Geometric and Topological
Methods in Machine Learning
2021-2022

Computational Topology: Simplicial Complexes and (Persistent) Homology

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Class outline: taking a step back...

My classes are about

Topological Data Analysis (TDA)

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Goal: Study geometric data sets with techniques coming from *topology*.

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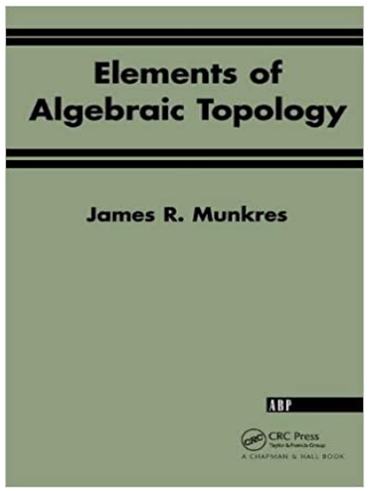
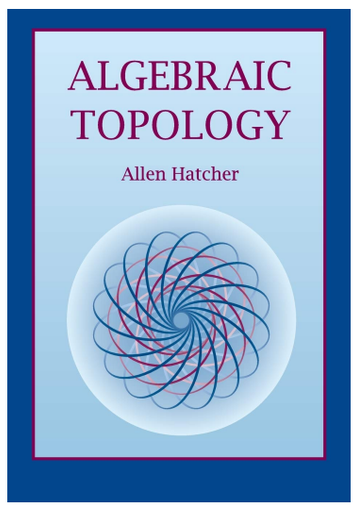
Question: What is topology?

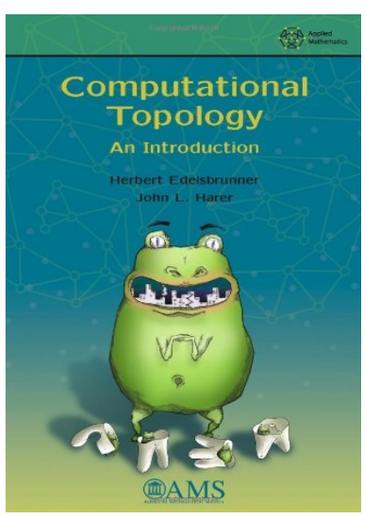
[*Elements of Algebraic Topology*, Munkres, CRC Press, 1984]

[*Algebraic Topology*, Hatcher, Cambridge University Press, 2002]

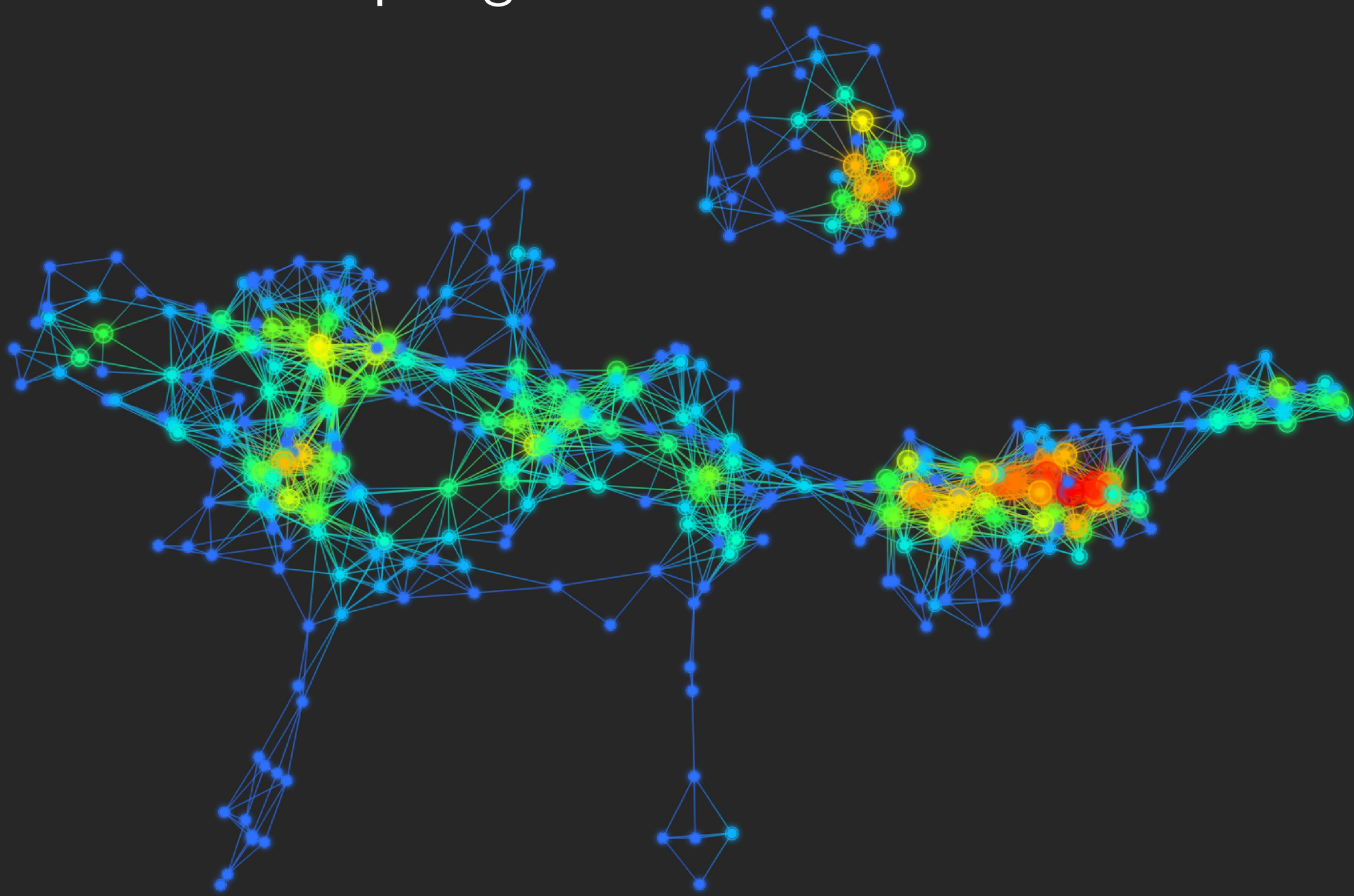
[*Computational Topology: an introduction*, Edelsbrunner, Harer, AMS, 2010]







Introduction: topological visualization



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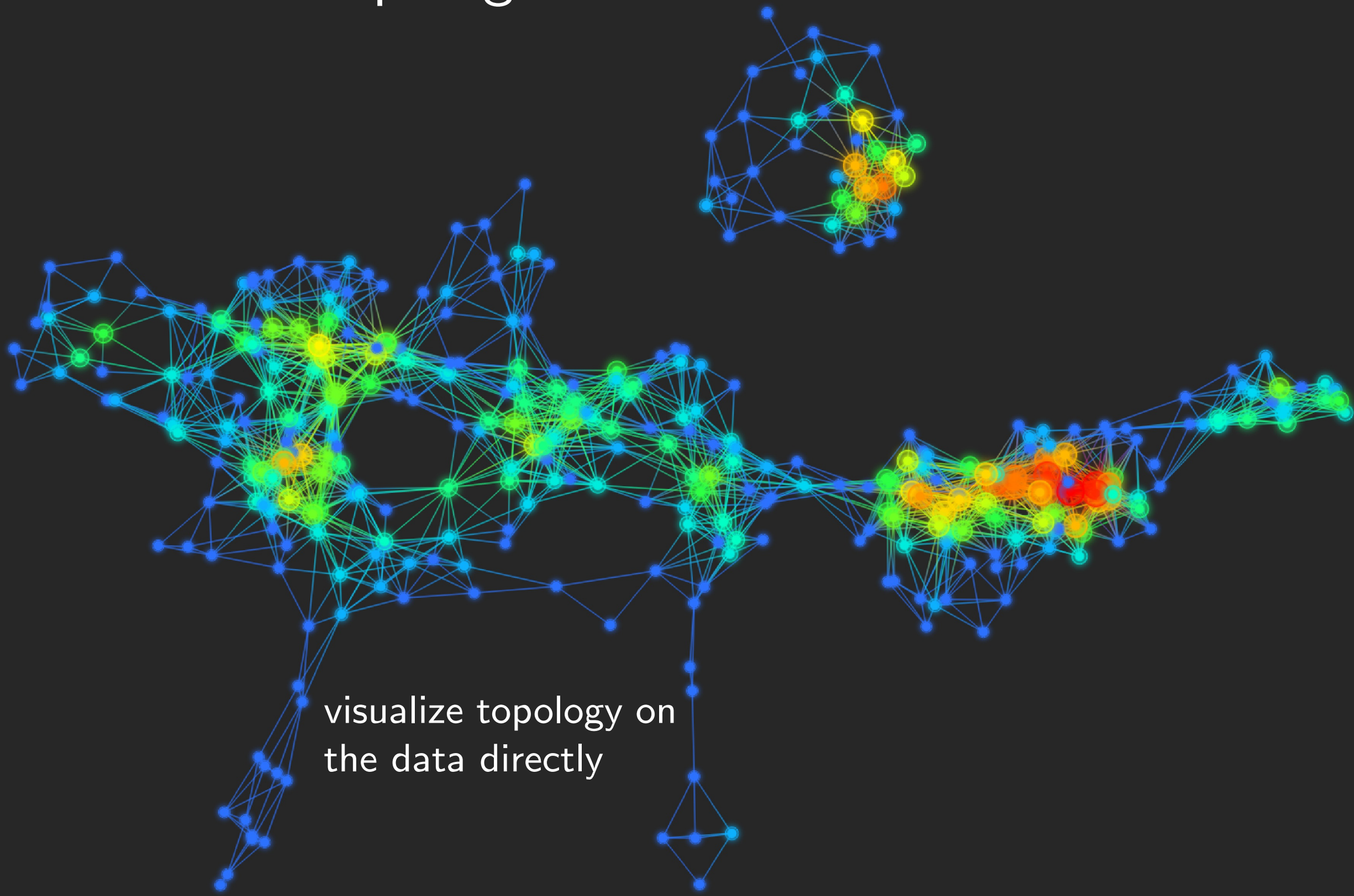


