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Winter School

An introduction to Topological Data Analysis through persistent homology: Intro and geometric inference

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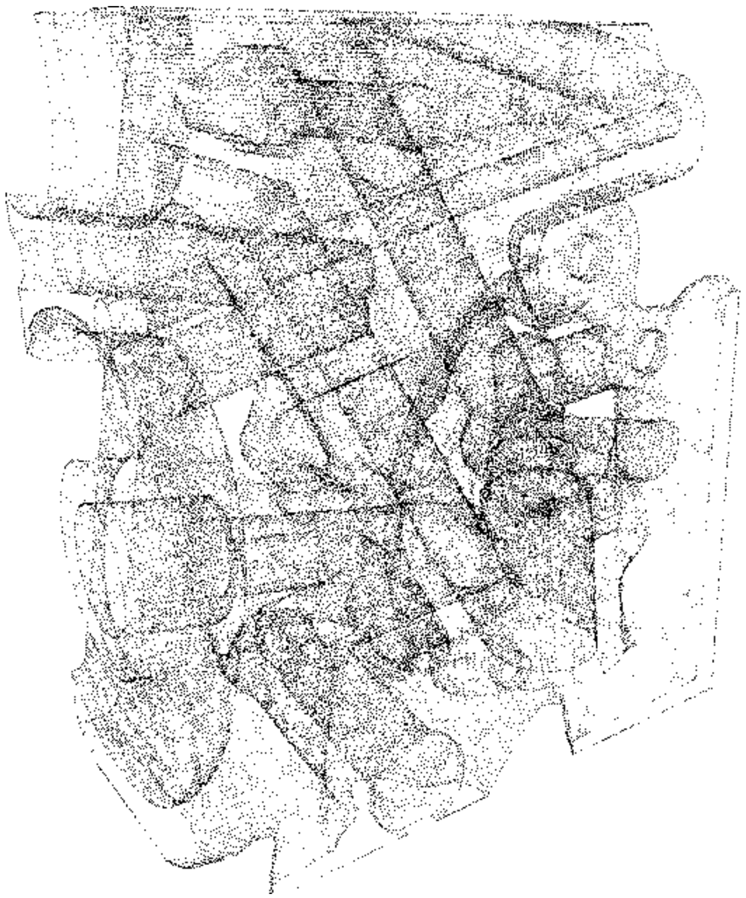
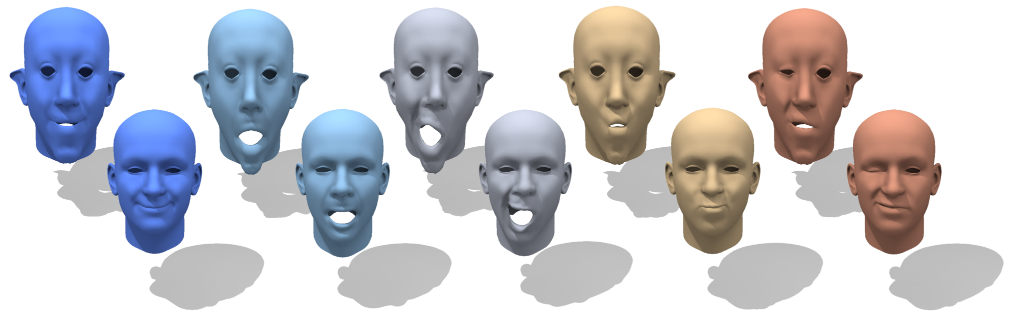
Some notes related to the course:
J-D. Boissonnat, F. Chazal, M. Yvinec, Computational Geometry and Topology for Data Analysis
http://geometrica.saclay.inria.fr/team/Fred.Chazal/

