Subdivide and Tile:
Triangulating spaces for understanding the world
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Geometric Inference

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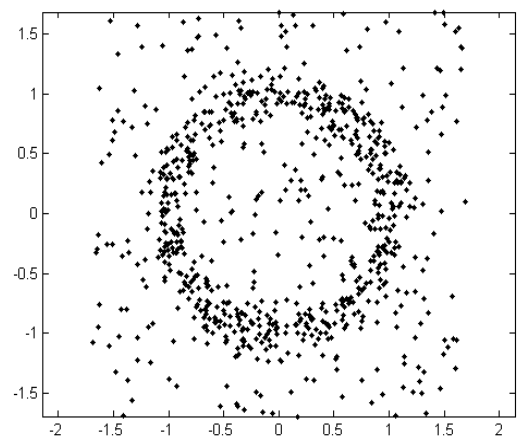
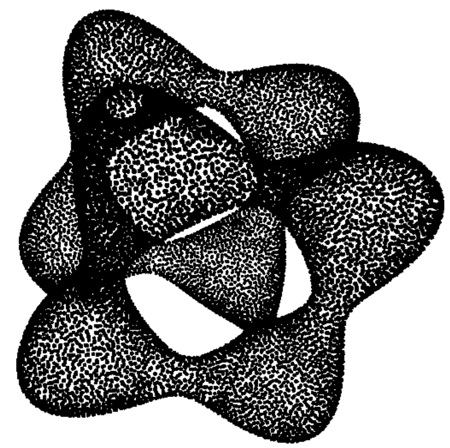
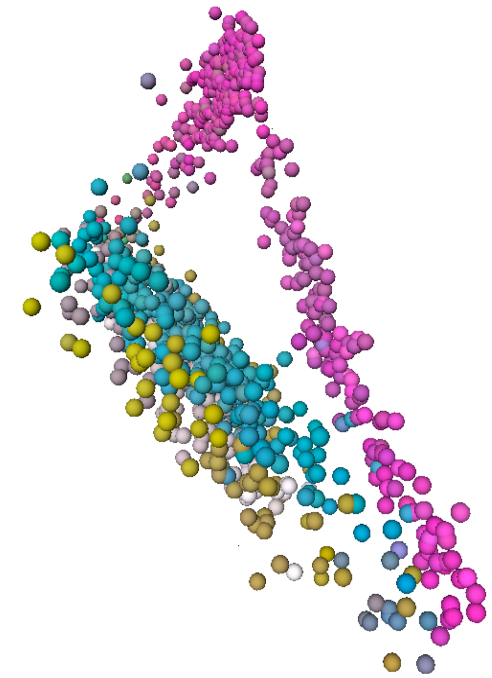
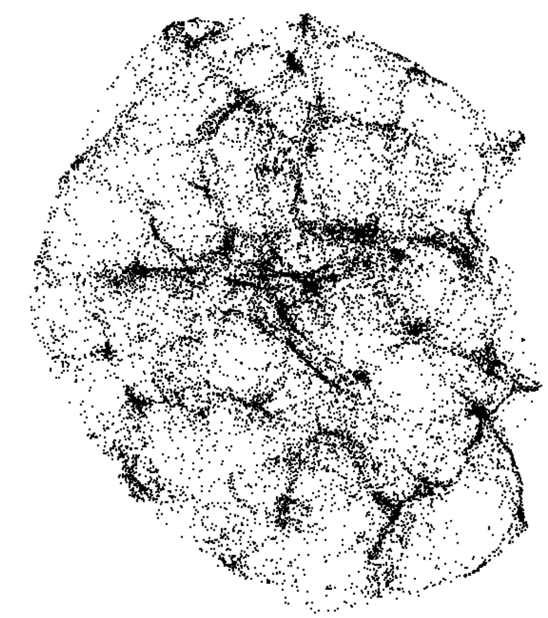
GEOMETRICA

Introduction and motivations



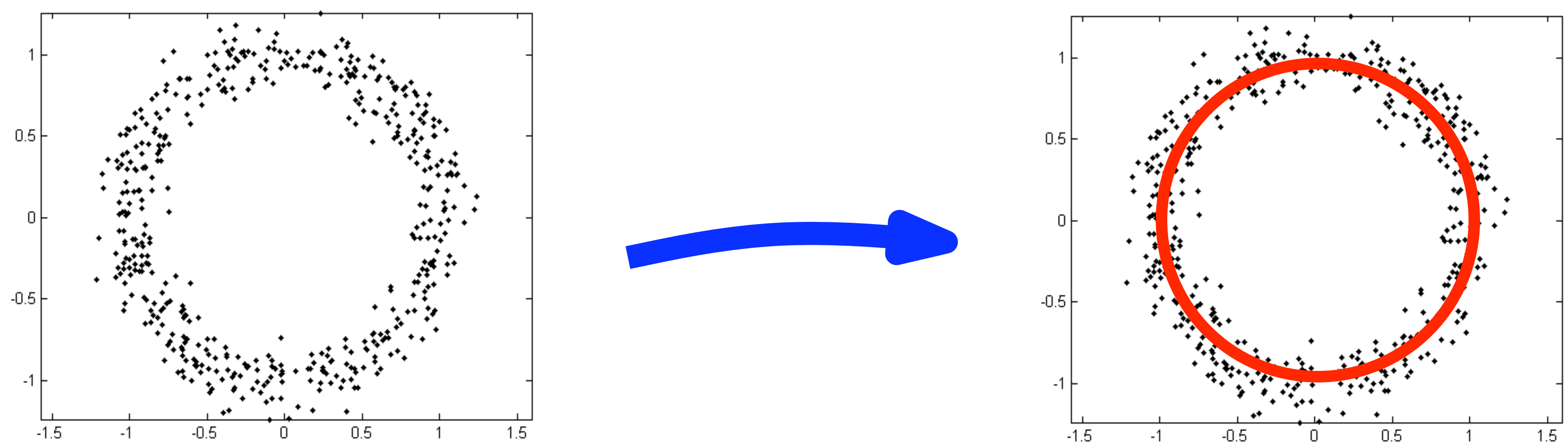




What can we say about the topology/geometry of spaces known only through a finite set of measurements?

What is the relevant topology/geometry of a point cloud data set?

Motivations: Reconstruction, Manifold Learning and NLDR, Clustering and Segmentation,...

Geometric Inference



Question: Given an approximation C of a geometric object K, is it possible to reliably estimate the topological and geometric properties of K, knowing only the approximation C?

Question *: Given a point cloud C (or some other more complicated set), is it possible to infer some robust topological or geometric information of C?

- The answer depends on:
  - the considered class of objects (no hope to get a positive answer in full generality),
  - a notion of distance between the objects (approximation).

Outline

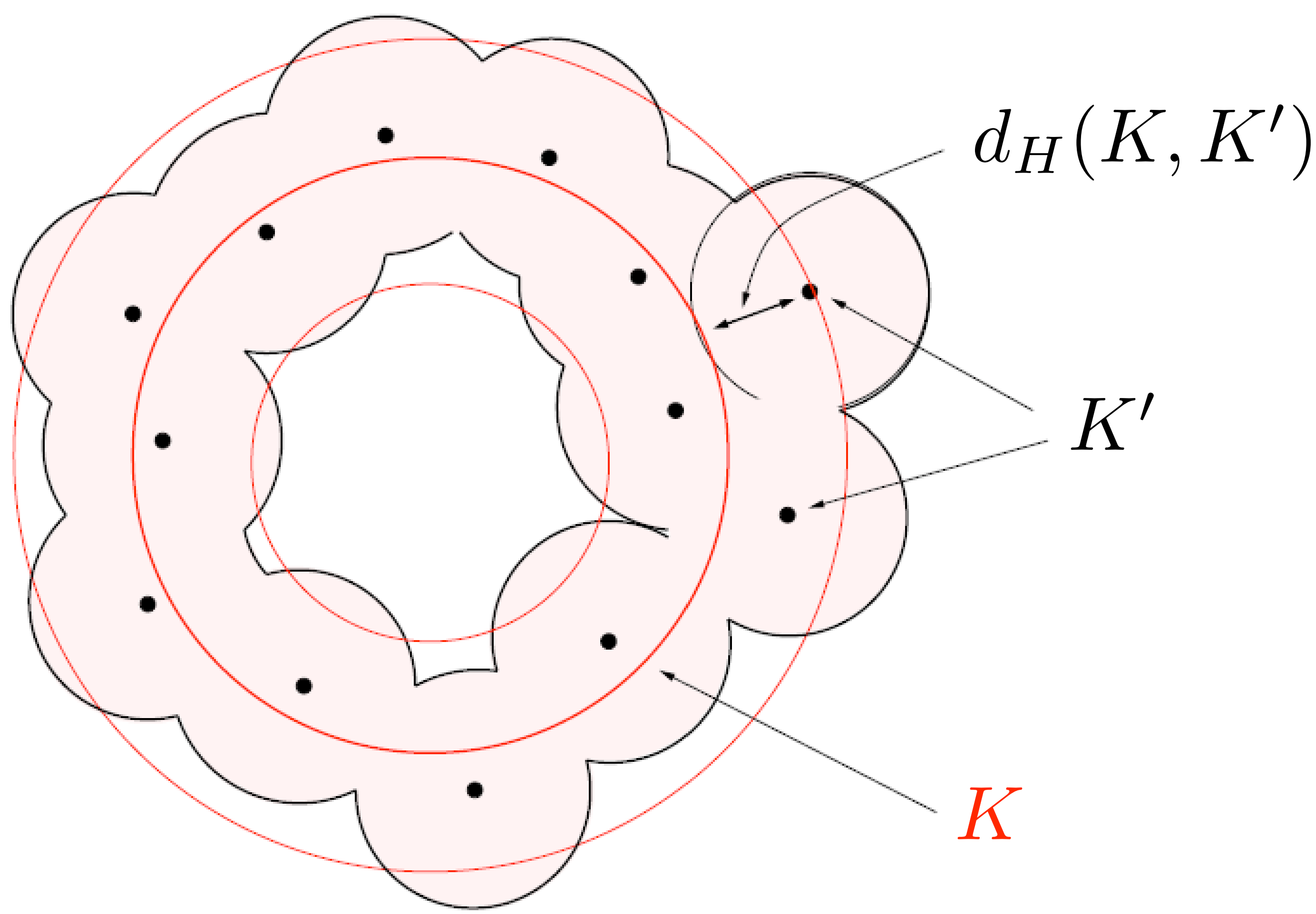
1. Distance functions for geometric inference
   - class of objects: (some) compact subsets of $\mathbb{R}^d$
   - approximation with respect to Hausdorff distance
2. (Practical) algorithms for topological inference
   - persistence-based algorithm
   - multiscale inference
3. Dealing with outliers: the measure point of view
   - class of objects: probability measures
   - approximation with respect to Wasserstein distance

Distance functions for geometric inference

Considered objects: compact subsets K of $\mathbb{R}^d$

Distance:
distance function to a compact $K \subset \mathbb{R}^d$: $d_K : x \to \inf_{p \in K} \|x - p\|$
Hausdorf distance between two compact sets:

$$d_H(K, K') = \sup_{x \in \mathbb{R}^d} |d_K(x) - d_{K'}(x)|$$



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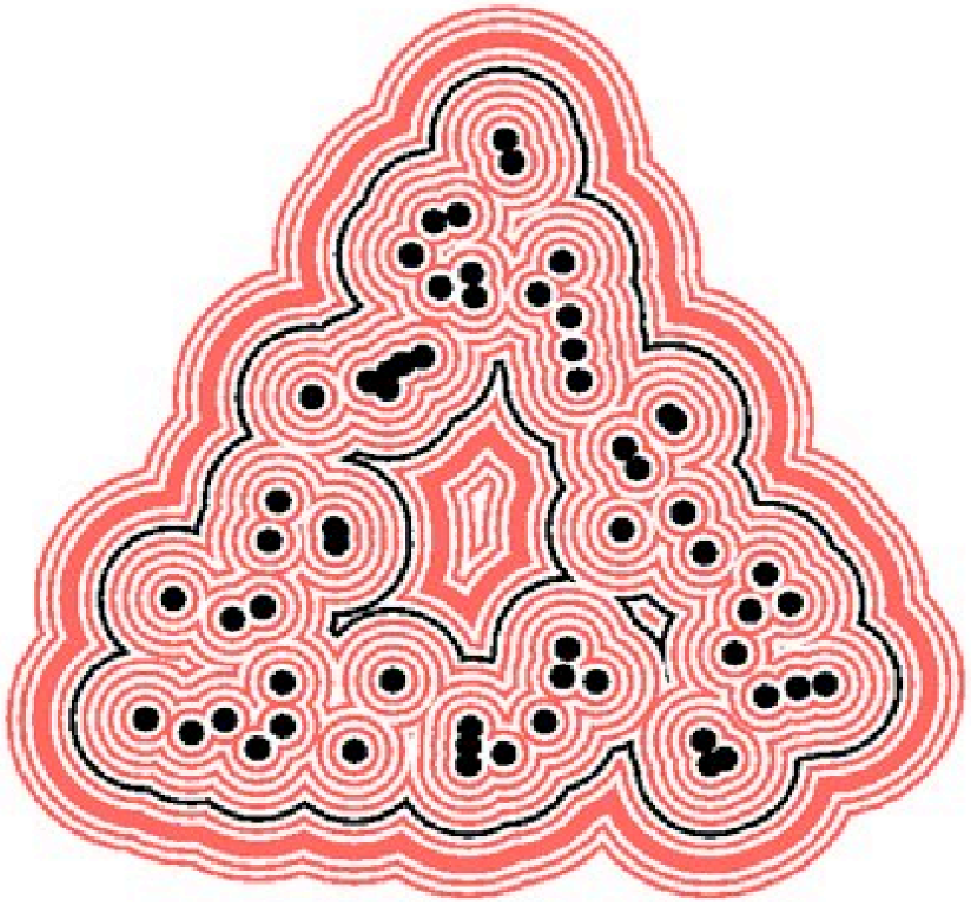
- Replace K and C by d_K and d_C
- Compare the topology of the offsets $K^r = d_K^{-1}([0, r])$ and $C^r = d_C^{-1}([0, r])$



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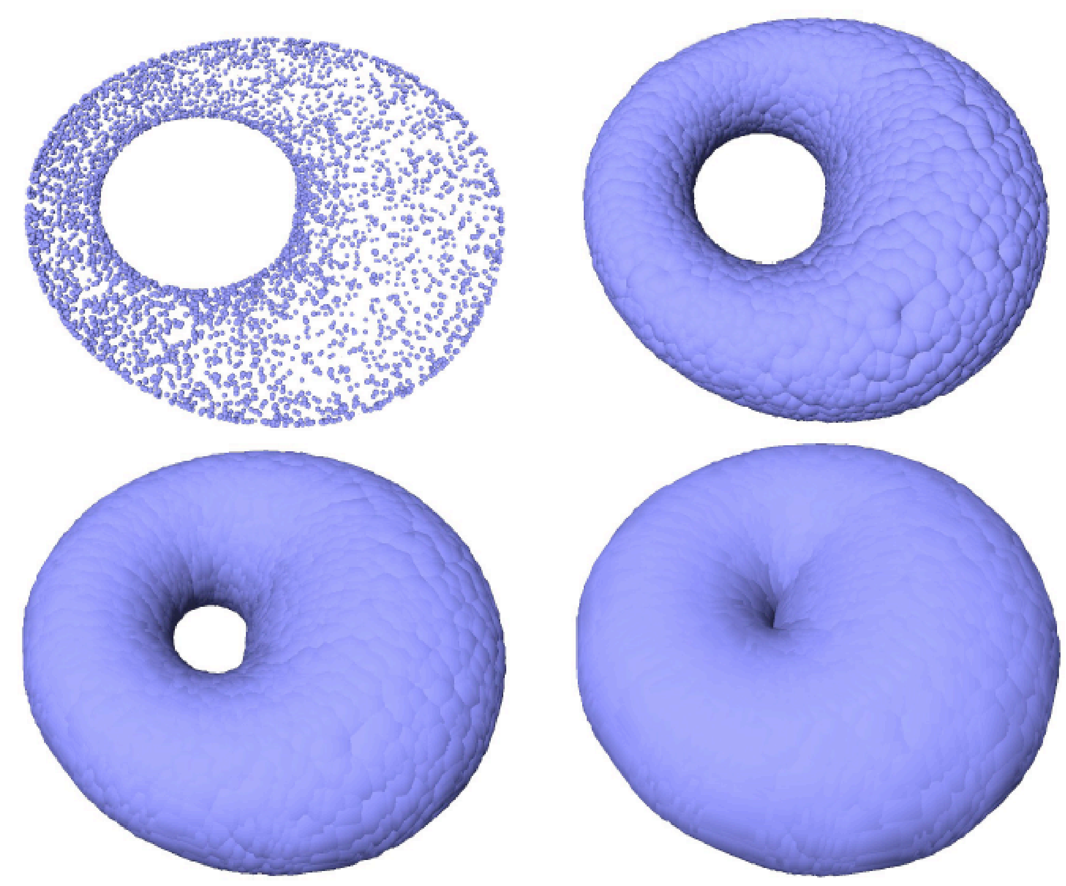

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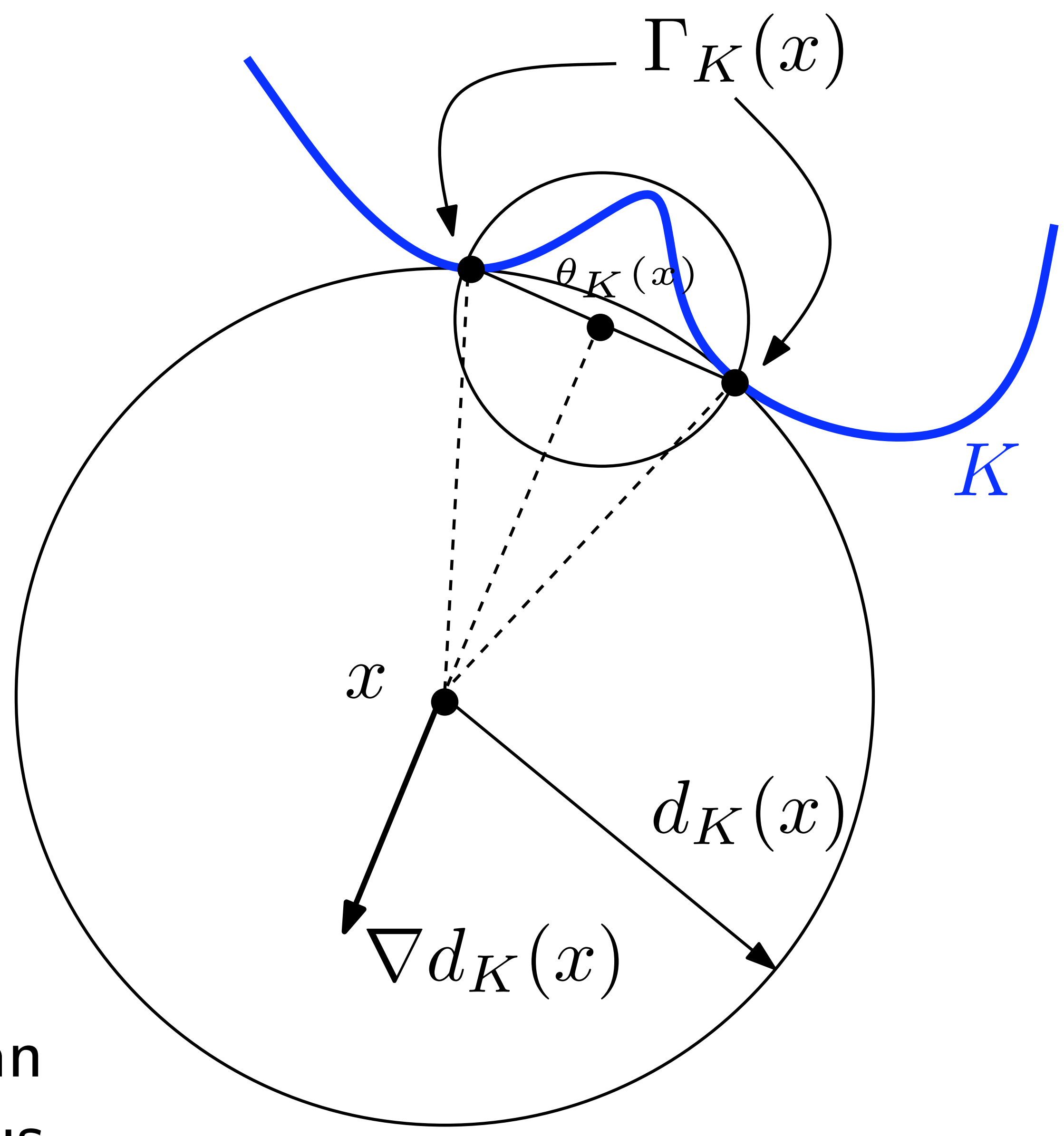
The gradient of the distance function

- $\Gamma_K(x) = \{y \in K : d(x,y) = d_K(x)\}$
- $\theta_K(x)$: center and radius of the smallest ball enclosing $\Gamma_K(x)$

$$\nabla d_K(x) = \frac{x - \theta_K(x)}{d_K(x)}$$

Although not continuous, it can be integrated in a continuous flow.



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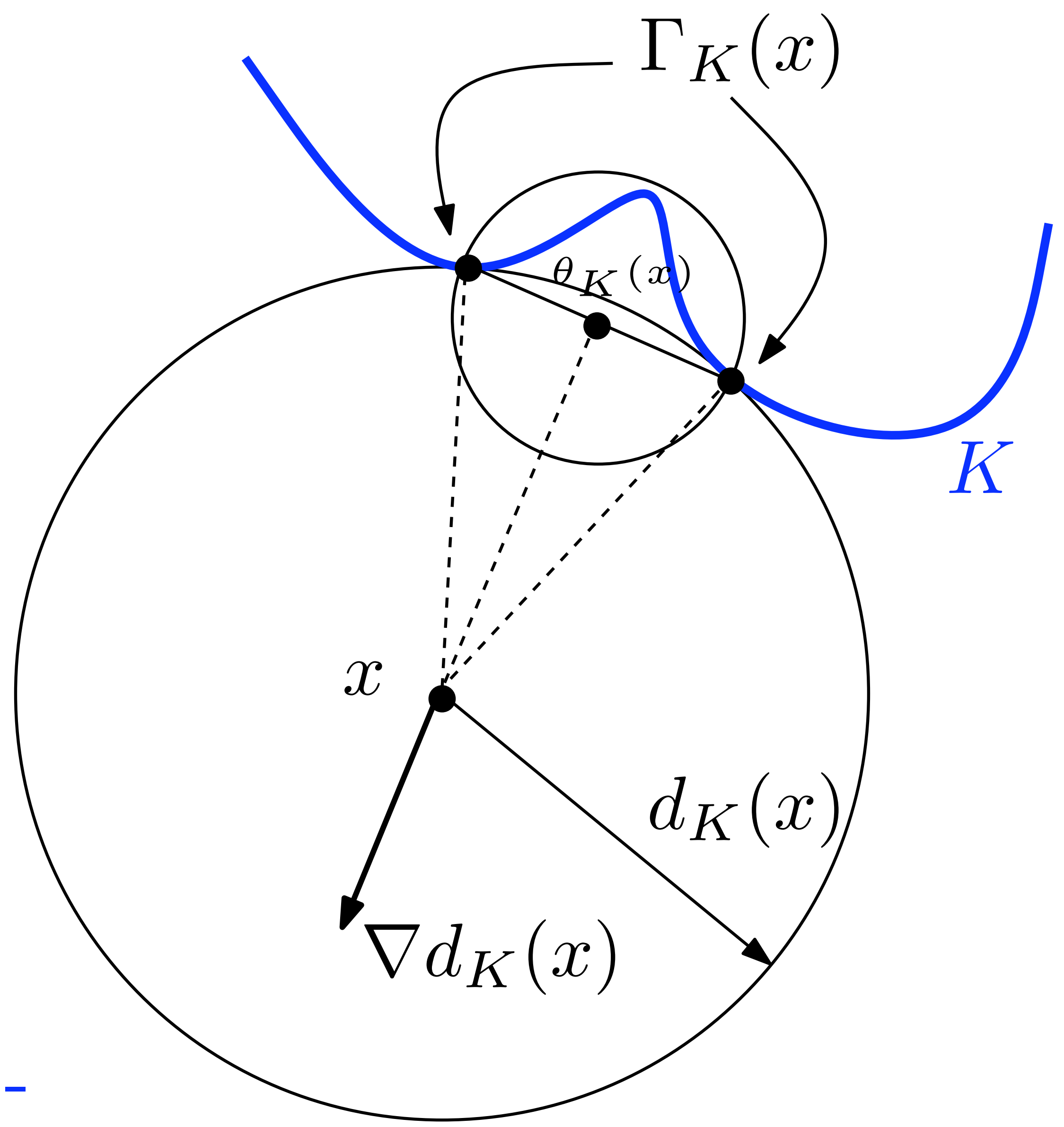
Can be generalized to distances to compact subsets of complete Riemannian manifolds



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Critical points and offsets topology

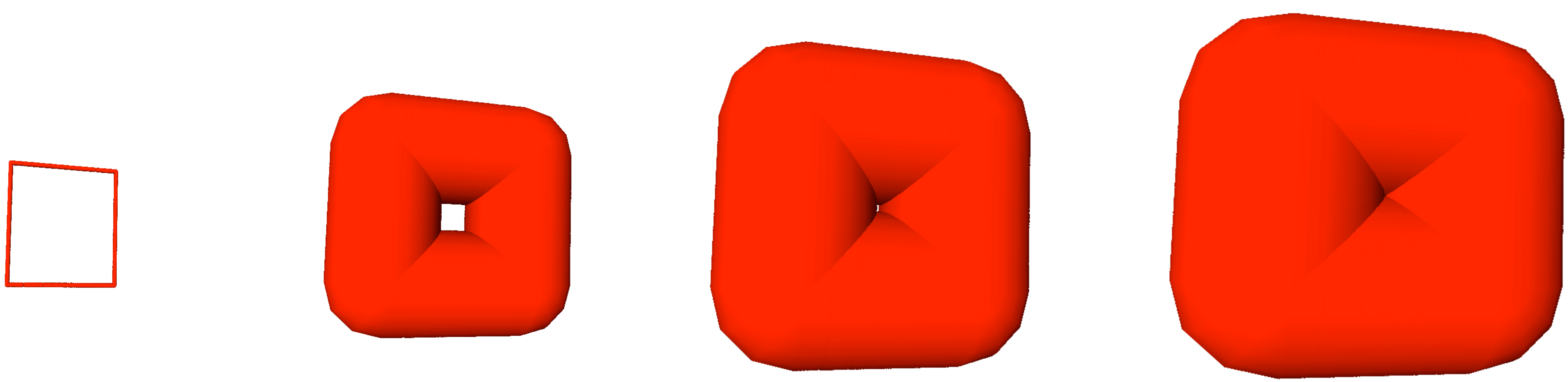
For $\alpha \geq 0$, the *α-offset of K* is $K^\alpha = \{x \in \mathbb{R}^d : d_K(x) \leq \alpha\}$

Theorem: [Grove, Cheeger,...] Let $K \subset \mathbb{R}^d$ be a compact set.

- Let r be a regular value of d_K. Then $d_K^{-1}(r)$ is a topological submanifold of $\mathbb{R}^d$ of codimension 1.
- Let $0 < r_1 < r_2$ be such that $[r_1, r_2]$ does not contain any critical value of d_K. Then all the level sets $d_K^{-1}(r)$, $r \in [r_1, r_2]$ are isotopic and

$$K^{r_2} \setminus K^{r_1} = \{x \in \mathbb{R}^d : r_1 < d_K(x) \leq r_2\}$$

is homeomorphic to $d_K^{-1}(r_1) \times (r_1, r_2]$.



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These results still hold for compact sets in (complete) Riemannian manifolds.

Weak feature size and stability

The *weak feature size* of a compact $K \subset \mathbb{R}^d$:

$$\text{wfs}(K) = \inf\{c > 0 : c \text{ is a critical value of } d_K\}$$

Proposition: [C-Lieutier'05] Let $K, K' \subset \mathbb{R}^d$ be such that

$$d_H(K, K') < \varepsilon := \frac{1}{2}\min(\text{wfs}(K), \text{wfs}(K'))$$

Then for all $0 < r \leq 2\varepsilon$, K^r and K'^r are homotopy equivalent.

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- Two continuous maps $f, f' : X \to Y$ are homotopic if there exist a continuous map $H : X \times [0,1] \to Y$ s.t. $H(.,0) = f$ and $H(.,1) = f'$.
- Two topological spaces X and Y are homotopy equivalent if there exist two continuous maps $f : X \to Y$ and $g : Y \to X$ s. t. $f \circ g$ and $g \circ f$ are homotopic to id_Y and id_X.

Weaker than homeomorphy but "share the same topological invariants" (e.g. Betti numbers)

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Proof: Use the gradient vector field (and its flow) to build an explicit homotopy equivalence.

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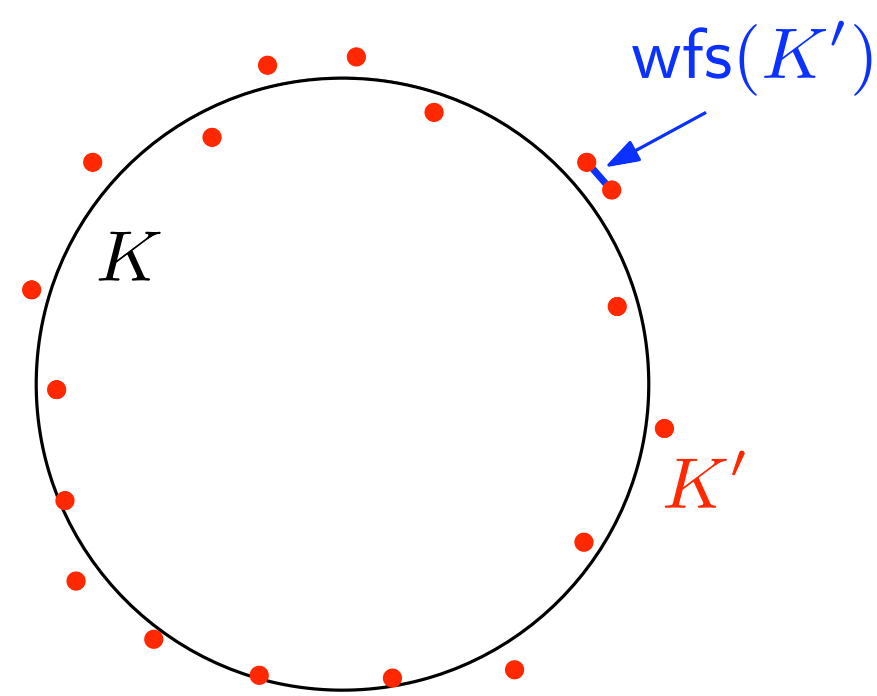
Compact set with positive wfs:

- Stability properties
- Large class of compact sets (including sub-analytic sets)
- $K \to \text{wfs}(K)$ is not continuous (unstability of critical points).



Overcoming the discontinuity of wfs

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Option 1:
Try to get topological information about K without any assumption on $\mathsf{wfs}(K')$.

Option 2:
Restrict to a smaller class of compact sets with some stability properties of the critical points.

Overcoming the discontinuity of wfs

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Try to get topological information about K without any assumption on $\mathsf{wfs}(K')$.

→ Persistence-based inference

Option 2:
Restrict to a smaller class of compact sets with some stability properties of the critical points.

→ Notion of μ-critical points. Strong reconstruction results.