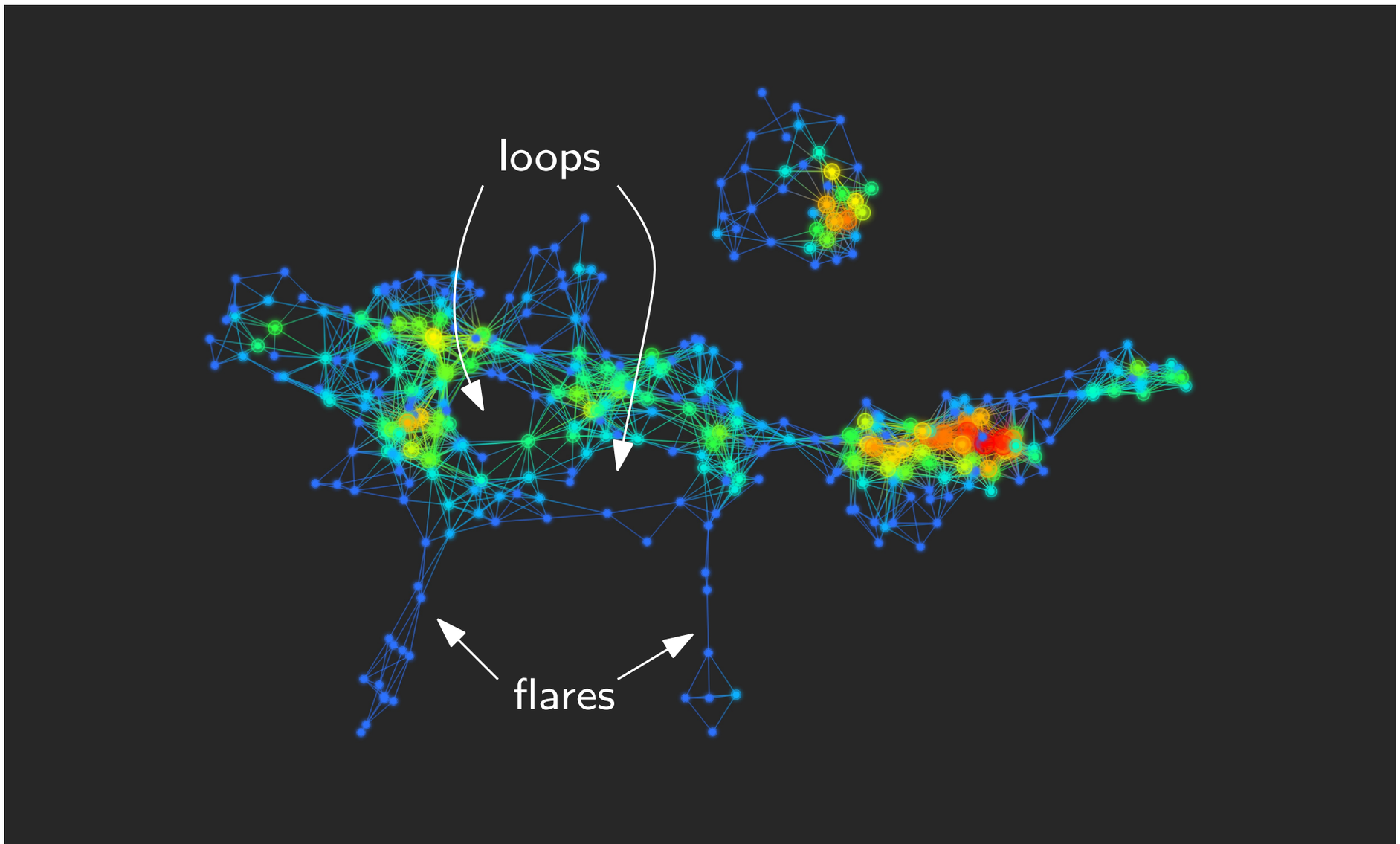
visualize topology on
the data directly

Introduction: topological visualization

Two types of applications:

- clustering
- feature selection

Principle: identify statistically relevant subpopulations through topological patterns (flares, loops).



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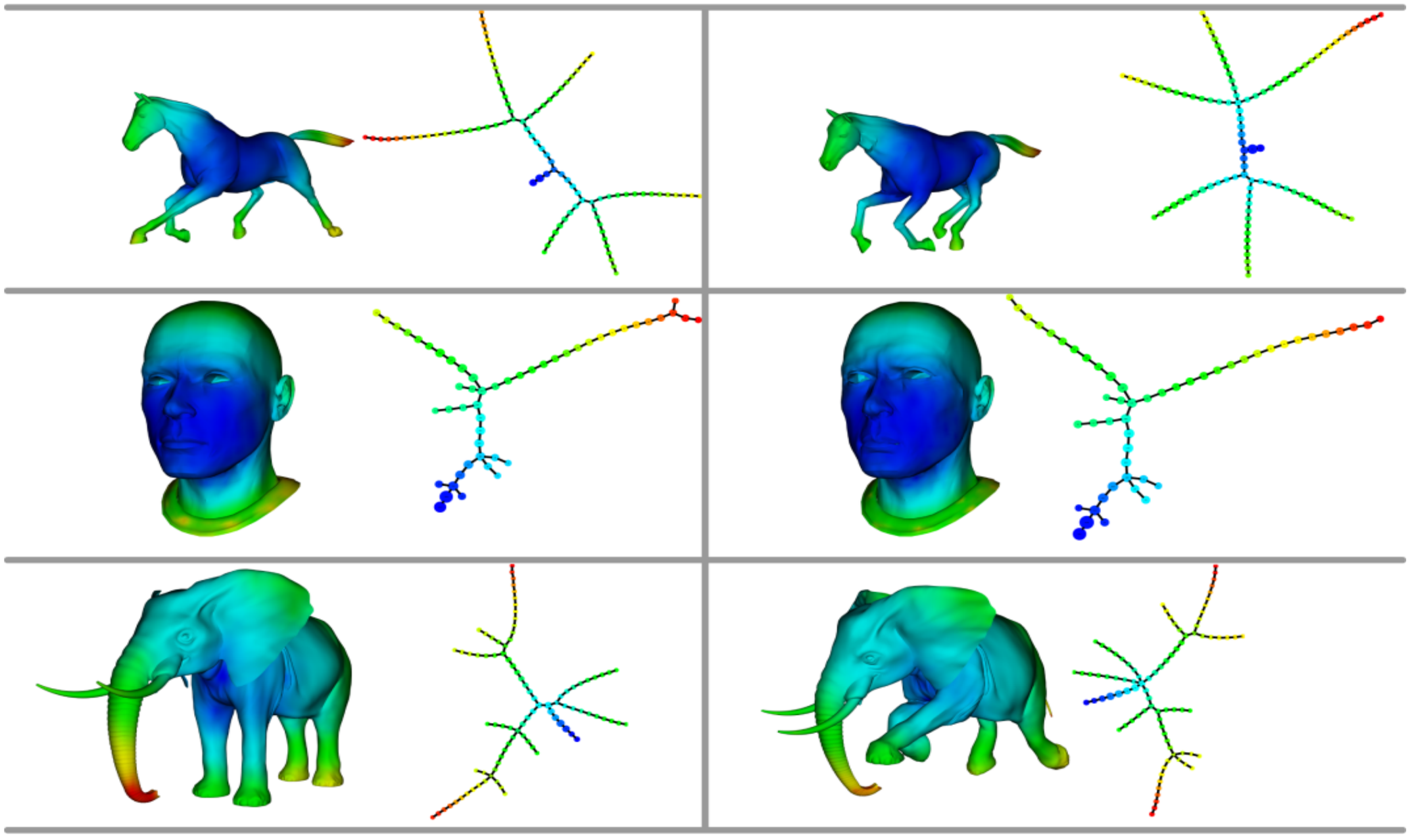


3d shapes classification

[*Topological Methods for the Analysis of High Dimensional Data Sets and 3D Object Recognition*, Singh, Mémoli, Carlsson, Symp. Point based Graphics, 2007]