informatics mathematics

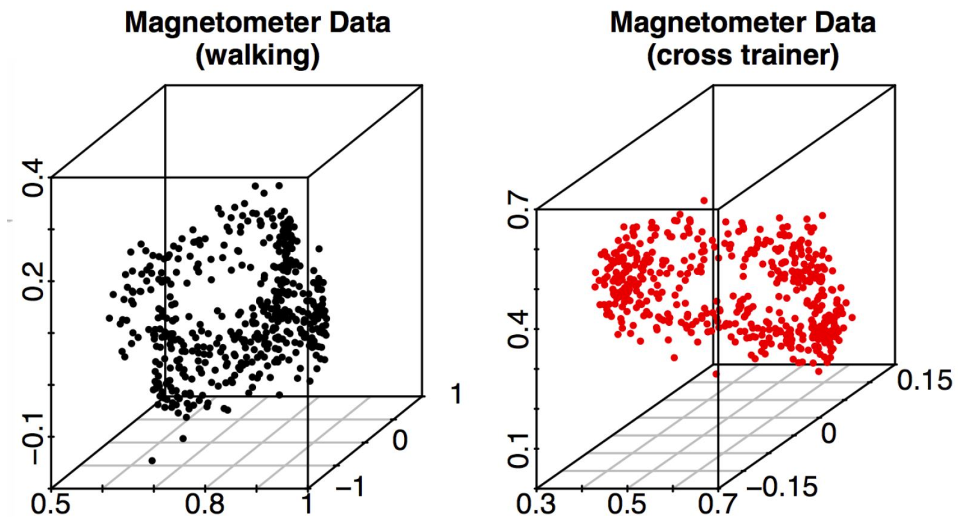
Introduction

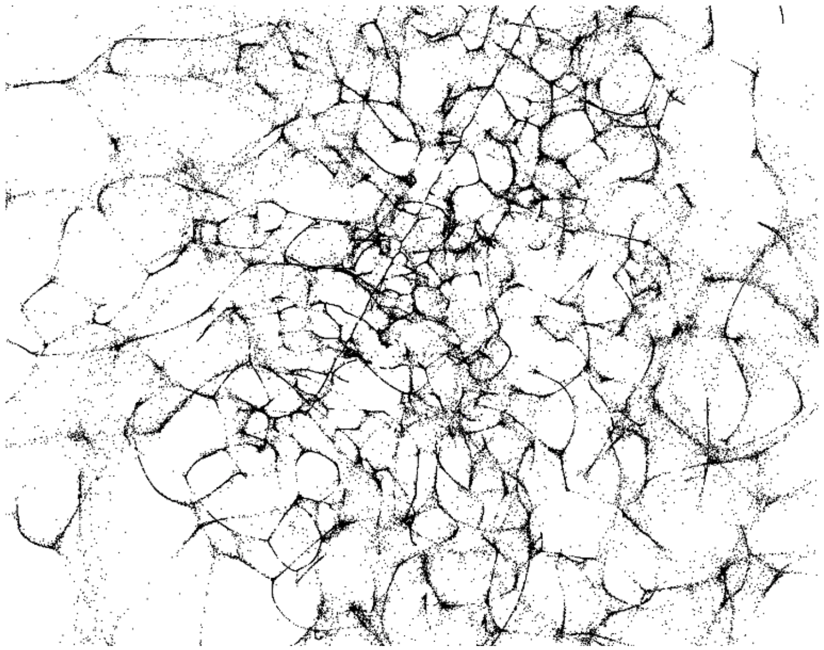


[Scanned 3D object]



[Shape database]



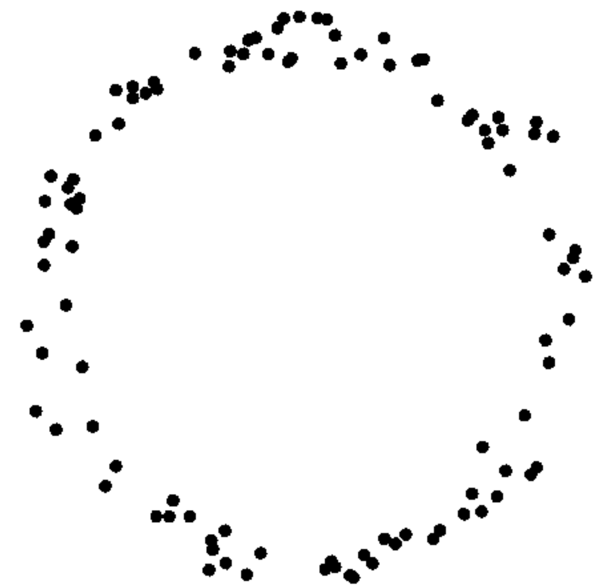


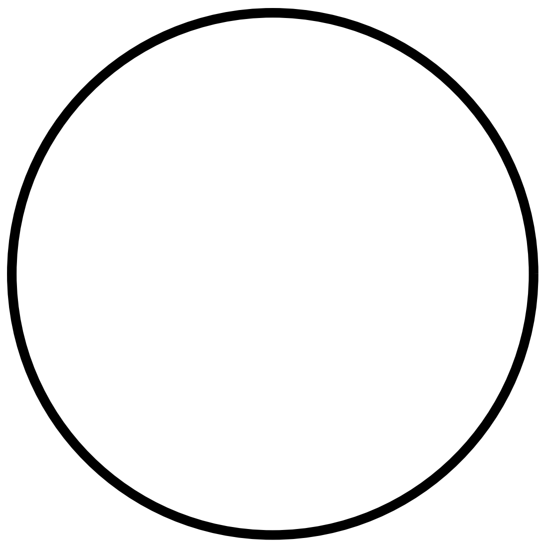
[Galaxies data]

- Data often come as (sampling of) metric spaces or sets/spaces endowed with a similarity measure with, possibly complex, topological/geometric structure.
- Data carrying geometric information are becoming high dimensional.
- Topological Data Analysis (TDA):
  - infer relevant topological and geometric features of these spaces.
  - take advantage of topol./geom. information for further processing of data (classification, recognition, learning, clustering, parametrization...).

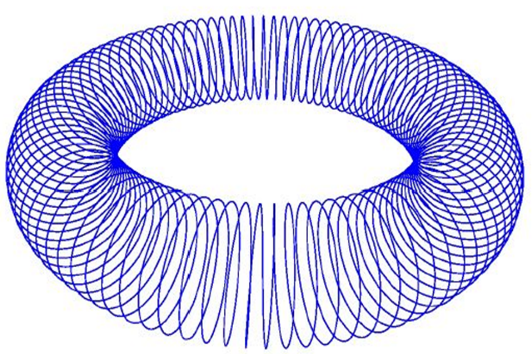
Introduction

Problem: how to compare topological properties of close shapes/data sets?

