(n) = \sqrt{2\log(n)}$ and thresholding Kolmnogorov signatures at $q = 1/2$ detects single mode of f with $\mathbb{P} \to 1$.

Thresholding metric signatures

Example 2: (decreasing signal to noise ratio)

$$f_n(x) = \begin{cases} \delta_n \text{ if } x \in [1/3, 2/3)\ , \\ 0 \text{ else}\ . \end{cases}$$

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Theorem (Bauer, Munk, Sieling, W.)

Let $\delta_n \sqrt{n} \to \infty$ and $\delta_n \sqrt{\log(n)} \to 0$. Then there exists no successful thresholding strategy for persistence signatures:

$$\limsup_{n\to\infty} \mathbb{P}\left(k^{\infty}_{q_n}(Y) = 1\right) < 1$$

for every possible thresholding sequence (q_n).

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Thresholding metric signatures

Example 3: (needle in heystack)

$$f_n(x) = \begin{cases} (1+\varepsilon)\sqrt{2\log(n)} \text{ if } x \in [j/n, (j+1)/n)\,, \\ 0 \text{ else}\,. \end{cases}$$

for $\varepsilon > 0$ and some j that is *not known a priori*.

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Observations:

- Sup-norm thresholding $(Y_1, \ldots, Y_n)$ minimax efficient for detecting single mode of f [Donoho/Jin, Ingster/Suslina].
- No thresholding known for persistence or Kolmogorov.

Empirical Kolmogorov signatures

Theorem (Bauer, Munk, Sieling, W.)

Let $\delta > 0$*. Then*

$$\mathbb{P}\left(\max_{k\in\mathbb{N}_0} |s_k(Y) - s_k(f)| \geq \delta\right) \leq 2\exp\left(-\frac{\delta^2 n}{2\nu + 2\kappa\delta}\right) .$$

Moreover, for given probability $\alpha \in (0, 1)$*, one can construct non-asymptotic confidence bands:*

$$\mathbb{P}\left(s_k(f) \in \left[(s_k(Y) - \tau_n(\alpha))_+ \,, s_k(Y) + \tau_n(\alpha)\right] \text{ for all } k \in \mathbb{N}_0\right) \geq 1 - \alpha \,,$$

where $(x)_+ = \max(0, x)$ *and* $\tau_n(\alpha)$ *can be explicitly computed. Asymptotically:* $\tau_n(\alpha) \approx 1/\sqrt{n}$*.*

Empirical Kolmogorov signatures

Remarks:

- These are "honest" (non-asymptotic) confidence bands.
- No a priori assumption on f required.

Thresholding K-signatures – overest. modes

Theorem (Bauer, Munk, Sieling, W.)

Let f have at most k modes, and let $\alpha \in (0, 1)$. Then

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Fact: $\tau_n(\alpha)$ is independent of the number and magnitude of the modes of f. In this sense the result is universal.

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- Without a priori information on the "smallest scales" of f, no method can provide a control for their underestimation [Donoho].
- *Only* possible to provide a bound for underestimating those signatures of f that are larger than a certain threshold.

Thresholding K-signatures – underest. modes

Theorem (Bauer, Munk, Sieling, W.)

Let $\alpha \in (0,1)$. *Then*

$$\mathbb{P}\left(k_{\tau_n(\alpha)}(Y) < k_{2\tau_n(\alpha)}(f)\right) \leq \alpha \ .$$

Let f *have at most* k *modes. Then one has two-sided bound:*

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Fixing α, one has $\tau_n(\alpha) \approx 1/\sqrt{n} \Rightarrow \exists C$ such that asymptotically by thresholding at $C/\sqrt{n}$, it can be guaranteed that all signatures of f above a certain threshold get detected with $\mathbb{P} \geq 1 - \alpha$.

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Number of modes of f can be estimated correctly from empirical signatures with $\mathbb{P} \to 1$ *under the assumption* of a lower bound on magnitude (in the Kolmogorov norm) of the smallest mode of f. This is independent of the number of modes of f.