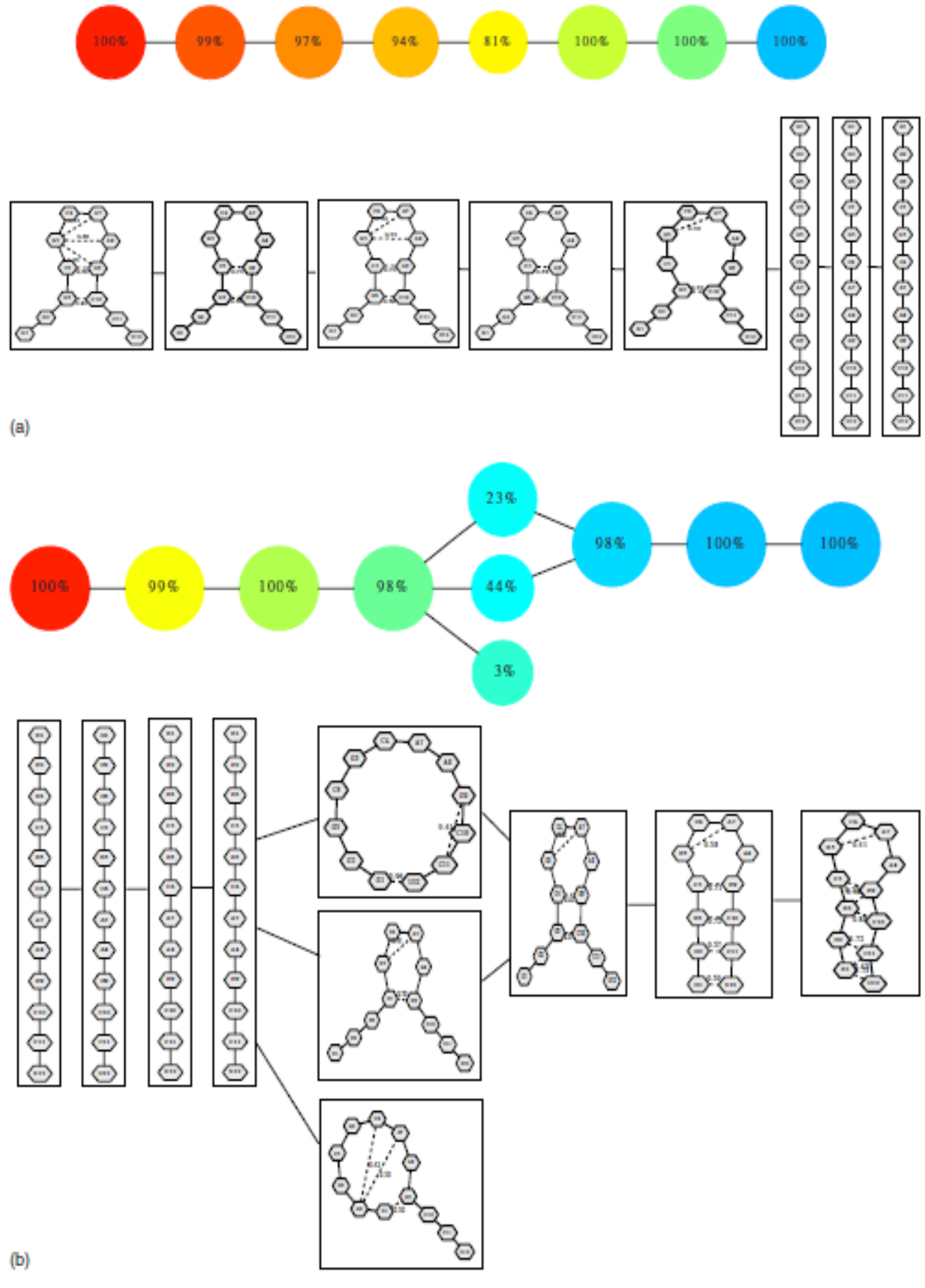
Introduction: topological visualization

[*Topological Methods for Exploring Low-density States in Biomolecular Folding Pathways*, Yao et al., J. Chemical Physics, 2009]

Data: conformations of molecules.

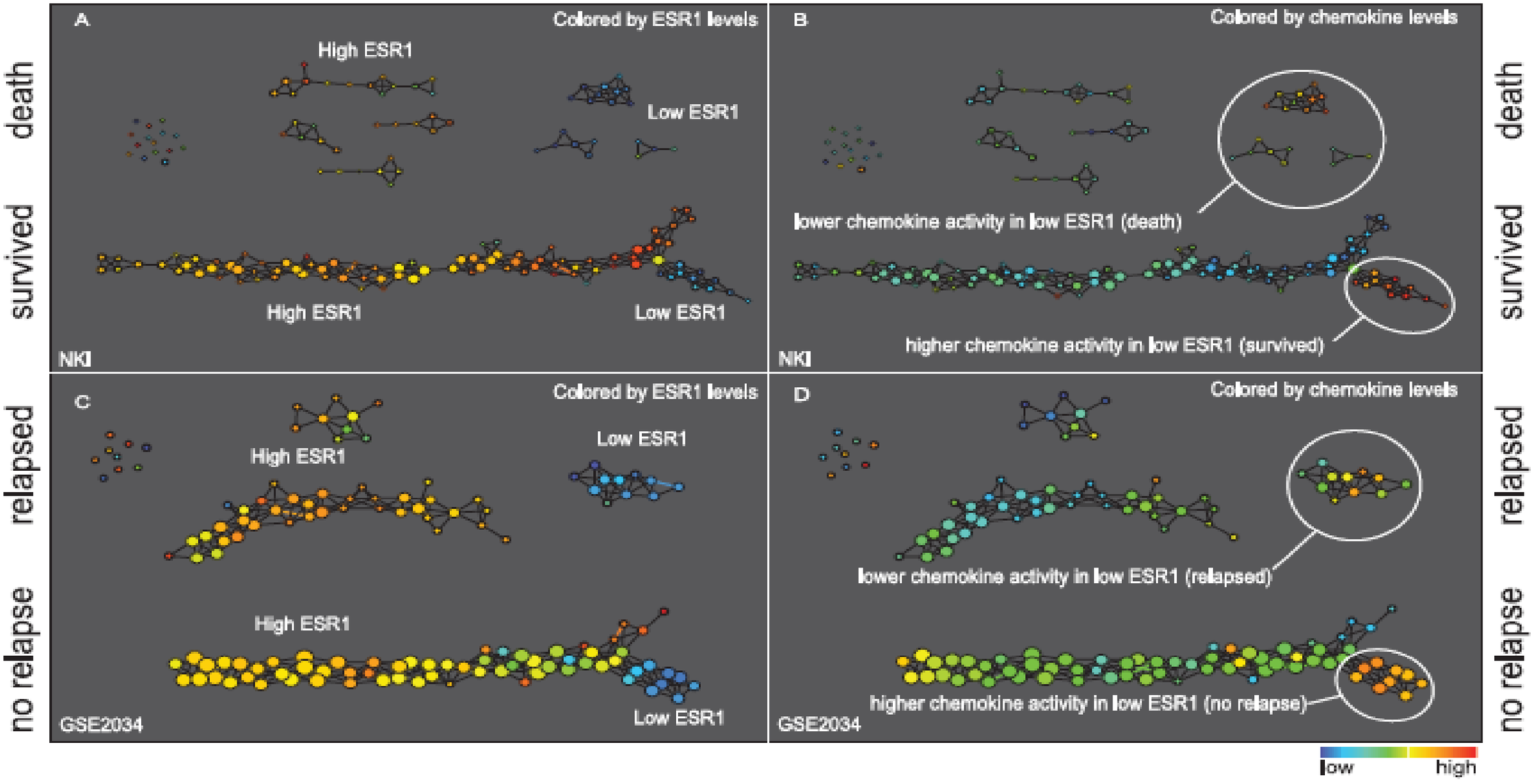
Goal: detect folding pathways.

Idea: 1 loop = 2 pathways.



Introduction: topological visualization

[*Extracting insights from the shape of complex data using topology*, Lum et al., Nature, 2013]



Data: breast cancer patients that went through specific therapy.

Goal: detect variables that influence survival after therapy in breast cancer.

Introduction: topological descriptors built from data

We will see how to build new topological features from data sets...

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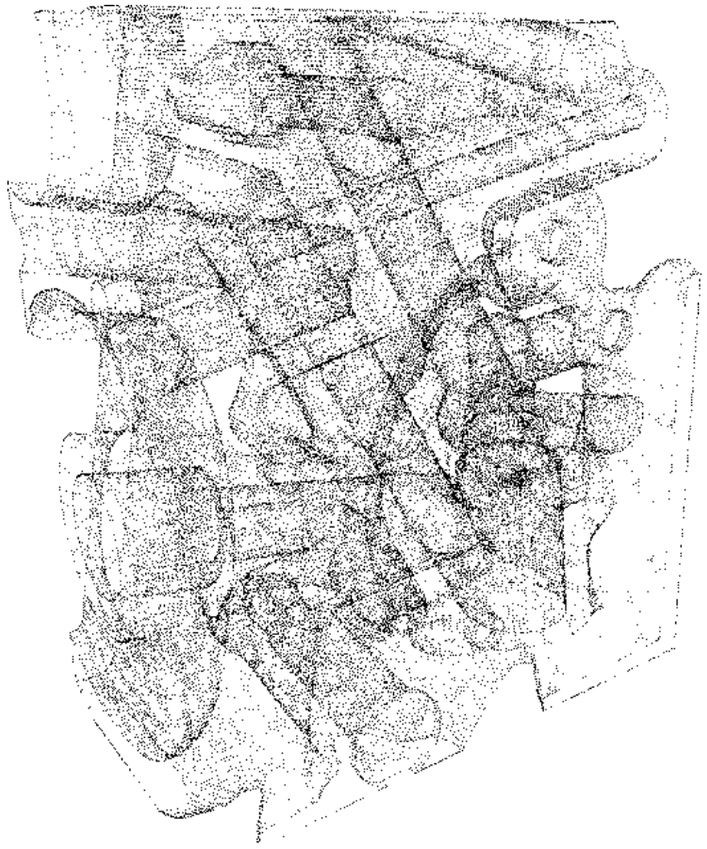
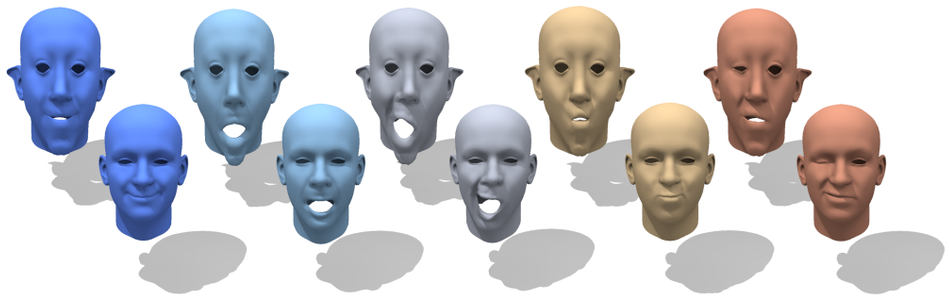
We will see how to build new topological features from data sets...