Option 1

Theorem: [C-Lieutier'05-Cohen-Steiner et al '05]
Let $K, K' \subset \mathbb{R}^d$ be compact and let $\varepsilon > 0$ be s.t. $d_H(K, K') < \varepsilon$ and wfs$(K) > 4\varepsilon$. For $\alpha > 0$ s.t. $\alpha + 4\varepsilon <$ wfs(K), let $i : K'^{\alpha+\varepsilon} \hookrightarrow K'^{\alpha+3\varepsilon}$ be the canonical inclusion.For any $0 < r < \mathrm{wfs}(K)$,

$$H_k(K^r) \cong im\left(i_* : H_k(K'^{\alpha+\varepsilon}) \to H_k(K'^{\alpha+3\varepsilon})\right)$$

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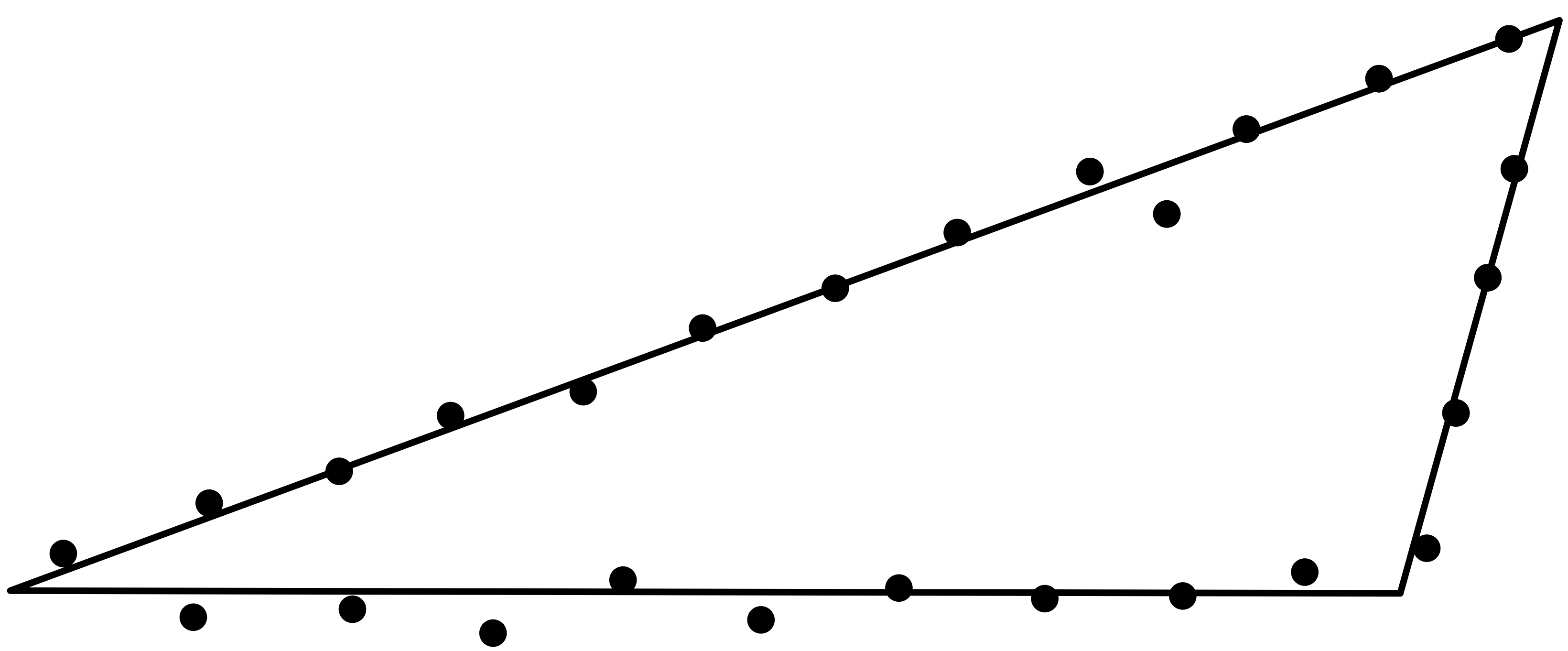

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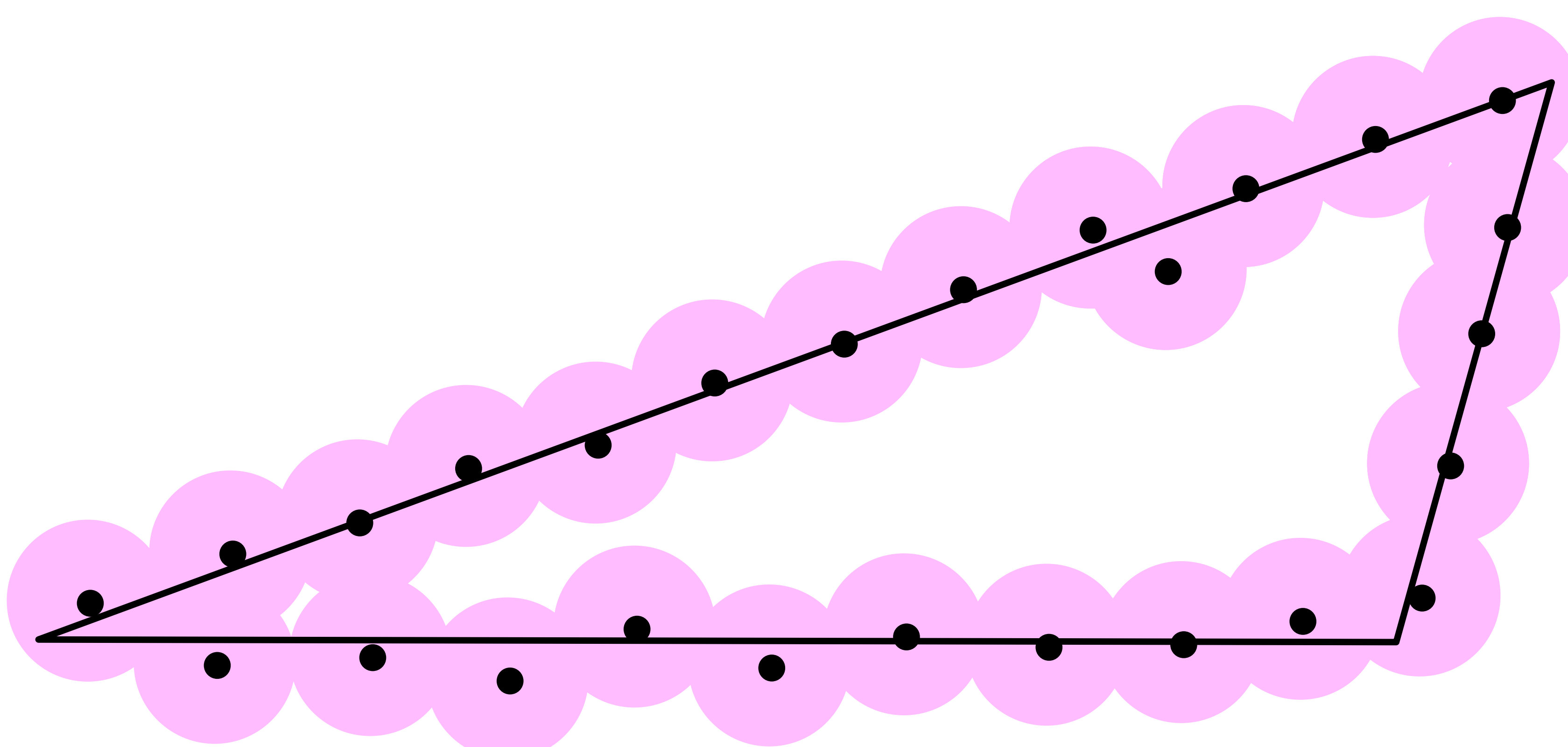

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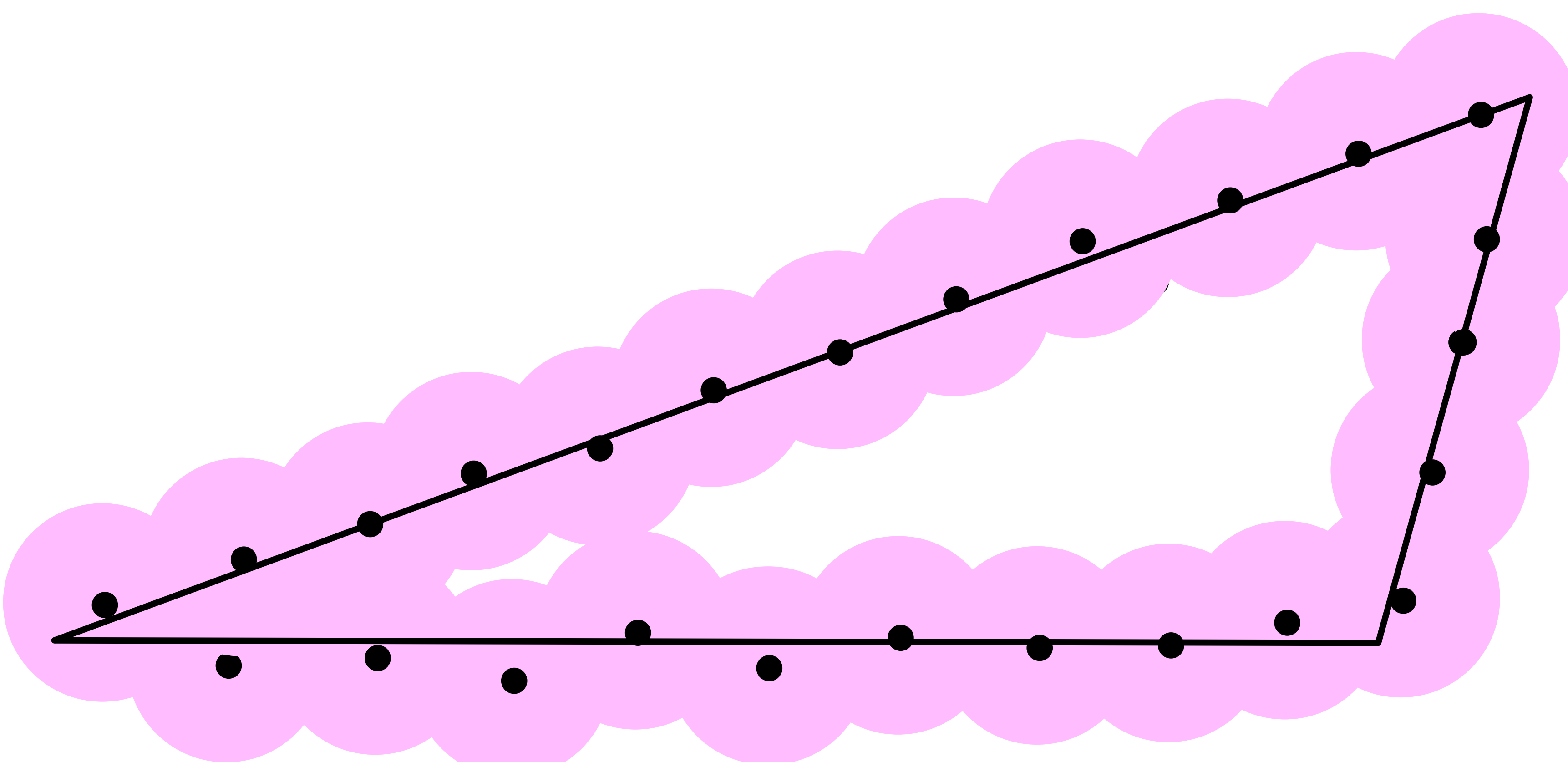

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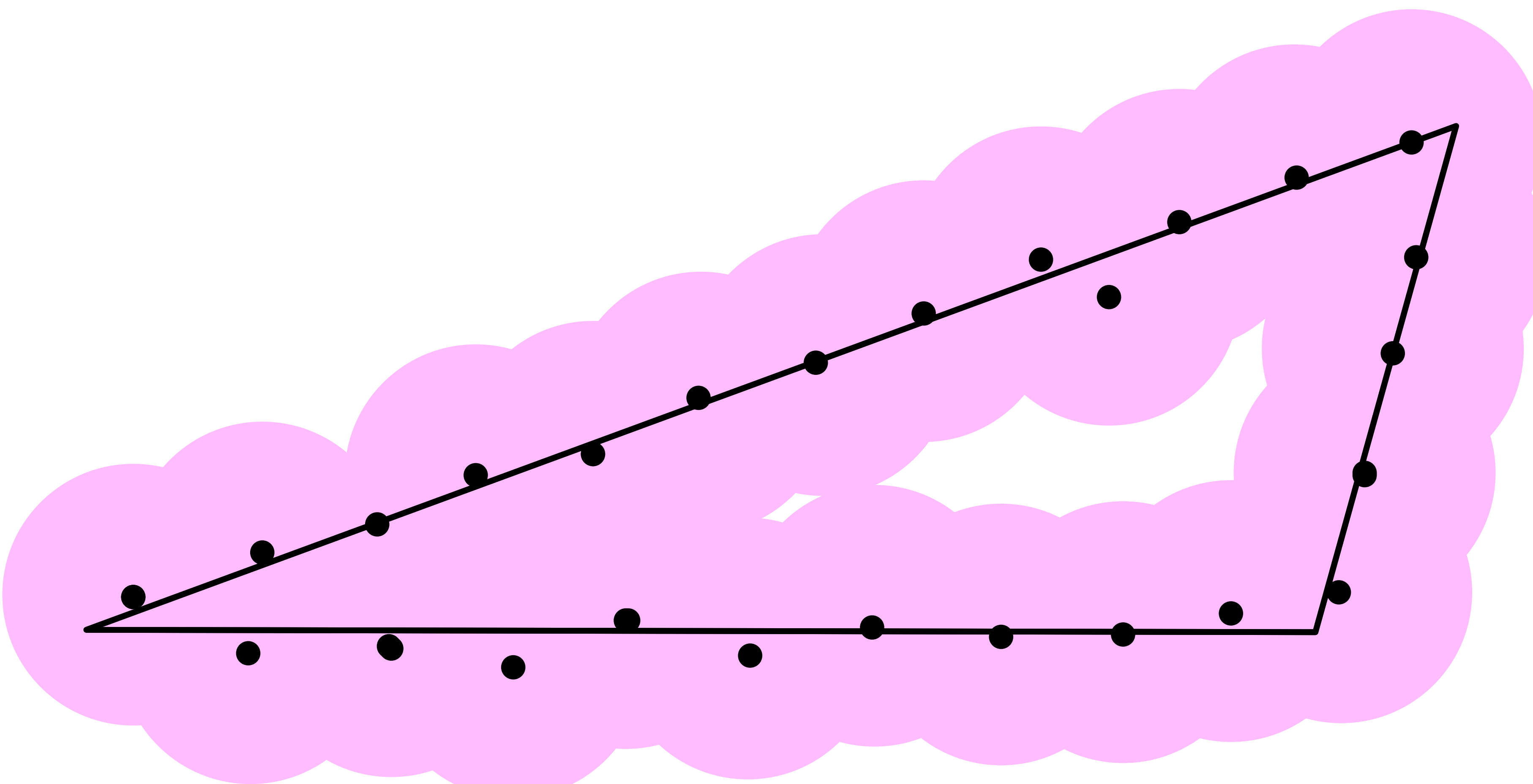
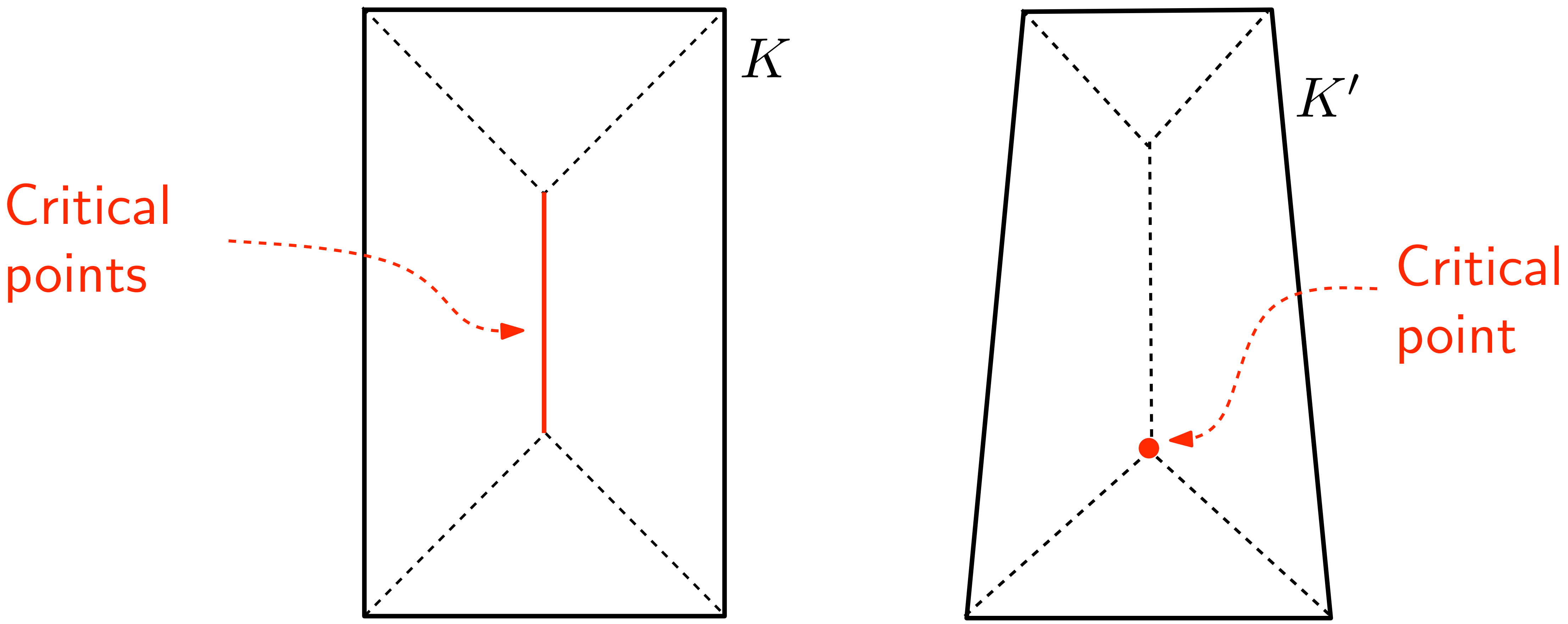


Option 2: μ-critical points and μ-reach



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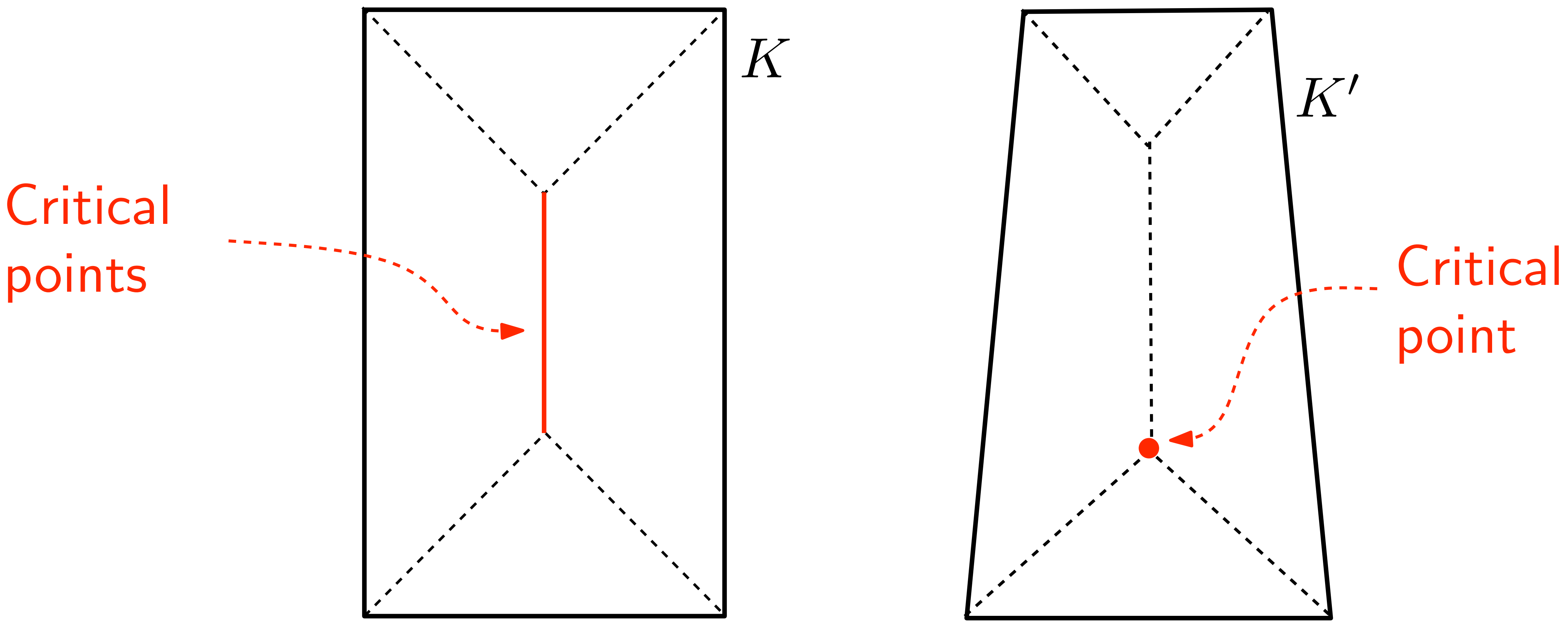
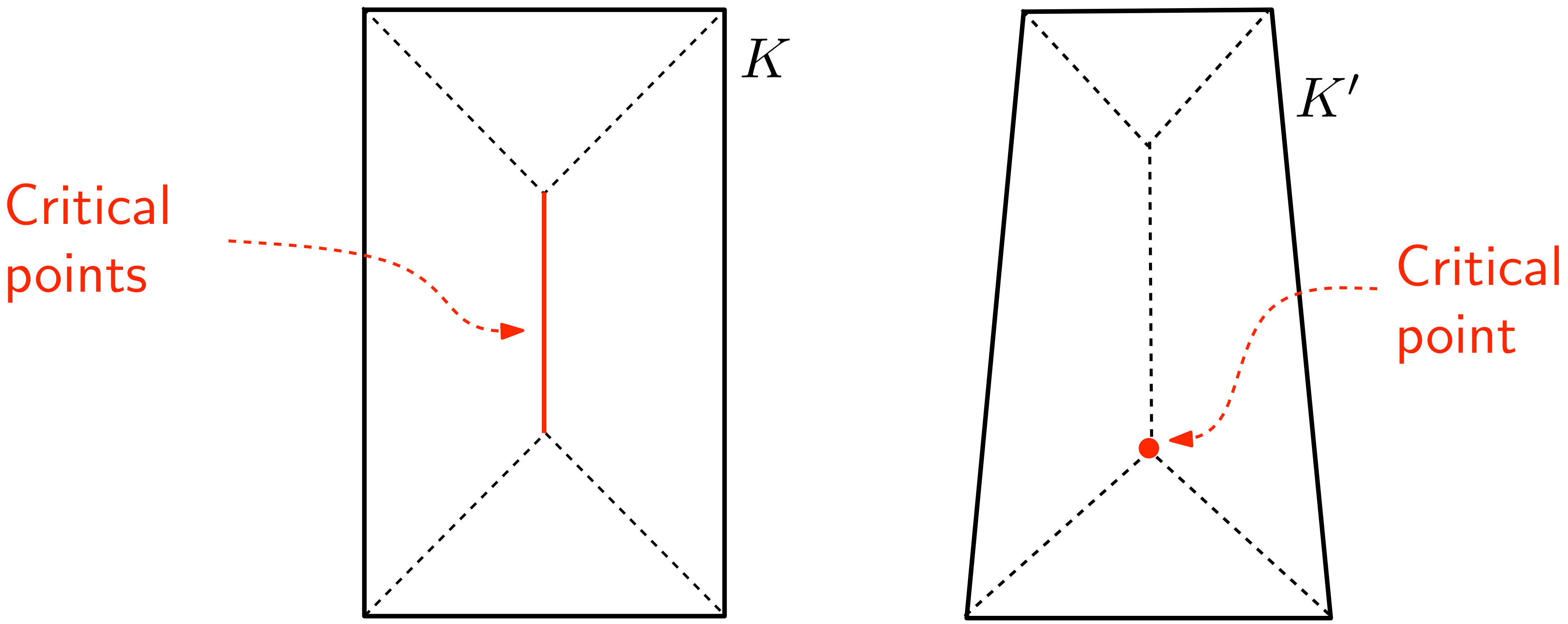
A point $x \in \mathbb{R}^d$ is *μ-critical* for K if $\|\nabla d_K(x)\| \leq \mu$



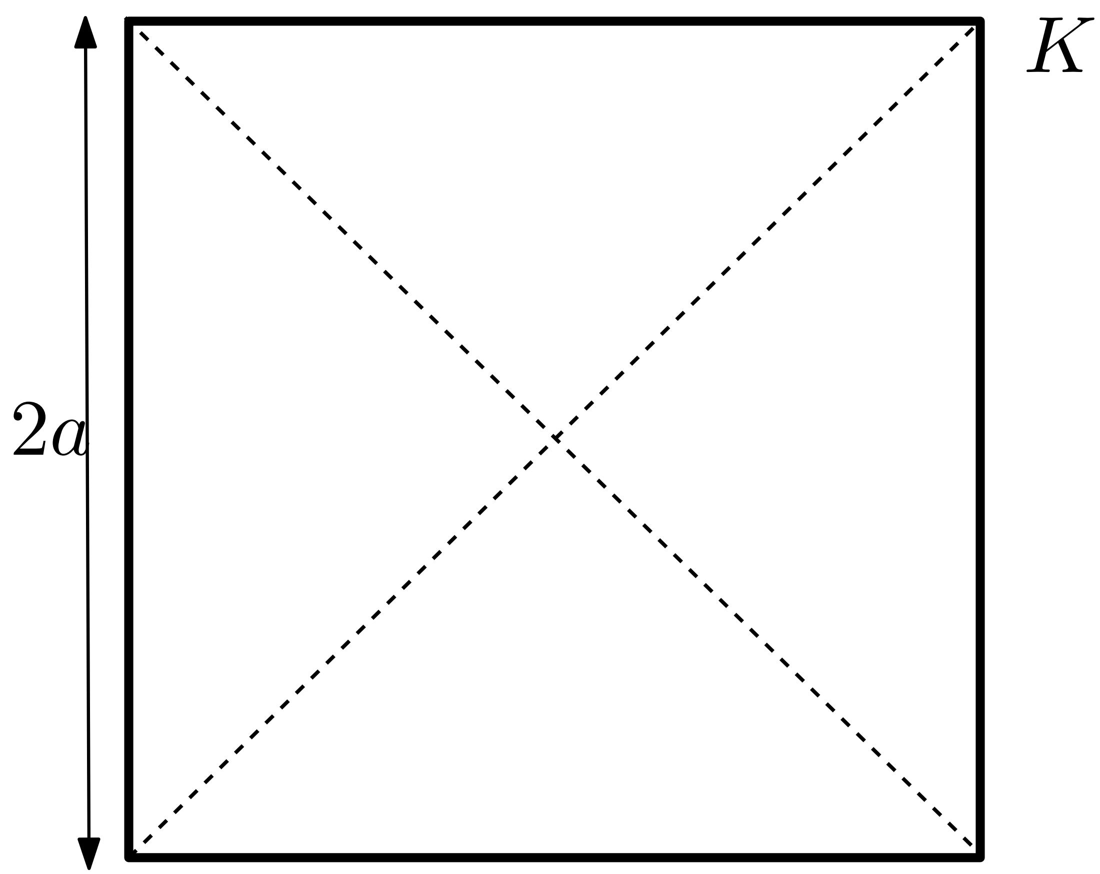
Option 2: μ-critical points and μ-reach

A point $x \in \mathbb{R}^d$ is μ-*critical* for K if $\|\nabla d_K(x)\| \leq \mu$



Theorem: [C-Cohen-Steiner-Lieutier'06] Let $K, K' \subset \mathbb{R}^d$ be two compact sets s. t. $d_H(K, K') \leq \varepsilon$. For any μ-critical point x for K, there exists a $(2\sqrt{\varepsilon / d_K(x)} + \mu)$-critical point for K' at distance at most $2\sqrt{\varepsilon d_K(x)}$ from x.

Option 2: μ-critical points and μ-reach



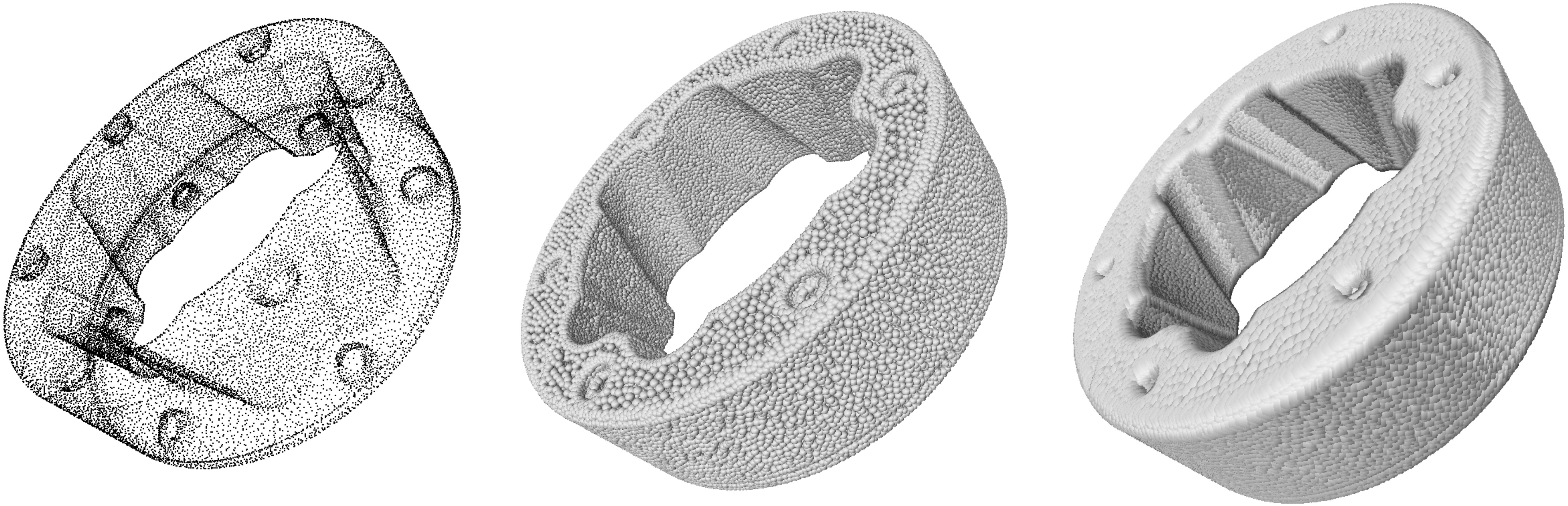
- $r_\mu(K) = 0$ if $\mu \geq \sqrt{2}/2$
- $r_\mu(K) = a$ if $\mu < \sqrt{2}/2$
- $\mathrm{wfs}(K) = a$

μ-*reach* of a compact $K \subset \mathbb{R}^d$:

$$r_\mu(K) = \inf\{d_K(x) : \|\nabla d_K(x)\| < \mu\}$$

- $\forall \mu \in (0, 1)$, $r_\mu(K) \leq$ wfs(K)
- for $\mu = 1$, $r_\mu(K)$ is the reach introduced by Federer in Geometric Measure Theory

Option 2: μ-critical points and μ-reach



A reconstruction theorem: [C-Cohen-Steiner-Lieutier'06]
Let $K \subset \mathbb{R}^d$ be a compact set s.t. $r_\mu = r_\mu(K) > 0$ for some $\mu > 0$. Let $K \subset \mathbb{R}^d$ be such that $d_H(K, K') < \kappa r_\mu(K)$ with $\kappa < \min(\frac{\sqrt{5}}{2} - 1, \frac{\mu^2}{16+2\mu^2})$
Then for any d, d' s.t.

$$0 < d < \text{wfs}(K) \;\; \text{and} \;\; \frac{4\kappa r_\mu}{\mu^2} \leq d' < r_\mu - 3\kappa r_\mu$$

the hypersurfaces $d_{K'}^{-1}(d')$ and $d_K^{-1}(d)$ are isotopic.

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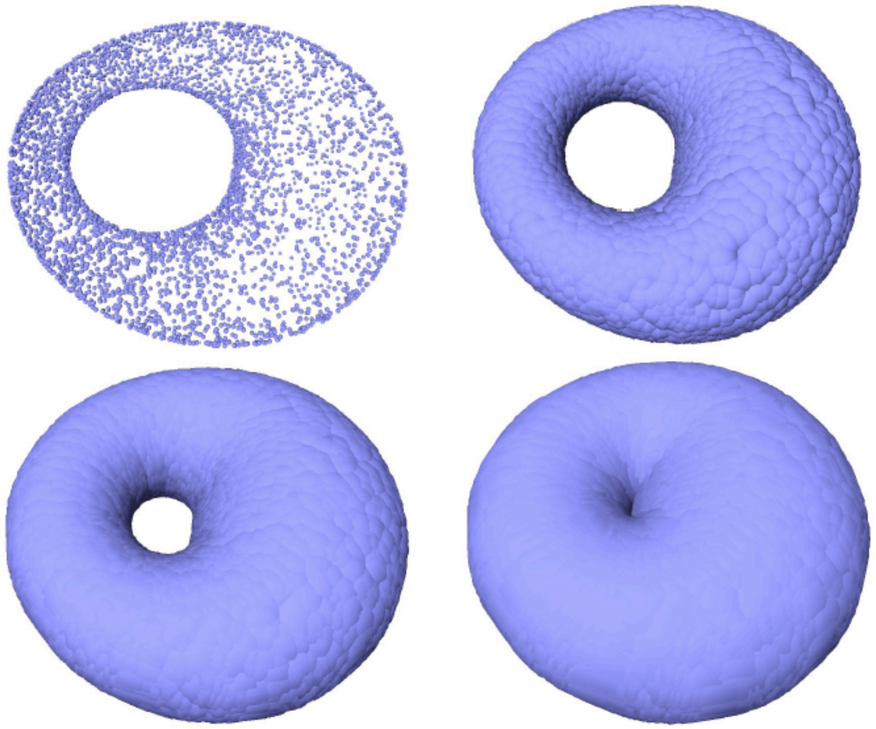

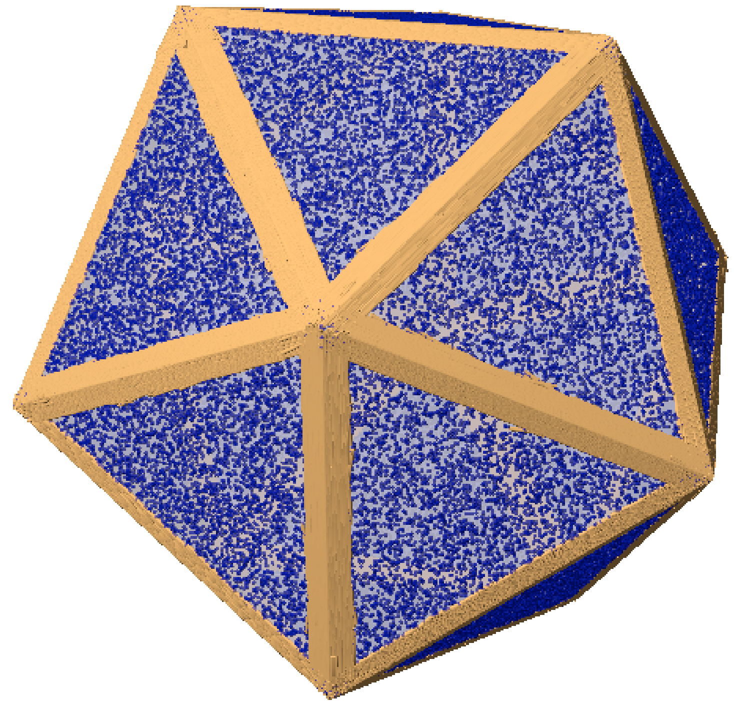

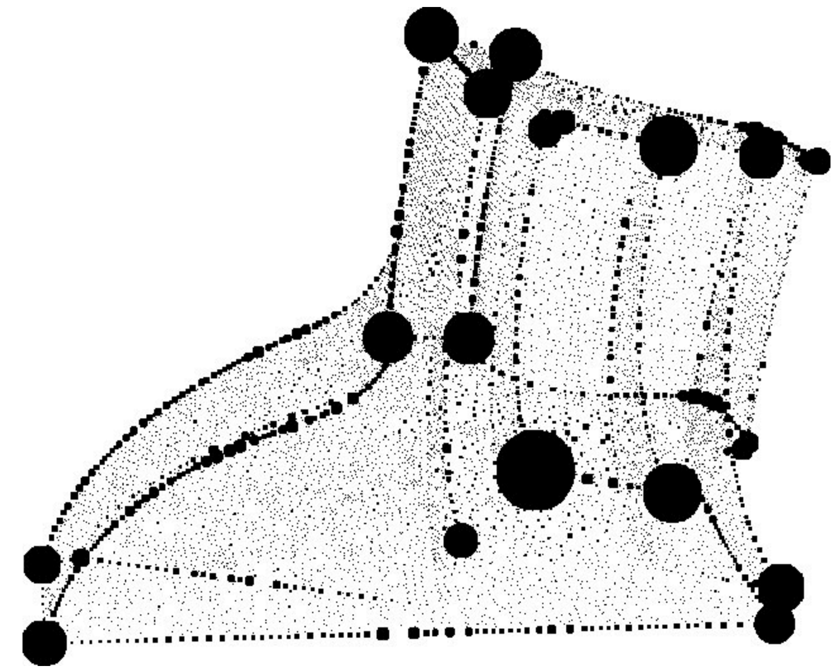

Topological/geometric properties of the offsets of K are stable with respect to Hausdorff approximation:

1. Topological stability of the offsets of K (CCSL'06, NSW'06).

2. Approximate normal cones (CCSL'08).

3. Boundary measures (CCSM'07), curvature measures (CCSLT'09), Voronoi covariance measures (GMO'09).

Distance-based inference: the algorithmic side

Topological/geometric inference in practice (from point cloud data sets) ?

Option 2: strong reconstruction results but.....

- Rely on the construction of Voronoï diagram and α-shapes.
- Critical issues in dimension > 3 and non-euclidean spaces.

Option 1:

- Rely on topological persistence theory (at least to infer the homology)
- Efficient algorithms in dimension > 3 and in Riemannian manifolds (or more general metric spaces).

An algorithm for geometric inference

- $X \subset \mathbb{R}^d$ be a compact set such that wfs$(X) > 0$.
- $L \subset \mathbb{R}^d$ be a finite set such that $d_H(X, L) < \varepsilon$ for some $\varepsilon > 0$.

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Can be replaced in the following by (complete) Riemannian manifold or a (totally bounded) metric space but require some extra assumptions $\longrightarrow$ see next slides.