Computing Kolmogorov signatures – Taut strings

Definition (Taut strings)

Let $f \in L^\infty[a, b]$ with antiderivative F. The taut string U_α is the minimizer of

$$\int_a^b \sqrt{1 + U'_\alpha(t)^2}\, \mathrm{d}t$$

subject to $U_\alpha(a) = F(a), \;\; U_\alpha(b) = F(b), \;\; \|U - F\|_\infty \leq \alpha.$

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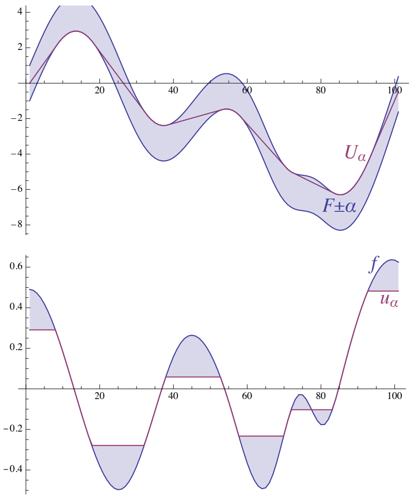
The function $u_\alpha = U_\alpha'$ minimizes the number of modes among all functions u with $d_{\mathrm{Kol}}(f, u) \leq \alpha$.

Taut strings continued



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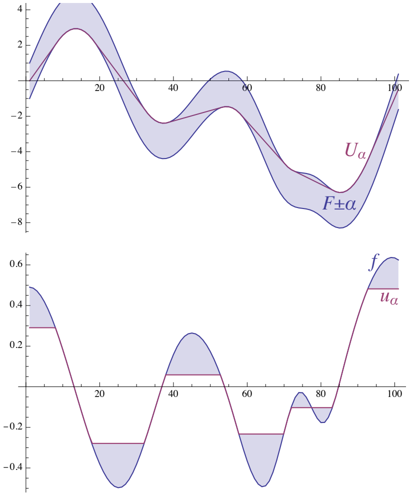

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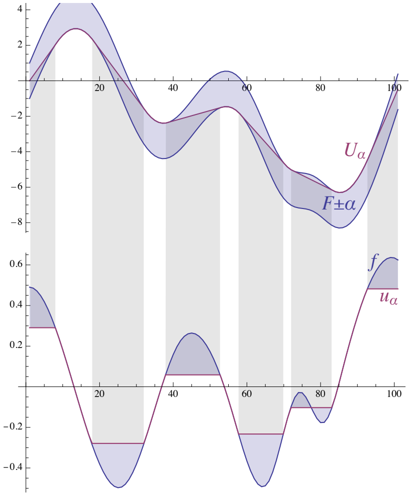

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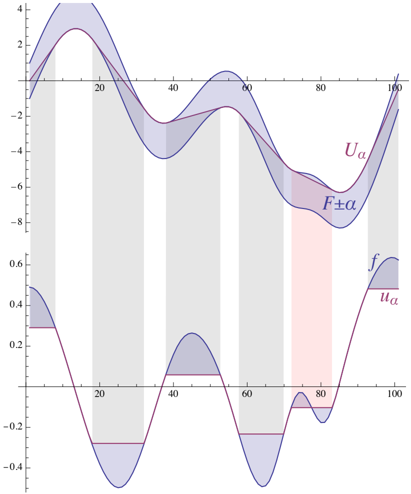

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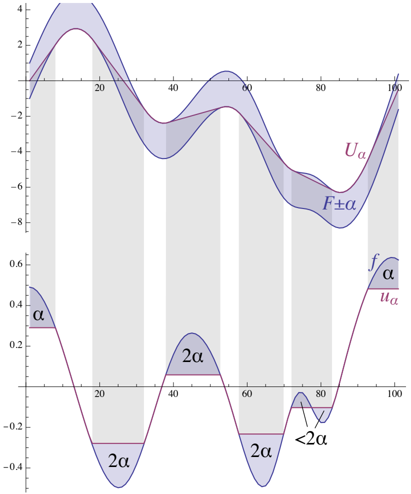

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- Kolmogorov signatures can be computed in $O(n \log(n))$.

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- But: Statistical questions persist for higher dim.
- Reference: Bauer, Munk, Sieling, W.: *Persistence Barcodes versus Kolmogorov Signatures: Detecting Modes of One-Dimensional Signals*. Found Comput Math, 2017.

Thank you for your attention!