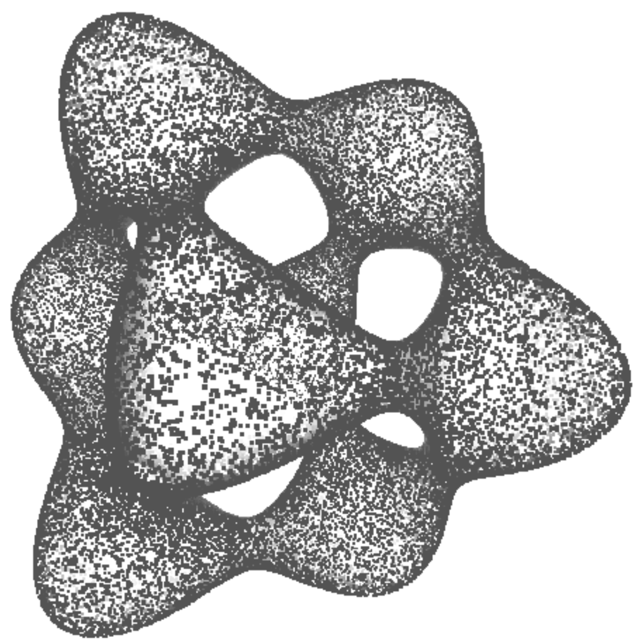


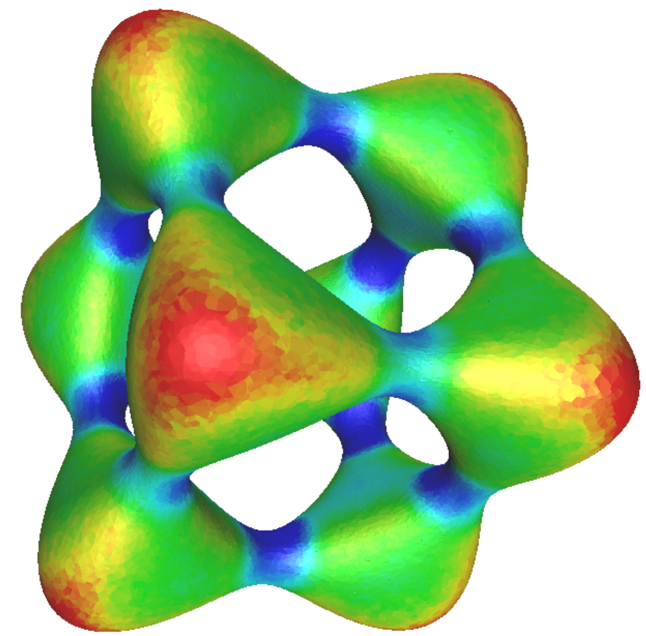


- Challenges and goals:
  $\rightarrow$ no direct access to topological/geometric information: need of intermediate constructions (simplicial complexes);
  $\rightarrow$ distinguish topological “signal” from noise;
  $\rightarrow$ topological information may be multiscale;
  $\rightarrow$ statistical analysis of topological information.



Topological and 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?

Challenges:
- define a relevant class of objects to be considered (no hope to get a positive answer in full generality);
- define a relevant notion of distance between the objects (approximation);
- topological and geometric properties cannot be directly infered from approximations.

Two strategies

1. **Reconstruction**

+ Full reconstruction of the underlying shape.
+ Strong topological and geometric information.
+ A well-developped theory.
- Strong regularity assumptions.
- Severe practical/algo issues in high dimensions.

1. **Topological inference**

+ Estimation of topological information without explicit reconstruction.
+ Lighter regularity assumptions.
+ A powerful theory that extends to general data.
- Weaker information.

This course

Background mathematical notions

Topological space

A topology on a set X is a family $\mathcal{O}$ of subsets of X that satisfies the three following conditions:
i) the empty set $\emptyset$ and X are elements of $\mathcal{O}$,
ii) any union of elements of $\mathcal{O}$ is an element of $\mathcal{O}$,
iii) any finite intersection of elements of $\mathcal{O}$ is an element of $\mathcal{O}$.
The set X together with the family $\mathcal{O}$, whose elements are called open sets, is a topological space. A subset C of X is closed if its complement is an open set.

A map $f : X \to X'$ between two topological spaces X and X' is continuous if and only if the pre-image $f^{-1}(O') = \{x \in X : f(x) \in O'\}$ of any open set $O' \subset X'$ is an open set of X. Equivalently, f is continuous if and only if the pre-image of any closed set in X' is a closed set in X (exercise).

A topological space X is a compact space if any open cover of X admits a finite subcover, i.e. for any family $\{U_i\}_{i \in I}$ of open sets such that $X = \cup_{i \in I} U_i$ there exists a finite subset $J \subseteq I$ of the index set I such that $X = \cup_{j \in J} U_j$.

Background mathematical notions

Metric space

A metric (or distance) on X is a map $d : X \times X \to [0, +\infty)$ such that:
i) for any $x, y \in X$, $d(x, y) = d(y, x)$,
ii) for any $x, y \in X$, $d(x, y) = 0$ if and only if $x = y$,
iii) for any $x, y, z \in X$, $d(x, z) \leq d(x, y) + d(y, z)$.
The set X together with d is a metric space.

The smallest topology containing all the open balls $B(x, r) = \{y \in X : d(x, y) < r\}$ is called the metric topology on X induced by d.

Example: the standard topology in an Euclidean space is the one induced by the metric defined by the norm: $d(x, y) = \|x - y\|$.

Compacity: a metric space X is compact if and only if any sequence in X has a convergent subsequence. In the Euclidean case, a subset $K \subset \mathbb{R}^d$ (endowed with the topology induced from the Euclidean one) is compact if and only if it is closed and bounded (Heine-Borel theorem).

Background mathematical notions

Shapes and Hausdorff distance

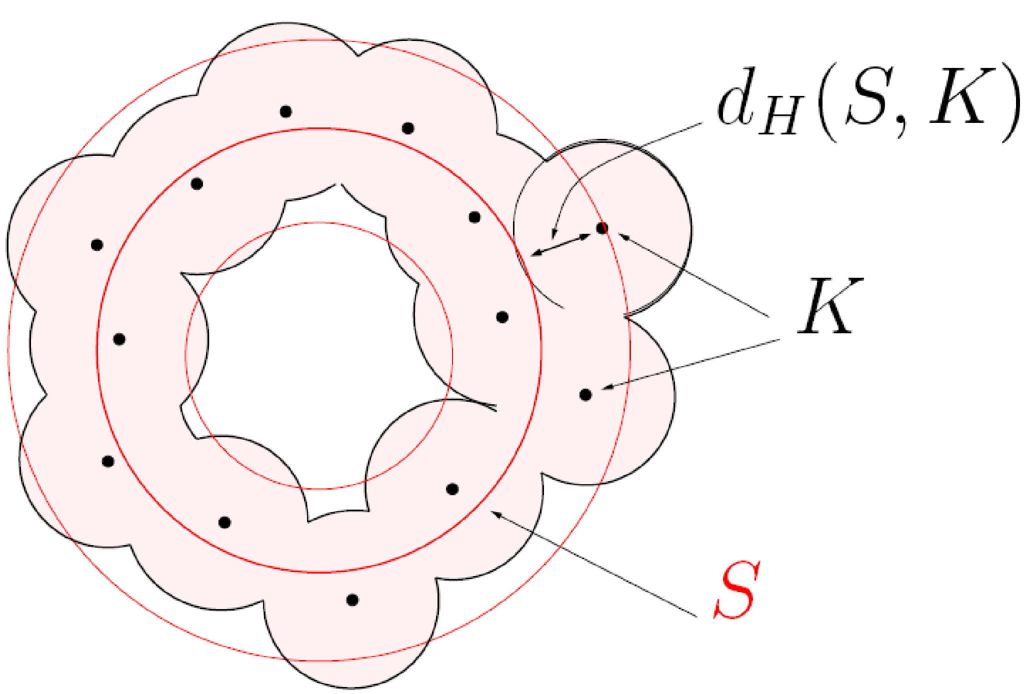
In the first lectures : shape = compact subset of $\mathbb{R}^d$