...but why is that interesting?

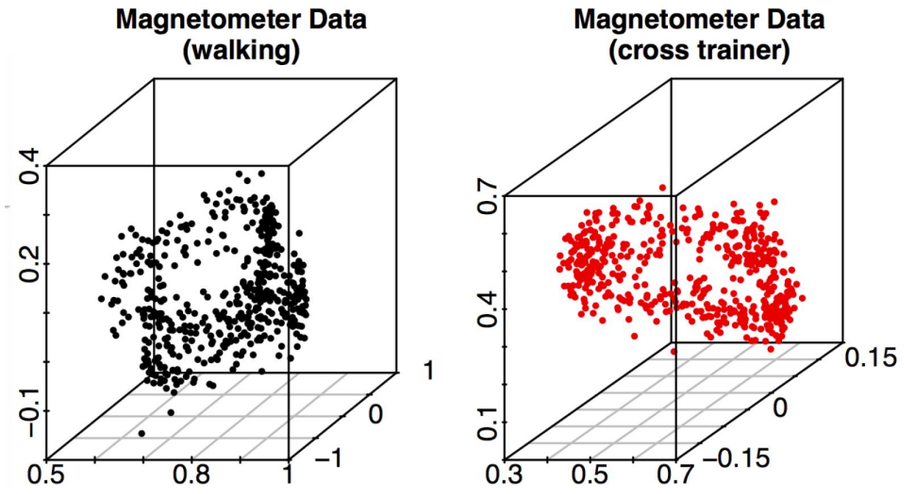
Introduction: topological descriptors built from data



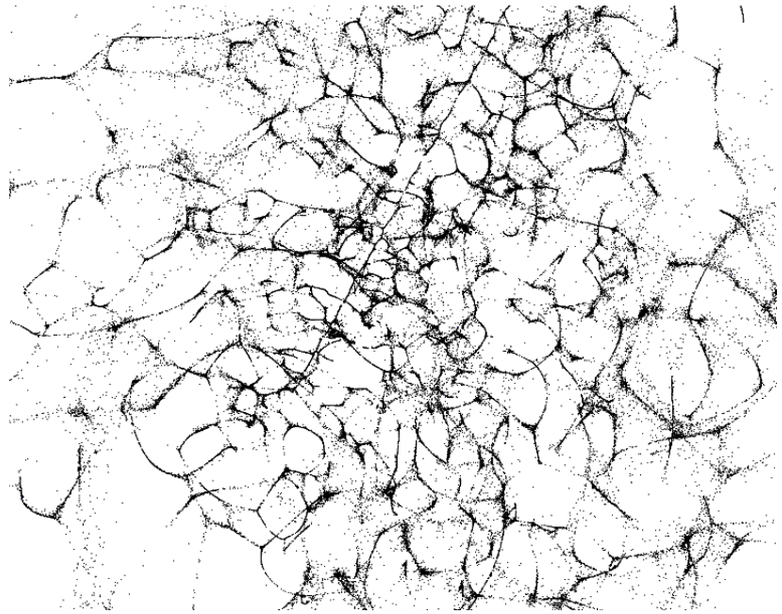
Scans



3D shapes

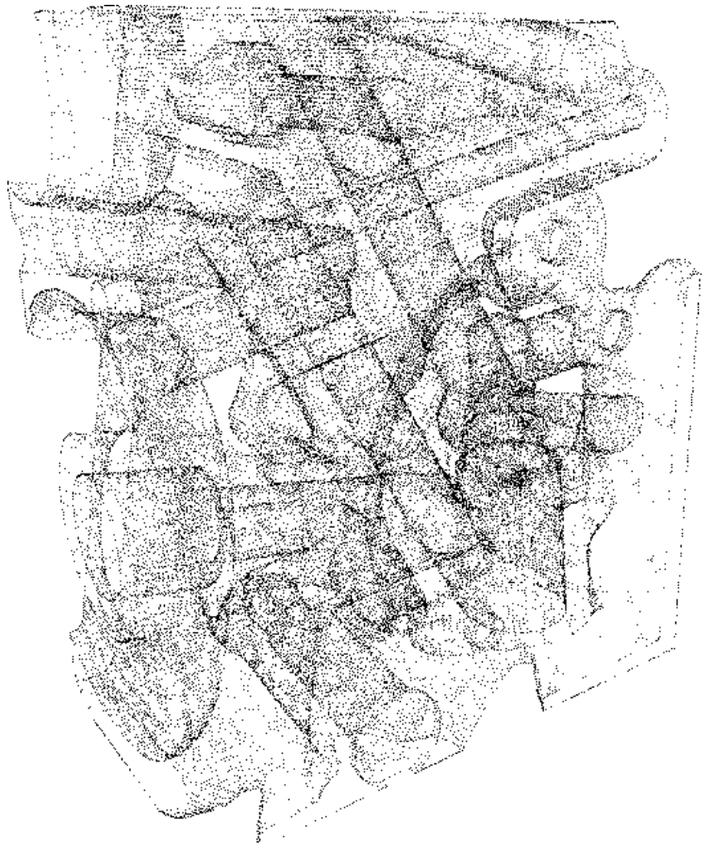


Magnetometer



Galaxies

Introduction: topological descriptors built from data



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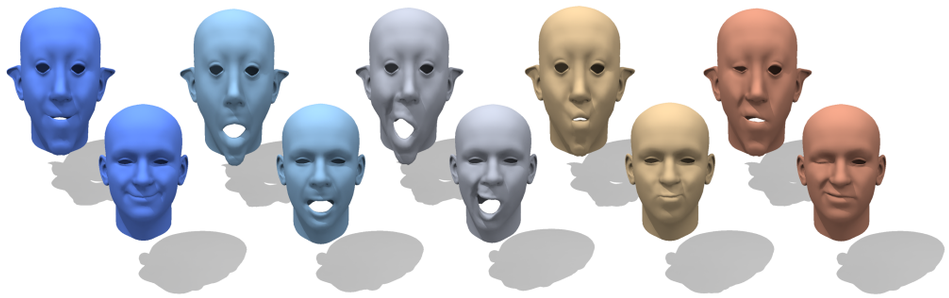

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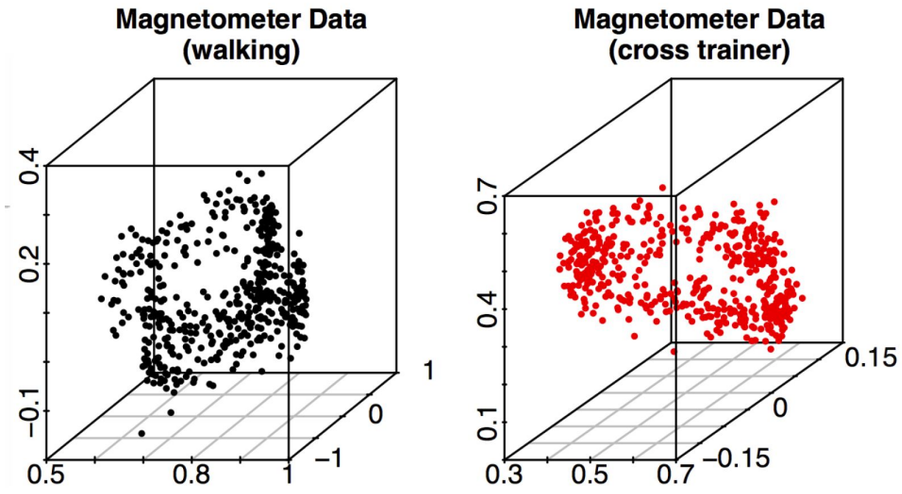