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Theorem:
Assume that wfs$(X) > 4\varepsilon$. For $\alpha > 0$ s.t. $\alpha + 4\varepsilon <$ wfs(X), let $i : L^{\alpha+\varepsilon} \hookrightarrow L^{\alpha+3\varepsilon}$ be the canonical inclusion.For any $0 < r < \mathrm{wfs}(X)$,

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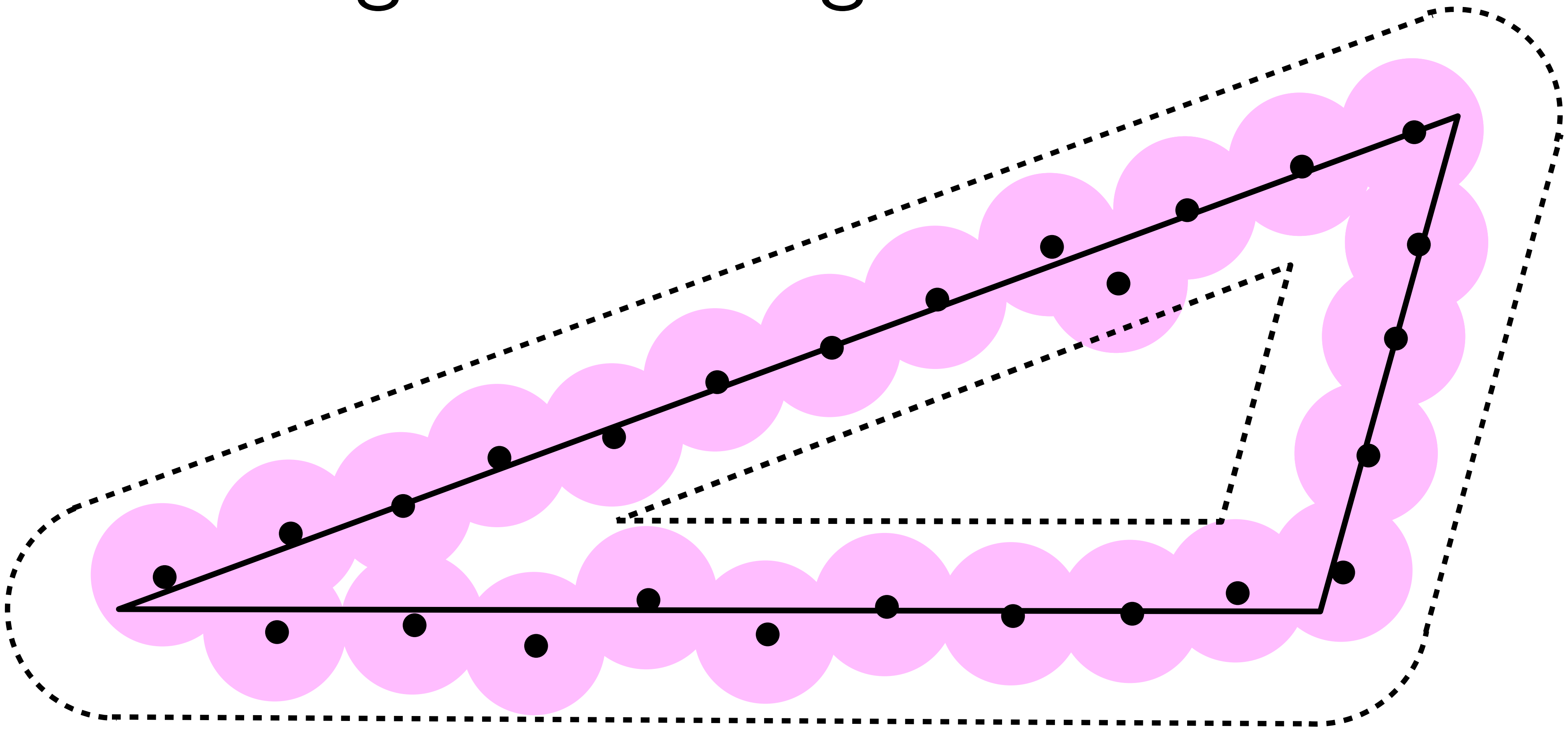
Theorem:
Assume that wfs$(X) > 4\varepsilon$. For $\alpha > 0$ s.t. $\alpha + 4\varepsilon <$ wfs(X), let $i : L^{\alpha+\varepsilon} \hookrightarrow L^{\alpha+3\varepsilon}$ be the canonical inclusion.For any $0 < r < \mathrm{wfs}(X)$,

$$H_k(X^r) \cong im\left(i_* : H_k(L^{\alpha+\varepsilon}) \to H_k(L^{\alpha+3\varepsilon})\right)$$

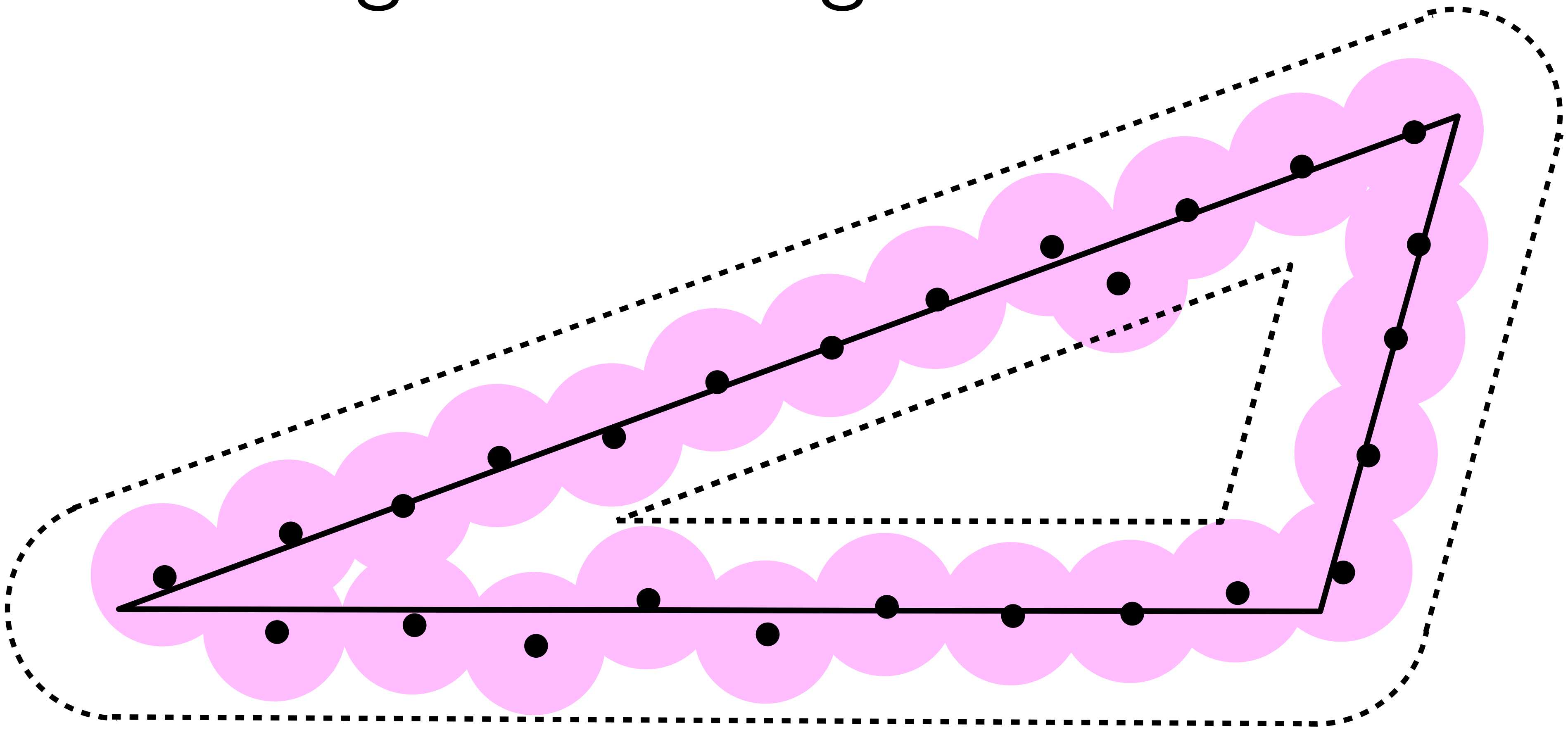
$$\pi_1(X^r, x) \cong im\left(i_* : \pi_1(L^{\alpha+\varepsilon}, x) \to \pi_1(L^{\alpha+3\varepsilon}, x)\right)$$

An algorithm for geometric inference



For any $\alpha > 0$, $\quad X^{\alpha} \subseteq L^{\alpha+\varepsilon} \subseteq X^{\alpha+2\varepsilon} \subseteq L^{\alpha+3\varepsilon} \subseteq X^{\alpha+4\varepsilon} \subseteq \cdots$

An algorithm for geometric inference



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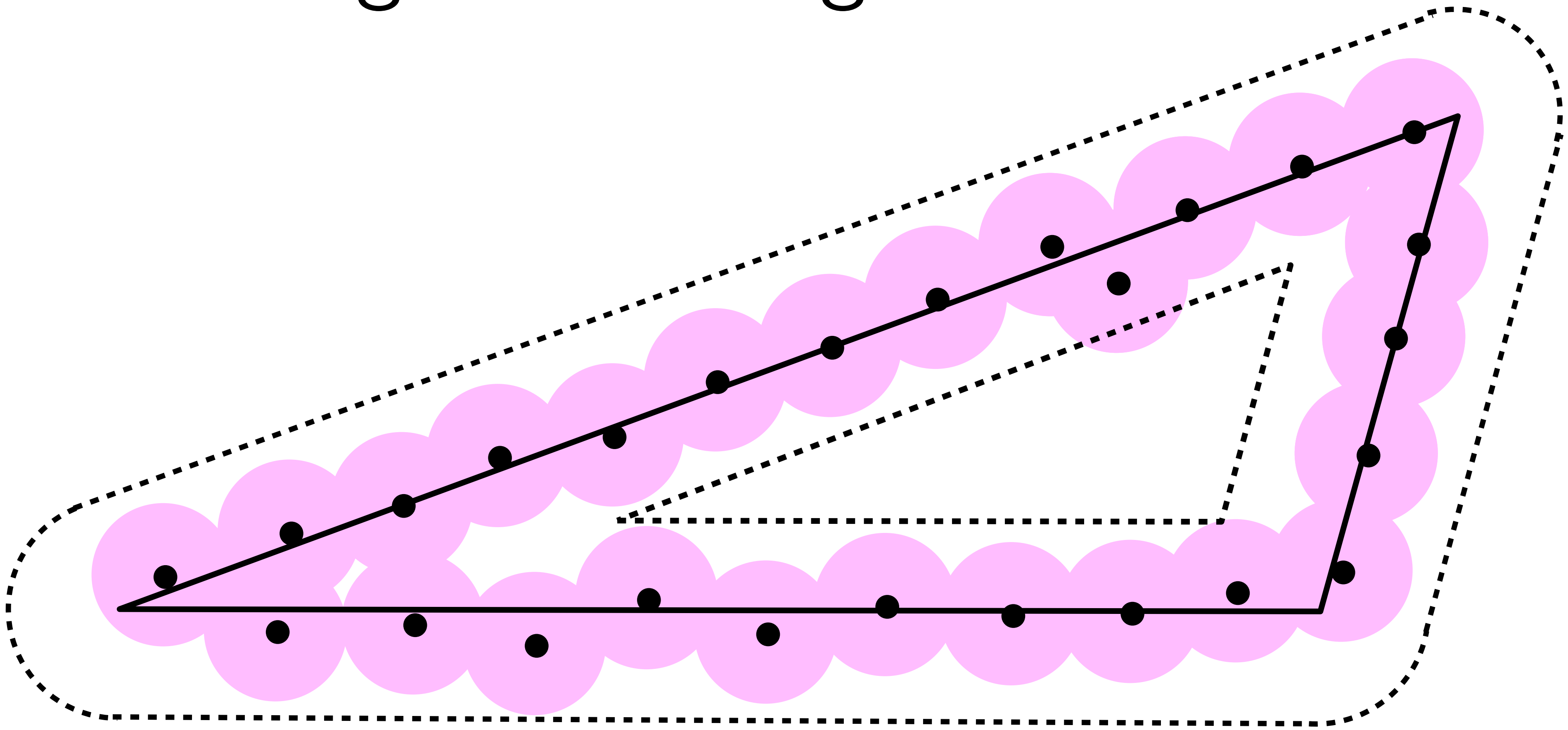
At homology level:

$$H_k(X^{\alpha}) \to H_k(L^{\alpha+\varepsilon}) \to H_k(X^{\alpha+2\varepsilon}) \to H_k(L^{\alpha+3\varepsilon}) \to H_k(X^{\alpha+4\varepsilon}) \to \cdots$$

An algorithm for geometric inference



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At homology level:

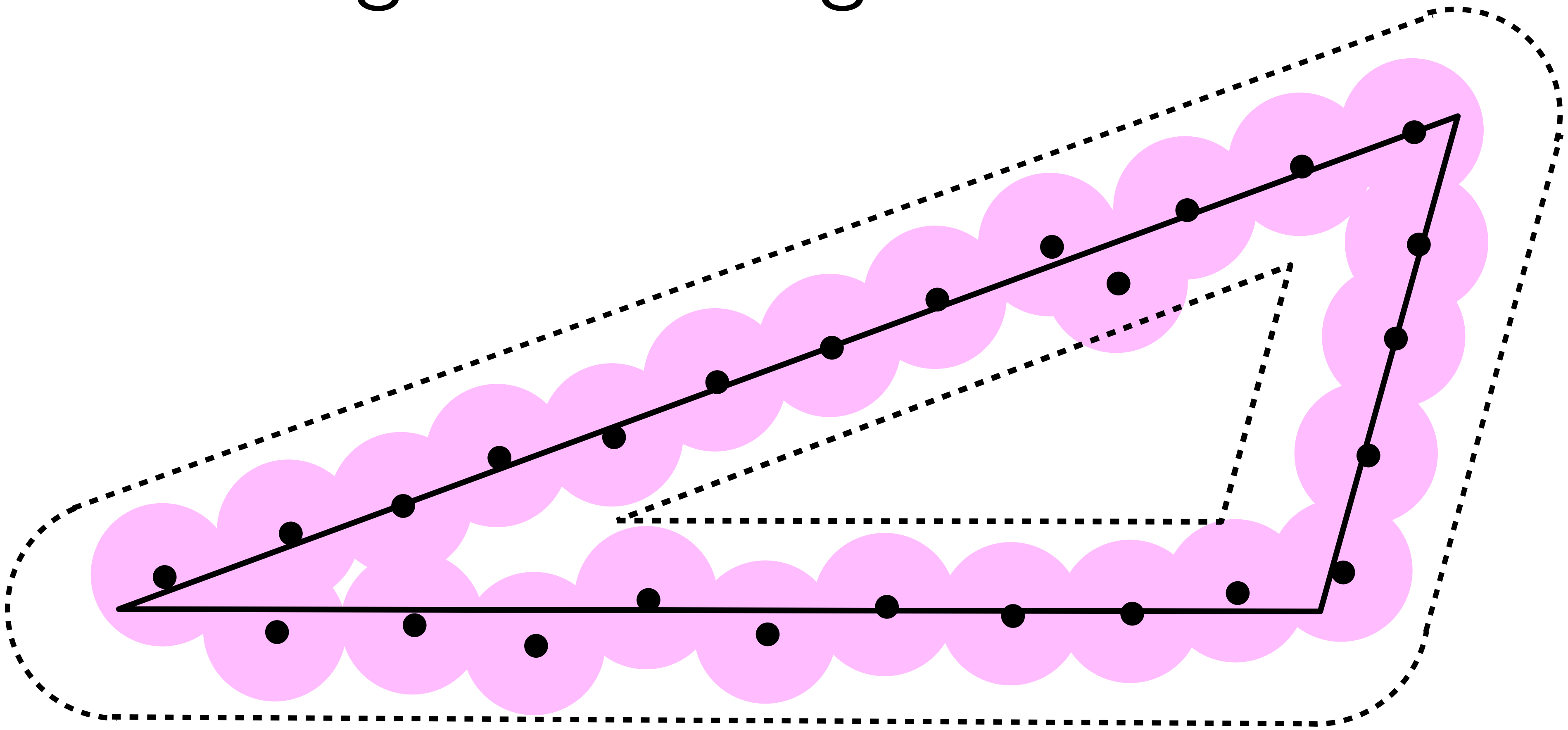
rank $= \dim H_k(X^{\alpha})$

$$H_k(X^{\alpha}) \to H_k(L^{\alpha+\varepsilon}) \to H_k(X^{\alpha+2\varepsilon}) \to H_k(L^{\alpha+3\varepsilon}) \to H_k(X^{\alpha+4\varepsilon}) \to \cdots$$

isomorphism

isomorphism

An algorithm for geometric inference



For any $\alpha > 0$, $\quad X^\alpha \subseteq L^{\alpha+\varepsilon} \subseteq X^{\alpha+2\varepsilon} \subseteq L^{\alpha+3\varepsilon} \subseteq X^{\alpha+4\varepsilon} \subseteq \cdots$

At homology level:

Cannot be directly computed !

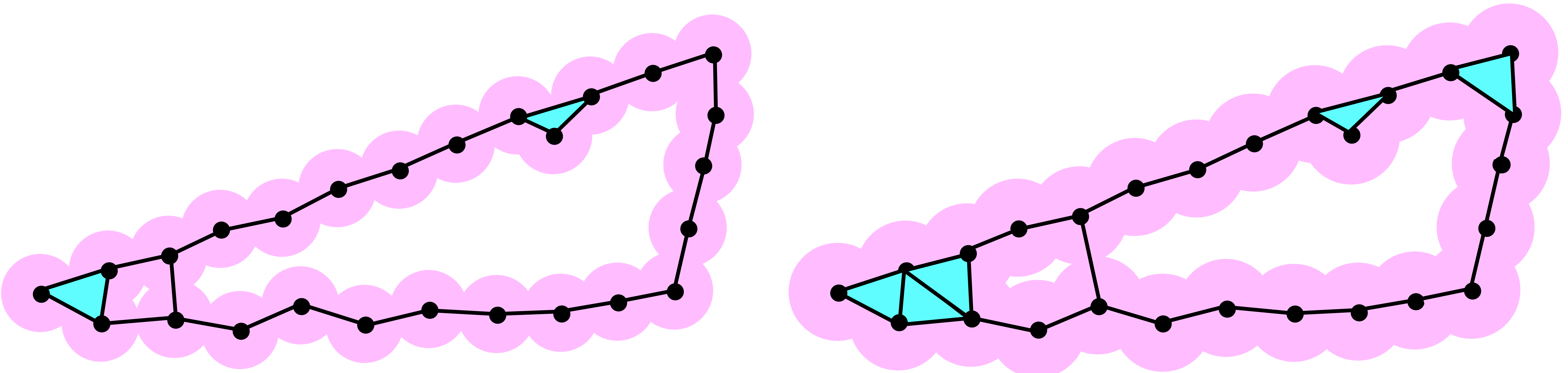
rank $= \dim H_k(X^\alpha)$

$$H_k(X^\alpha) \to H_k(L^{\alpha+\varepsilon}) \to H_k(X^{\alpha+2\varepsilon}) \to H_k(L^{\alpha+3\varepsilon}) \to H_k(X^{\alpha+4\varepsilon}) \to \cdots$$

isomorphism

isomorphism

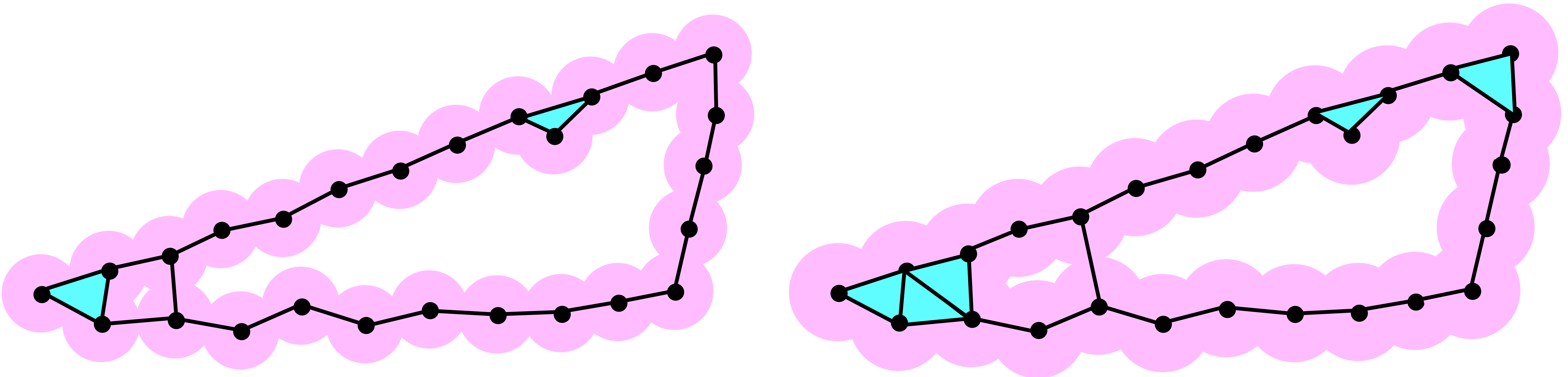
Using the Čech complex



The Čech complex $\mathcal{C}^\alpha(L)$:

$$\text{for } p_0, \cdots p_k \in L, \quad \sigma = [p_0 p_1 \cdots p_k] \in \mathcal{C}^\alpha(L) \;\text{ iff }\; \bigcap_{i=0}^{k} B(p_i, \alpha) \neq \emptyset$$

Using the Čech complex



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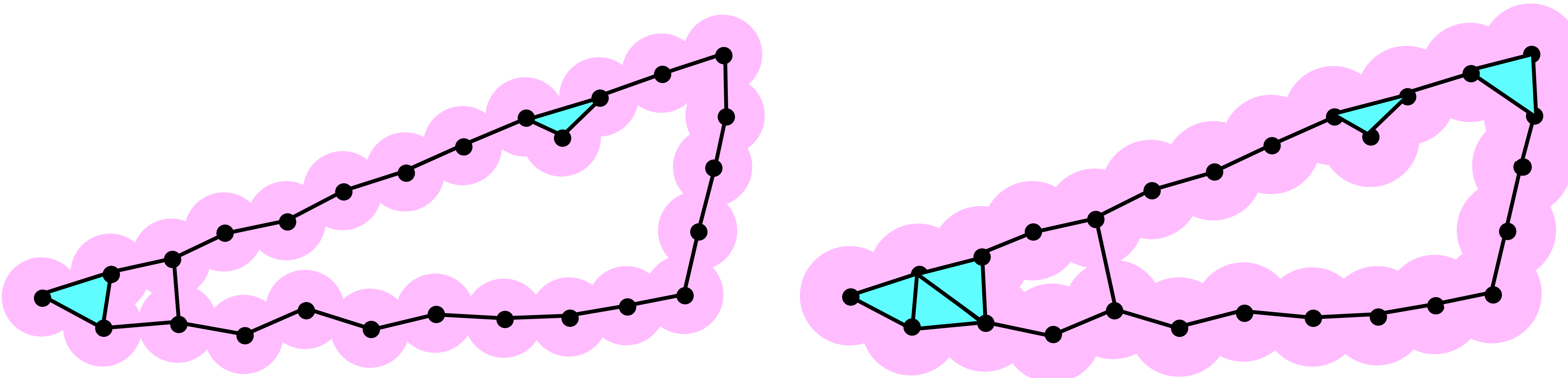
Nerve theorem: For any $\alpha > 0$, L^α and $\mathcal{C}^\alpha(L)$ are homotopy equivalent and the homotopy equivalences can be chosen to commute with inclusions.

Using the Čech complex



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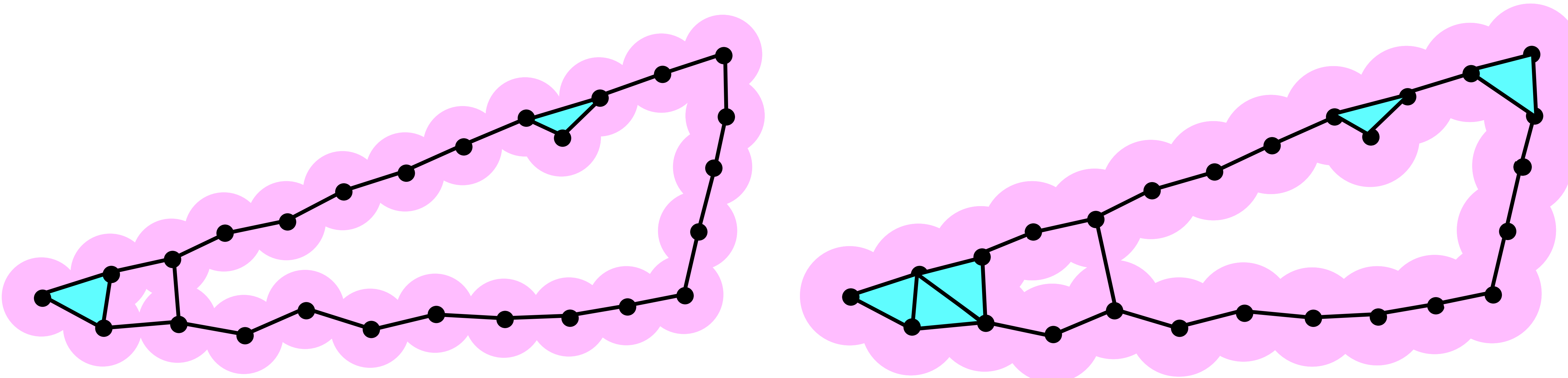
Nerve theorem: For any $\alpha > 0$, L^α and $\mathcal{C}^\alpha(L)$ are homotopy equivalent and the homotopy equivalences can be chosen to commute with inclusions.

Still true when L is a subset of a Riemannian manifold or a metric space
IF all the intersections $\cap_{i=0}^{k} B(p_i, \alpha)$ are either empty or contractible!

Using the Čech complex



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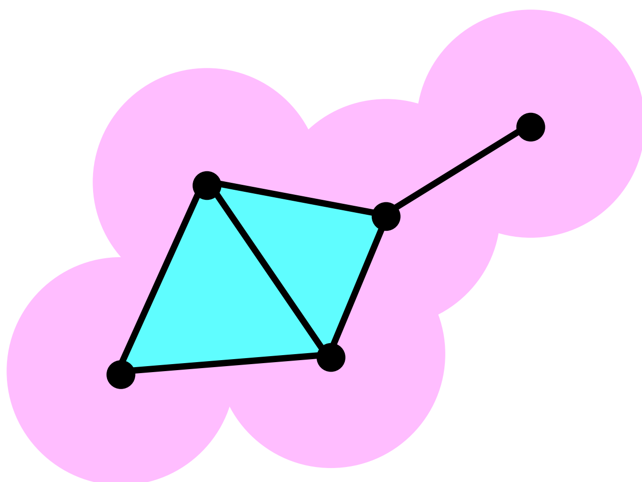
Nerve theorem: For any $\alpha > 0$, L^α and $\mathcal{C}^\alpha(L)$ are homotopy equivalent and the homotopy equivalences can be chosen to commute with inclusions.

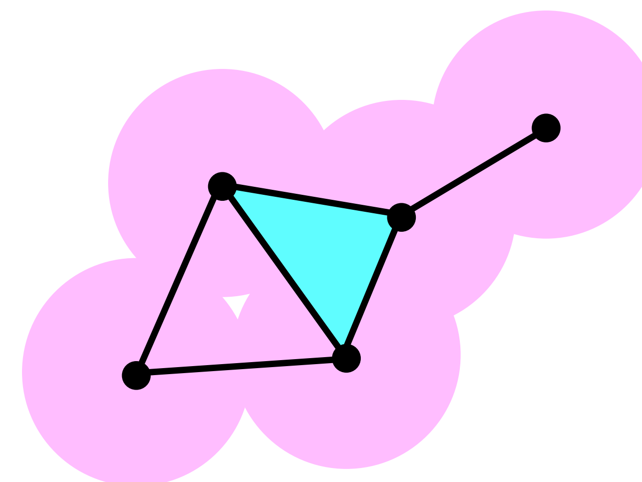
$$\begin{array}{ccccccc} \cdots & \to & H_k(L^{\alpha+\varepsilon}) & \to & H_k(L^{\alpha+3\varepsilon}) & \to & \cdots \\ & & \downarrow & & \downarrow & & \\ \cdots & \to & H_k(\mathcal{C}^{\alpha+\varepsilon}(L)) & \to & H_k(\mathcal{C}^{\alpha+3\varepsilon}(L)) & \to & \cdots \end{array}$$

Allow to work with simplicial complexes but... still too difficult to compute

Using the Rips complex



Rips vs Čech



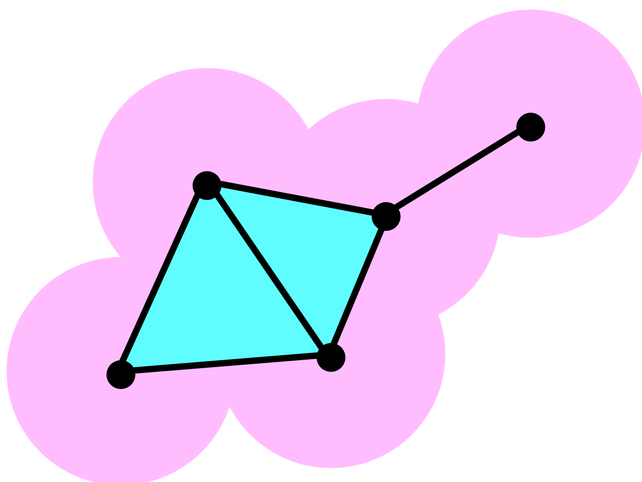
The Rips complex $\mathcal{R}^\alpha(L)$: for $p_0, \cdots p_k \in L$,

$$\sigma = [p_0 p_1 \cdots p_k] \in \mathcal{R}^\alpha(L) \ \text{ iff } \ \forall i, j \in \{0, \cdots k\}, \ d(p_i, p_j) \leq \alpha$$

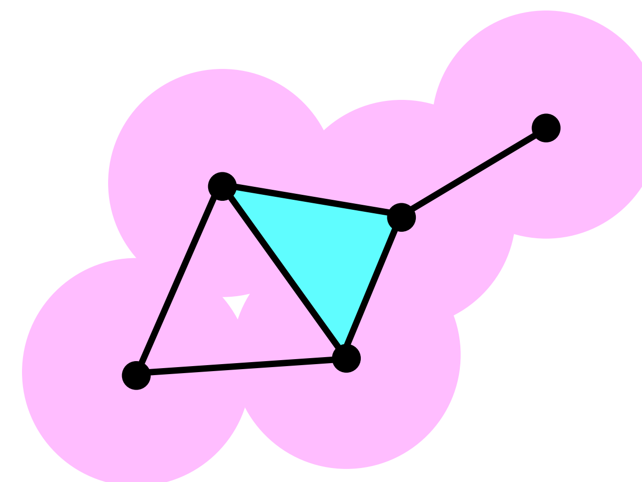
- Easy to compute and fully determined by its 1-skeleton
- Rips-Čech interleaving: for any $\alpha > 0$,

$$\mathcal{C}^{\frac{\alpha}{2}}(L) \subseteq \mathcal{R}^\alpha(L) \subseteq \mathcal{C}^\alpha(L) \subseteq \mathcal{R}^{2\alpha}(L) \subseteq \cdots$$

Using the Rips complex



Rips vs Čech



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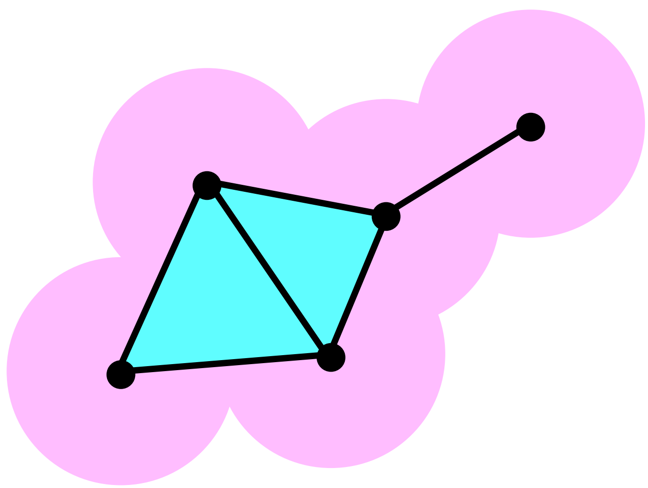
Theorem: [C-Oudot'08]
Let $X \subset \mathbb{R}^d$ be a compact set and $L \subset \mathbb{R}^d$ a finite set such that $d_H(X, L) < \varepsilon$ for some $\varepsilon < \frac{1}{9}$ wfs(X). Then for all $\alpha \in [2\varepsilon, \frac{1}{4}(\mathrm{wfs}(X) - \varepsilon)]$ and all $\lambda \in (0, \mathrm{wfs}(X)))$, one has: $\forall k \in \mathbb{N}$

$$\beta_k(X^\lambda) = \dim(H_k(X^\lambda)) = \mathsf{rk}(\mathcal{R}^\alpha(L) \to \mathcal{R}^{4\alpha}(L))$$

Using the Rips complex



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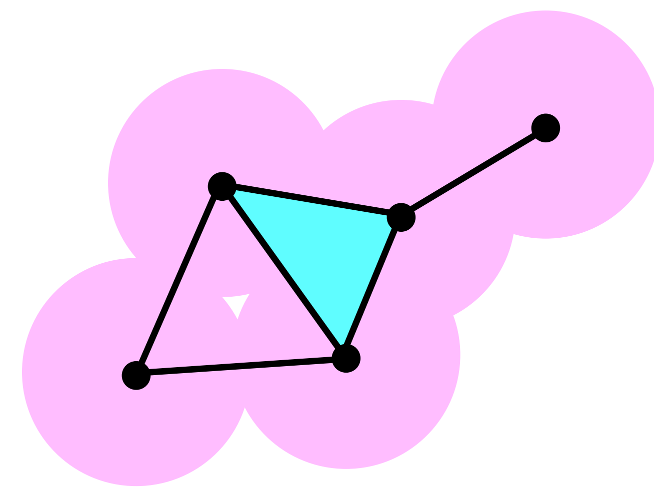

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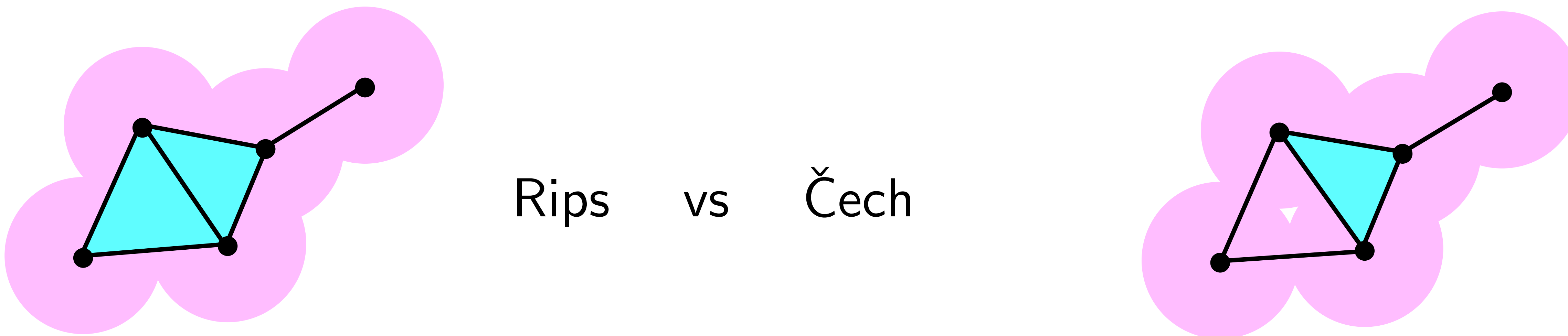
Easy to compute using persistence algo.

Using the Rips complex



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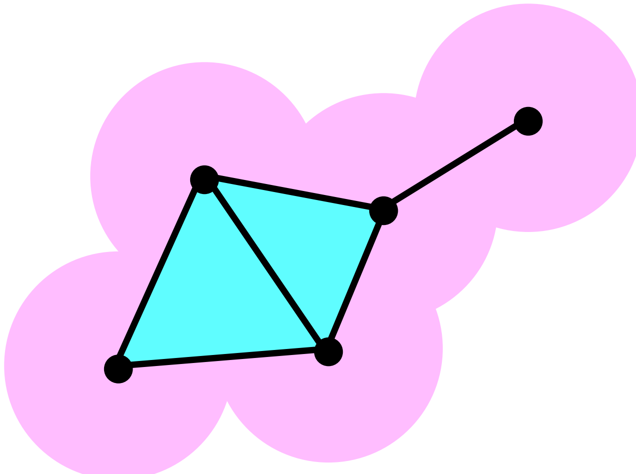
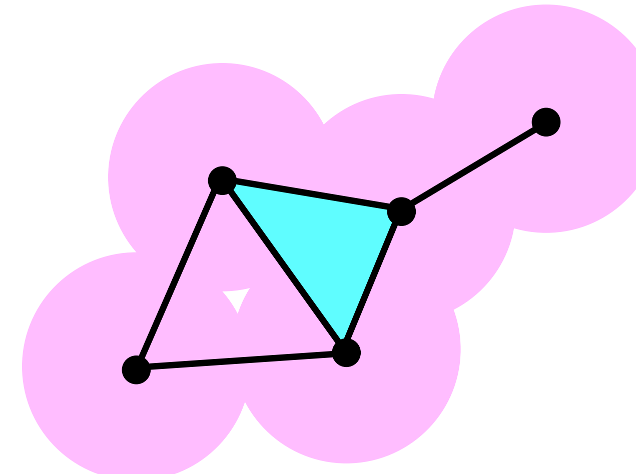
Can be replace by a Riemmanian manifold
BUT take care of convexity radius!
Also some stability results in metric spaces...