The distance function to a compact $K \subset \mathbb{R}^d$, $d_K : \mathbb{R}^d \to \mathbb{R}_+$ is defined by

$$d_K(x) = \inf_{p \in K} \|x - p\|$$

The Hausdorf distance between two compact sets $K, K' \subset \mathbb{R}^d$:

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



Exercise: Show that

$$d_H(K, K') = \max\left(\sup_{y \in K'} d_K(y), \sup_{z \in K} d_{K'}(z)\right)$$

Distance functions and geometric inference

The distance function to a compact $K \subset \mathbb{R}^d$, $d_K : \mathbb{R}^d \to \mathbb{R}_+$ is defined by

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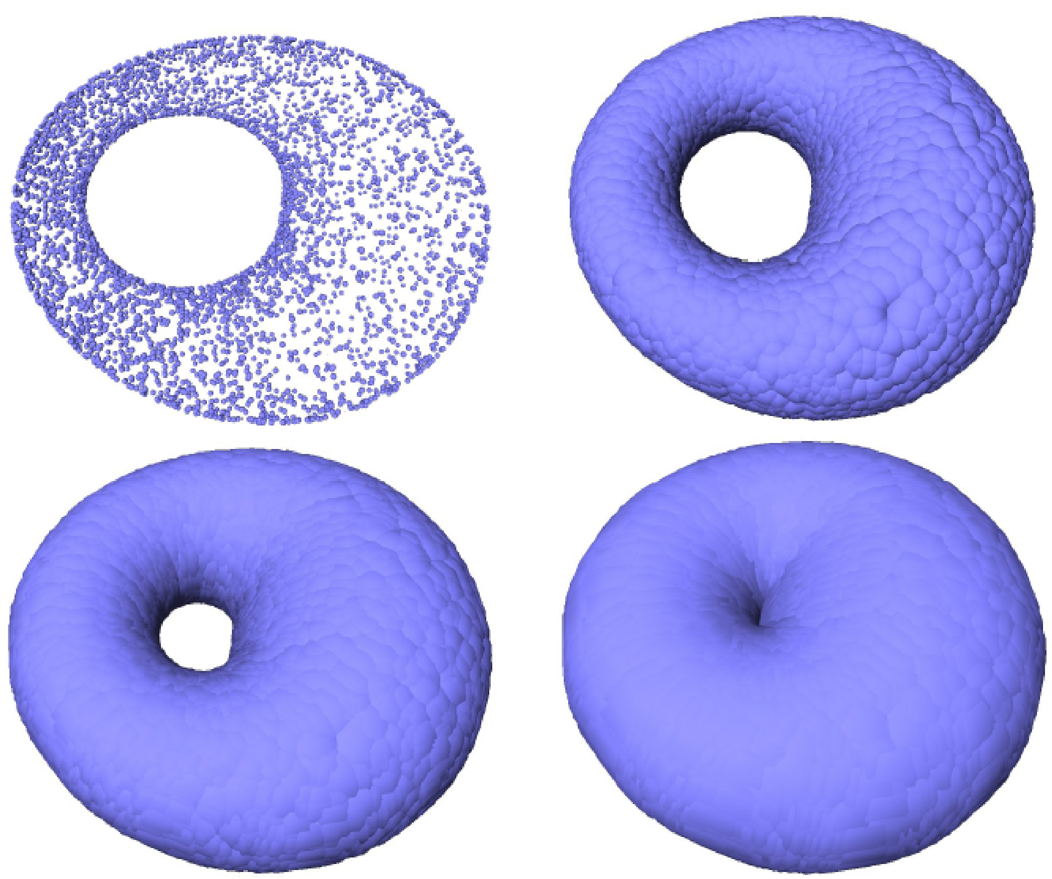
The Hausdorf distance between two compact sets $K, K' \subset \mathbb{R}^d$:

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

The idea:

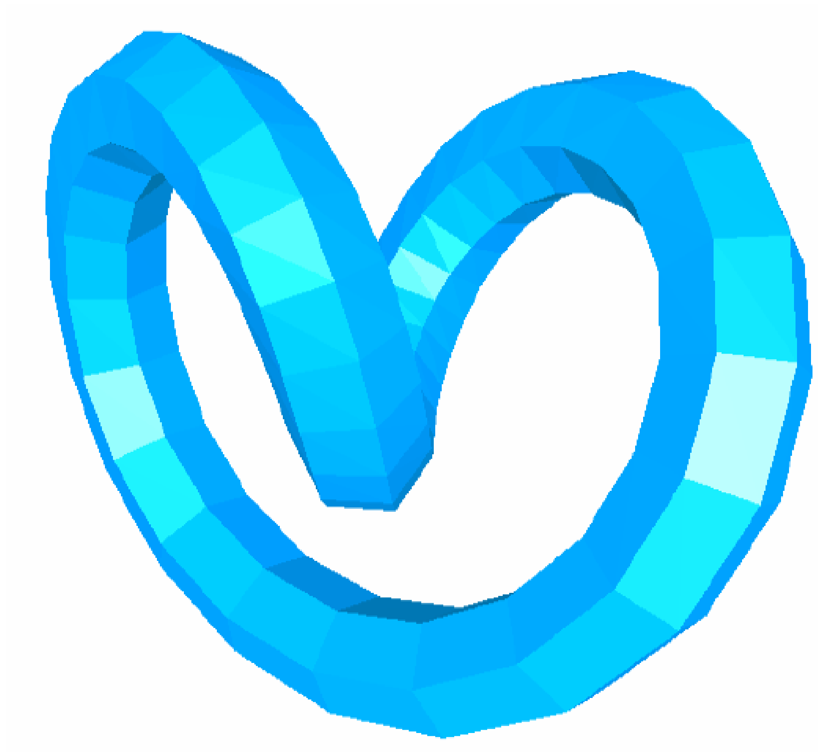
- Replace K and C by d_K and d_C
- Compare the topology of the offsets