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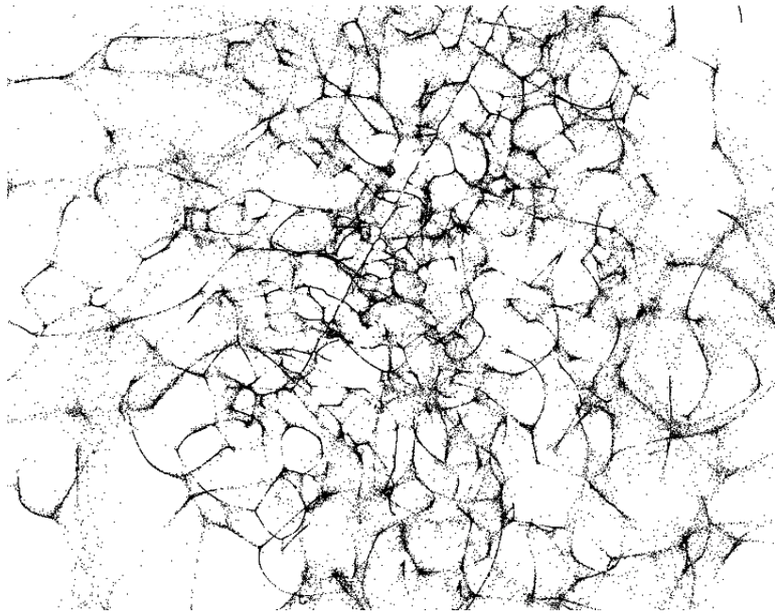
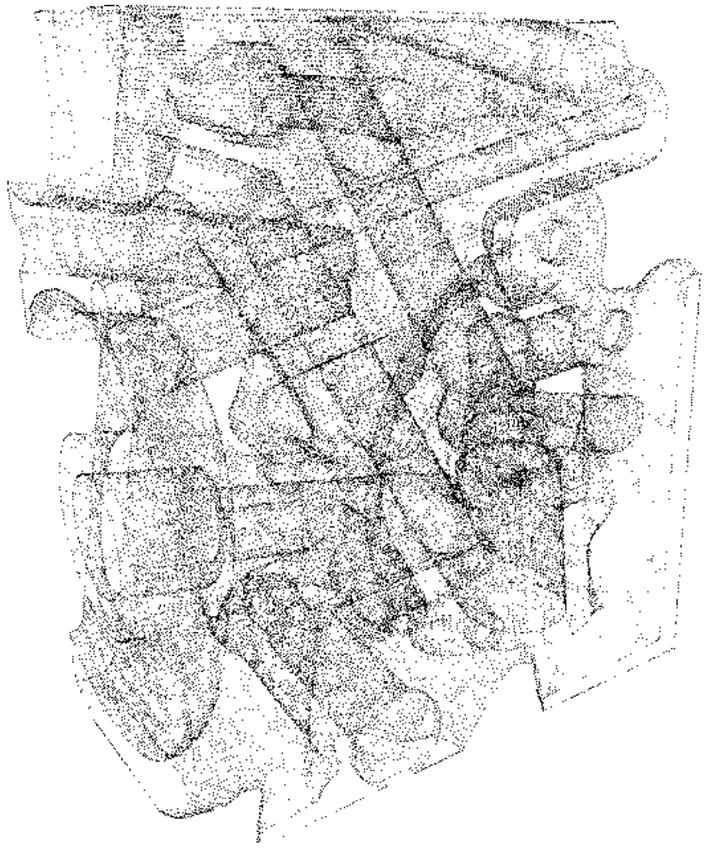


Galaxies

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 is usually high dimensional.

Introduction: topological descriptors built from data



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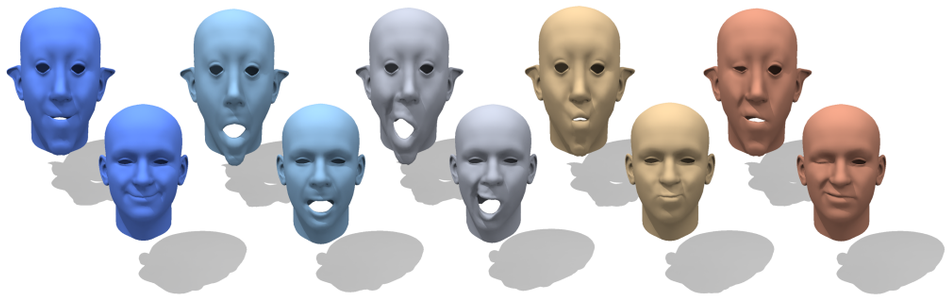

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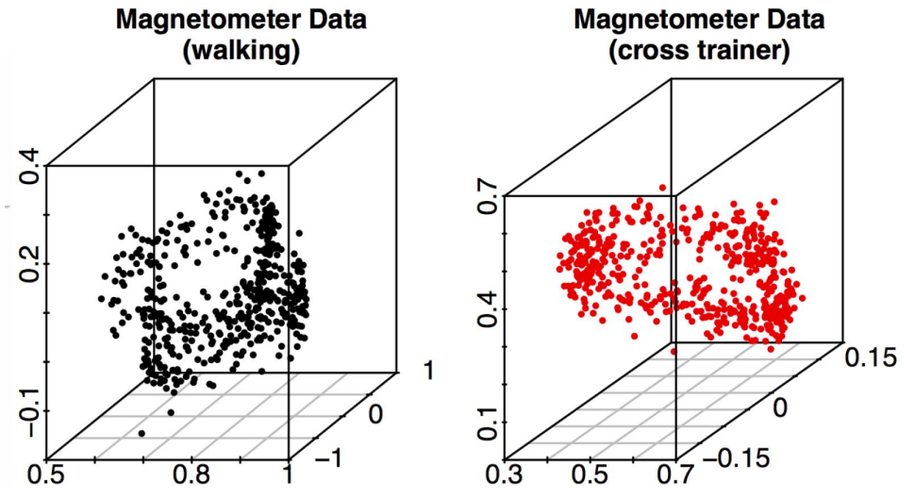

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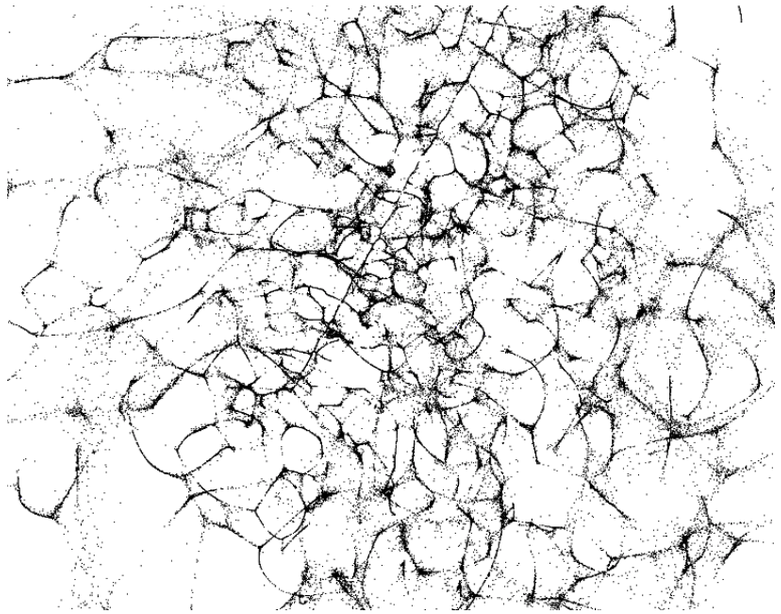
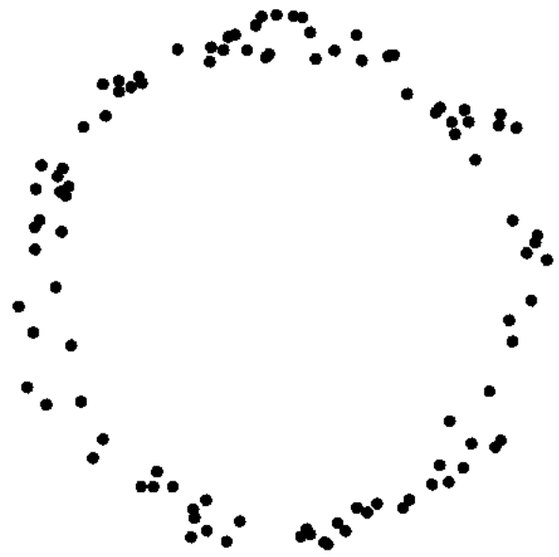


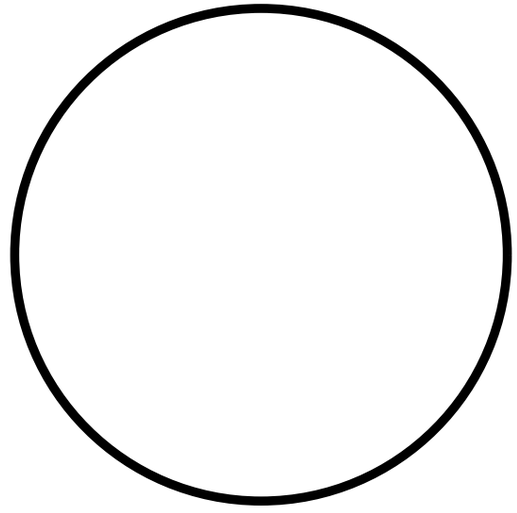
Galaxies

Features from Topological Data Analysis allow to:
- 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...).

Challenges and advantages

Problem: how to define the *topology* of a data set?