Easy to compute using persistence algo.

Using the Rips complex



Rips vs Čech



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Pb: Choice of α when wfs(X) is unknown?

Multiscale inference

Input: A point cloud W and its pairewise distances $\{d(w,w')\}_{w,w'\in W}$.
$\rightarrow$ Maintain a nested pair $\mathcal{R}^{4\varepsilon}(L) \hookrightarrow \mathcal{R}^{16\varepsilon}(L)$ where $L = L(\varepsilon)$.

Init.: $L = \emptyset$; $\varepsilon = +\infty$

WHILE $L \subset W$
insert $p = argmax_{w\in W} d(w, L)$ in L
update $\varepsilon = \max_{w\in W} d(w, L)$
update $\mathcal{R}^{4\varepsilon}(L)$ and $\mathcal{R}^{16\varepsilon}(L)$
Persistence($\mathcal{R}^{4\varepsilon}(L) \hookrightarrow \mathcal{R}^{16\varepsilon}(L)$)
END_WHILE

Output: Sequence of persitent Betti numbers
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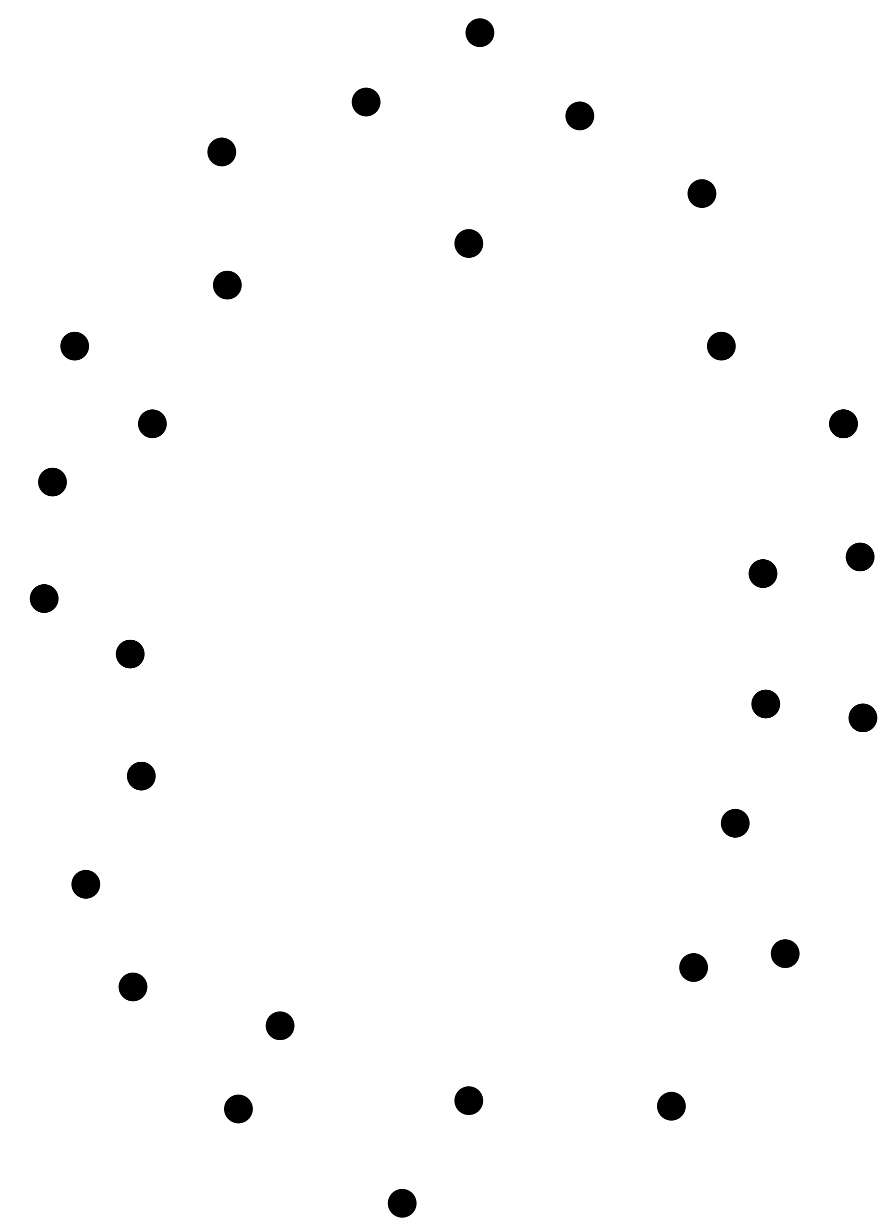

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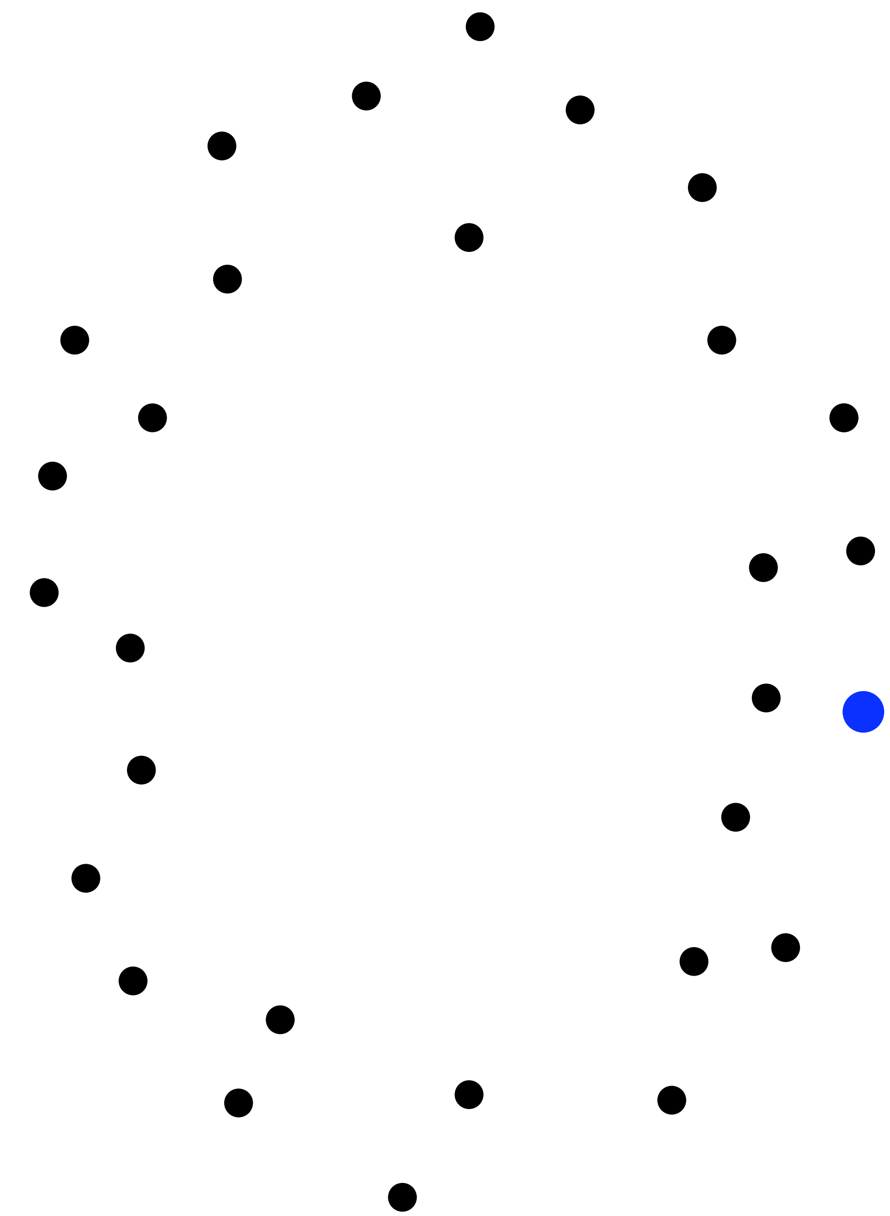

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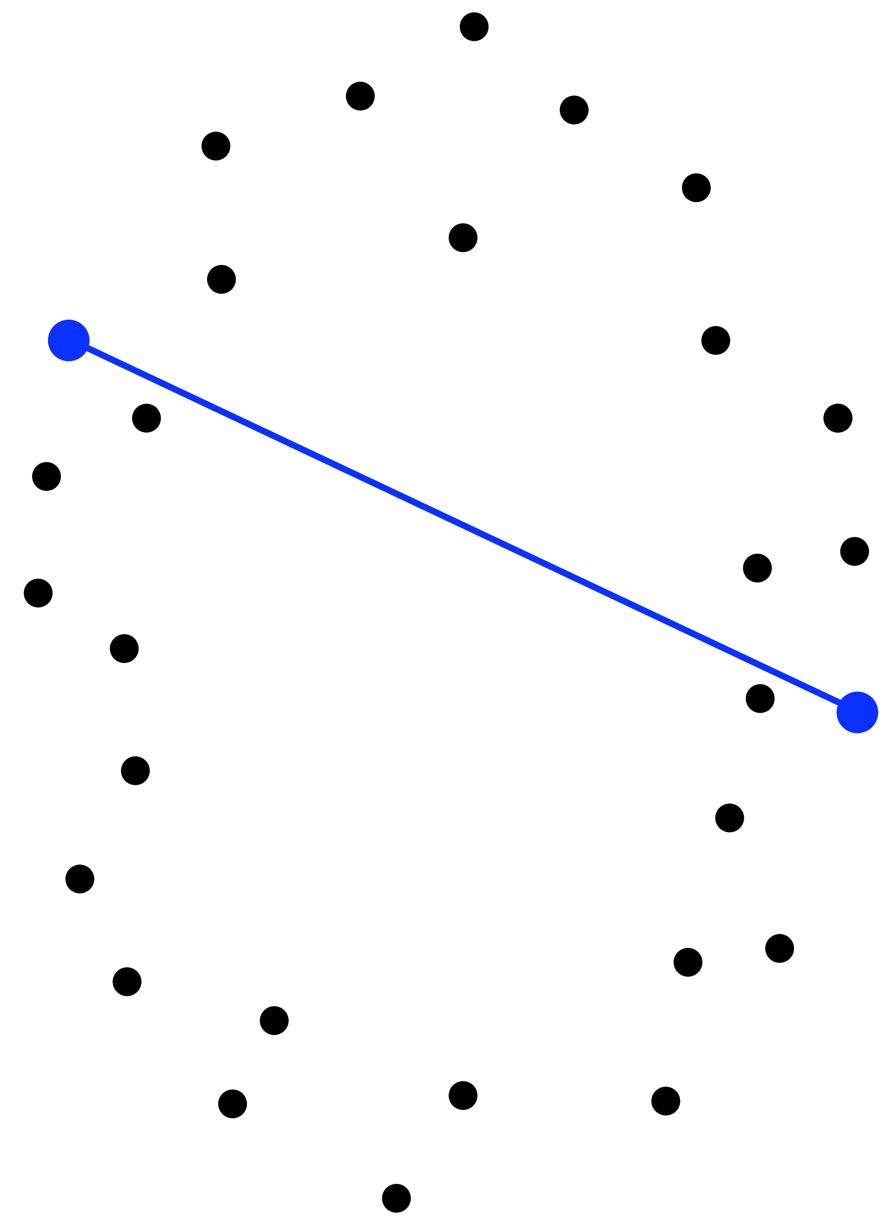

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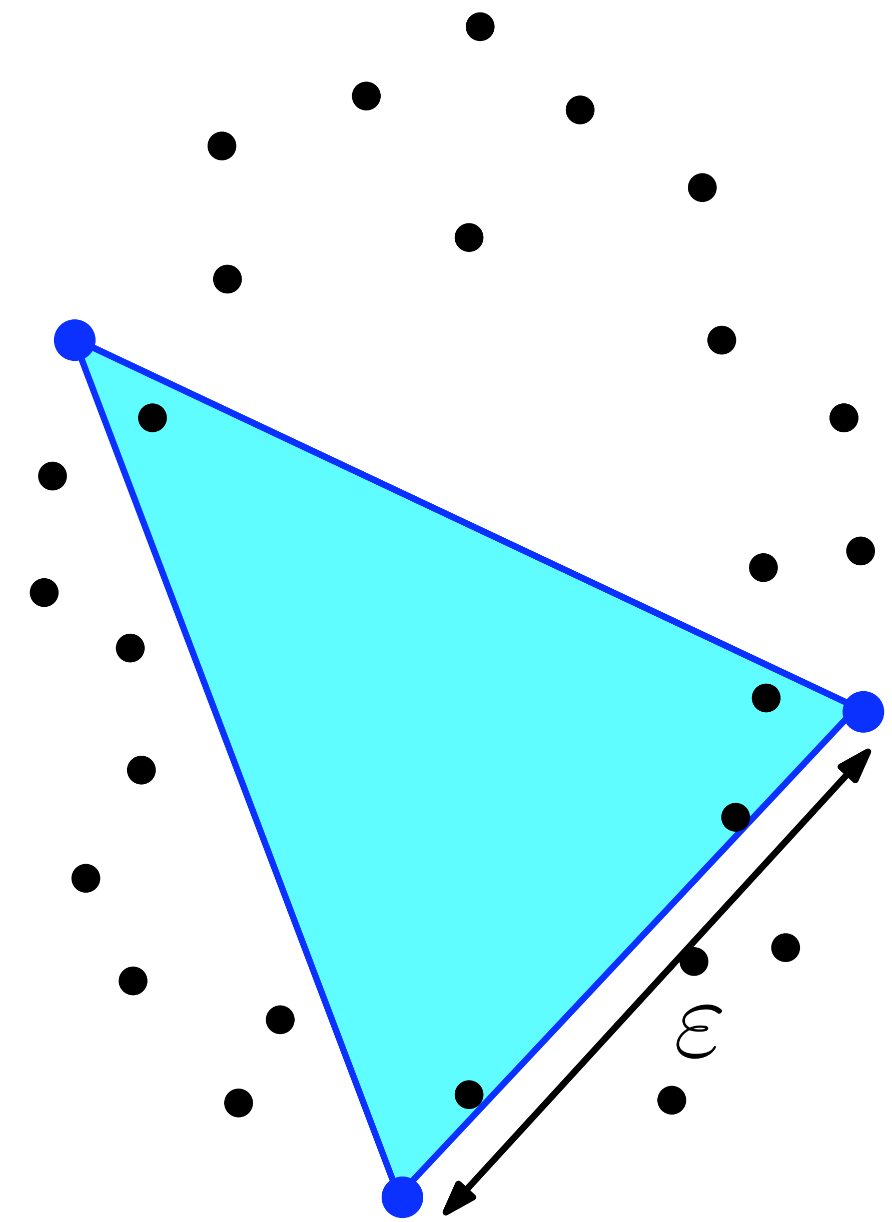

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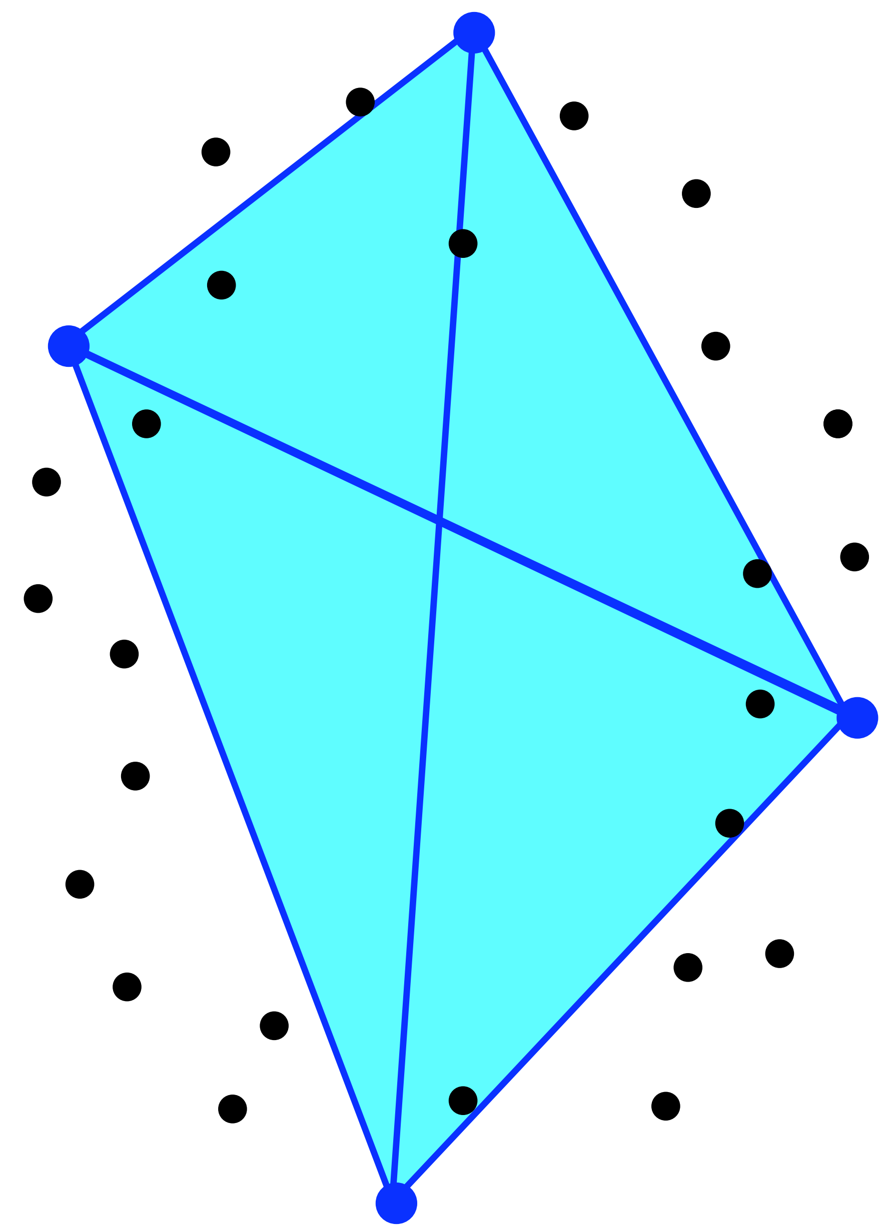

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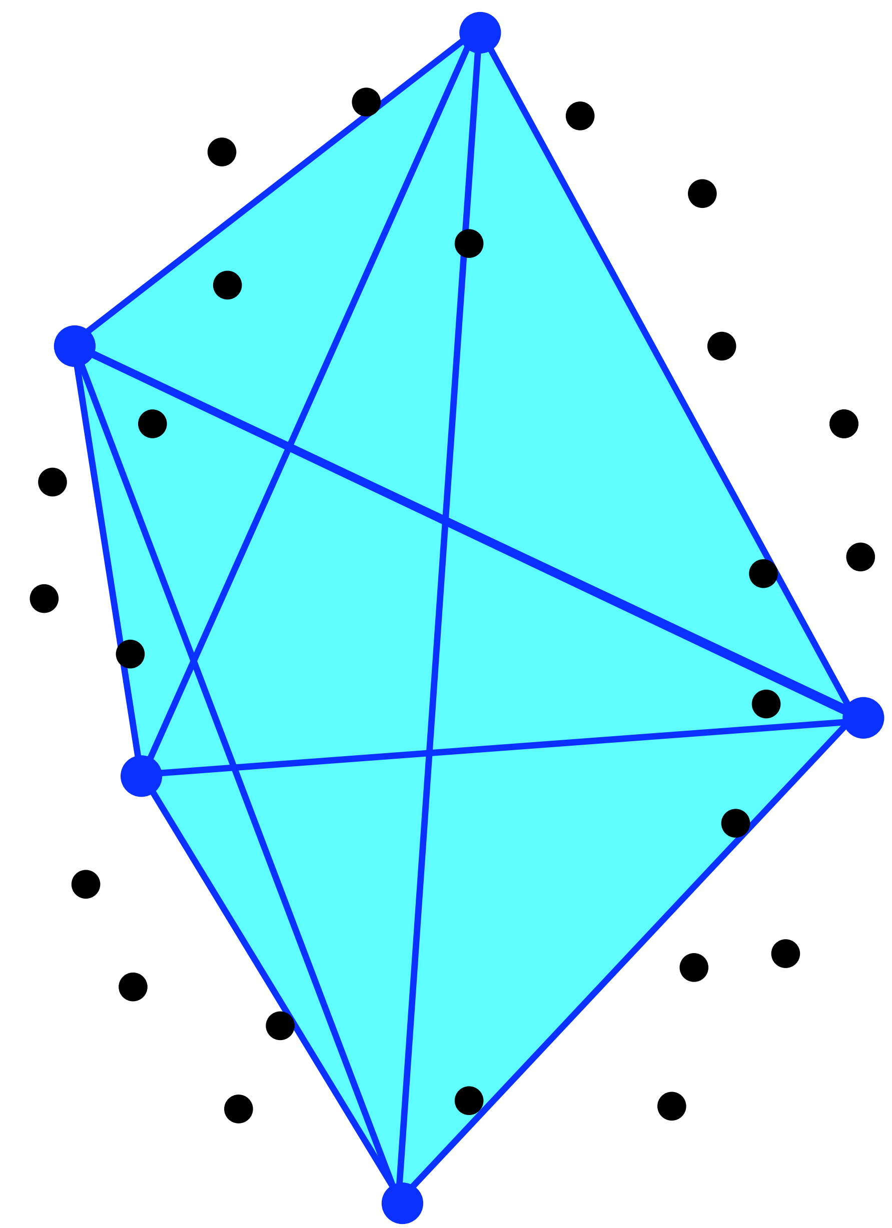

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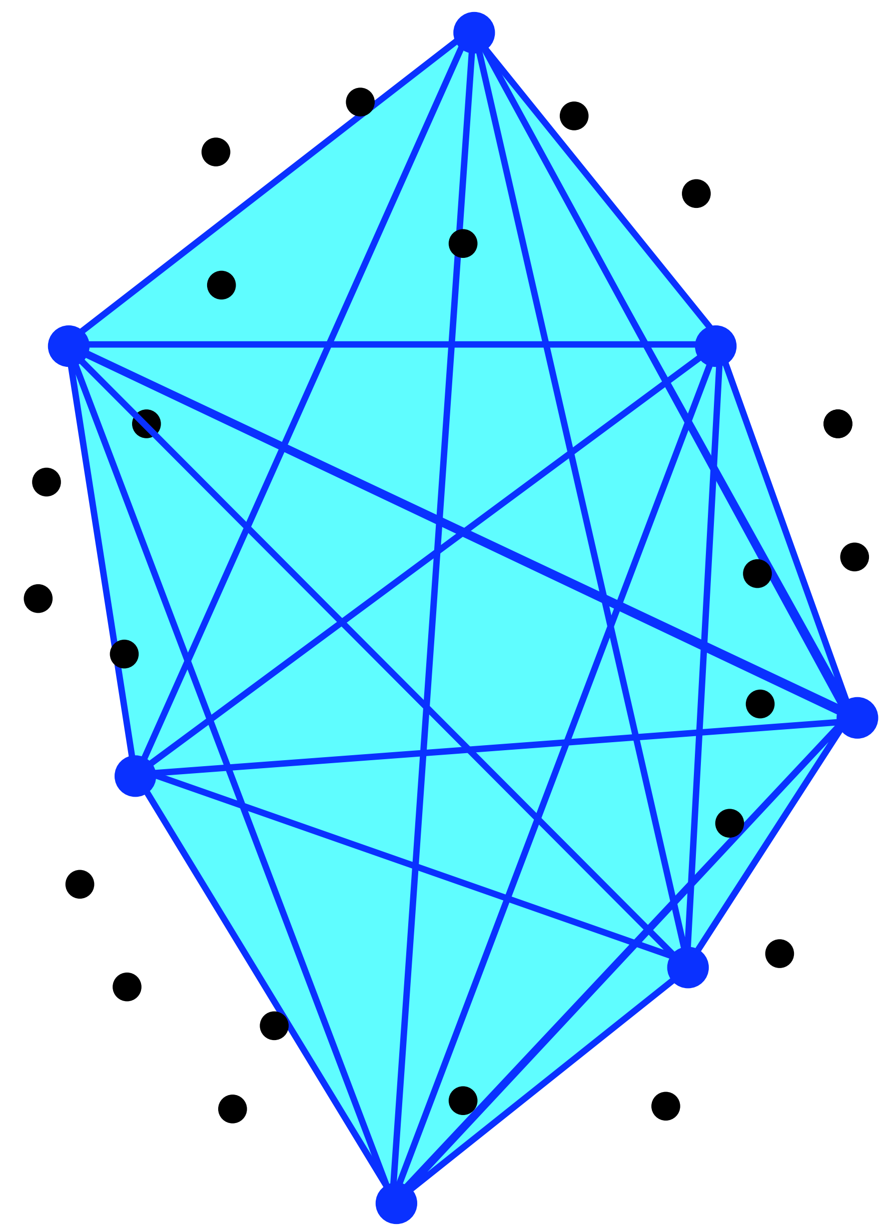

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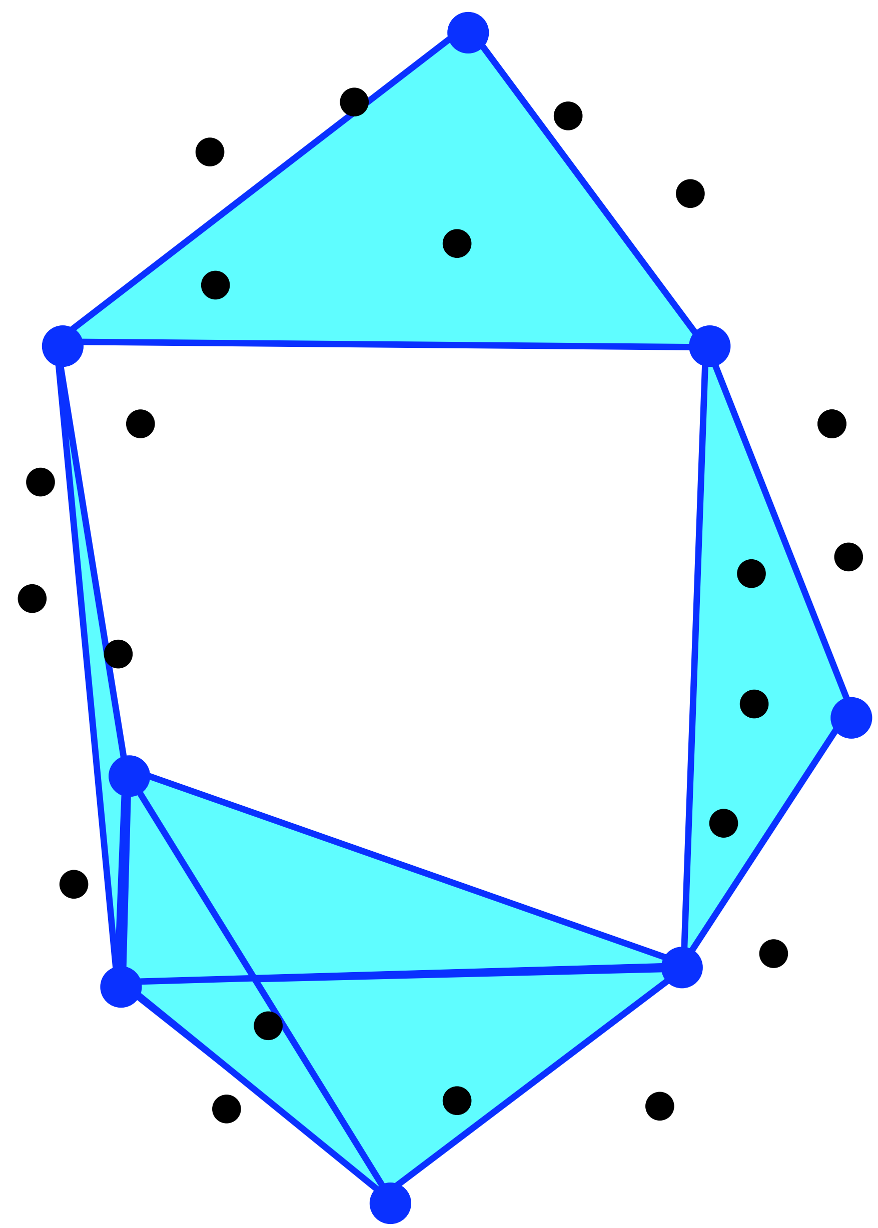
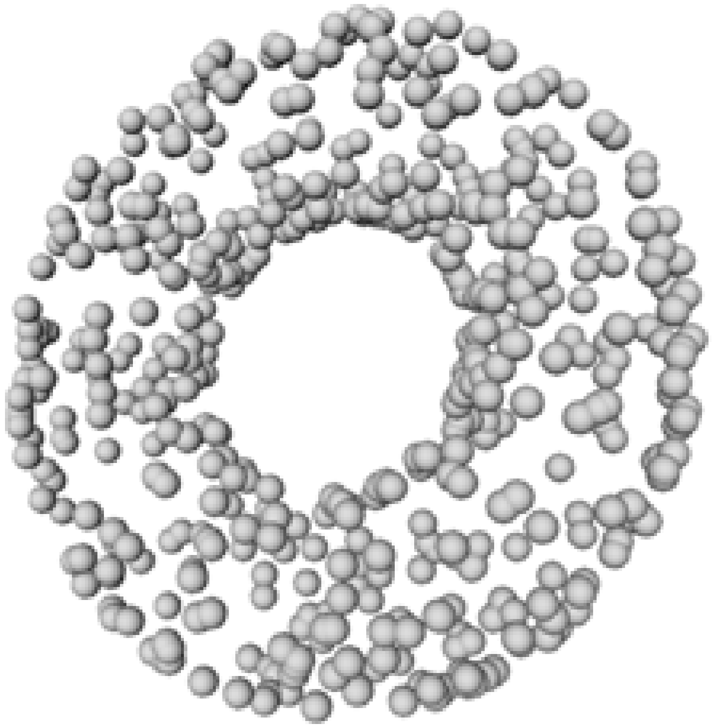
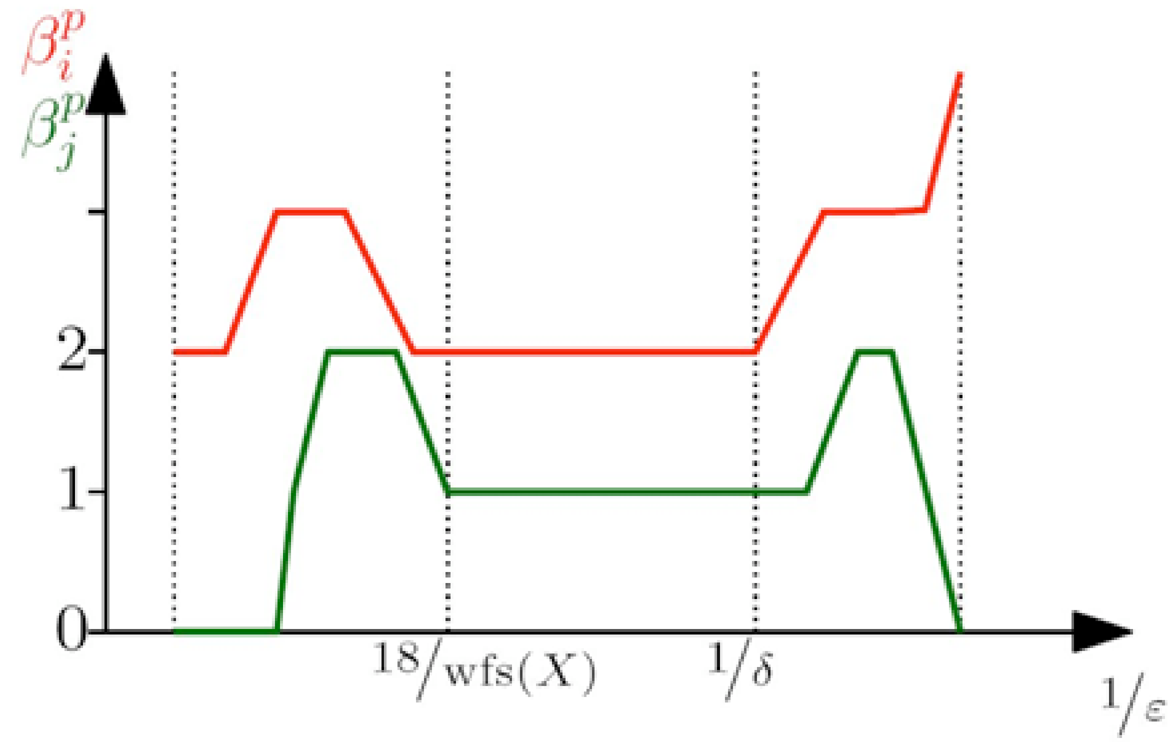


Multiscale inference



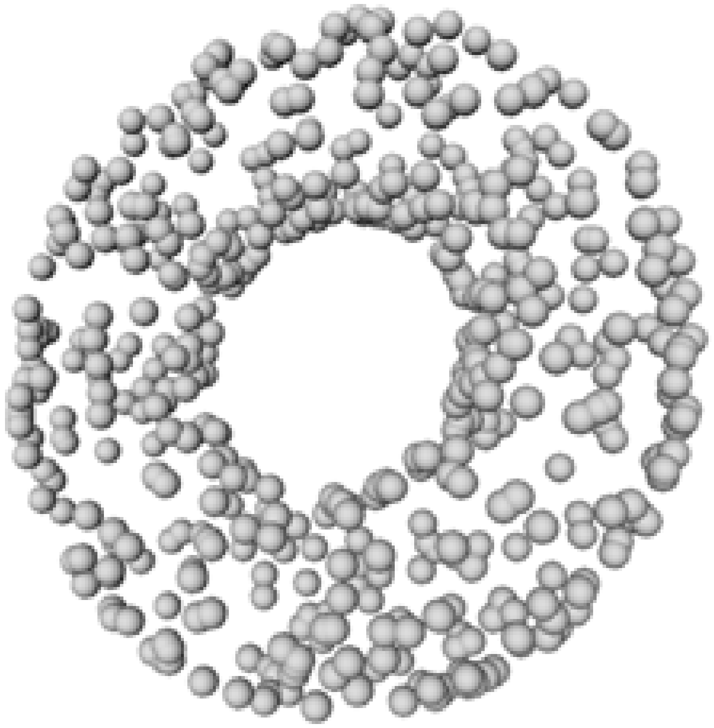


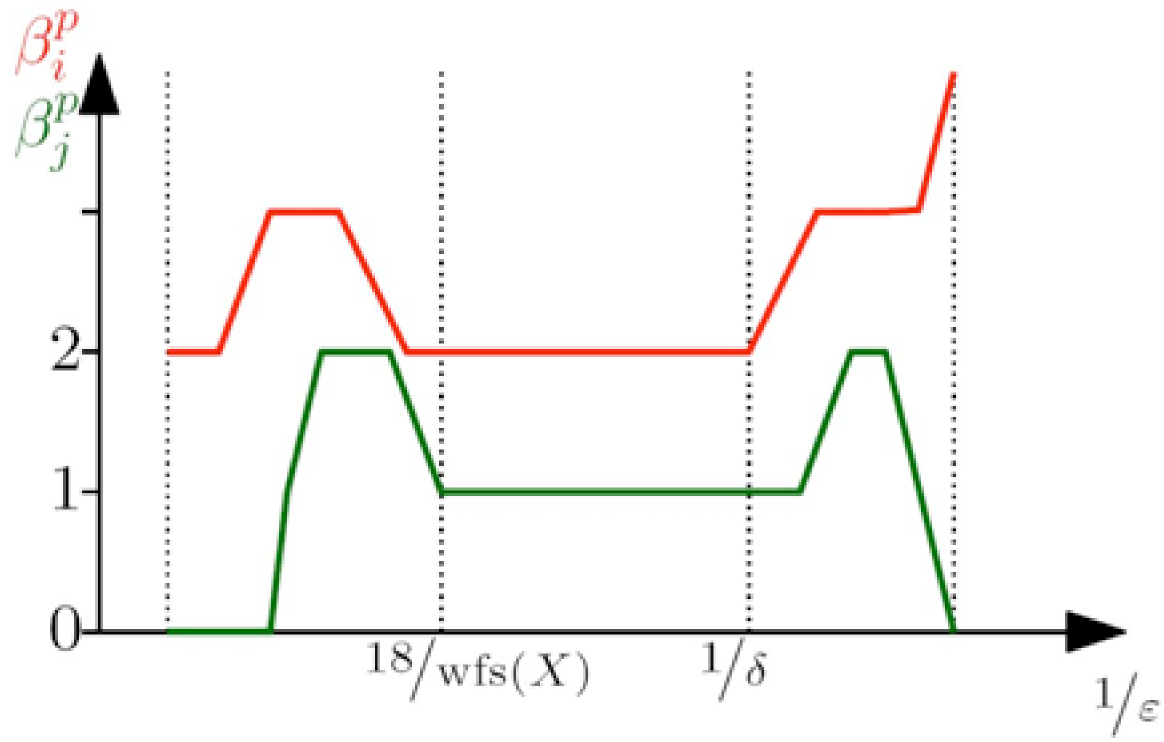
Theorem: [C-Oudot'08]
If $d_H(W, X) < \delta$ for $\delta < \frac{1}{18}\mathrm{wfs}(X)$, than at every iteration of the algorithm such that $\delta < \varepsilon < \frac{1}{18}\mathrm{wfs}(X)$,

$$\beta_k(X^\lambda) = \dim H_k(X^\lambda) = rk(H_k(\mathcal{R}^{4\varepsilon}(L)) \to H_k(\mathcal{R}^{4\varepsilon}(L)))$$

for any $\lambda \in (0, \mathrm{wfs}(X))$ and any $k \in \mathbb{N}$.