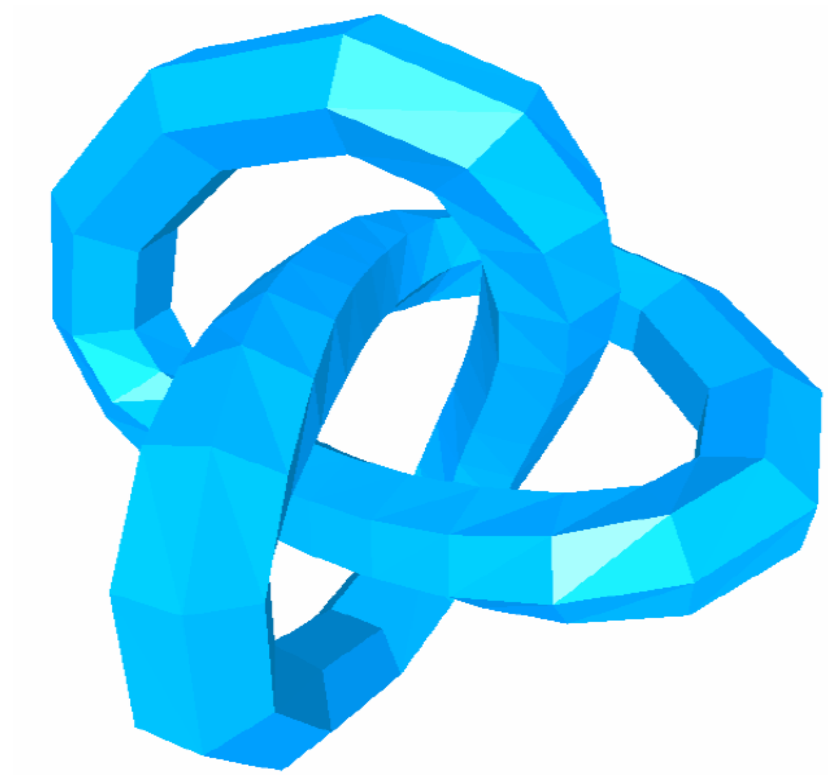
$K^r = d_K^{-1}([0, r])$ and $C^r = d_C^{-1}([0, r])$



Comparing topological spaces

Homeomorphy and isotopy

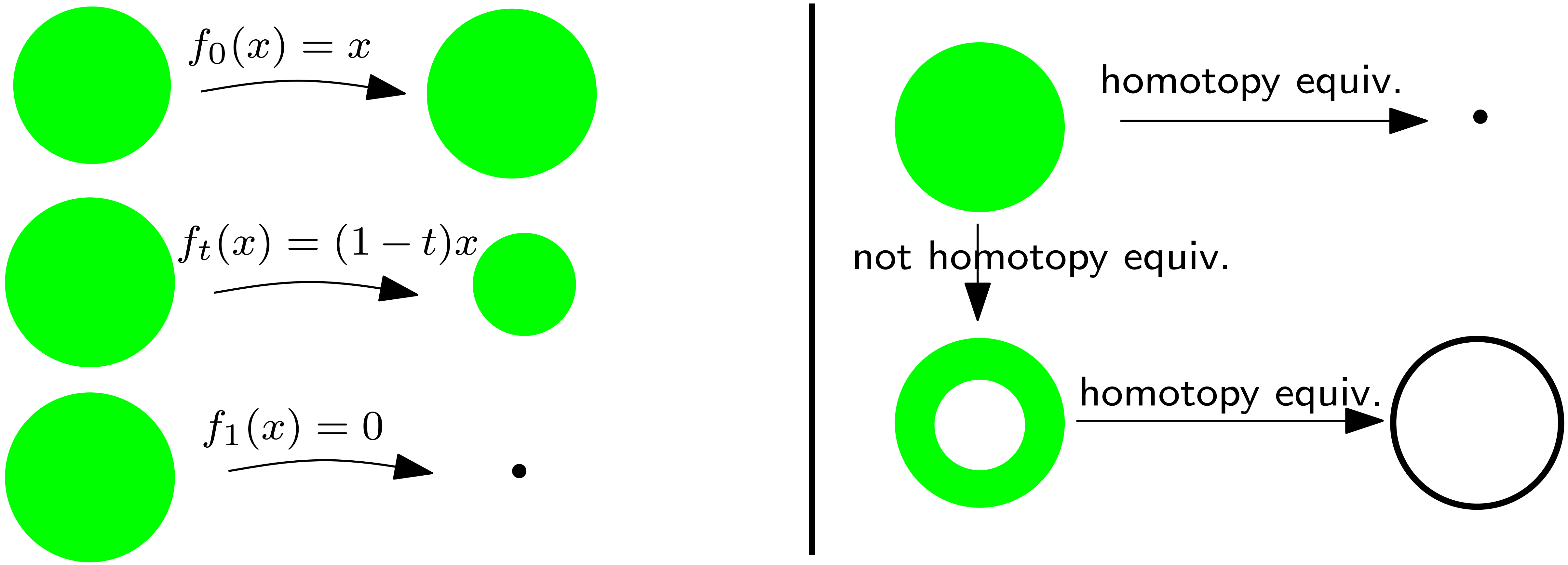




- X and Y are homeomorphic if there exists a bijection $h : X \to Y$ s. t. h and h^{-1} are continuous.
- $X, Y \subset \mathbb{R}^d$ are ambient isotopic if there exists a continuous map $F : \mathbb{R}^d \times [0,1] \to \mathbb{R}^d$ s. t. $F(.,0) = Id_{\mathbb{R}^d}$, $F(X,1) = Y$ and $\forall t \in [0,1]$, $F(.,t)$ is an homeomorphim of $\mathbb{R}^d$.