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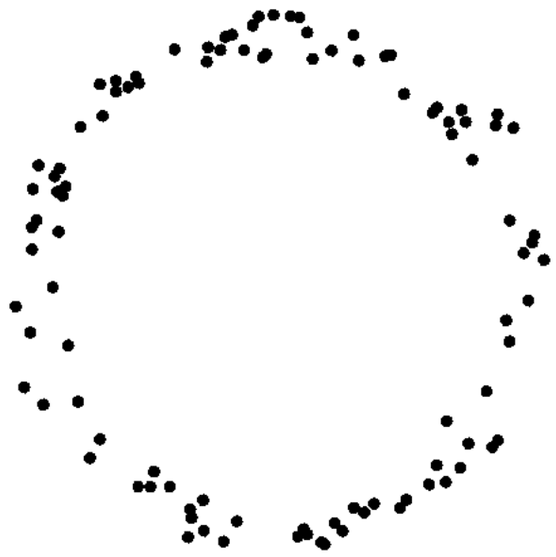
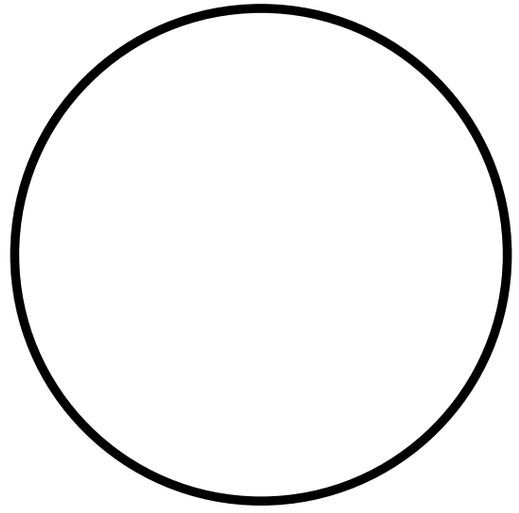




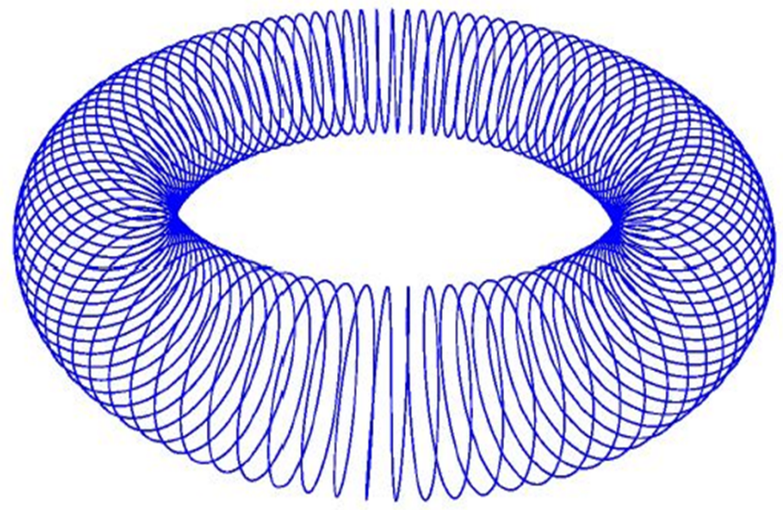
Challenges and goals:

$\rightarrow$ no direct access to topological/geometric information: need of intermediate constructions with *simplicial complexes*;

$\rightarrow$ distinguish topological "signal" from noise;

$\rightarrow$ topological information may be multiscale;

$\rightarrow$ statistical analysis of topological information.



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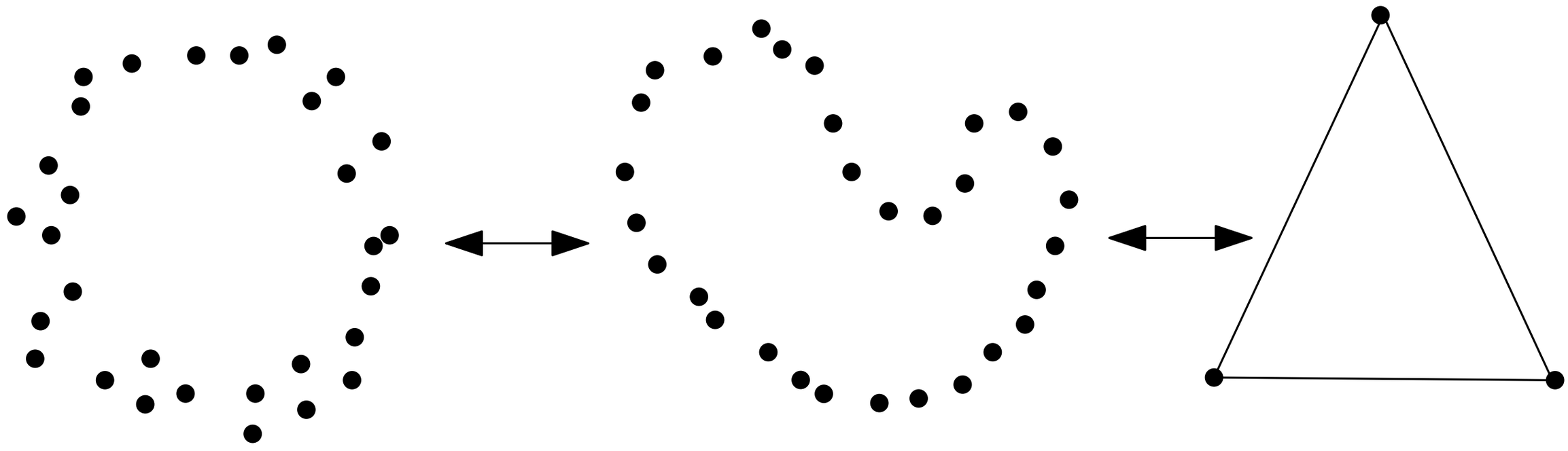

Advantages:

→ **coordinate invariance:** topological features/invariants do not rely on any coordinate system ⇒ no need to have data with coordinates, or to embed data in spaces with coordinates... but the metric (distance/similarity between data points) is important.

→ **deformation invariance:** topological features are invariant under homeomorphism and reparameterization.

→ **compressed representation:** topology offers a set of tools to summarize the data in compact ways while preserving its topological structure.

A brief look at topology

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A: The so-called *topological spaces*.

Def: A *topological space* is a set X equipped with a *topology*, i.e., a family $\mathcal{O}$ of subsets of X, called the *open sets* of X, such that:
(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 $\mathcal{O}$.

Open sets are the tools that allow to define *continuity*, which is the primary notion that allow to compare spaces in topology.

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Def: a map $f : X \to Y$ is *continuous* if and only if the pre-image $f^{-1}(O_Y) = \{x \in X : f(x) \in O_Y\}$ of any open set $O_Y \subseteq Y$ is an open set of X.

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A very common family of topological spaces is comprised of the *metric spaces*.

Def: 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.

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

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Def: Here are the main comparison tools of topology:

- Two maps $f_0 : X \to Y$ and $f_1 : X \to Y$ are *homotopic* if $\exists$ a continuous map $F : [0,1] \times X \to Y$ s.t. $\forall x \in X$, $F(0,x) = f_0(x)$ and $F_1(1,x) = f_1(x)$. X and Y are homotopy equivalent if $\exists$ 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.
- X and Y are homeomorphic if $\exists$ a bijection (homeomorphism) $h : X \to Y$ s.t. h and h^{-1} are continuous.
- X and Y are isotopic if $\exists$ a continuous map (isotopy) $F : X \times [0,1] \to Y$ s.t. $F(.,0) = \mathrm{id}_X$, $F(X,1) = Y$ and $\forall t \in [0,1]$, $F(.,t)$ is an homeomorphism.

Q: Which notion is stronger/weaker?

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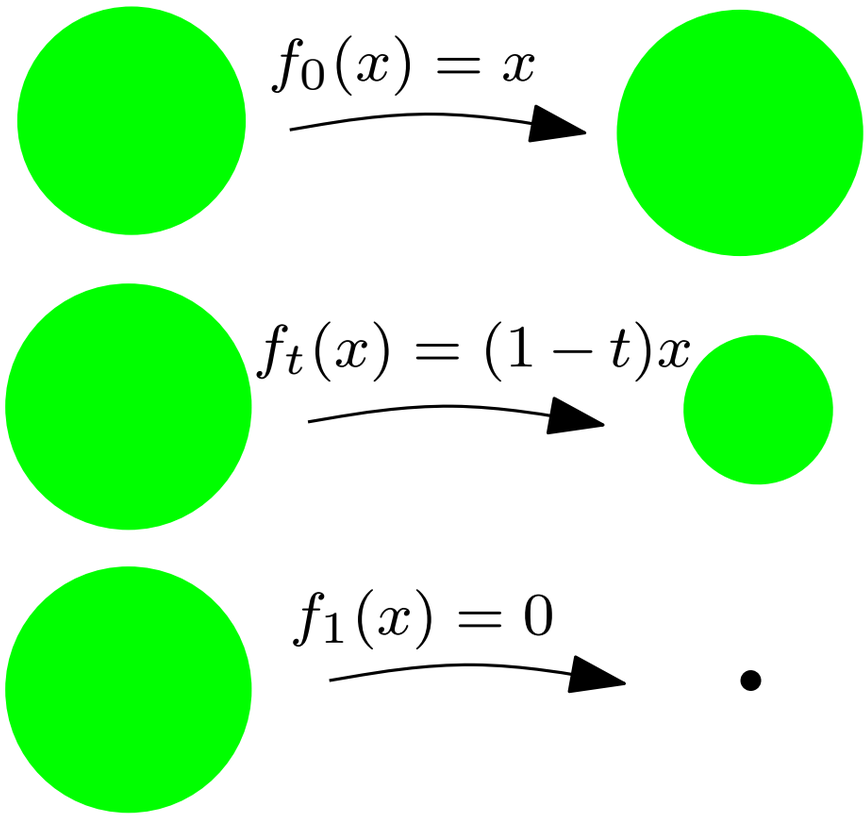