Multiscale inference





Complexity of the algorithm:

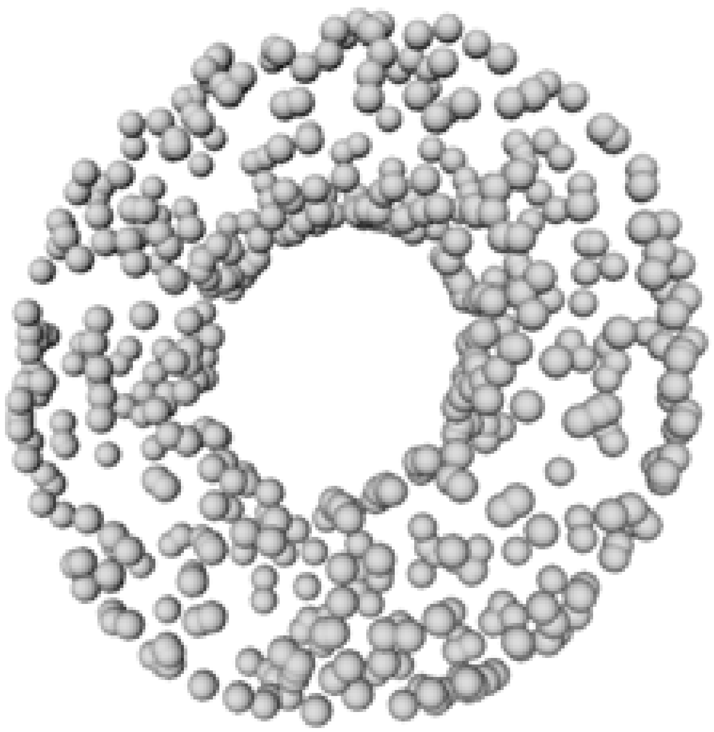
- If $X \subset \mathbb{R}^d$ is non smooth the running time of the algorithm is

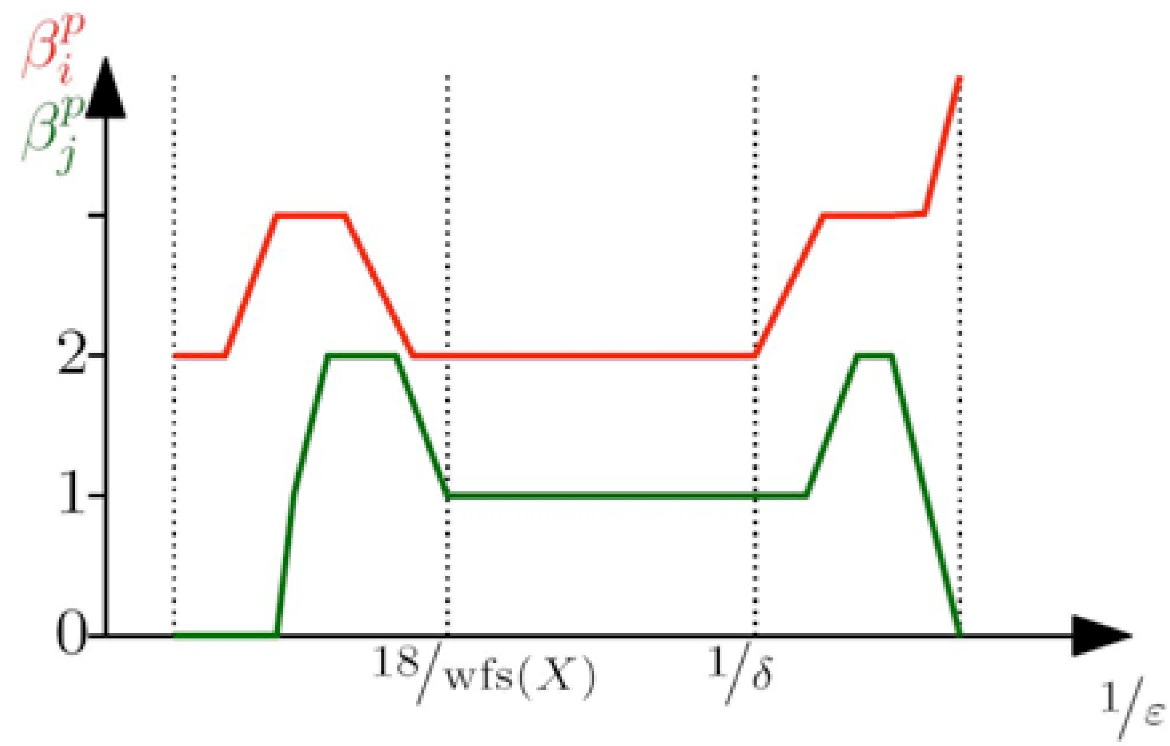
$$O(8^{33^d}|W|^5)$$

- If X is a smooth submanifold of $\mathbb{R}^d$ dimension m the running time is

$$O(8^{35^m}|W|)$$

Multiscale inference





Complexity of the algorithm:

- If $X \subset \mathbb{R}^d$ is non smooth the running time of the algorithm is

$$O(8^{33^d}|W|^5)$$

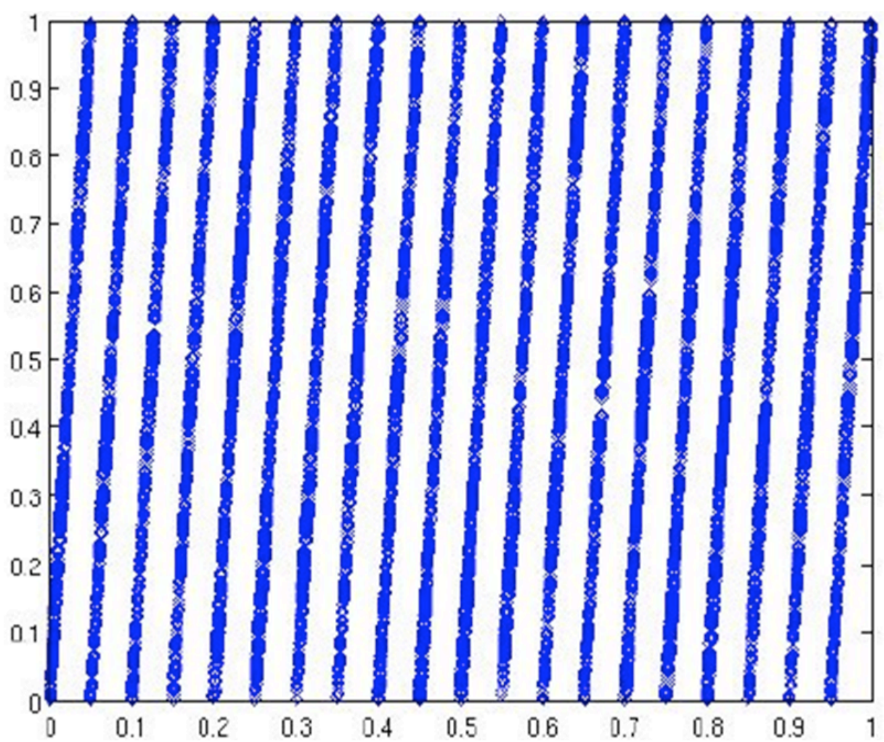
- If X is a smooth submanifold of $\mathbb{R}^d$ dimension m the running time is

$$O(8^{35^m}|W|)$$

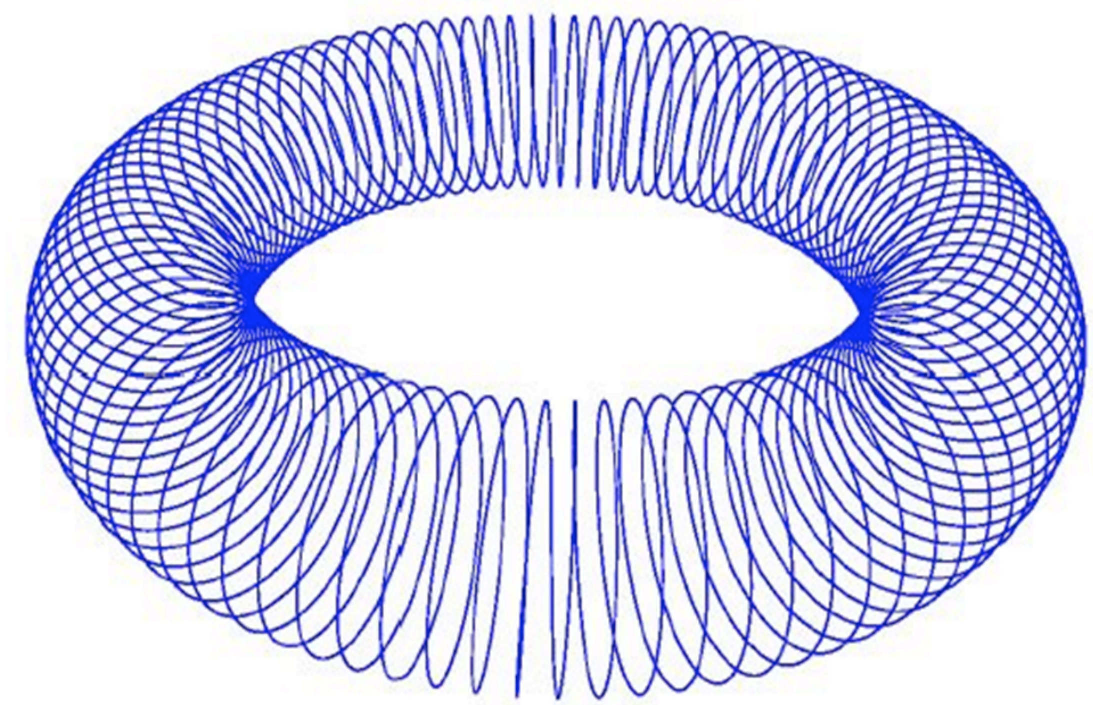
Depend on the intrinsic dimension of X

A synthetic example

$[0, 1] \times [0, 1]$



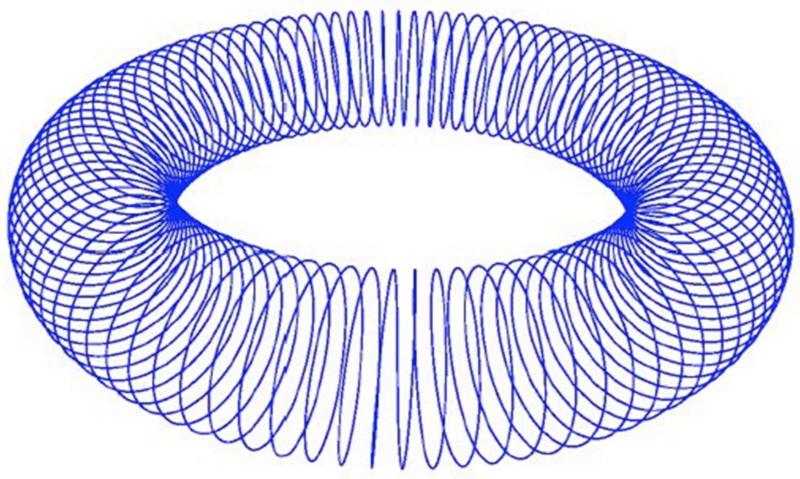
$\mathbb{R}^{1000}$

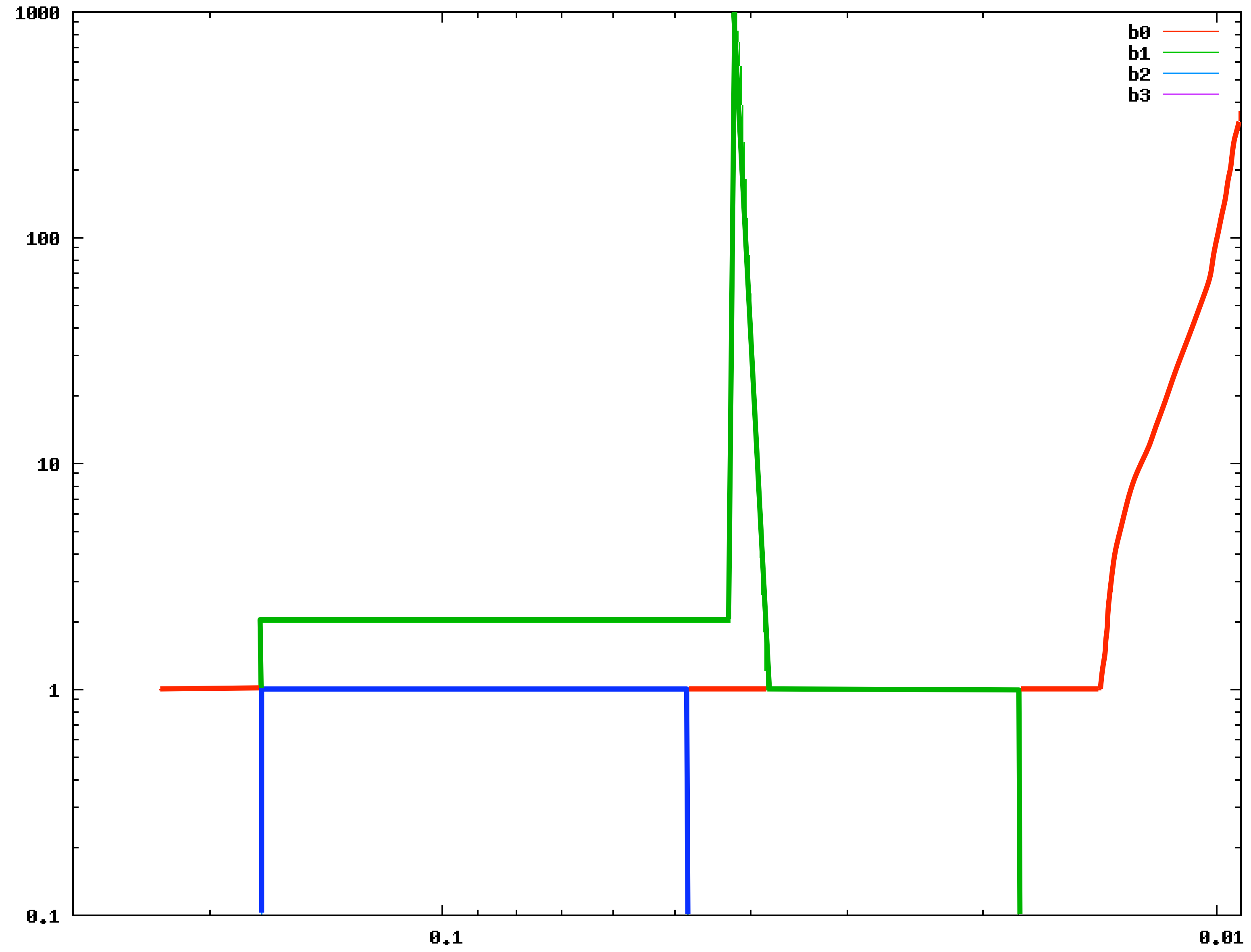


Non-linear embedding of $\mathbb{S}^1 \times \mathbb{S}^1$ in $\mathbb{R}^{1000}$

$50,000$ points sampled uniformly at random from a curve drawn on the 2-torus $\mathbb{S}^1 \times \mathbb{S}^1$.

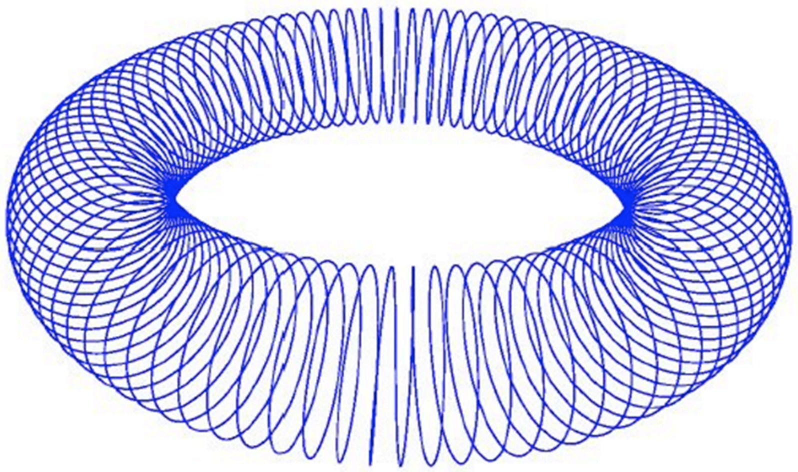
A synthetic example

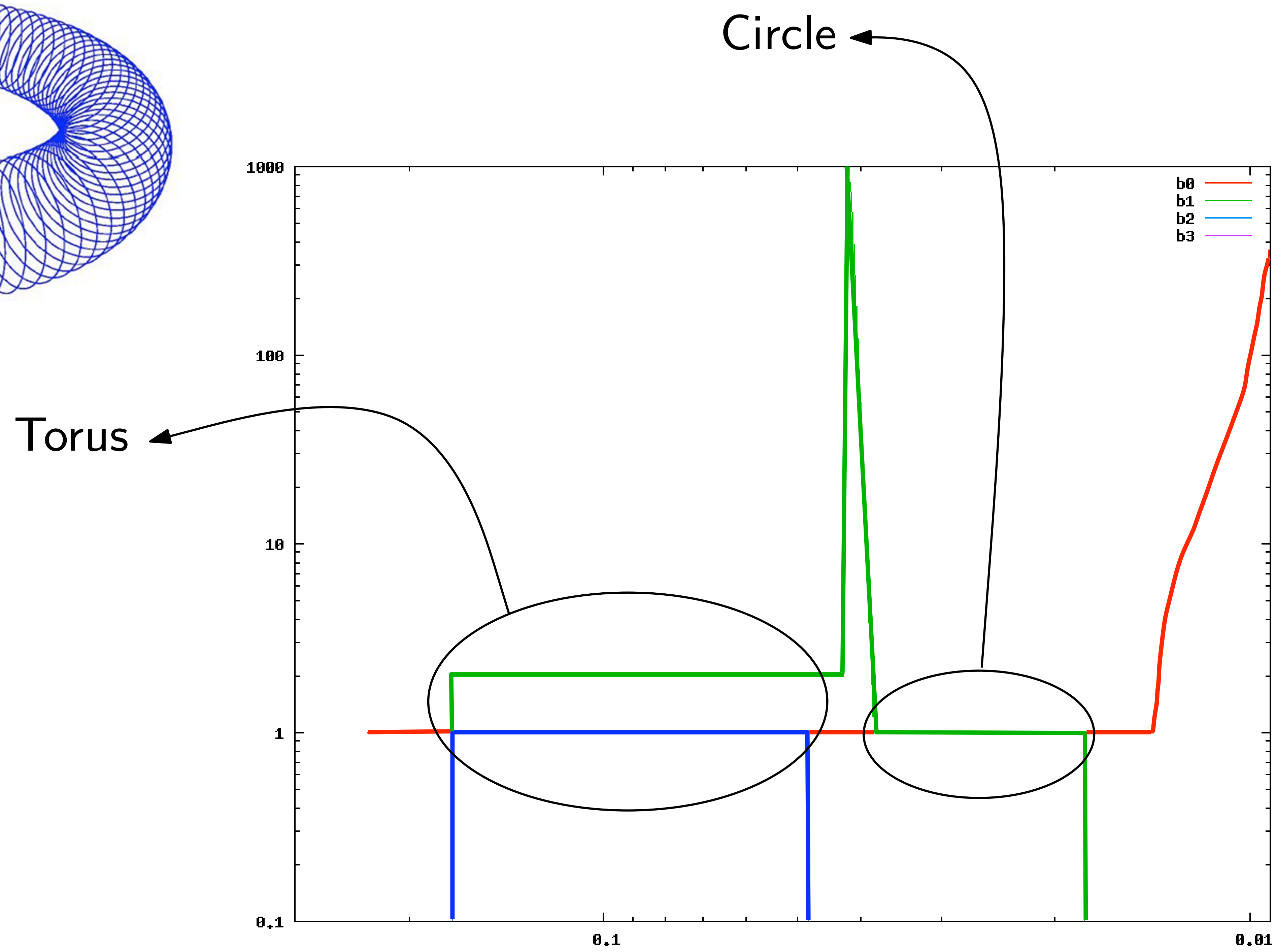




Output: sequence of Betti numbers on a log-log scale

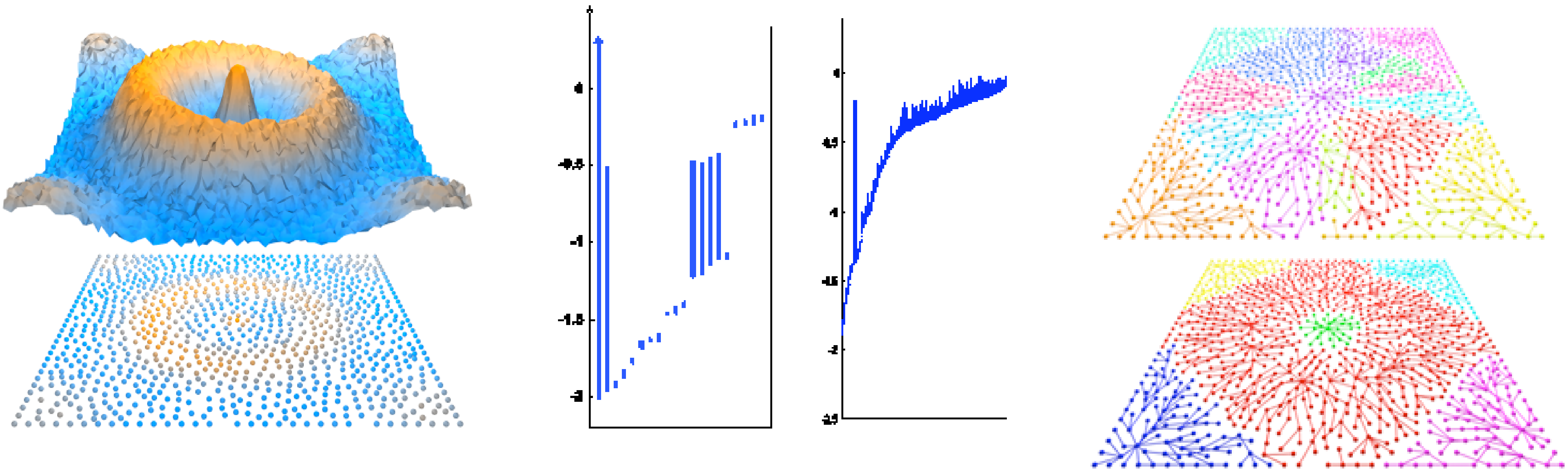
A synthetic example





Output: sequence of Betti numbers on a log-log scale

Generalization(s)

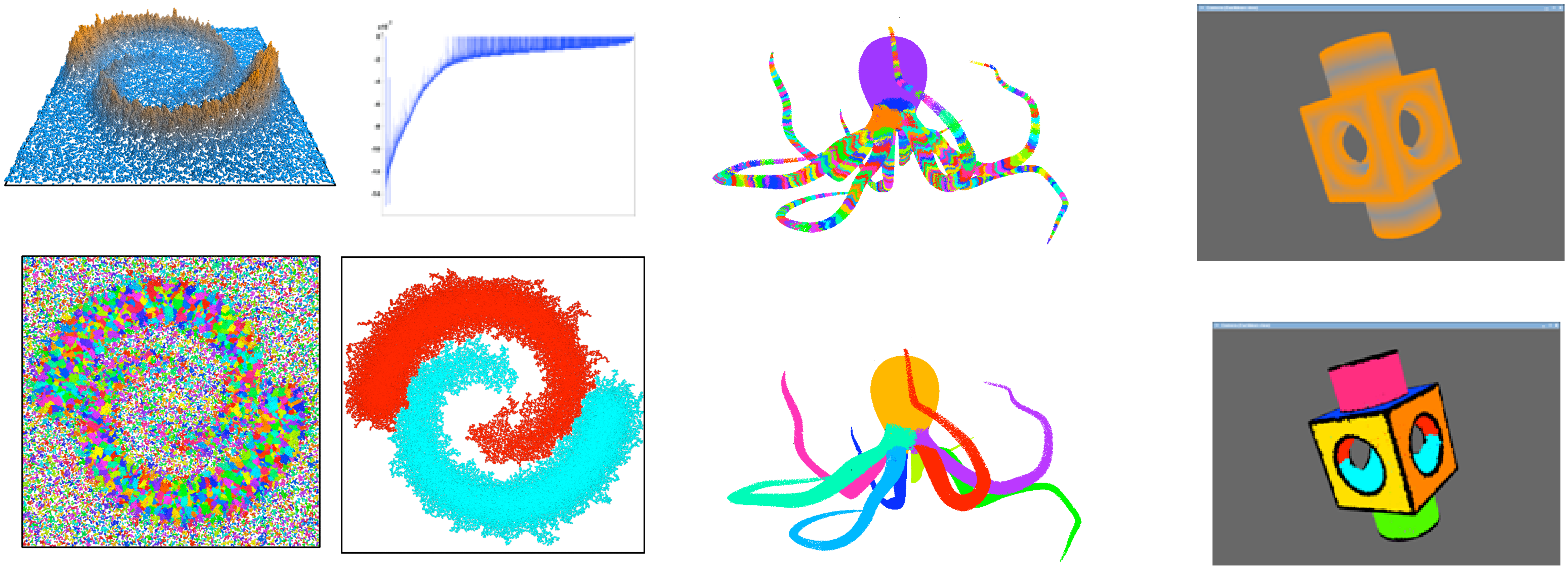


Previous approach can be generalized, leading to robust algorithms to compute the topological persistence of functions defined over point clouds sampled around unknown shapes

Ref:

- F. Chazal, L. Guibas, S. Oudot, P. Skraba, *Analysis of Scalar Fields over Point Cloud Data*, proc. ACM Symposium on Discrete Algorithms 2009.
- F. Chazal, S. Oudot, *Toward Persistence-Based Reconstruction in Euclidean Spaces*, proc. ACM Symposium on Computational Geometry 2008.

Generalization(s)



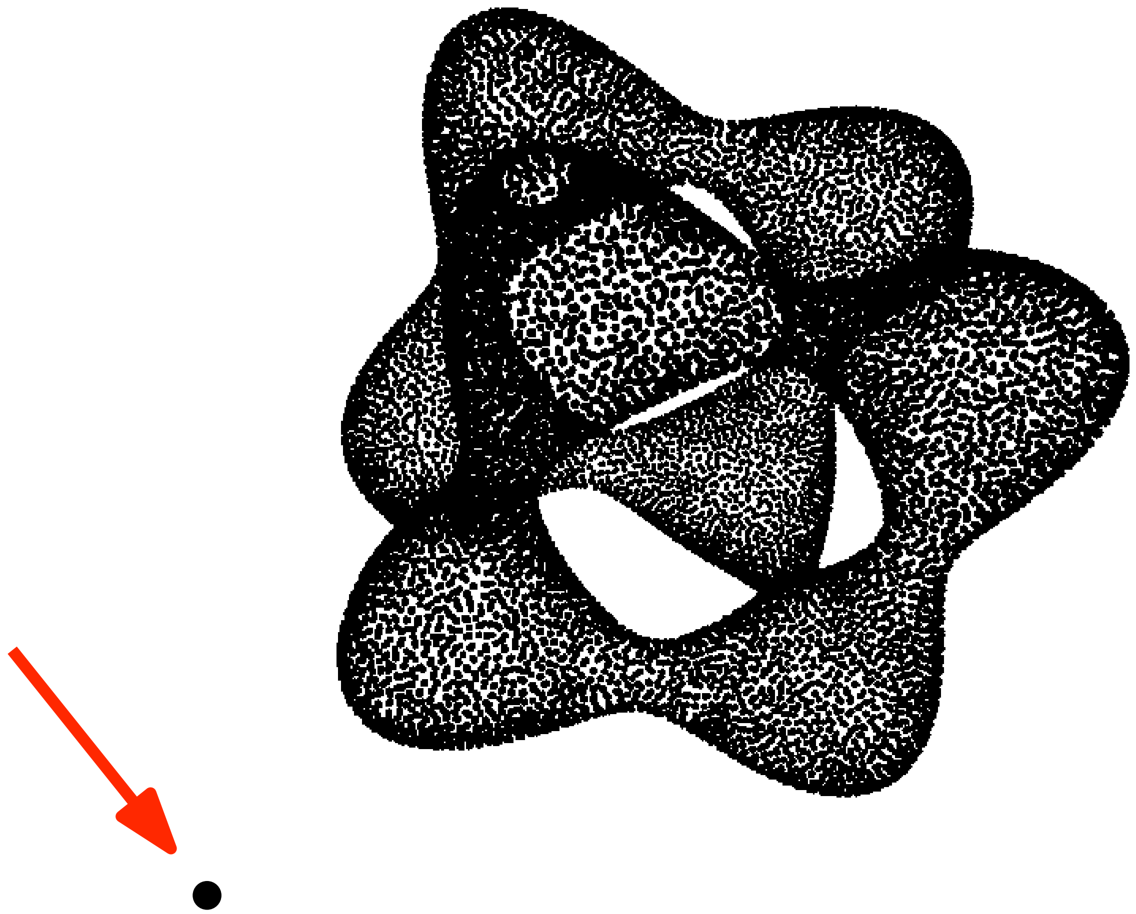
Applications to clustering, segmentations, sensor networks,...

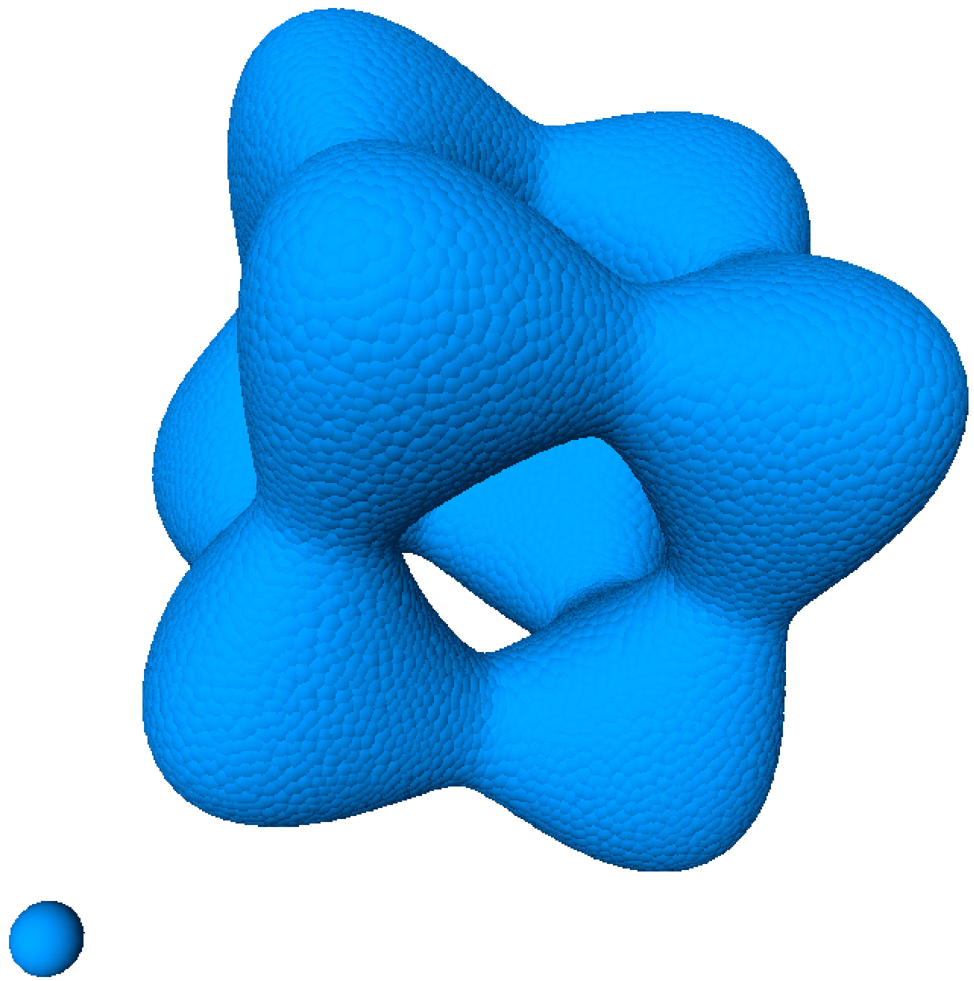
Ref:

- F. Chazal, L. Guibas, S. Oudot, P. Skraba, *Analysis of Scalar Fields over Point Cloud Data*, proc. ACM Symposium on Discrete Algorithms 2009.

- F. Chazal, S. Oudot, *Toward Persistence-Based Reconstruction in Euclidean Spaces*, proc. ACM Symposium on Computational Geometry 2008.

The problem of “outliers”





If $K' = K \cup \{x\}$ where $d_K(x) > R$, then $\|d_K - d_{K'}\|_\infty > R$: offset-based inference methods fail!

Question: Can we generalized the previous approach by replacing the distance function by a “distance-like” function having a better behavior with respect to “'noise” and “outliers”?

Distance-like functions: the three main ingredients of stability

- the stability of the map $K \mapsto d_K$:
  $\|d_K - d_{K'}\|_\infty = d_H(K, K')$

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Distance-like functions: the three main ingredients of stability

- the stability of the map $K \mapsto d_K$:
  $\|d_K - d_{K'}\|_\infty = d_H(K, K')$

- the 1-Lipschitz property for d_K; $\longrightarrow$ d_K is differentiable almost everywhere.

- the 1-concavity of the function d_K^2:
  $x \to \|x\|^2 - d_K^2(x)$ is convex. $\longrightarrow$
  - the gradient vector field ∇d_K is well defined and integrable (although not continuous).
  - d_K admits a second derivative almost everywhere.