Comparing topological spaces

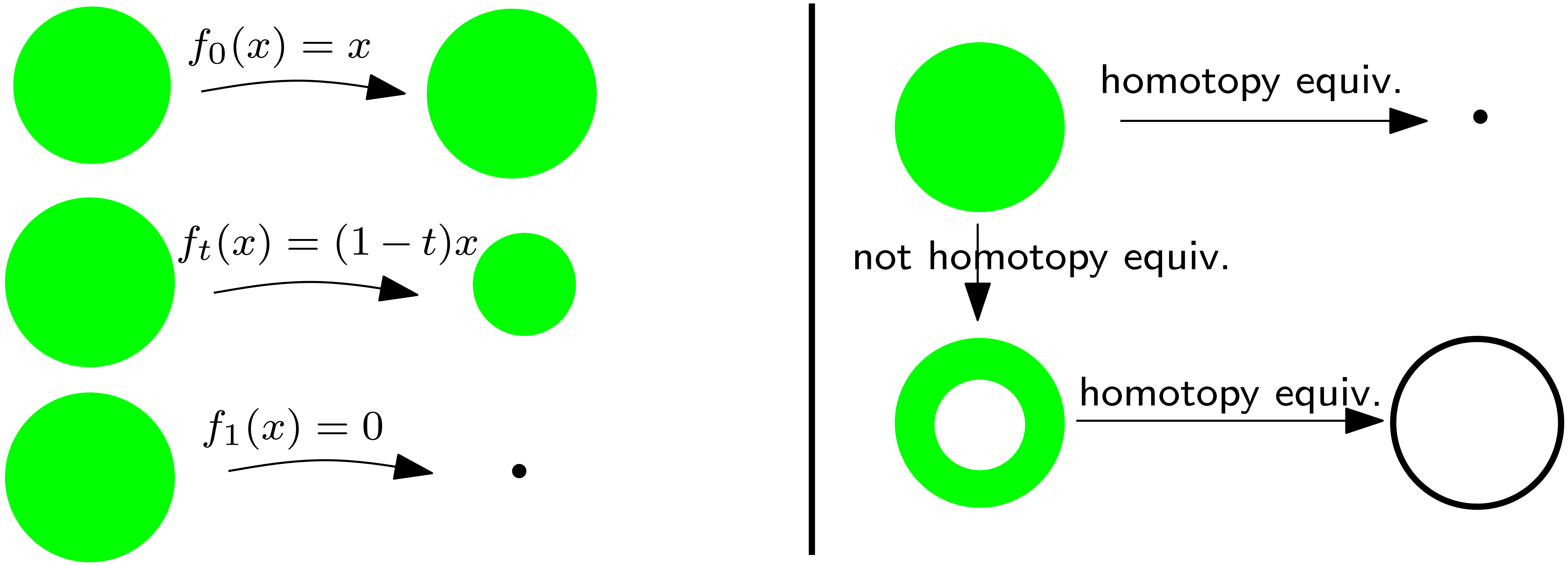
Homotopy, homotopy type



- Two maps $f_0 : X \to Y$ and $f_1 : X \to Y$ are homotopic if there exists a continuous map $H : [0,1] \times X \to Y$ s. t. $\forall x \in X$, $H(0,x) = f_0(x)$ and $H_1(1,x) = f_1(x)$.
- X and Y have the same homotopy type (or are homotopy equivalent) if there exists continuous maps $f : X \to Y$ and $g : Y \to X$ s. t. $g \circ f$ is homotopic to Id_X and $f \circ g$ is homotopic to Id_Y.

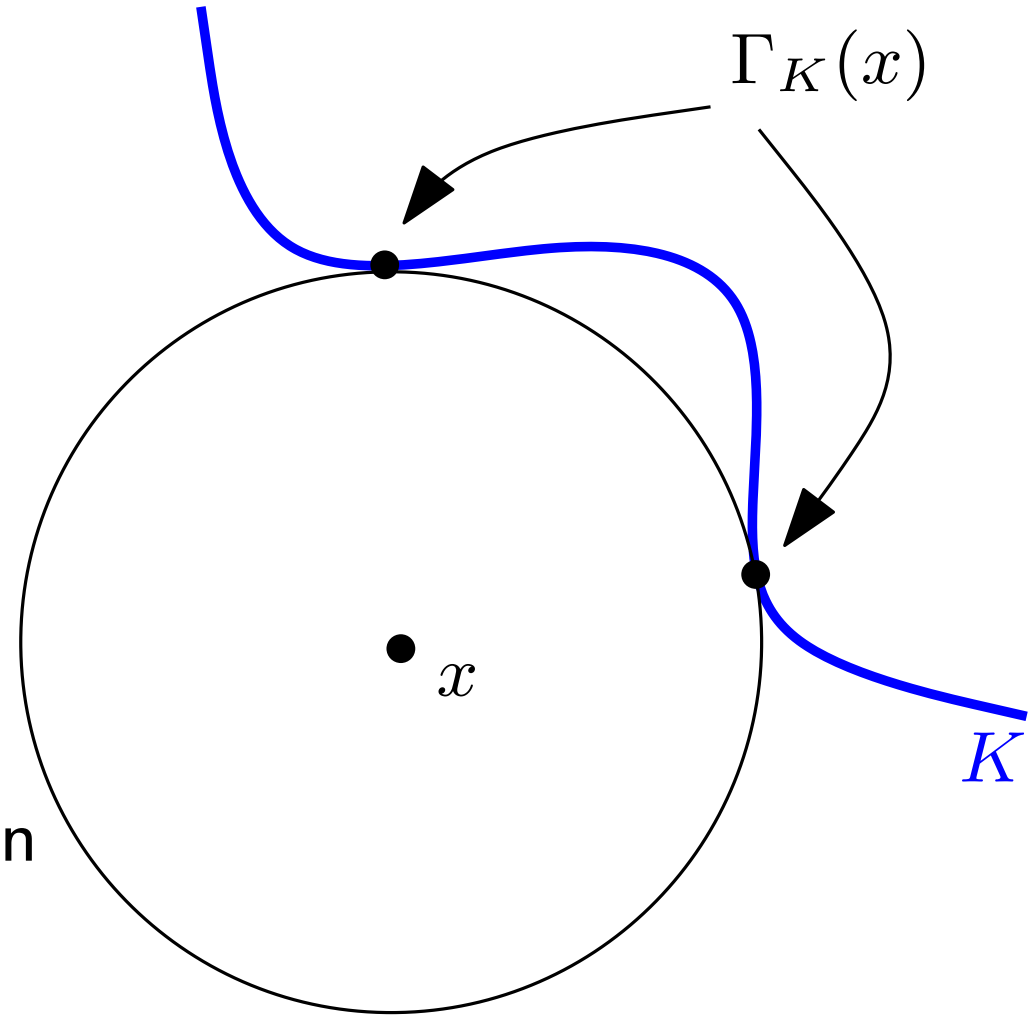
Comparing topological spaces

Homotopy, homotopy type



If $X \subset Y$ and if there exists a continuous map $H : [0,1] \times X \to X$ s.t.:
i) $\forall x \in X$, $H(0,x) = x$,
ii) $\forall x \in X$, $H(1,x) \in Y$
iii) $\forall y \in Y$, $\forall t \in [0,1]$, $H(t,y) \in Y$,
then X and Y are homotopy equivalent. If one replaces condition *iii)* by $\forall y \in Y$, $\forall t \in [0,1]$, $H(t,y) = y$ then H is a deformation retract of X onto Y.