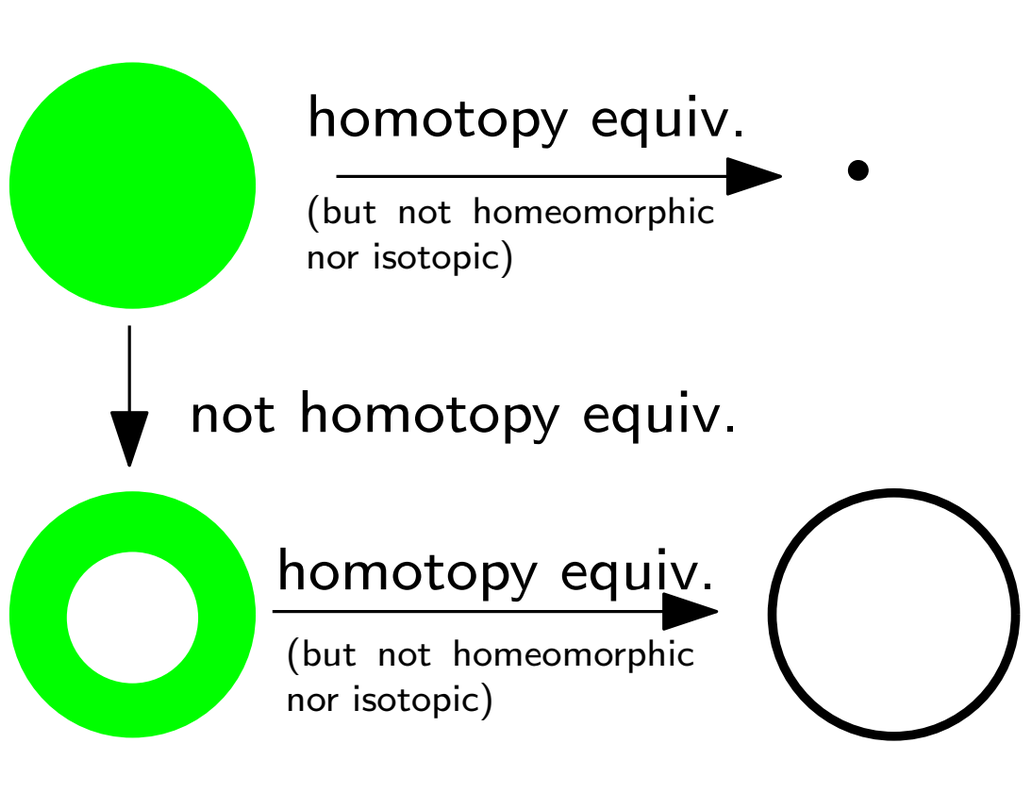

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Previous examples are particular homotopy equivalences called *deformation retracts*.

Def: If $Y \subseteq X$ and if there exists a continuous map $F : [0,1] \times X \to X$ s.t.:
(i) $\forall x \in X,\ F(0,x) = x$
(ii) $\forall x \in X,\ F(1,x) \in Y$
(iii) $\forall y \in Y,\ \forall t \in [0,1],\ F(t,y) \in Y$
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.

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Q: Can you find two spaces that are homeomorphic but not isotopic?

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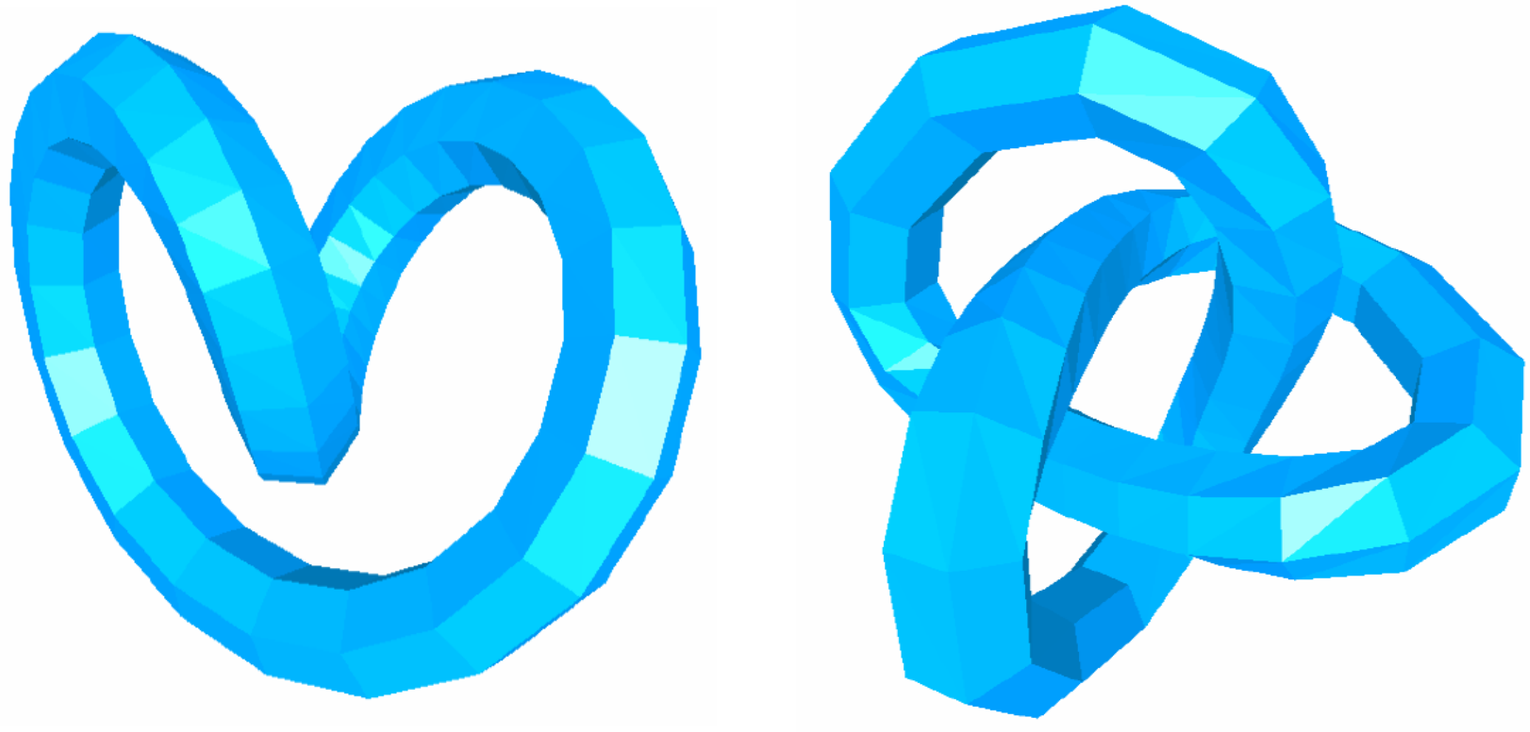
A: Torus and trefoil knot.



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Q: Can you find an isotopy between these guys?

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Pb 1: How to encode topological spaces for computational purposes?

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Pb 1: How to encode topological spaces for computational purposes?

Pb 2: Looking for homotopy equivalences/homeomorphisms/isotopies is extremely difficult. Are there mathematical quantities that are invariant to homotopy equivalences **and** easy to compute?

A topological space fit for computation

Pb 1: How to encode topological spaces for computational purposes?

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A: Using spaces made of small convex bricks, namely the *simplicial complexes* made of *simplices*.

Simplex and simplicial complex

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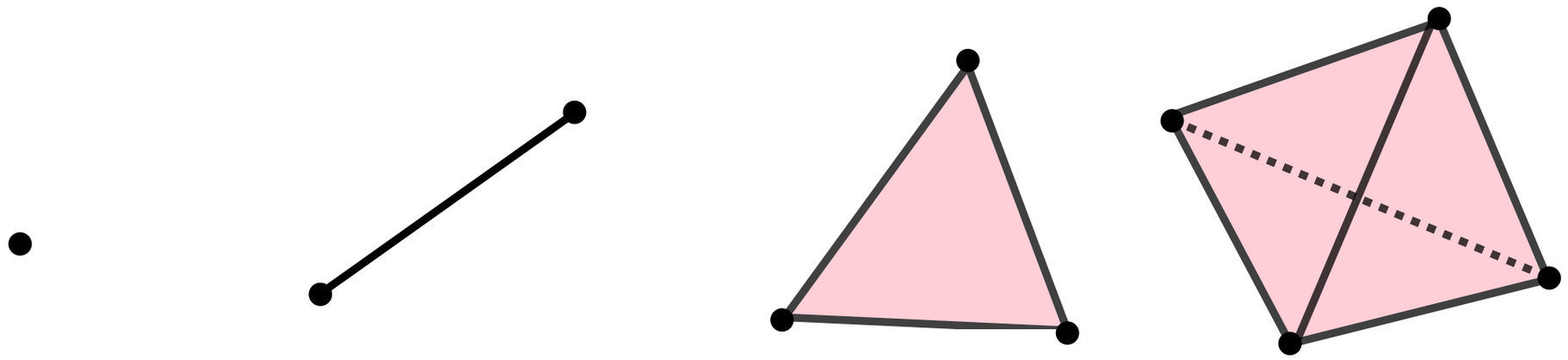