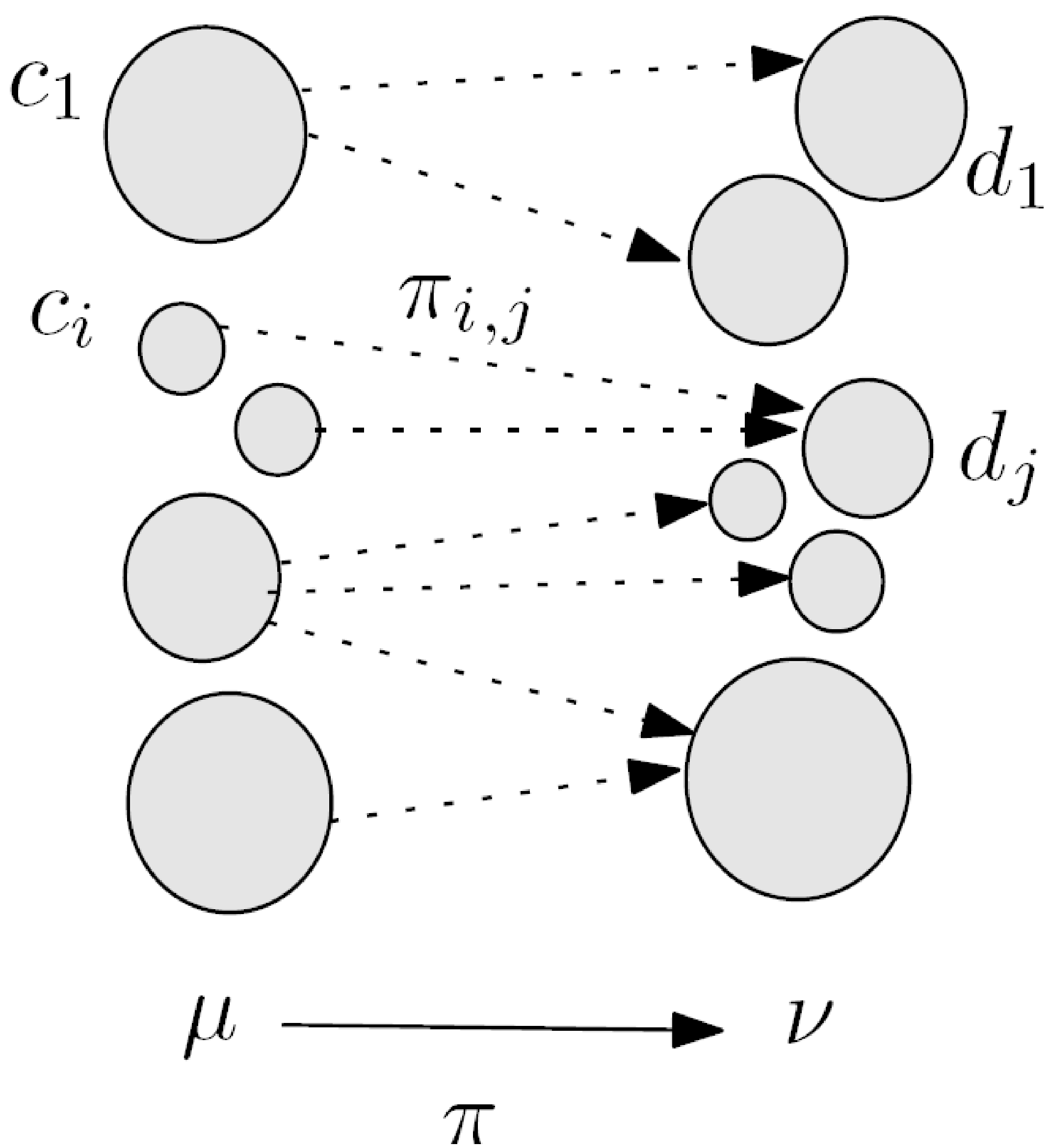
Replacing compact sets by measures

A **measure** μ is a mass distribution on $\mathbb{R}^d$:
mathematically, it is defined as a map μ that takes a (Borel) subset $B \subset \mathbb{R}^d$ and outputs a nonnegative number $\mu(B)$. Moreover we ask that if (B_i) are disjoint subsets, $\mu\left(\bigcup_{i\in\mathbb{N}} B_i\right) = \sum_{i\in\mathbb{N}} \mu(B_i)$.

- $\mu(B)$ corresponds to to the mass of μ contained in B
- a point cloud $C = \{p_1, \ldots, p_n\}$ defines a measure $\mu_C = \frac{1}{n}\sum_i \delta_{p_i}$
- the volume form on a k-dimensional submanifold M of $\mathbb{R}^d$ defines a measure $\mathrm{vol}_{k|M}$.
- etc...

Distance between measures

The **Wasserstein distance** $d_W(\mu,\nu)$ between two probability measures μ,ν quantifies the optimal cost of pushing μ onto ν, the cost of moving a small mass dx from x to y being $\|x-y\|^2 dx$.



1. μ and ν are discrete measures: $\mu = \sum_i c_i \delta_{x_i}$, $\nu = \sum_j d_j \delta_{y_j}$ with $\sum_j d_j = \sum_i c_i$.
2. *Transport plan*: set of coefficients $\pi_{ij} \geq 0$ with $\sum_i \pi_{ij} = d_j$ and $\sum_j \pi_{ij} = c_i$.
3. Cost of a transport plan
   $$C(\pi) = \left(\sum_{ij} \|x_i - y_j\|^2 \pi_{ij} \right)^{1/2}$$
4. $d_W(\mu,\nu) := \inf_\pi C(\pi)$

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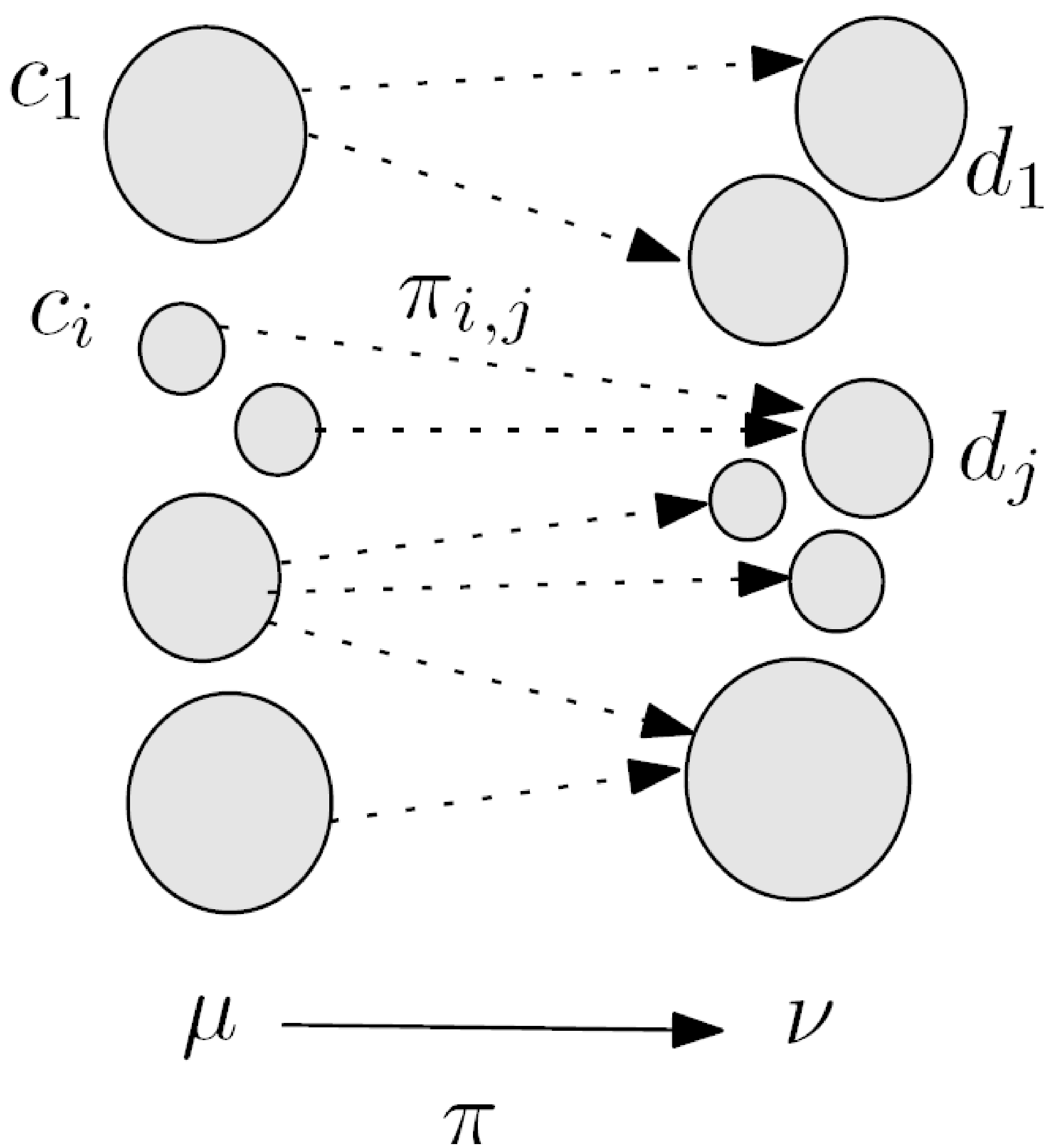
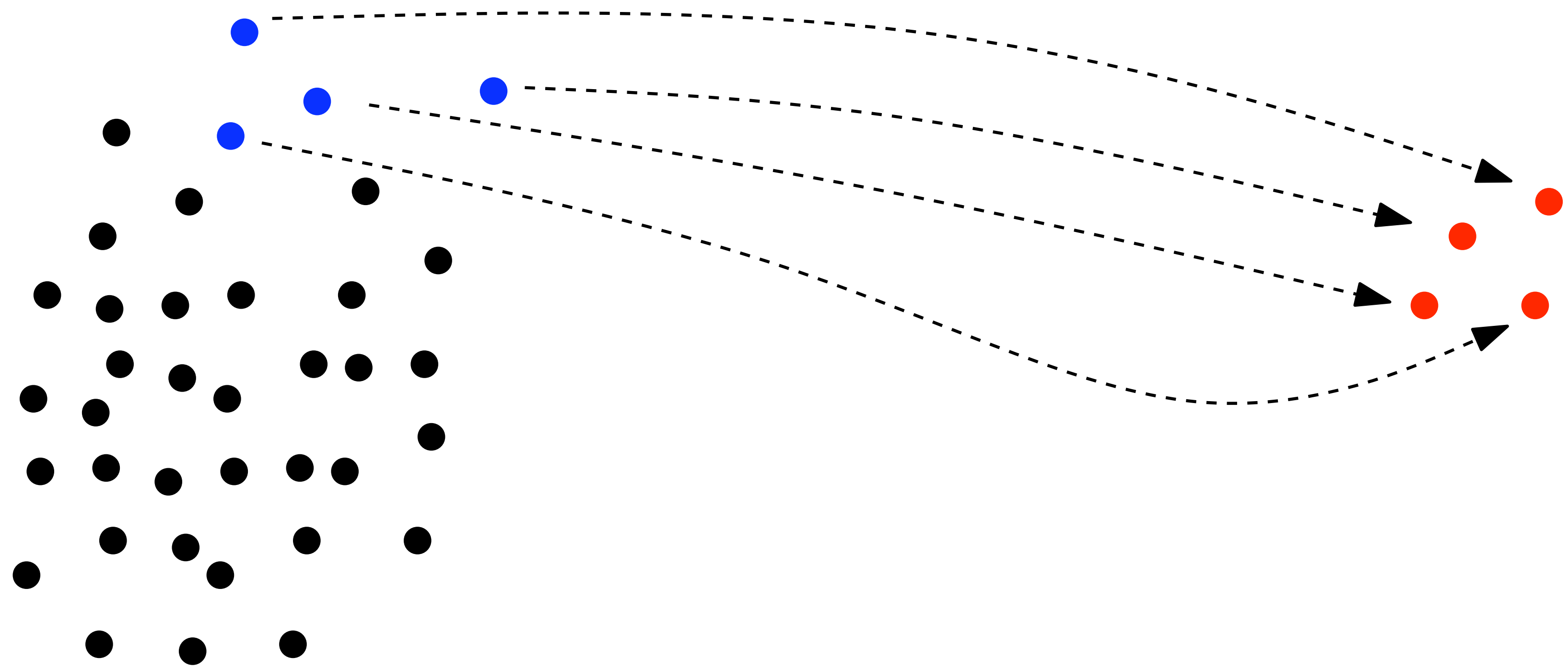


1. μ and ν are proba measures in $\mathbb{R}^d$
2. *Transport plan*: π a proba measure on $\mathbb{R}^d \times \mathbb{R}^d$ s.t. $\pi(A \times \mathbb{R}^d) = \mu(A)$ and $\pi(\mathbb{R}^d \times B) = \nu(B)$.
3. Cost of a transport plan
   $C(\pi) = \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 d\pi(x, y) \right)^{\frac{1}{2}}$
4. $d_W(\mu, \nu) := \inf_\pi C(\pi)$

Wasserstein distance



Examples:

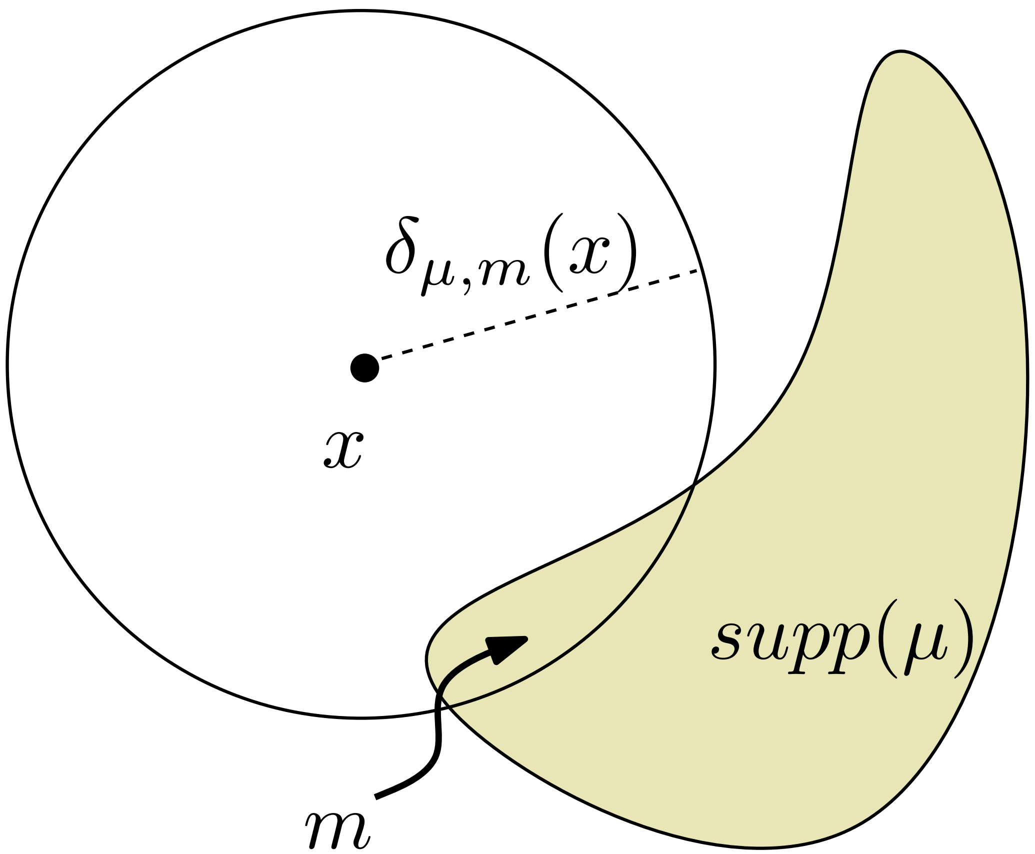
- If C_1 and C_2 are two point clouds, with $\#C_1 = \#C_2$, then $d_W(\mu_{C_1}, \mu_{C_2})$ is the square root of the cost of a minimal least-square matching between C_1 and C_2.

- If $C = \{p_1, \ldots, p_n\}$ is a point cloud, and $C' = \{p_1, \ldots, p_{n-k-1}, o_1, \ldots, o_k\}$ with $d(o_i, C) = R$, then

$$d_H(C, C') \geq R \qquad \text{but} \qquad d_W(\mu_C, \mu_{C'}) \leq \frac{k}{n}(R + \mathrm{diam}(C))$$

The distance to a measure

Distance function to a measure, first attempt:
Let $m \in]0,1[$ be a positive mass, and μ a probability measure on $\mathbb{R}^d$: $\delta_{\mu,m}(x) = \inf\{r > 0 : \mu(\mathbb{B}(x,r)) > m\}$.



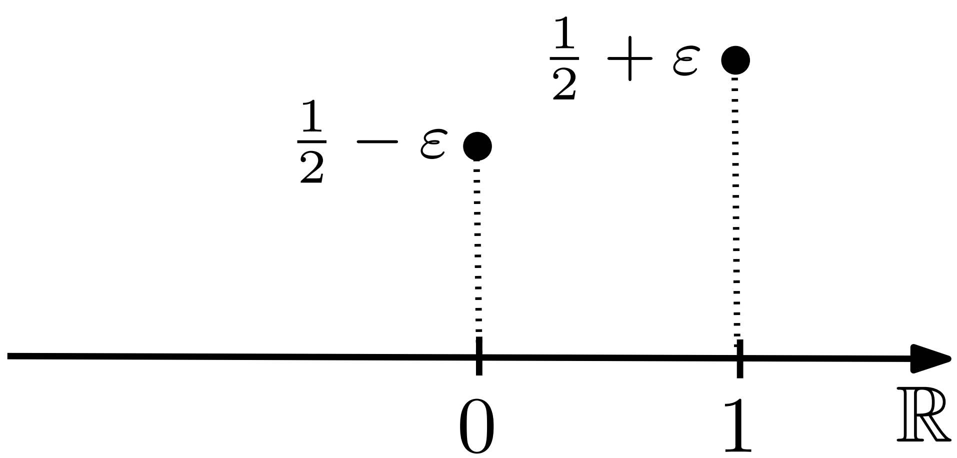
- $\delta_{\mu,m}$ is the smallest distance needed to capture a mass of at least m;
- Coincides with the distance to the k-th neighbor when $m = k/n$ and $\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{p_i}$:

$$\delta_{\mu,k/n}(\mu) = \|x - p_C^k(x)\|$$

Unstability of $\mu \mapsto \delta_{\mu,m}$

Distance function to a measure, first attempt:
Let $m \in]0,1[$ be a positive mass, and μ a probability measure on $\mathbb{R}^d$: $\delta_{\mu,m}(x) = \inf\{r > 0 : \mu(\mathbb{B}(x,r)) > m\}$.

Unstability under Wasserstein perturbations:



$$\mu_\varepsilon = (1/2 - \varepsilon)\delta_0 + (1/2 + \varepsilon)\delta_1$$

for $\varepsilon > 0 :\ \forall x < 0,\ \delta_{\mu_\varepsilon,1/2}(x) = |x - 1|$

for $\varepsilon = 0 :\ \forall x < 0,\ \delta_{\mu_0,1/2}(x) = |x - 0|$

Consequence: the map $\mu \mapsto \delta_{\mu,m} \in \mathcal{C}^0(\mathbb{R}^d)$ is discontinuous whatever the (reasonable) topology on $\mathcal{C}^0(\mathbb{R}^d)$.

The distance function to a measure

Definition: If μ is a probability measure on $\mathbb{R}^d$ and $m_0 > 0$, one let:

$$d_{\mu,m_0} : x \in \mathbb{R}^d \mapsto \left(\frac{1}{m_0} \int_0^{m_0} \delta_{\mu,m}^2(x) dm \right)^{1/2}$$

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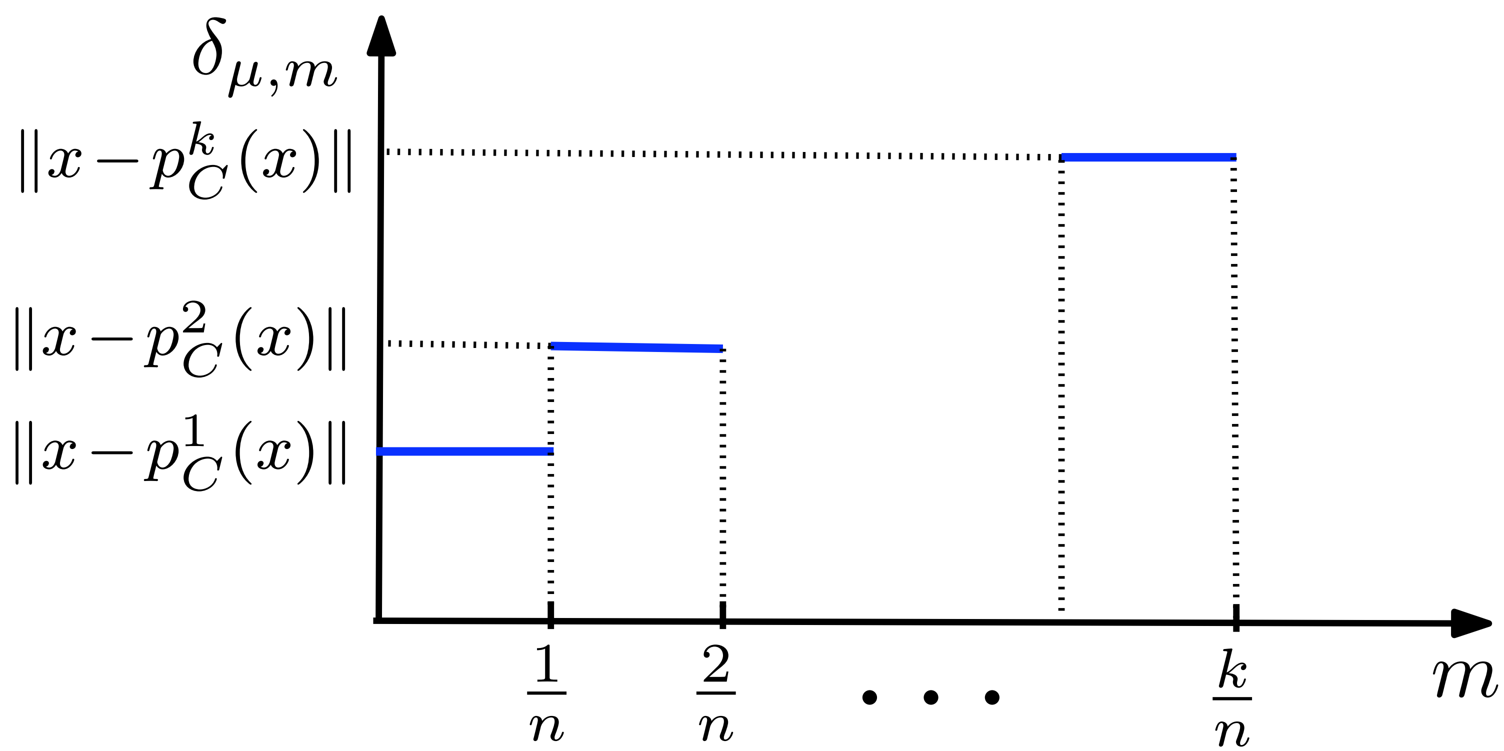

Example. Let $C = \{p_1, \dots, p_n\}$ and $\mu = \frac{1}{n}\sum_{i=1}^n \delta_{p_i}$. Let $p_C^k(x)$ denote the kth nearest neighbor to x in C, and set $m_0 = k_0/n$:

$$d_{\mu,m_0}(x) = \left(\frac{1}{k_0} \sum_{k=1}^{k_0} \|x - p_C^k(x)\|^2 \right)^{1/2}$$

Another expression for d_{μ,m_0}

$$d_{\mu,m_0}(x) = \min_{\tilde{\mu}} \left\{ d_W\left(\delta_x, \frac{1}{m_0}\tilde{\mu}\right) : \tilde{\mu}(\mathbb{R}^d) = m_0 \text{ and } \tilde{\mu} \leq \mu \right\}$$

"The projection submeasure": $\tilde{\mu}_{x,m_0}$ = the restriction of μ on the ball $B = \mathbb{B}(x, \delta_{\mu,m_0}(x))$, whose trace on the sphere ∂B has been rescaled so that the total mass of $\tilde{\mu}_{x,m_0}$ is m_0.

$$d^2_{\mu,m_0}(x) = \frac{1}{m_0} \int_{h \in \mathbb{R}^d} \|h - x\|^2 \, d\tilde{\mu}_{x,m_0} = d^2_W\left(\delta_x, \frac{1}{m_0}\tilde{\mu}_{x,m_0}\right)$$

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Proof:

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Proof:

Only one transport plan : $y \in \mathbb{R}^d \to x$

$$\int_{\mathbb{R}^d} \|h - x\|^2 d\tilde{\mu}(h)$$

Another expression for d_{μ,m_0}

$$d_{\mu,m_0}(x) = \min_{\tilde{\mu}} \left\{ d_W\left(\delta_x, \frac{1}{m_0}\tilde{\mu}\right) : \tilde{\mu}(\mathbb{R}^d) = m_0 \text{ and } \tilde{\mu} \leq \mu \right\}$$

Proof:

$$\int_{\mathbb{R}^d} \|h-x\|^2 d\tilde{\mu}(h) = \int_{\mathbb{R}_+} t^2 d\tilde{\mu}_x(t) = \int_0^{m_0} F_{\tilde{\mu}_x}^{-1}(m)^2 dm$$

pushforward of $\tilde{\mu}$ by the distance function to x.

$F_{\tilde{\mu}_x}(t) = \tilde{\mu}_x([0,t))$ is the cumulative function of $\tilde{\mu}_x$ and $F_{\tilde{\mu}_x}^{-1}(m) = \inf\{t \in \mathbb{R} : F_{\tilde{\mu}_x}(t) > m\}$ is its generalized inverse

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- $\tilde{\mu} \leq \mu \Rightarrow F_{\tilde{\mu}_x}(t) \leq F_{\mu_x}(t) \Rightarrow F_{\tilde{\mu}_x}^{-1}(m) \geq F_{\mu_x}^{-1}(m)$
- $F_{\tilde{\mu}_x}(t) = \mu(\mathbb{B}(x,t))$ and $F_{\tilde{\mu}_x}^{-1}(m) = \delta_{\mu,m}(x)$

$$\int_{\mathbb{R}^d} \|h - x\|^2 d\tilde{\mu}(h) \geq \int_0^{m_0} F_{\mu_x}^{-1}(m)^2 dm = \int_0^{m_0} \delta_{\mu,m}(x)^2 dm$$

Another expression for d_{μ,m_0}

$$d_{\mu,m_0}(x) = \min_{\tilde\mu} \left\{ d_W\left(\delta_x, \frac{1}{m_0}\tilde\mu\right) : \tilde\mu(\mathbb{R}^d) = m_0 \text{ and } \tilde\mu \leq \mu \right\}$$

Proof:

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Equality iff $F_{\tilde\mu_x}^{-1}(m) = F_{\mu_x}^{-1}(m)$ for almost every m
$\Rightarrow$ equality if $\tilde\mu = \tilde\mu_{x,m_0}$

$$\int_{\mathbb{R}^d} \|h-x\|^2 d\tilde\mu(h) \geq \int_0^{m_0} F_{\mu_x}^{-1}(m)^2 dm = \int_0^{m_0} \delta_{\mu,m}(x)^2 dm$$

Semiconcavity of d^2_{μ,m_0}

Theorem: Let μ be a probability measure in $\mathbb{R}^d$ and let $m_0 \in (0,1)$.

1. d^2_{μ,m_0} is 1-semiconcave, i.e. x $\in \mathbb{R}^d \mapsto \|x\|^2 - d^2_{\mu,m_0}$ is convex.
2. d^2_{μ,m_0} is differentiable almost everywhere in $\mathbb{R}^d$, with gradient defined by
$$\nabla_x d^2_{\mu,m_0} = \frac{2}{m_0} \int_{h \in \mathbb{R}^d} (x-h)\, d\tilde{\mu}_{x,m_0}(h)$$
3. the function $x \in \mathbb{R}^d \mapsto d_{\mu,m_0}(x)$ is 1-Lipschitz.

Example. Let $C = \{p_1, \ldots, p_n\}$ and $\mu = \frac{1}{n}\sum_{i=1}^n \delta_{p_i}$. Let $p_C^k(x)$ denote the kth nearest neighbor to x in C, and set $m_0 = k_0/n$:

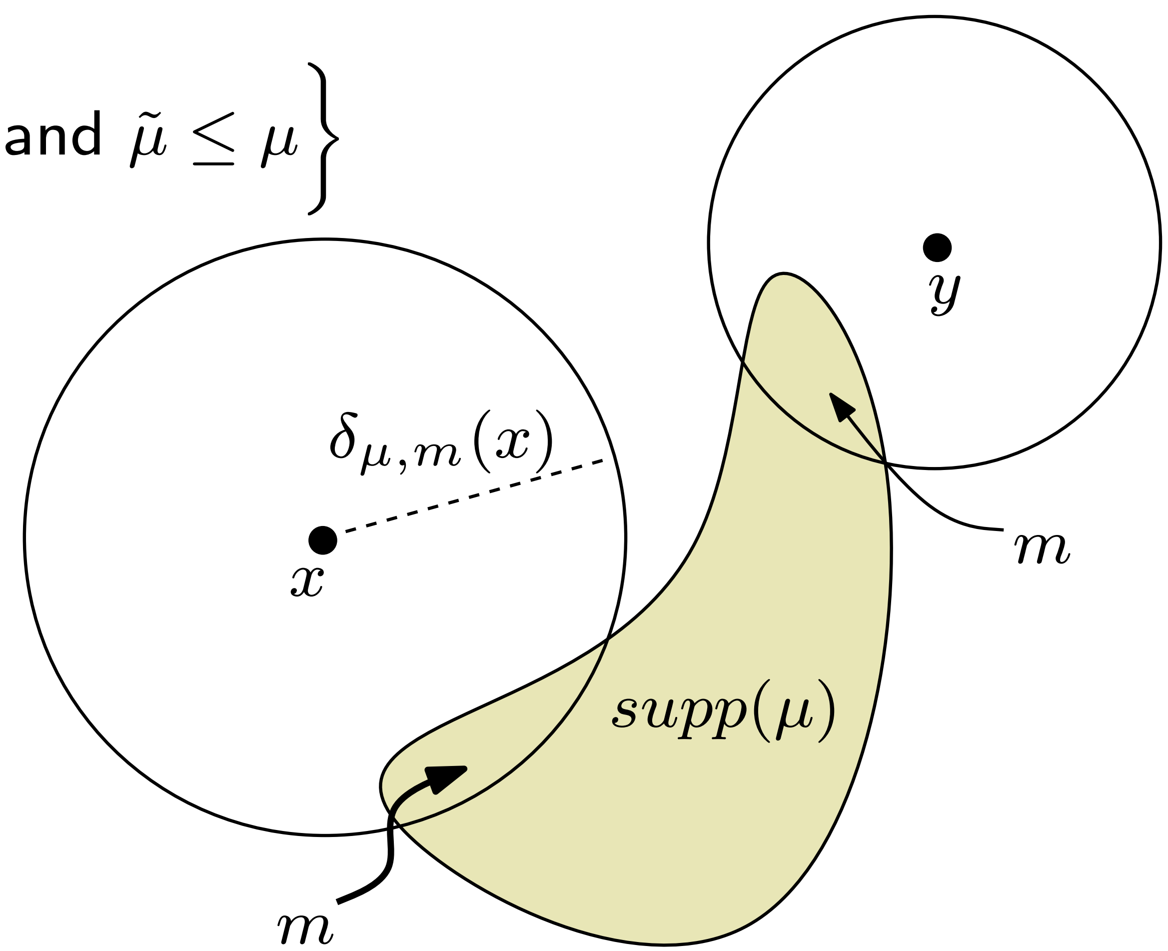
$$\nabla d^2_{\mu,m_0}(x) = 2 d_{\mu,m_0} \nabla d_{\mu,m_0} = \frac{2}{k_0} \sum_{k=1}^{k_0} (x - p_C^k(x))$$

Semiconcavity of d^2_{μ,m_0}

Proof:

$$d^2_{\mu,m_0}(y) = \frac{1}{m_0}\int_{h\in\mathbb{R}^d} \|y-h\|^2\, d\tilde{\mu}_{y,m_0}(h)$$
$$\leq \frac{1}{m_0}\int_{h\in\mathbb{R}^d} \|y-h\|^2\, d\tilde{\mu}_{x,m_0}(h)$$

$$d_{\mu,m_0}(x) = \min_{\tilde{\mu}} \left\{ d_W\left(\delta_x, \frac{1}{m_0}\tilde{\mu}\right) : \tilde{\mu}(\mathbb{R}^d) = m_0 \text{ and } \tilde{\mu} \leq \mu \right\}$$



Semiconcavity of d^2_{μ,m_0}

Proof:

$$\begin{aligned}
d^2_{\mu,m_0}(y) &= \frac{1}{m_0}\int_{h\in\mathbb{R}^d} \|y-h\|^2\, d\tilde{\mu}_{y,m_0}(h) \\
&\leq \frac{1}{m_0}\int_{h\in\mathbb{R}^d} \|y-h\|^2\, d\tilde{\mu}_{x,m_0}(h) \\
&= \frac{1}{m_0}\int_{h\in\mathbb{R}^d} \left(\|x-h\|^2 + 2\langle x-h, y-x\rangle + \|y-x\|^2\ \right)\, d\tilde{\mu}_{x,m_0}(h) \\
&= d^2_{\mu,m_0}(x) + \|y-x\|^2 + \langle V, y-x\rangle
\end{aligned}$$

with $V = \frac{2}{m_0}\int_{h\in\mathbb{R}^d}[x-h]\, d\tilde{\mu}_{x,m_0}(h)$.

Semiconcavity of d^2_{μ,m_0}

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&= \frac{1}{m_0}\int_{h\in\mathbb{R}^d} \left(\|x-h\|^2 + 2\langle x-h, y-x\rangle + \|y-x\|^2\right)\, d\tilde{\mu}_{x,m_0}(h) \\
&= d^2_{\mu,m_0}(x) + \|y-x\|^2 + \langle V, y-x\rangle
\end{aligned}$$

with $V = \frac{2}{m_0}\int_{h\in\mathbb{R}^d}[x-h]\, d\tilde{\mu}_{x,m_0}(h)$.

$$\Rightarrow (\|y\|^2 - d^2_{\mu,m_0}(y)) - (\|x\|^2 - d^2_{\mu,m_0}(x)) \geq \langle 2x - V, x-y\rangle$$

This is the gradient!

Stability of of $\mu \rightarrow d_{\mu,m_0}$

Theorem: If μ and ν are two probability measures on $\mathbb{R}^d$ and $m_0 > 0$, then $\|d_{\mu,m_0} - d_{\nu,m_0}\|_\infty \leq \frac{1}{\sqrt{m_0}} d_W(\mu, \nu)$.

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Proof: for $x \in \mathbb{R}^d$, let $\mu^x = (d_x)_\sharp \mu$, $\nu^x = (d_x)_\sharp \nu$ where $d_x : y \in \mathbb{R}^d \mapsto \|y - x\|$.

- $d_W(\mu^x, \nu^x) = \|F_{\mu^x}^{-1} - F_{\nu^x}^{-1}\|_{L^2([0,1])}$

Classical result for measures on $\mathbb{R}$

Stability of of $\mu \to d_{\mu,m_0}$

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- $d_W(\mu^x, \nu^x) = \|F_{\mu^x}^{-1} - F_{\nu^x}^{-1}\|_{L^2([0,1])}$ $+ \ \delta_{\mu^x,m}(0) = F_{\mu^x}^{-1}(m)$
- $\left| \sqrt{\int_0^{m_0} \delta^2_{\mu^x,m}(0) dm} - \sqrt{\int_0^{m_0} \delta^2_{\nu^x,m}(0) dm} \right| \leq d_W(\mu^x, \nu^x)$

Stability of of $\mu \to d_{\mu,m_0}$

Theorem: If μ and ν are two probability measures on $\mathbb{R}^d$ and $m_0 > 0$, then $\|d_{\mu,m_0} - d_{\nu,m_0}\|_\infty \leq \frac{1}{\sqrt{m_0}} d_W(\mu,\nu)$.

Proof: for $x \in \mathbb{R}^d$, let $\mu^x = (d_x)_\sharp \mu$, $\nu^x = (d_x)_\sharp \nu$ where $d_x : y \in \mathbb{R}^d \mapsto \|y - x\|$.

- $d_W(\mu^x, \nu^x) = \|F_{\mu^x}^{-1} - F_{\nu^x}^{-1}\|_{L^2([0,1])}$
- $\left| \sqrt{\int_0^{m_0} \delta^2_{\mu^x,m}(0)dm} - \sqrt{\int_0^{m_0} \delta^2_{\nu^x,m}(0)dm} \right| \leq d_W(\mu^x, \nu^x)$
- $d_W(\mu^x, \nu^x) \leq d_W(\mu, \nu)$ ⟵ Any transport plan π between μ and ν induces a transport plan $\pi_x = (d_x, d_x)_\sharp \pi$ between μ^x and ν^x

Stability of of $\mu \to d_{\mu,m_0}$

Theorem: If μ and ν are two probability measures on $\mathbb{R}^d$ and $m_0 > 0$, then $\|d_{\mu,m_0} - d_{\nu,m_0}\|_\infty \leq \frac{1}{\sqrt{m_0}} d_W(\mu,\nu)$.