Medial axis and critical points



$$\Gamma_K(x) = \{y \in K : d_K(x) = d(x,y)\}$$

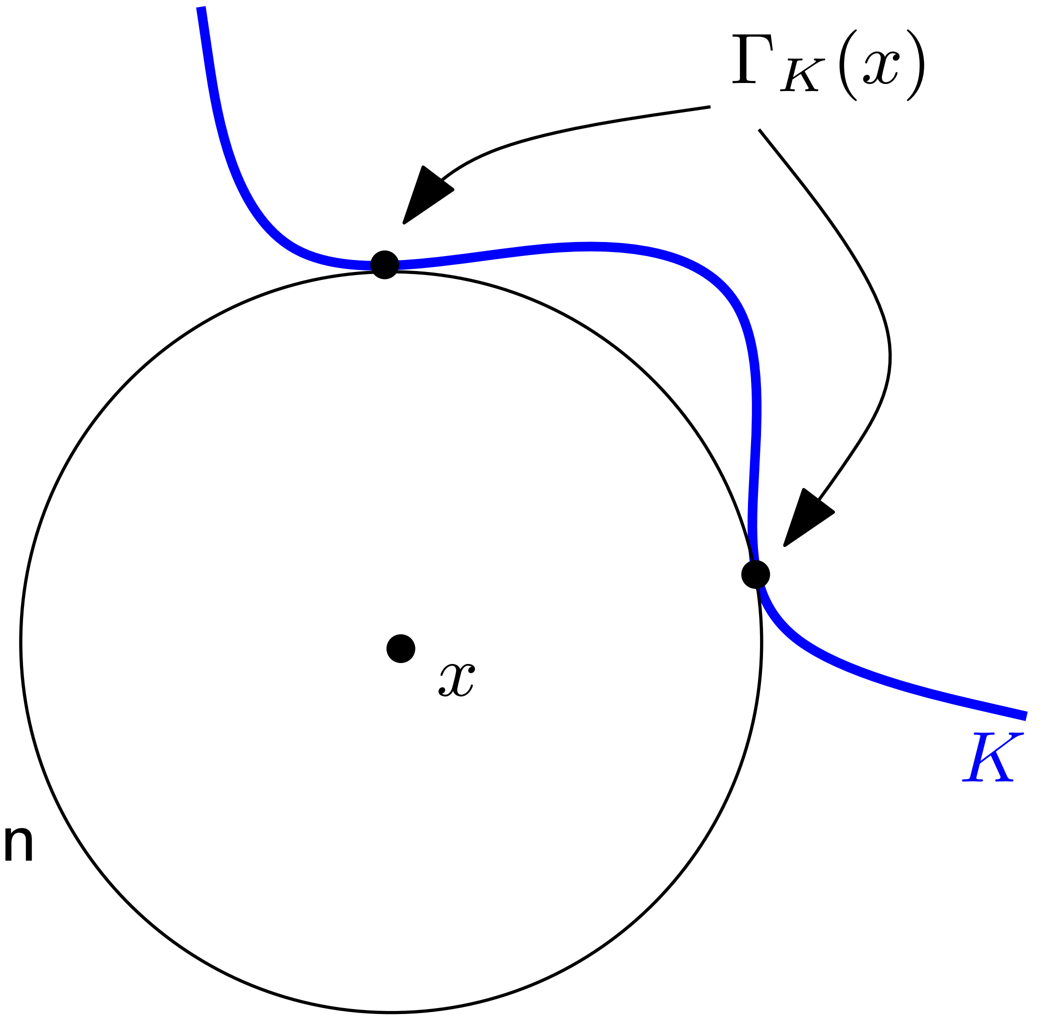
The Medial axis of K:

$$\mathcal{M}(K) = \{x \in \mathbb{R}^d : |\Gamma_K(x)| \geq 2\}$$

$x \in \mathbb{R}^d$ is a critical point of d_K iff x is contained in the convex hull of $\Gamma_K(x)$.

Exercise: What is the medial axis of a finite set of point $K = \{p_1, \cdots p_n\} \subset \mathbb{R}^d$? What are the critical points of d_K?

Medial axis and critical points



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$x \in \mathbb{R}^d$ is a critical point of d_K iff x is contained in the convex hull of $\Gamma_K(x)$.