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- $d_W(\mu^x, \nu^x) = \|F^{-1}_{\mu^x} - F^{-1}_{\nu^x}\|_{L^2([0,1])}$
- $\left| \sqrt{\int_0^{m_0} \delta^2_{\mu^x,m}(0) dm} - \sqrt{\int_0^{m_0} \delta^2_{\nu^x,m}(0) dm} \right| \leq d_W(\mu^x, \nu^x)$
- $d_W(\mu^x, \nu^x) \leq d_W(\mu, \nu)$
- $|d_{\mu,m_0}(x) - d_{\nu,m_0}(x)| \leq \frac{1}{\sqrt{m_0}} d_W(\mu^x, \nu^x) \leq \frac{1}{\sqrt{m_0}} d_W(\mu, \nu)$

To summarize

Theorem [C-Cohen-Steiner-Mérigot'09]

1. the function $x \mapsto d_{\mu,m_0}(x)$ is 1-Lipschitz;
2. the function $x \mapsto \|x\|^2 - d^2_{\mu,m_0}(x)$ is convex;
3. the map $\mu \mapsto d_{\mu,m_0}$ from probability measures to continuous functions is $\frac{1}{\sqrt{m_0}}$–Lipschitz, ie

$$\|d_{\mu,m_0} - d_{\mu',m_0}\|_\infty \leq \frac{1}{\sqrt{m_0}} d_W(\mu, \mu')$$

In practice: d_{μ,m_0} and $\nabla d_{\mu,m_0}$ are very easy to compute for $\mu = \sum_{i=1}^n \delta_{p_i}$, $C = \{p_1, \cdots p_n\} \subset \mathbb{R}^d$!

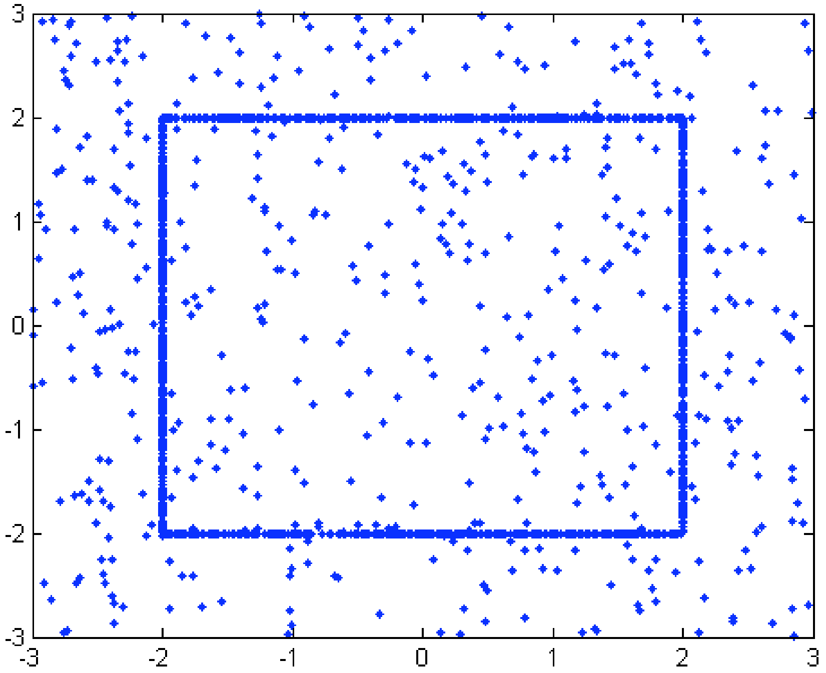
Consequences

Most of the topological and geometric inference for distance functions transpose to distance to a measure functions!

$\Longrightarrow$ This gives a way to associate robust geometric features to any probability measure in an Euclidean space:

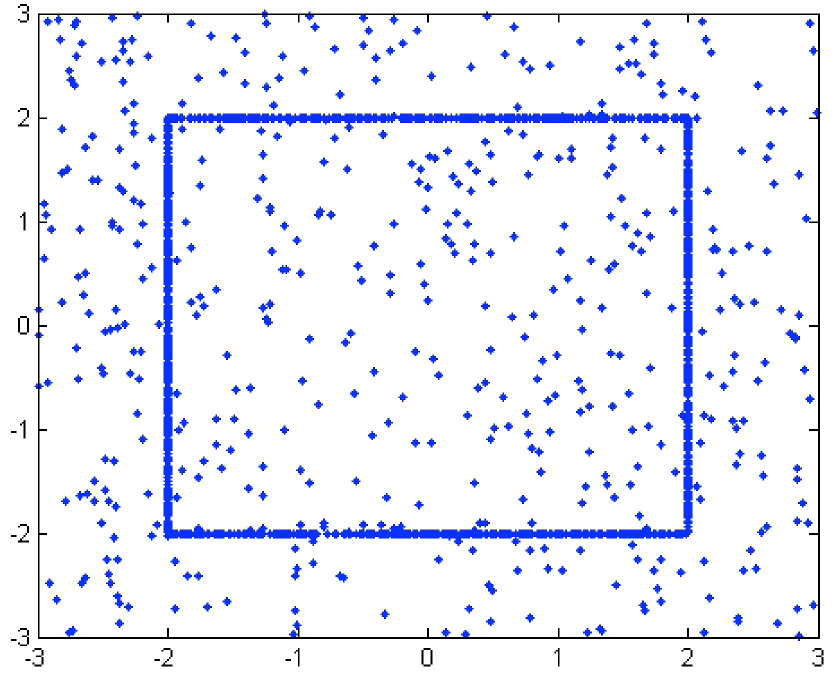
- offsets topology and geometry,
- analogous of the notions of medial axes,
- L^1 stability of $\nabla d_{\mu,m_0}$
- $\cdots$

Example: a square with outliers

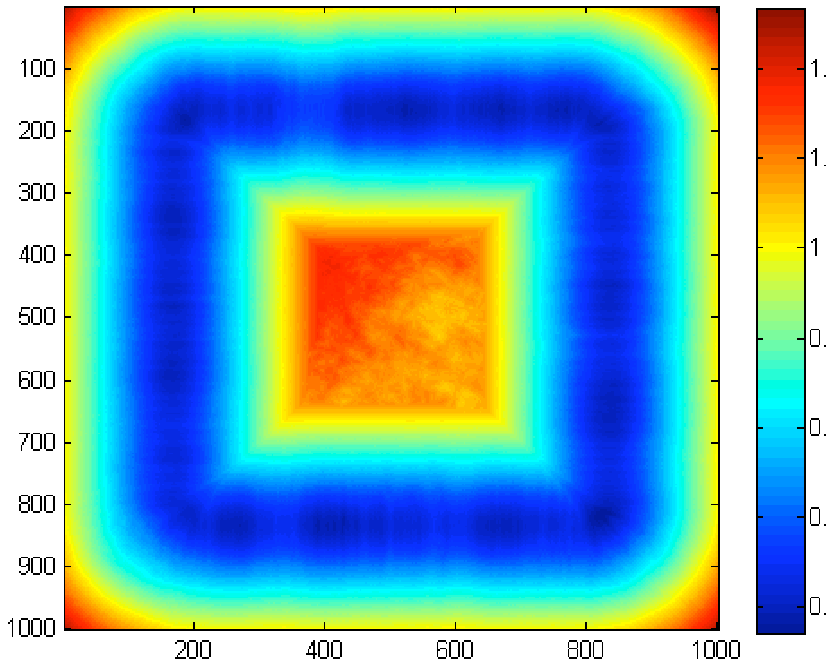


2300 points, 20% outliers

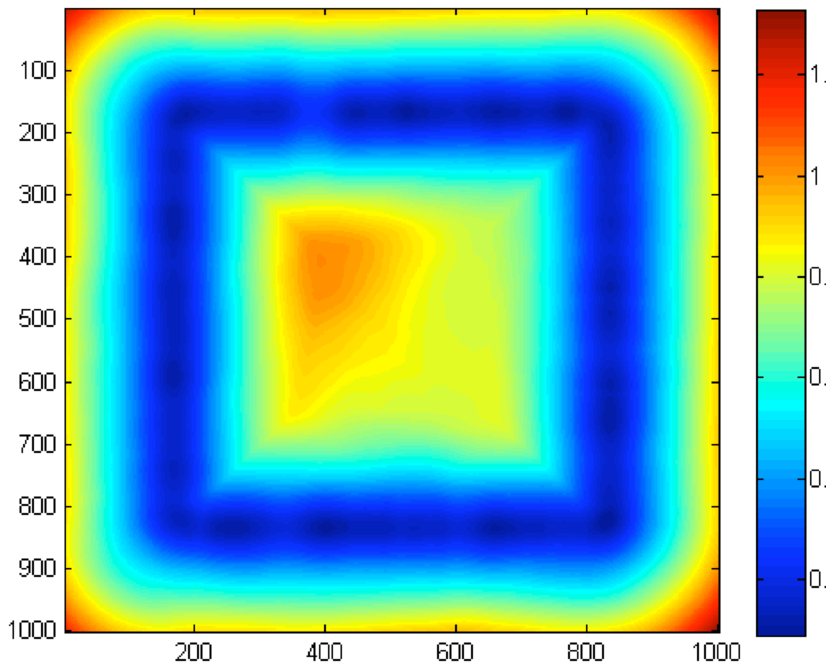
Example: a square with outliers



2300 points, 20% outliers



δ_{μ,m_0}, $m_0 = 0.023$ $(k = 50)$



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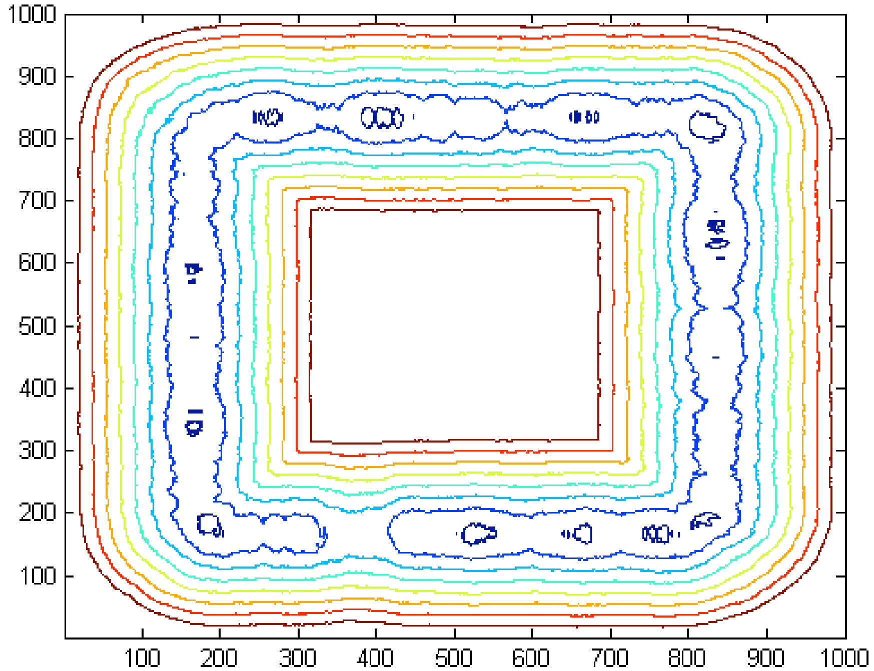

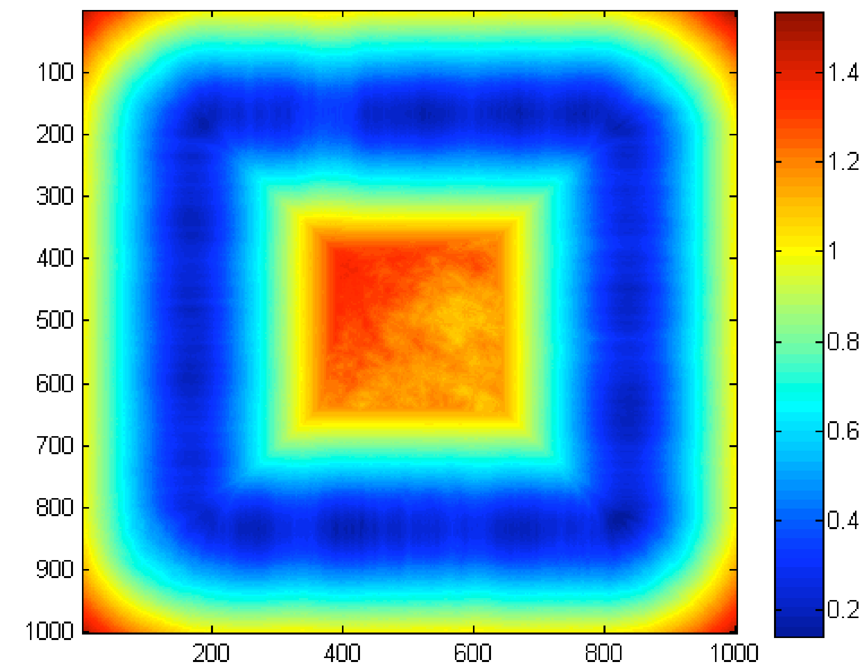

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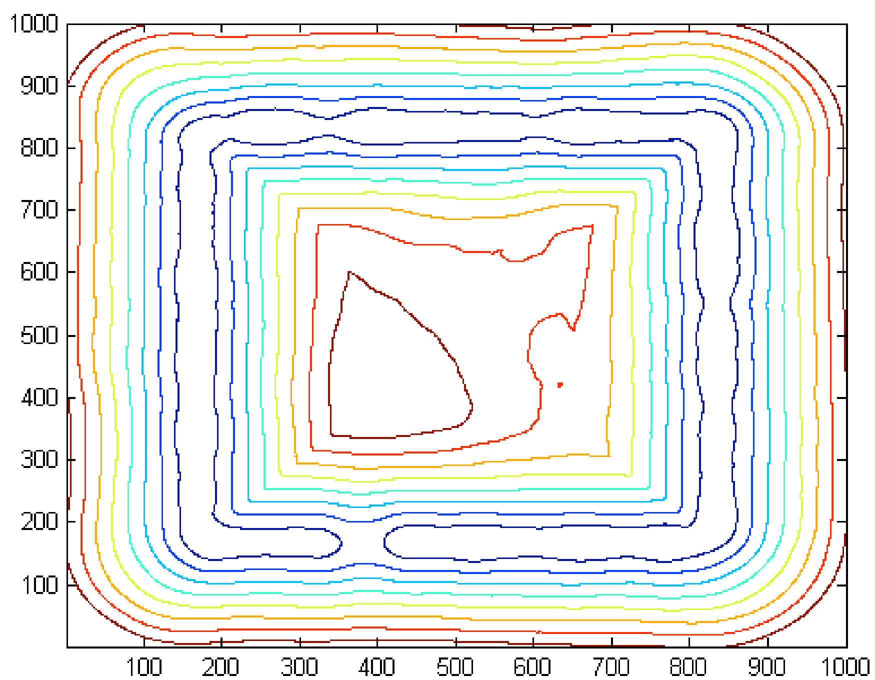

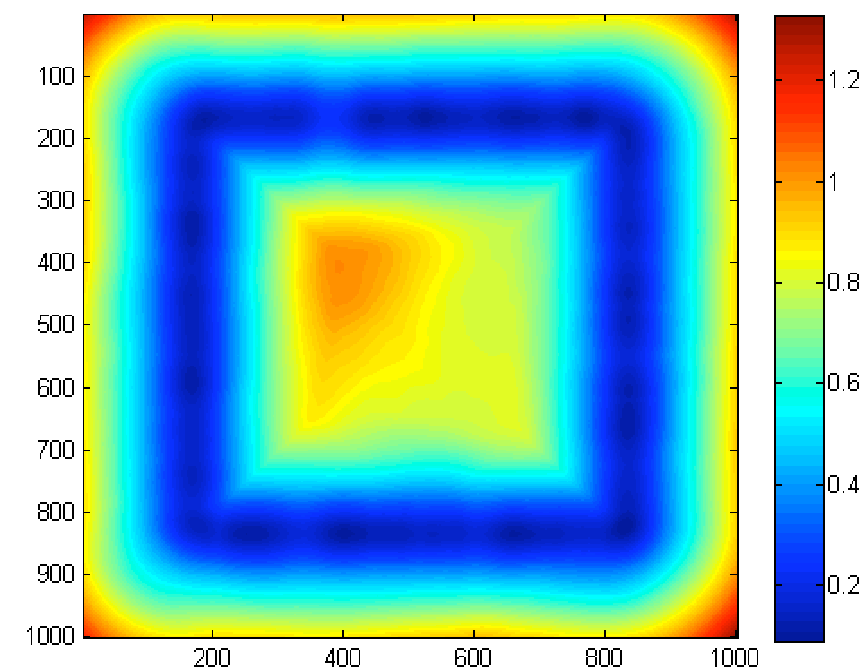

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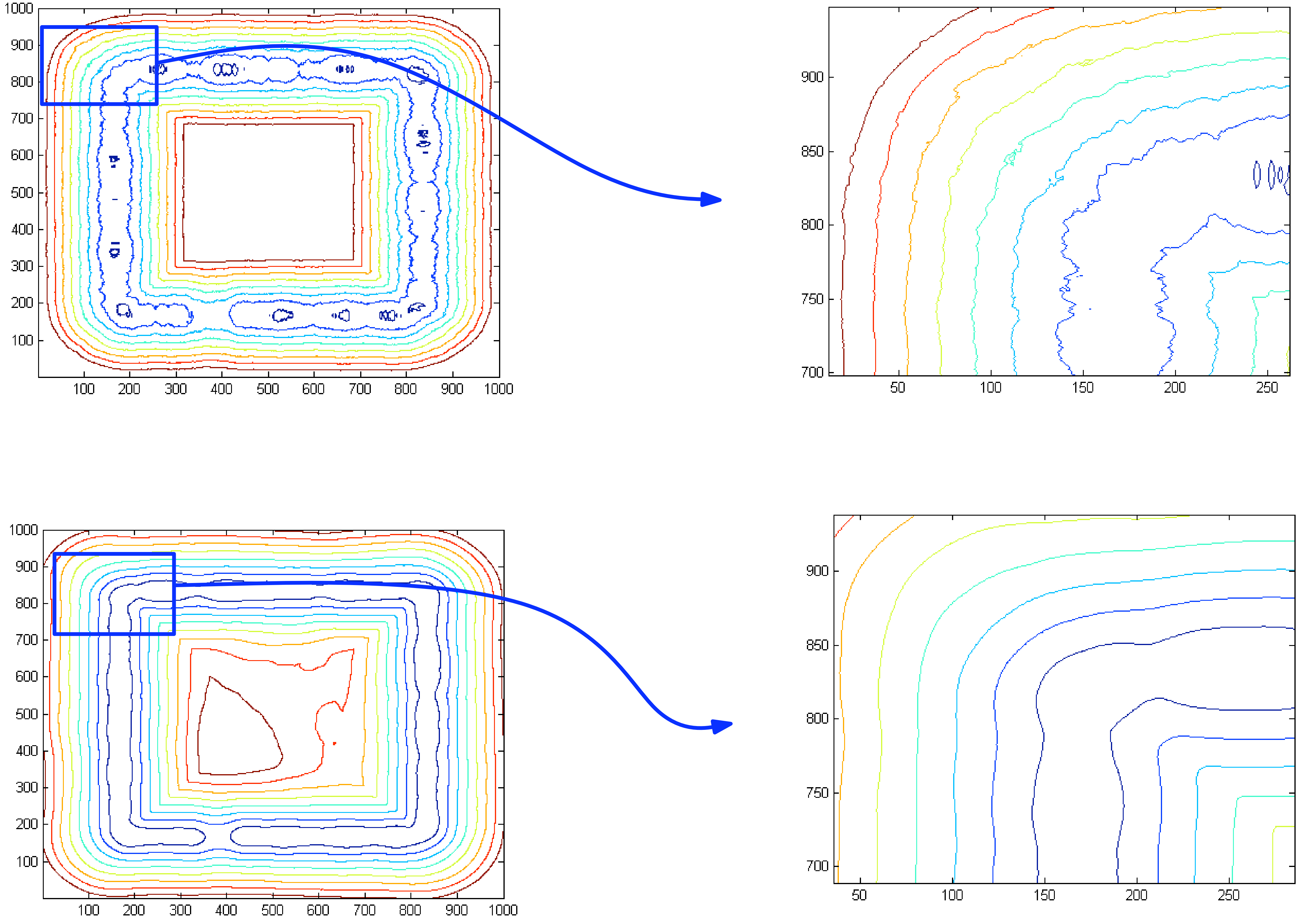
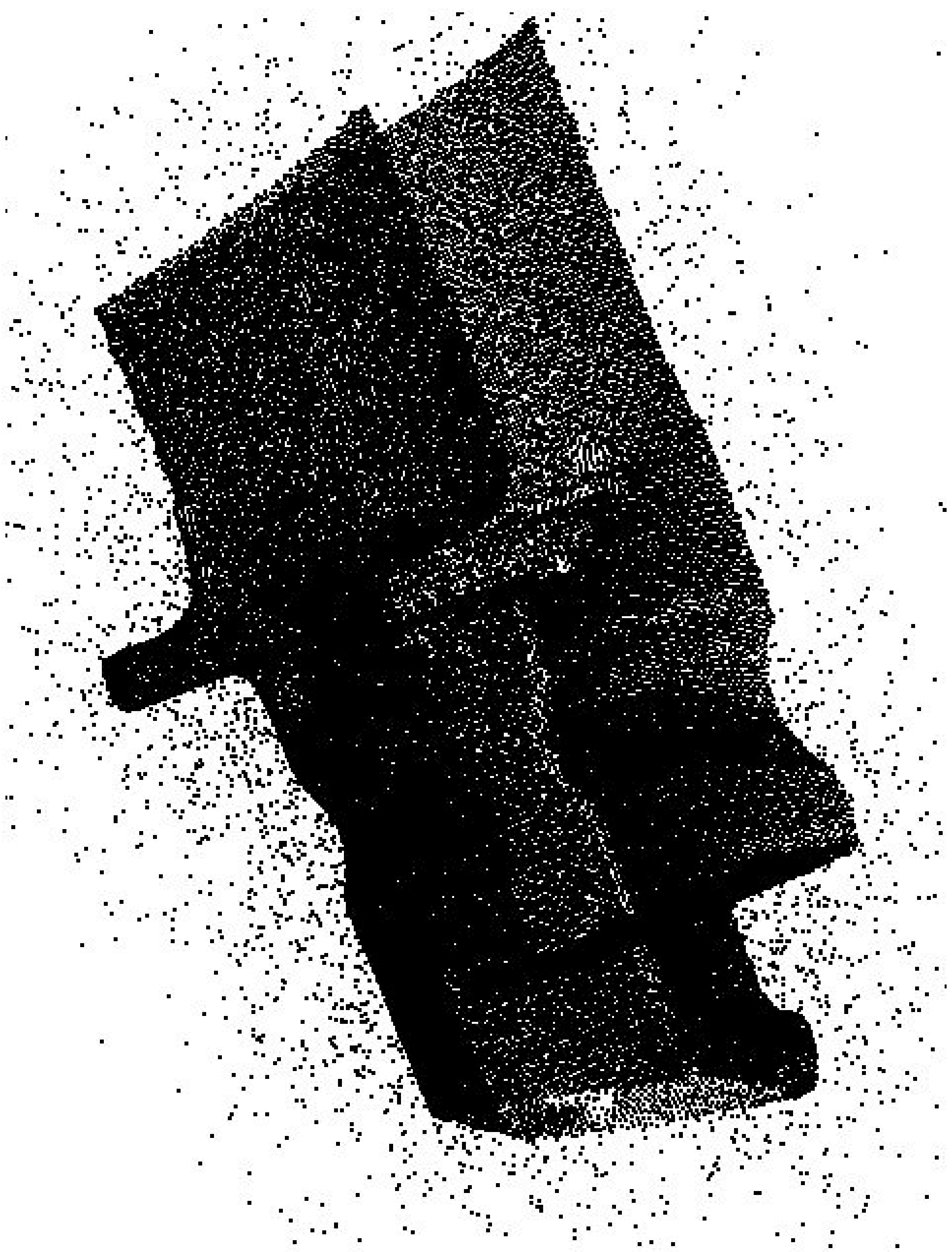
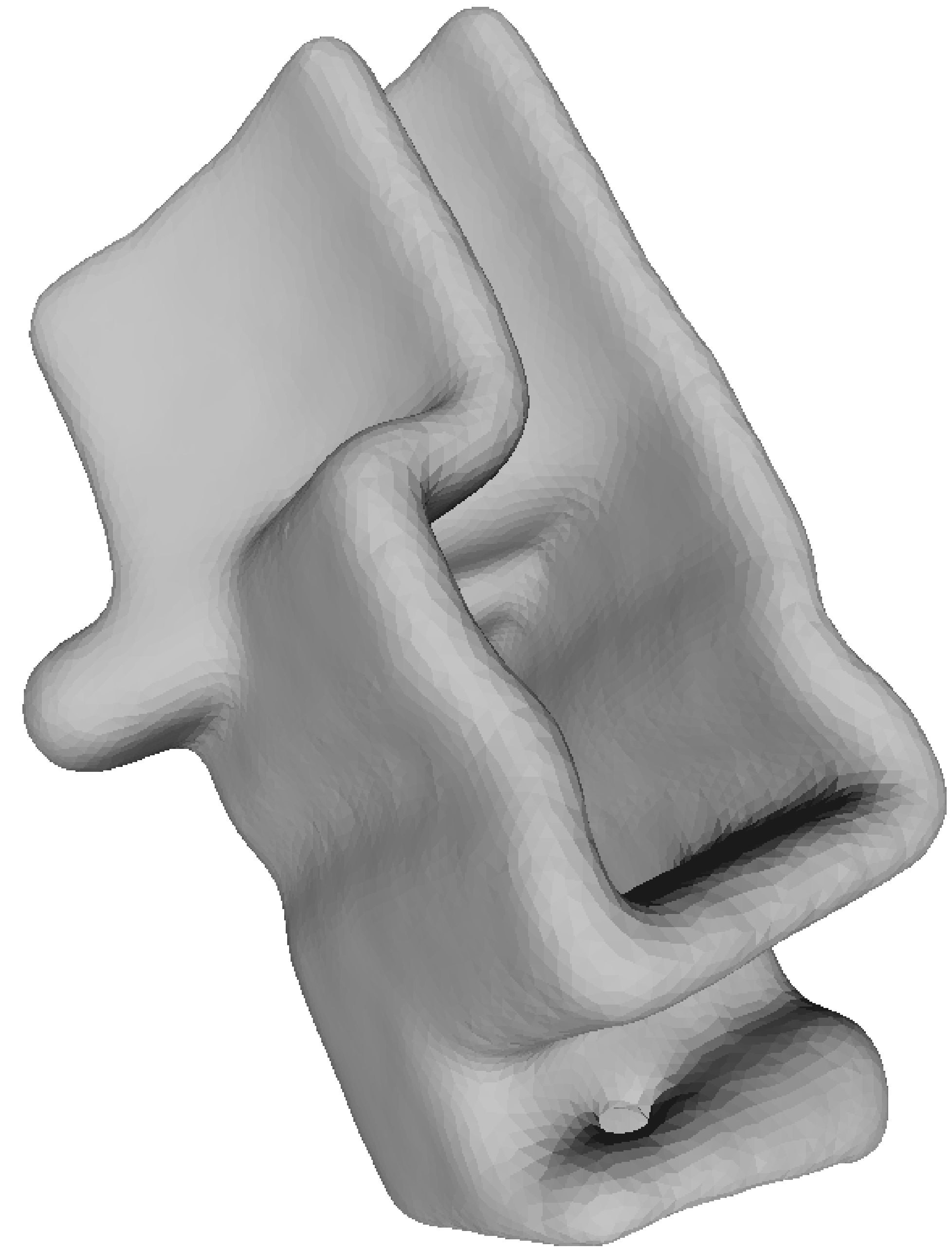


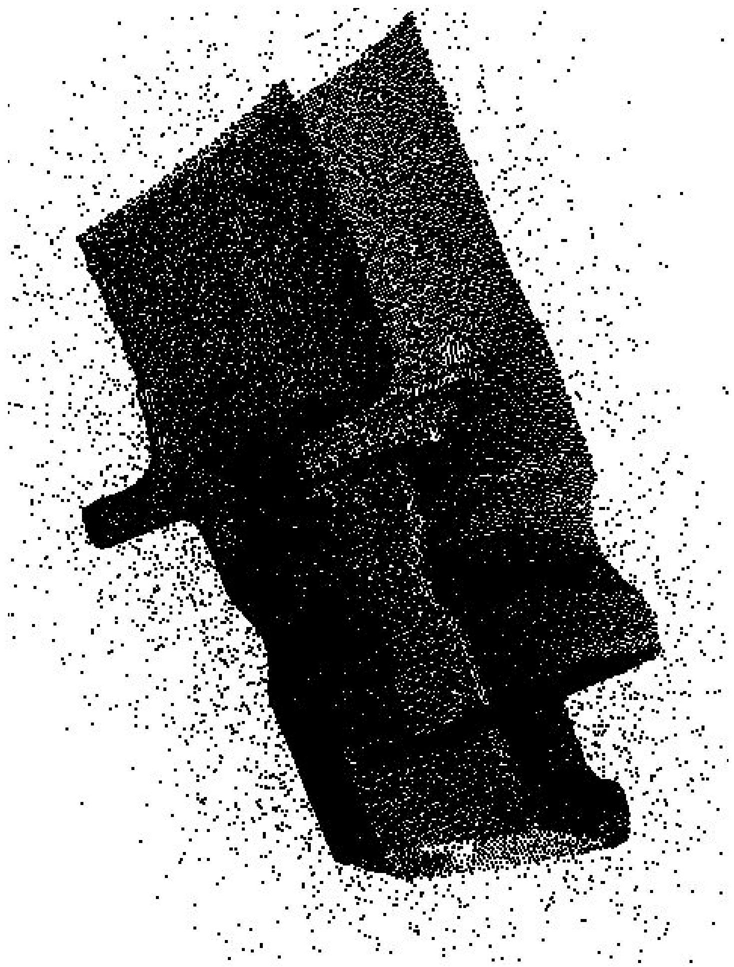
A 3D example

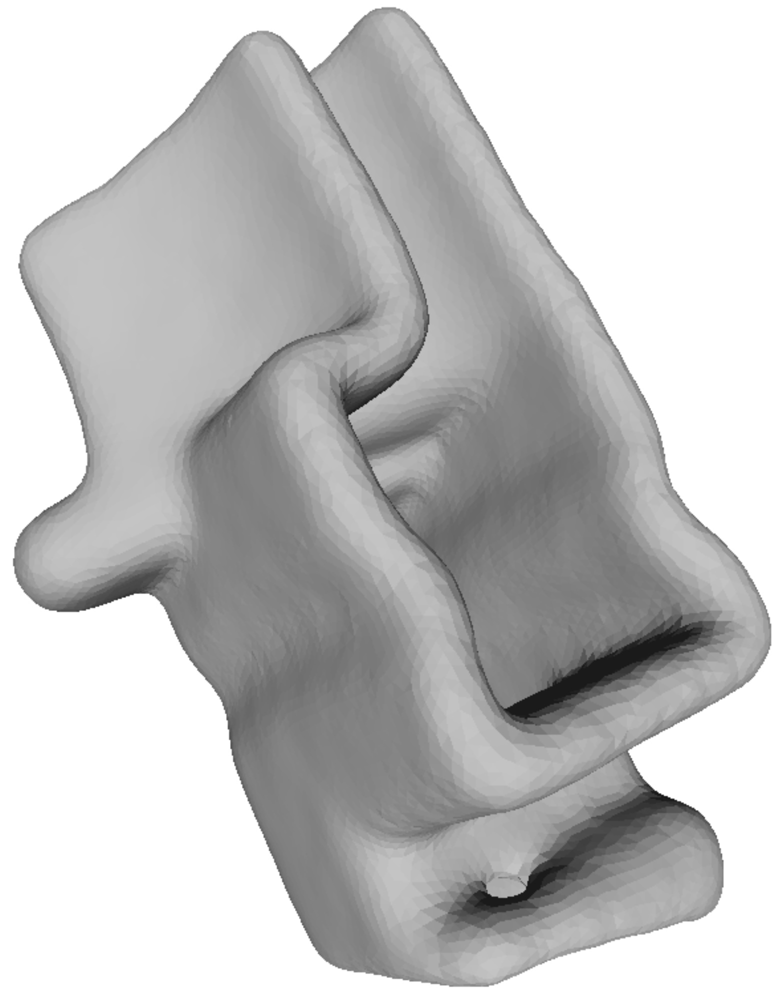




Reconstruction of an offset of a mechanical part from a noisy approximation with 10% outliers

A reconstruction theorem

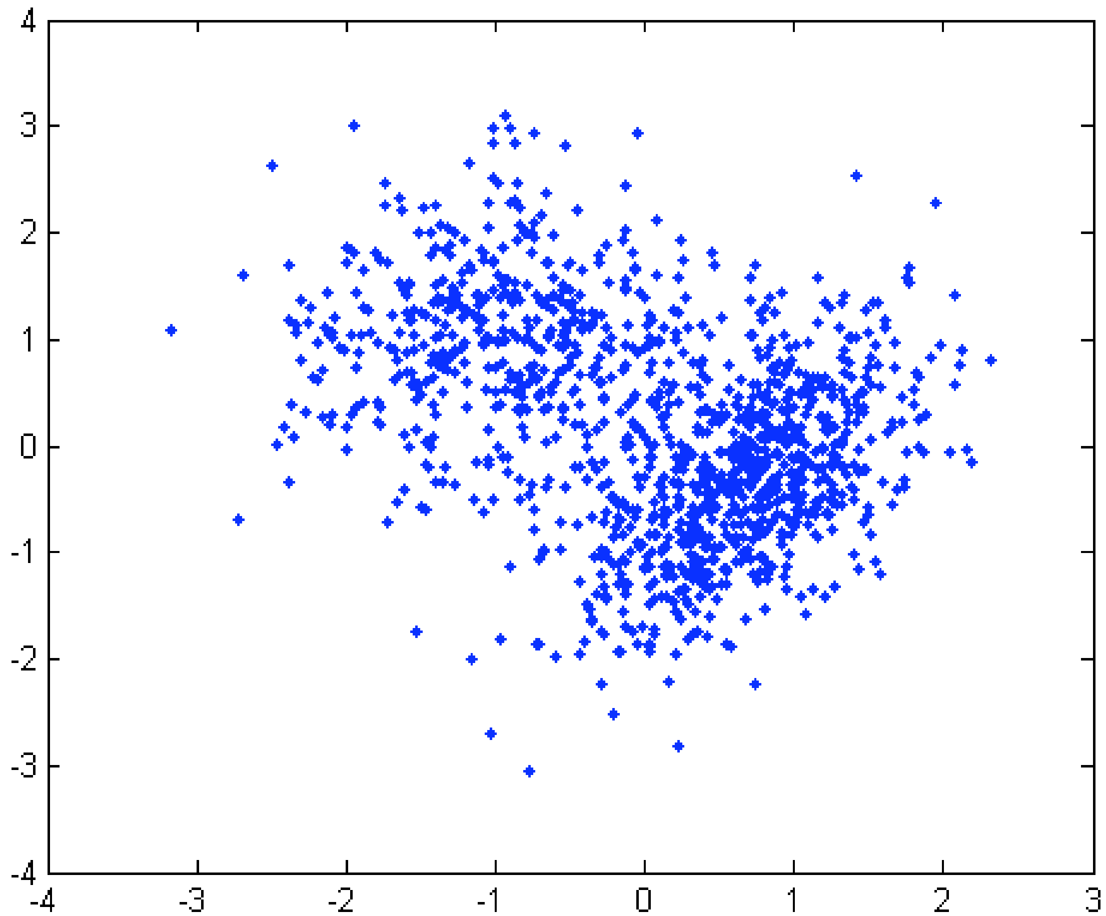




$\exists C > 0$ s.t. $\forall x \in K$, $\mu(\mathbb{B}(x,\varepsilon)) \geq C\varepsilon^k$ as soon as ε is small enough.

Theorem: Let μ be a probability measure *of dimension at most* $k > 0$ with compact support $K \subset \mathbb{R}^d$ such that $r_\alpha(K) > 0$ for some $\alpha \in (0,1]$. For any $0 < \eta < r_\alpha(K)$, there exists positive constants $m_1 = m_1(\mu,\alpha,\eta) > 0$ and $C = C(m_1) > 0$ such that:
for any $m_0 < m_1$ and any probability measure μ' such that $W_2(\mu,\mu') < C\sqrt{m_0}$, the sublevel set $d_{\mu',m_0}^{-1}((-\infty,\eta])$ is isotopic to the offsets $d_K^{-1}([0,r])$ of K for $0 < r < r_\alpha(K)$.

Comparison to kNN density estimation



$$\hat{\mu} = \frac{1}{1200} \sum_{i=1}^{1200} \delta_{p_i}$$

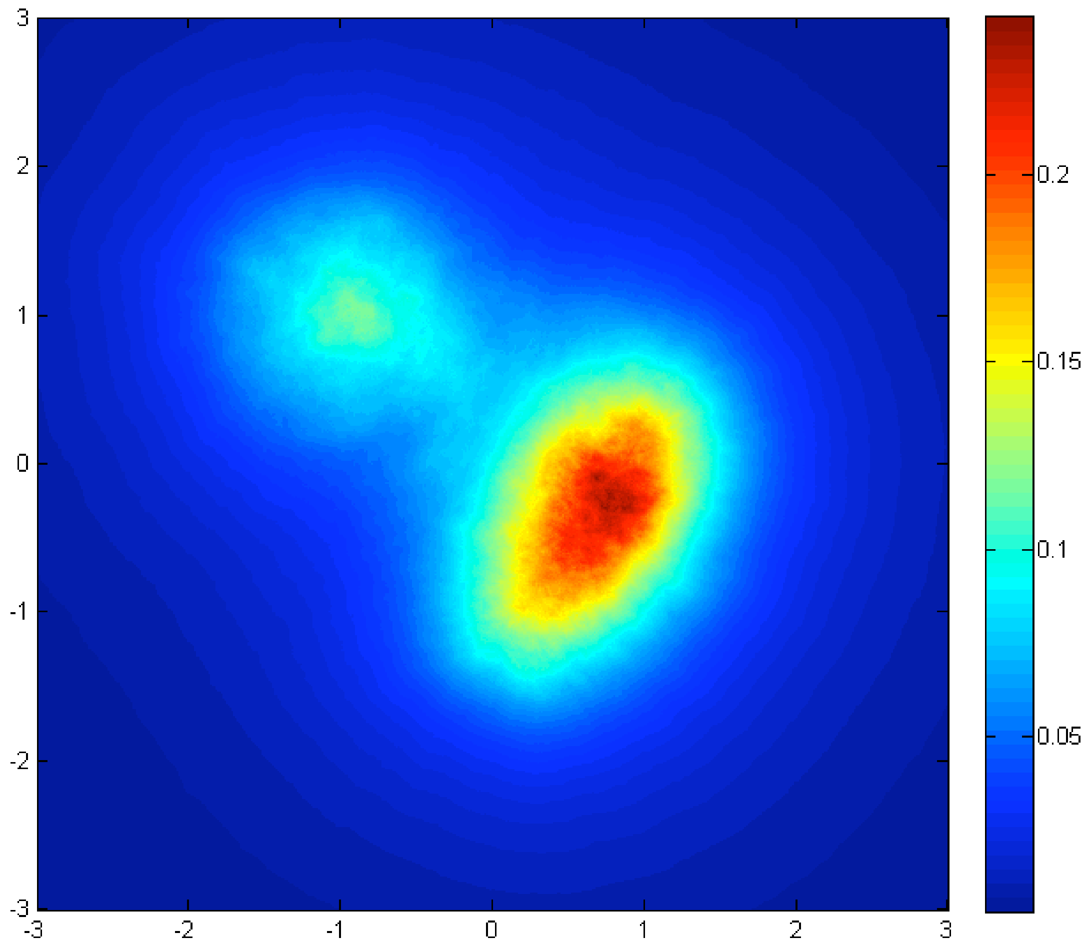
Data: 1200 points $p_1, \cdots, p_{1200}$

Density is estimated using

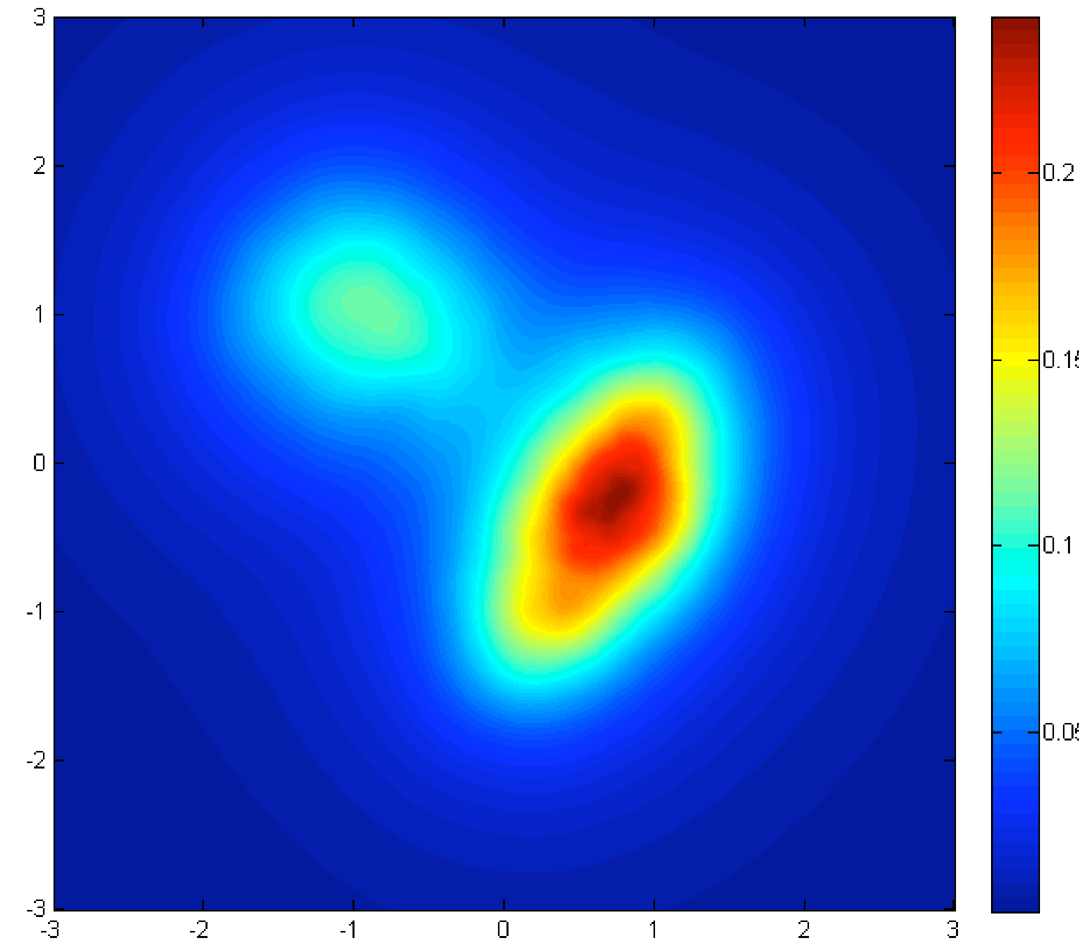
1. $x \mapsto \frac{m_0}{\omega_{d-1}(\delta_{\hat{\mu},m_0}(x))}$, $m_0 = 150/1200$ ($k = 150$) (Devroye-Wagner'77).

2. $\frac{m_0}{2\pi d_{\hat{\mu},m_0}(x)^2}$, $m_0 = 150/1200$ ($k = 150$).

Comparison to kNN density estimation



1.



2.

Density is estimated using

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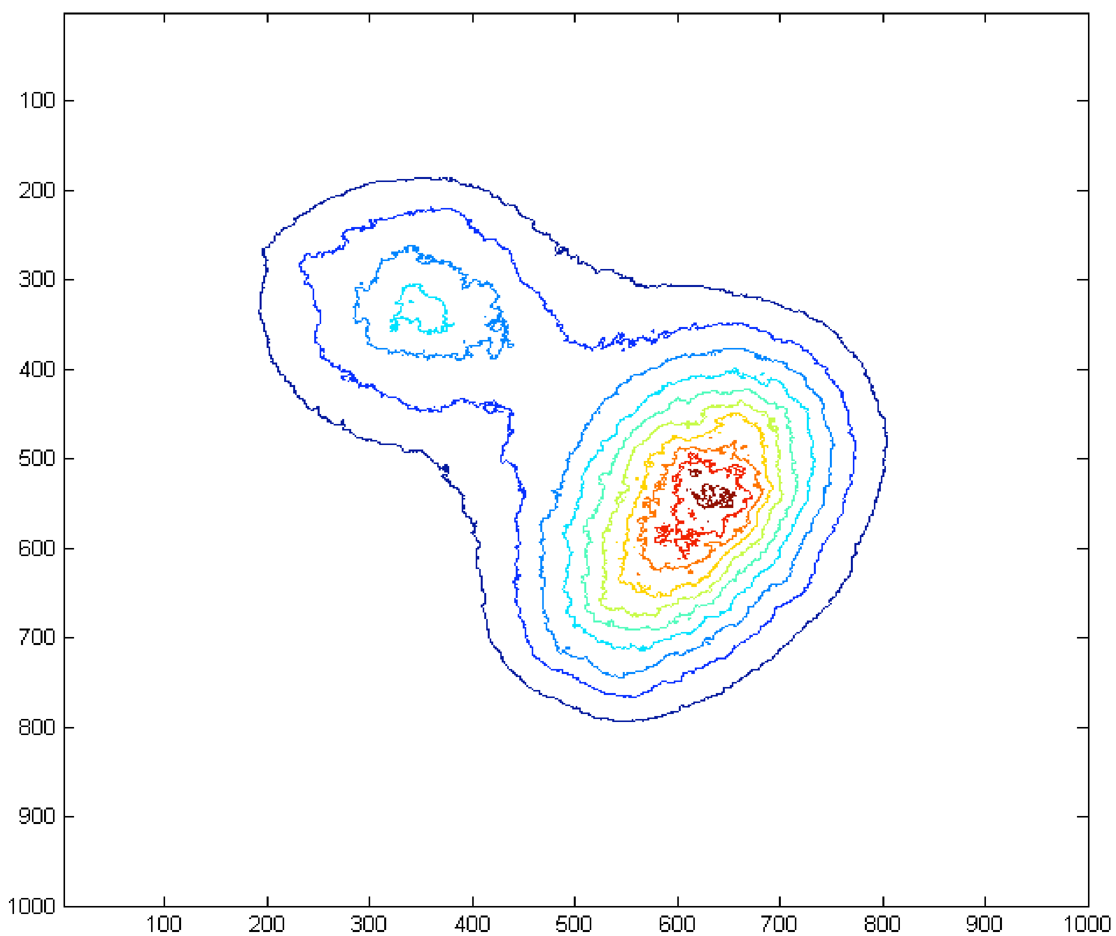

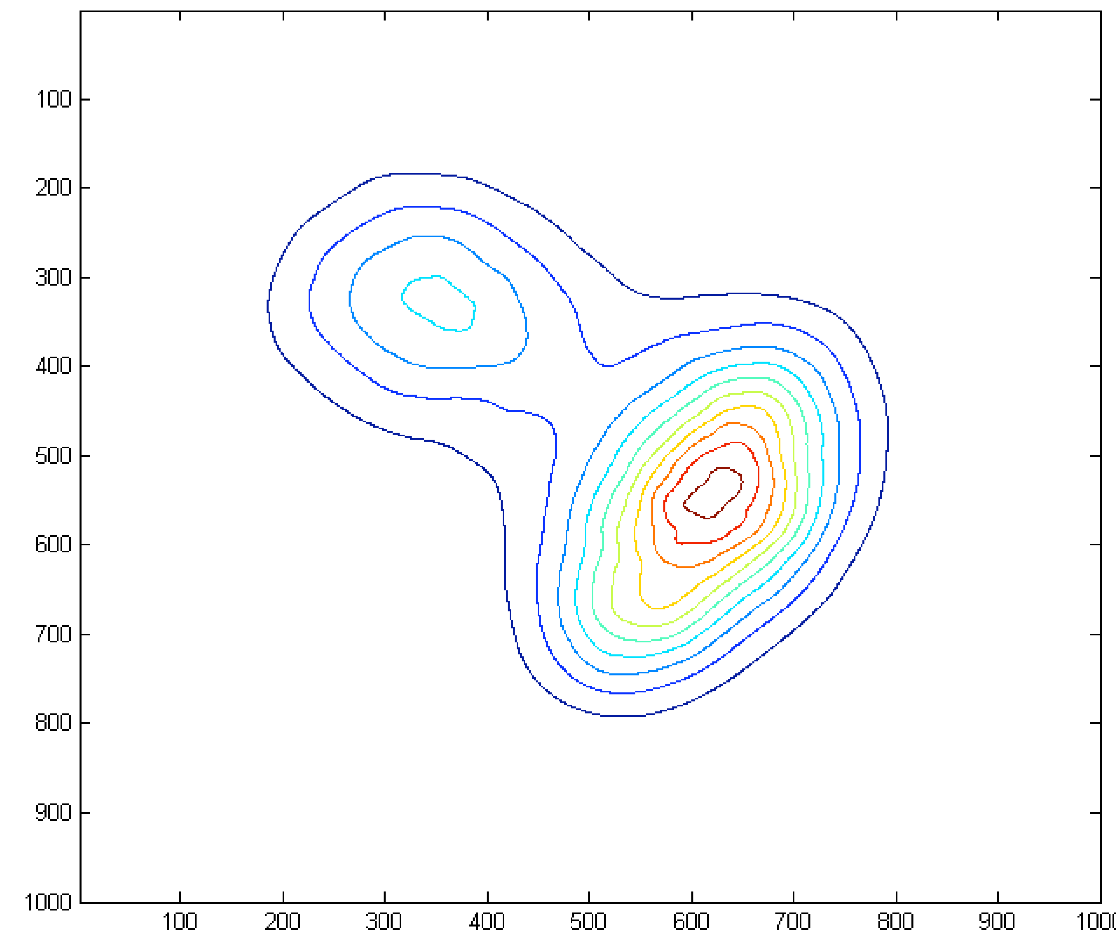

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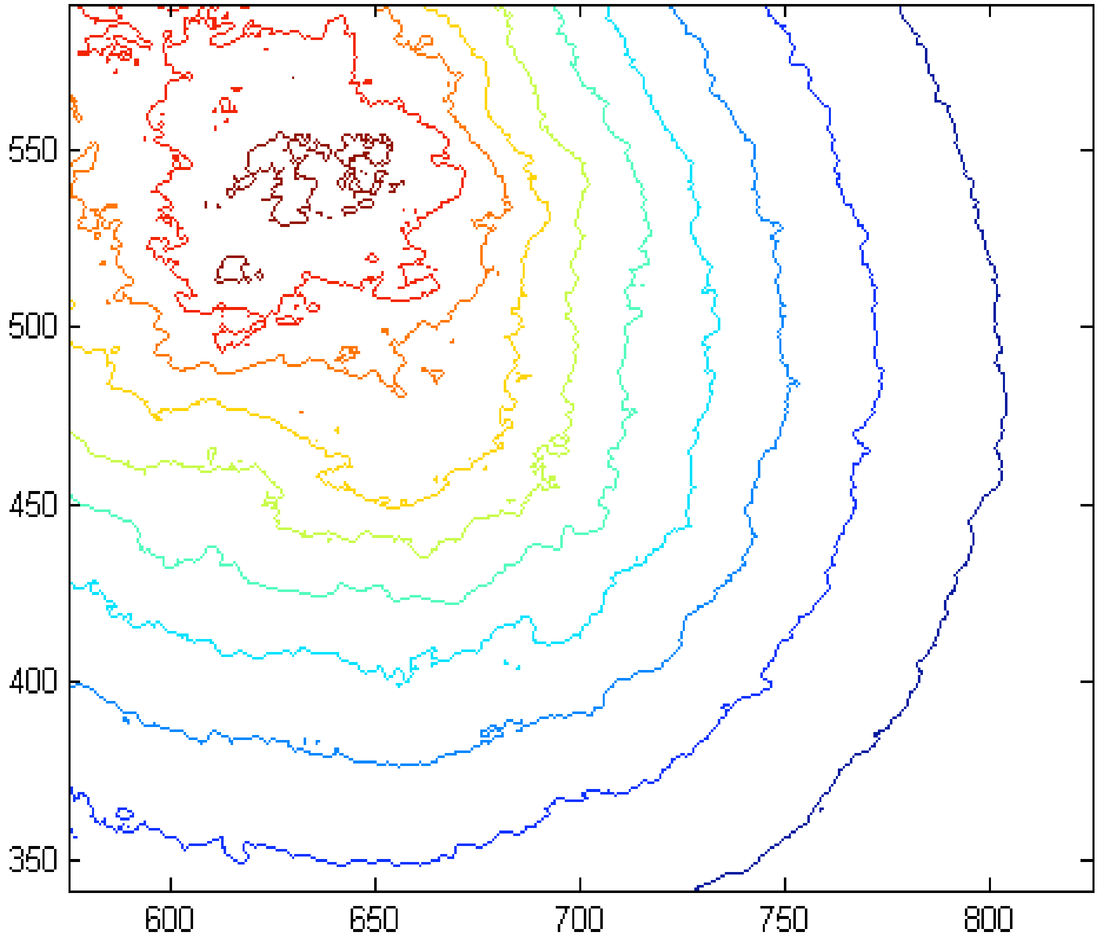

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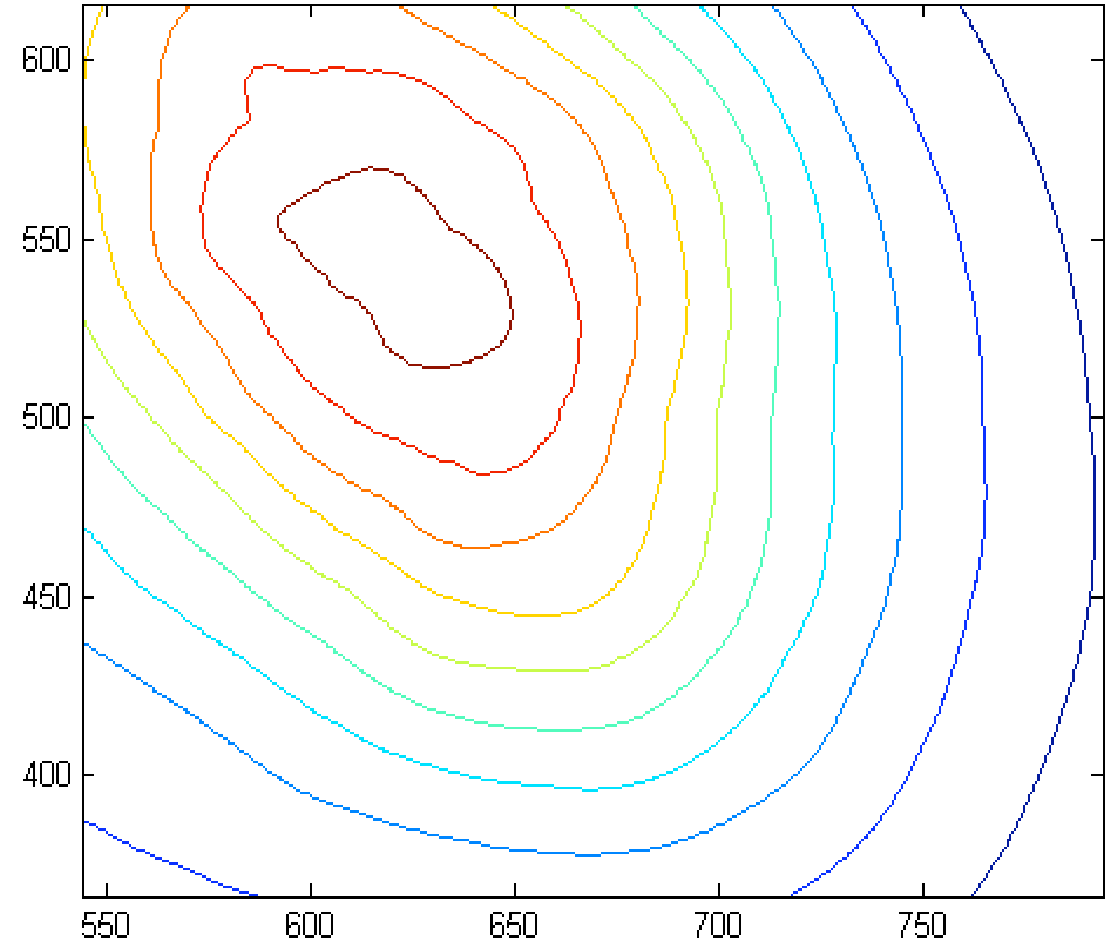

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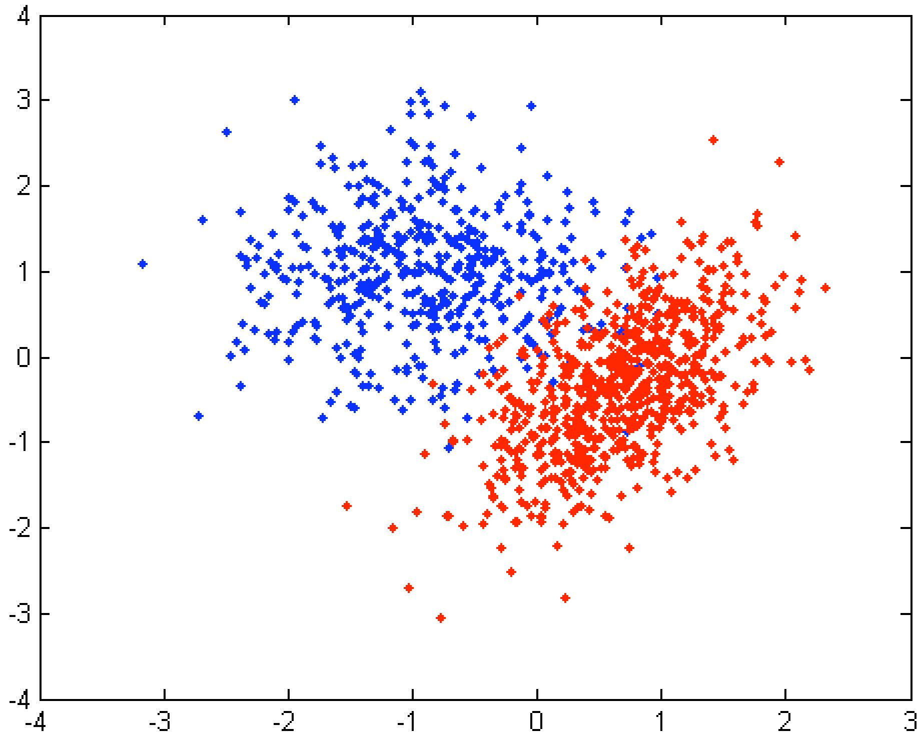
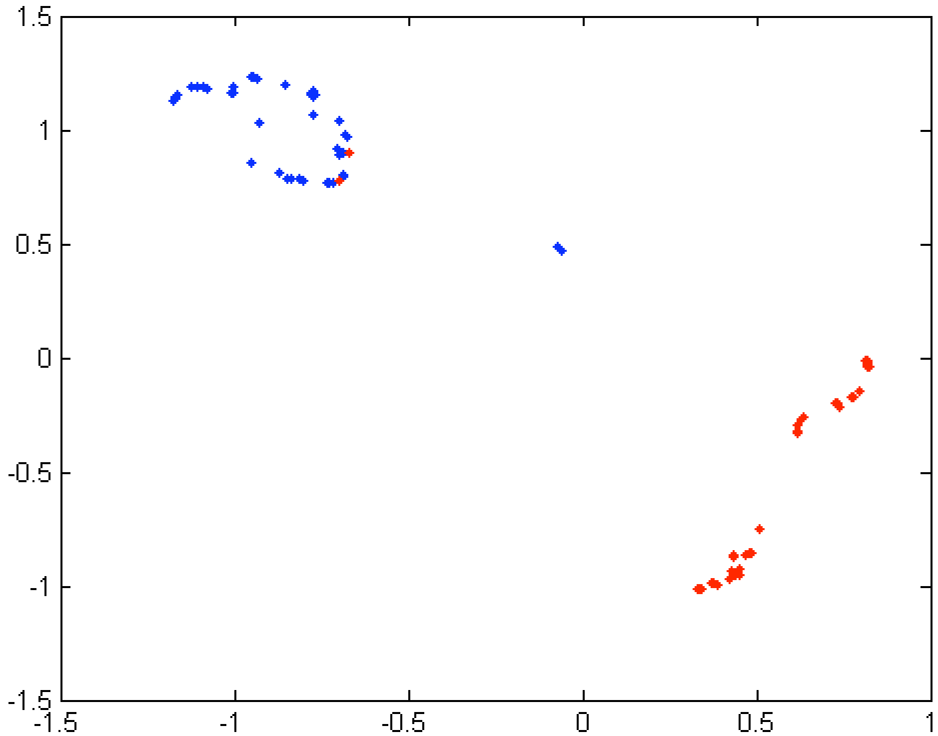
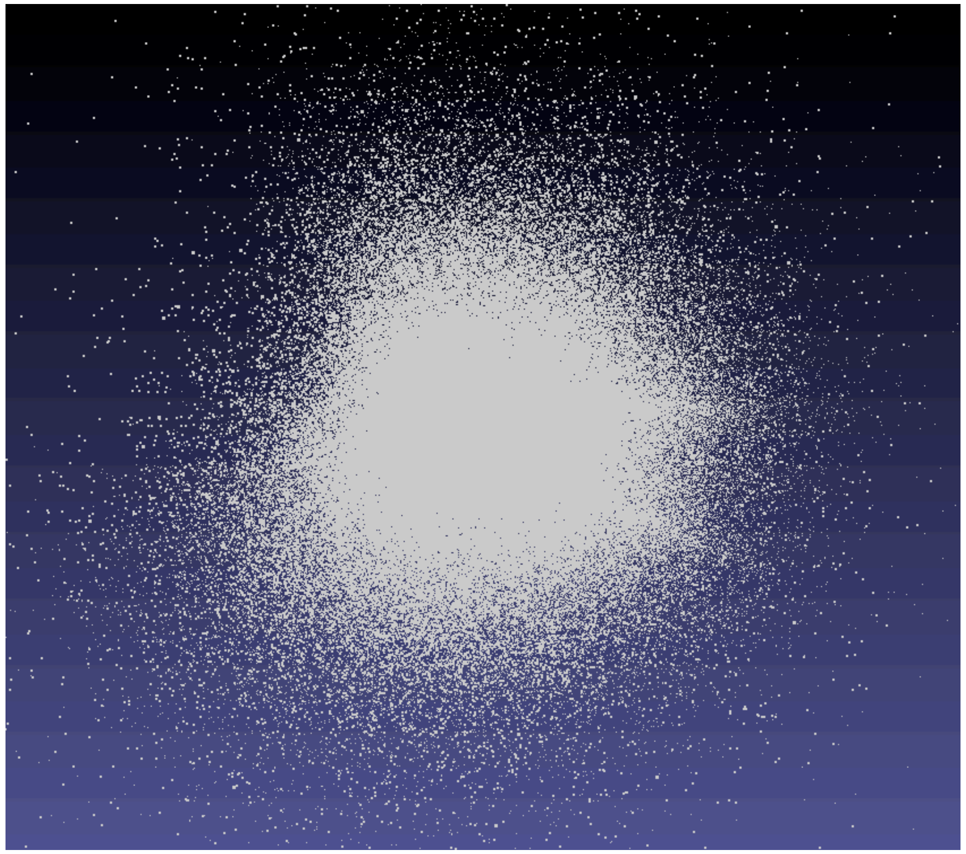
Pushing data along the gradient of d_{μ,m_0}

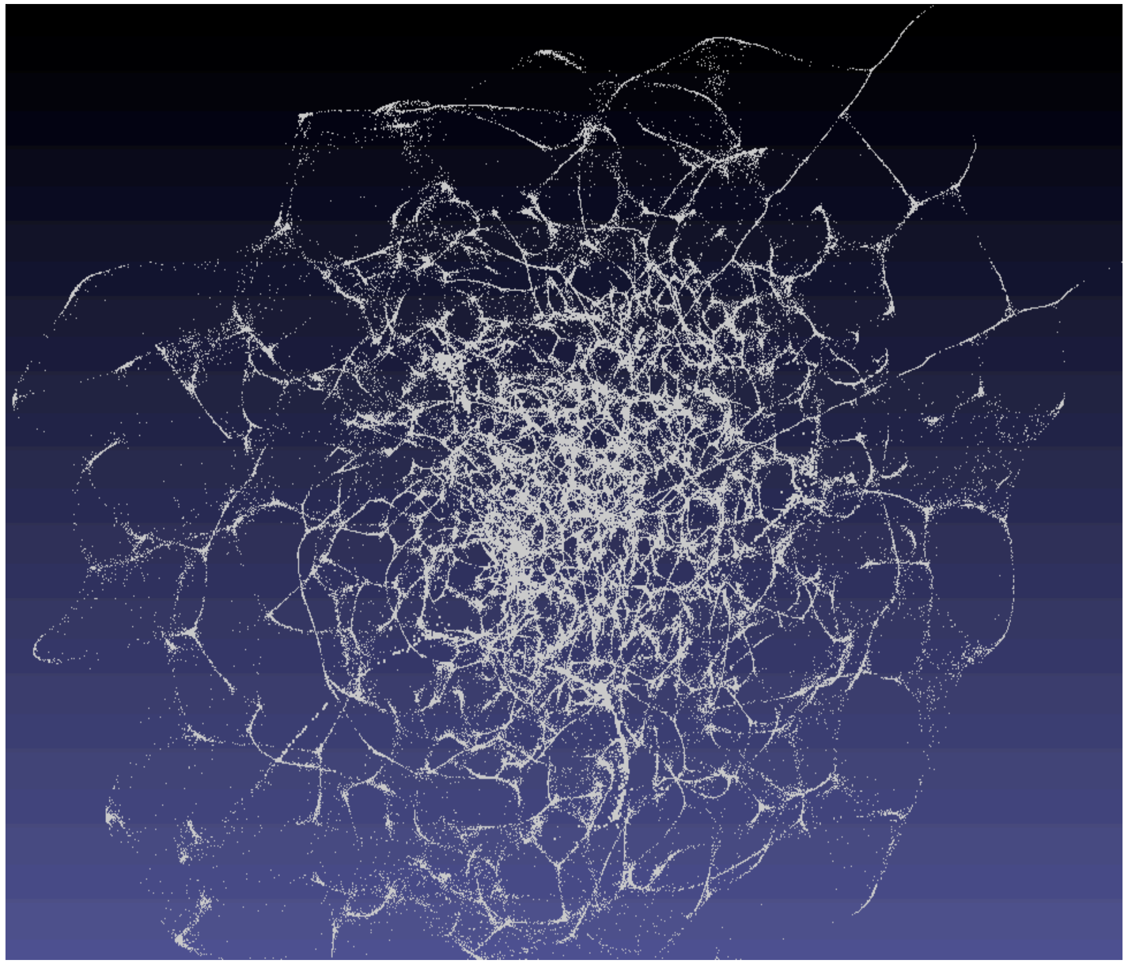


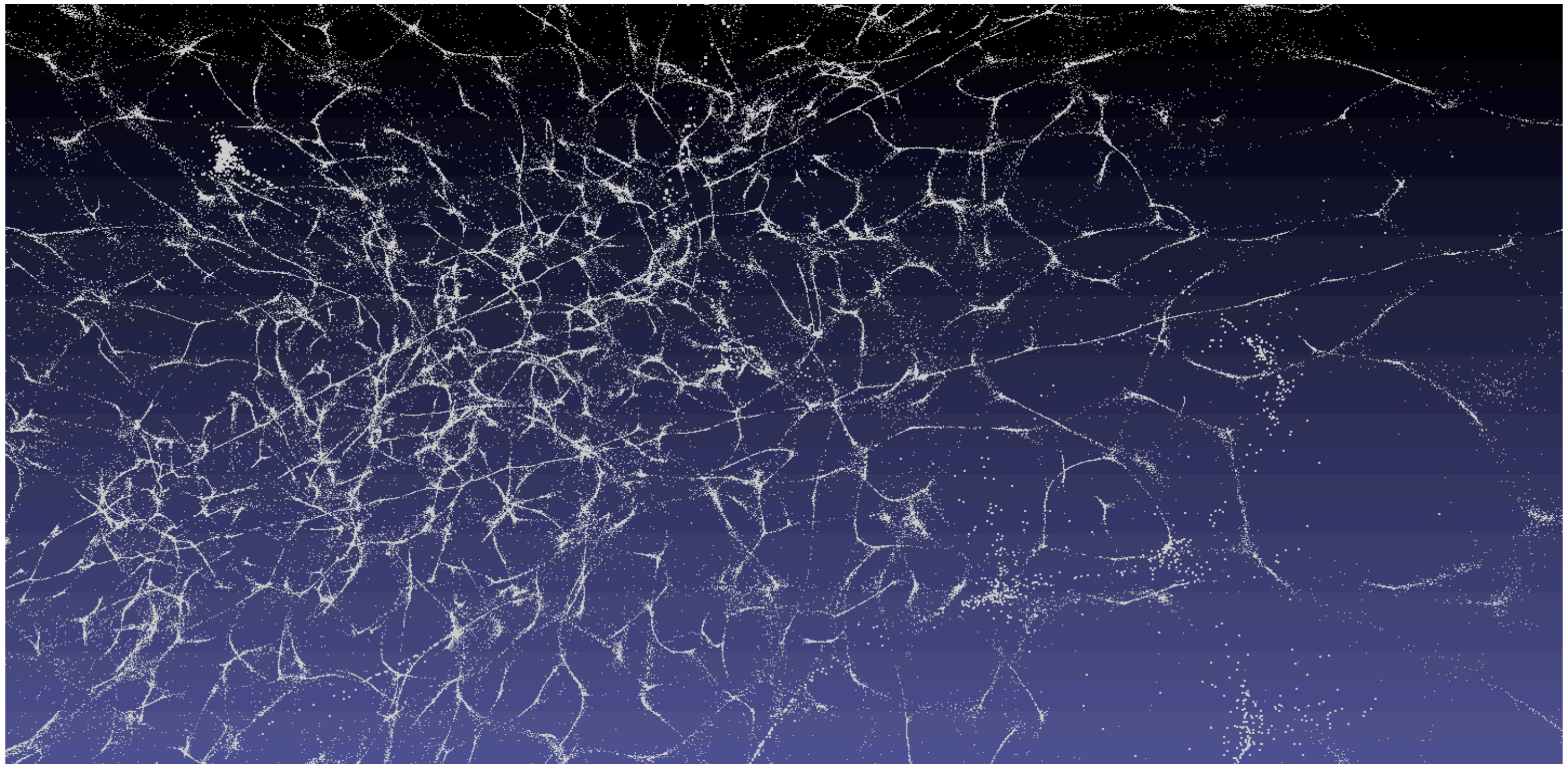


- Mean-Shift like algorithm (Fukunaga-Hostetler'75, Comaniciu-Meer '02)
- Theoretical guarantees on the convergence of the algorithm and "smoothness" of trajectories.

Pushing data along the gradient of d_{μ,m_0}







Take-home messages

- $\mu \mapsto d_{\mu,m_0}$ provide a way to associate geometry to a measure in Euclidean space.
- d_{μ,m_0} is robust to Wasserstein perturbations : outliers and noise are easily handled (no assumption on the nature of the noise).
- d_{μ,m_0} shares regularity properties with the usual distance function to a compact.
- Geometric stability results in this measure-theoretic setting : topology/geometry of the sublevel sets of d_{μ,m_0}, stable notion of persistence diagram for μ,...
- Algorithm: for finite point clouds d_{μ,m_0} and $\nabla(d_{\mu,m_0})$ can be easily and efficiently computed in any dimension.

To get more details:
http://geometrica.saclay.inria.fr/team/Fred.Chazal/papers/RR-6930.pdf