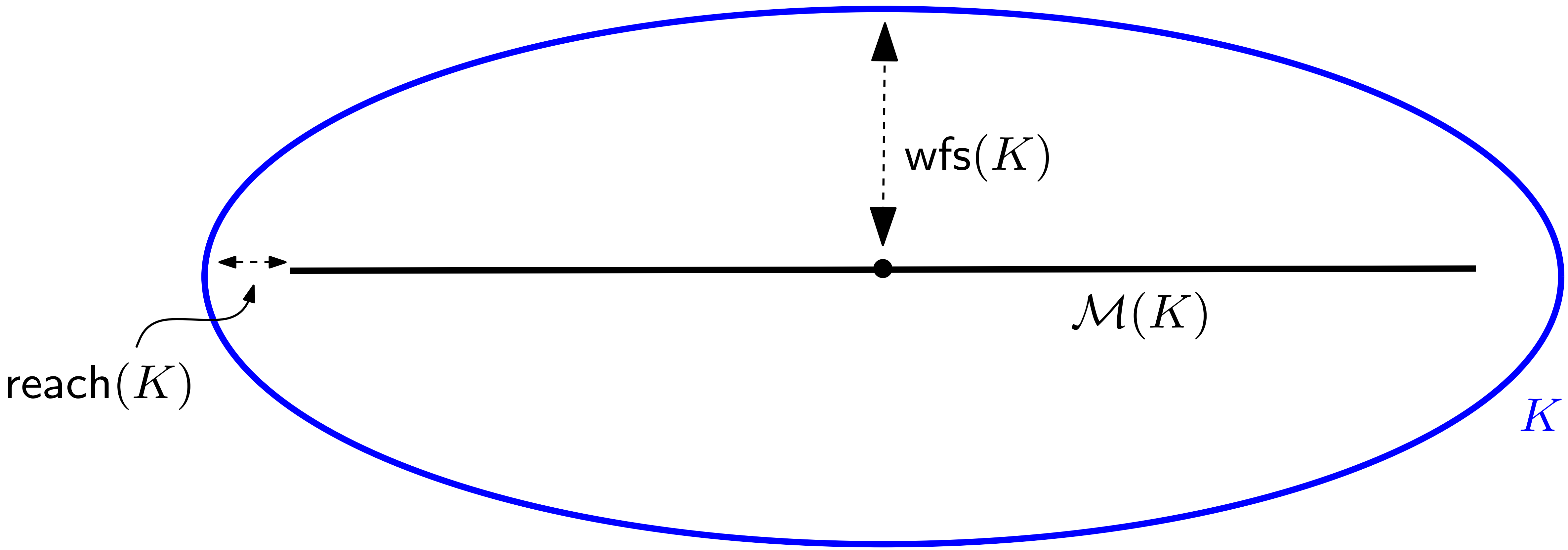
Theorem: [Grove, Cheeger,...] Let $K \subset \mathbb{R}^d$ be a compact set.

- if r is a regular value of d_K, then $d_K^{-1}(r)$ is a topological submanifold of $\mathbb{R}^d$ of codim 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 $d_K^{-1}(r_1) \times (r_1, r_2]$.

Reach and weak feature size



The reach of K, $\tau(K)$ is the smallest distance from $\mathcal{M}(K)$ to K:

$$\tau(K) = \inf_{y \in \mathcal{M}(K)} d_K(y)$$

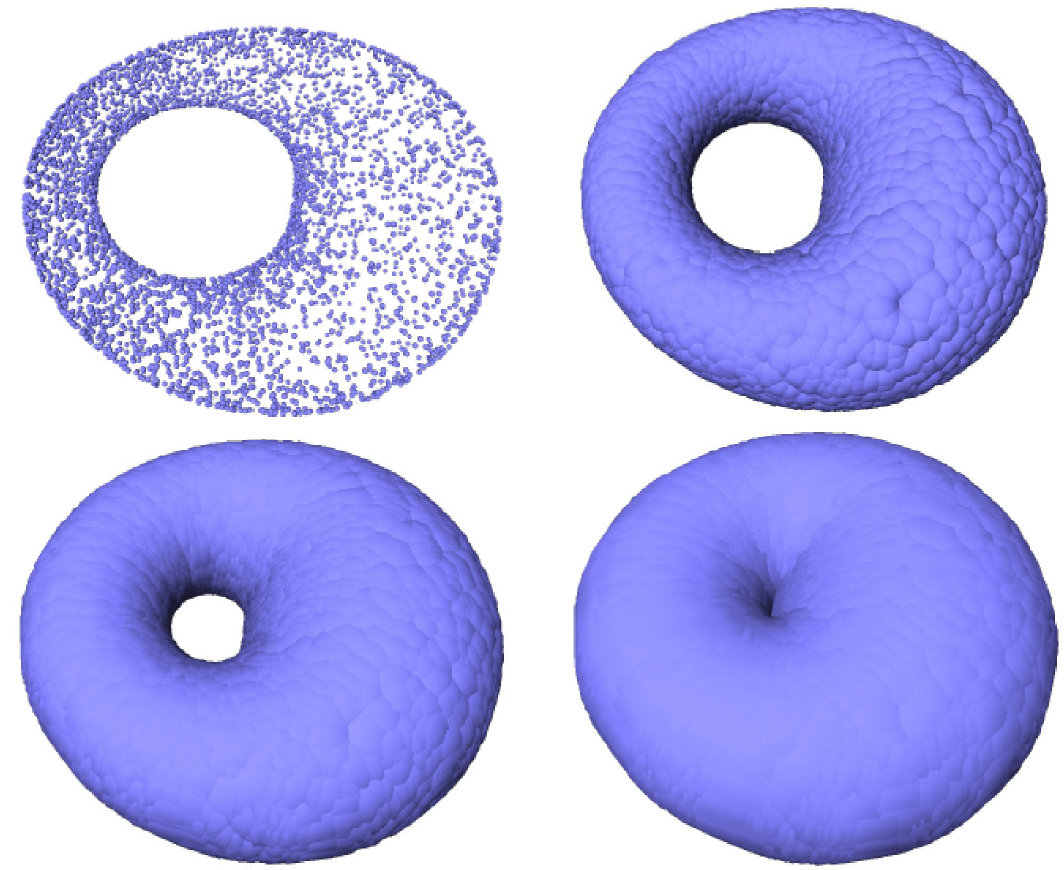
The weak feature size of K, wfs(K), is the smallest distance from the set of critical points of d_K to K:

$$\text{wfs}(K) = \inf\{d_K(y) : y \in \mathbb{R}^d \setminus K \text{ and } y \text{ crit. point of } d_K\}$$

Reach, μ-reach and geometric inference

(Not considered in this course - see course notes for details)

"Theorem:" Let $K \subset \mathbb{R}^d$ be such that $\tau = \tau(K) > 0$ and let $C \subset \mathbb{R}^d$ be such that $d_H(K, C) < c\tau$ for some (explicit) constant c. Then, for well-chosen (and explicit) r, C^r is homotopy equivalent to K.



More generally, for compact sets with positive μ-reach (wfs$(K) \leq r_\mu(K) \leq \tau(K)$):

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).