0-simplex:
vertex

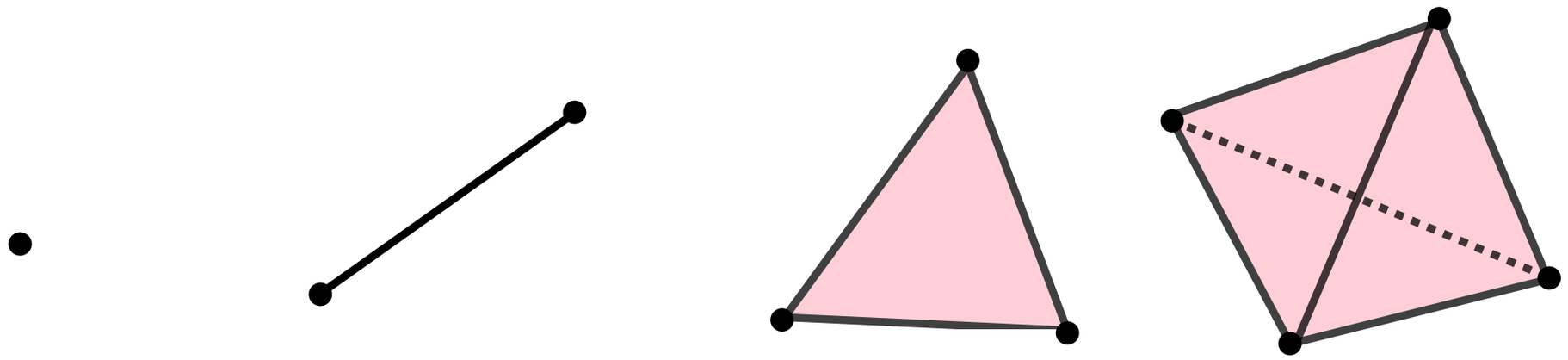
1-simplex:
edge

2-simplex:
triangle

3-simplex:
tetrahedron

etc...

Simplex and simplicial complex



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etc...

Def: Given a set $P = \{p_0, \ldots, p_k\} \subset \mathbb{R}^d$ of $k+1$ affinely independent points, the k-dimensional simplex σ (or k-simplex for short) spanned by P is the set of convex combinations

$$\sum_{i=0}^{k} \lambda_i \, p_i, \quad \text{with} \quad \sum_{i=0}^{k} \lambda_i = 1 \quad \text{and} \quad \lambda_i \geq 0.$$

The points $p_0, \ldots, p_k$ are called the vertices of σ.

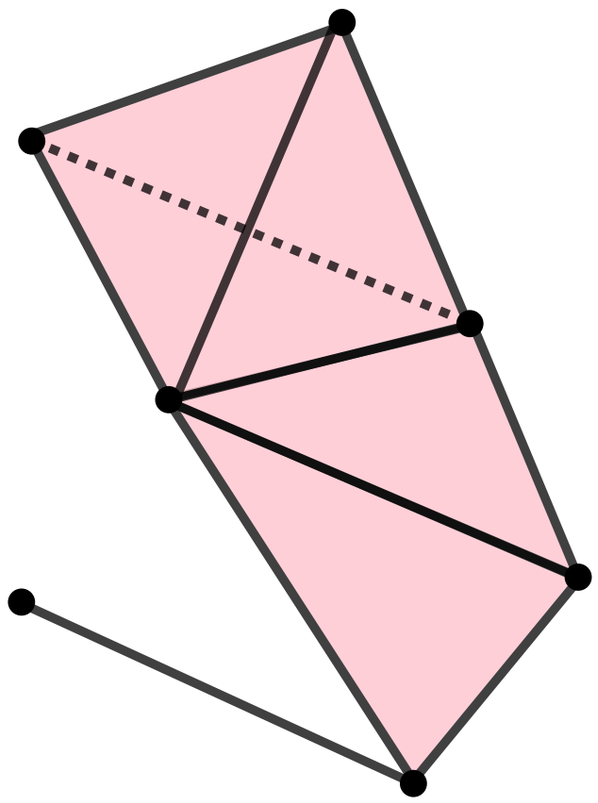
Simplex and simplicial complex

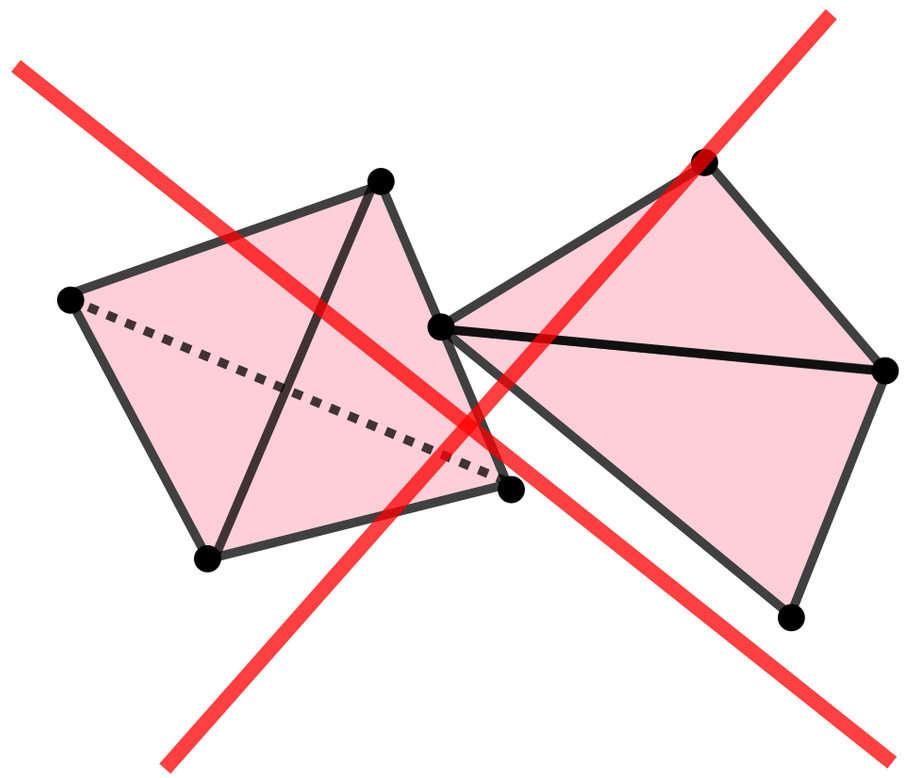
Def: A simplicial complex K in $\mathbb{R}^d$ is a collection of simplices s.t.:

- *(i)* any face of a simplex of K is a simplex of K,
- *(ii)* the intersection of any two simplices of K is either empty or a common face of both.

The underlying space of K (written $|K| \subseteq \mathbb{R}^d$) is the union of its simplices.

Simplex and simplicial complex





Def: A simplicial complex K in $\mathbb{R}^d$ is a collection of simplices s.t.:

- *(i)* any face of a simplex of K is a simplex of K,
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Def: A simplicial complex of dimension d is pure if every simplex is the face of a d-simplex.

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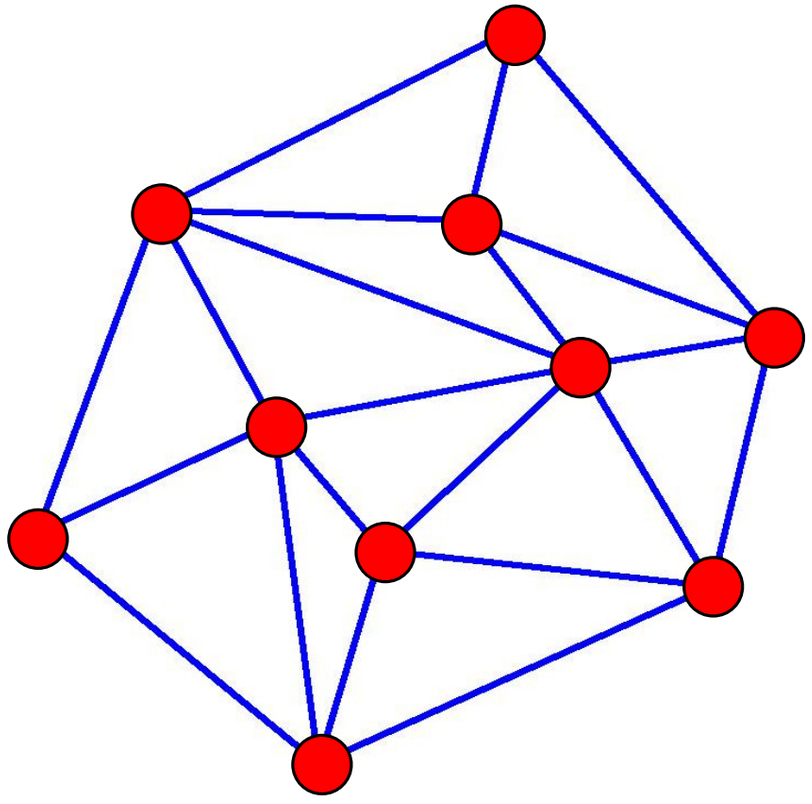

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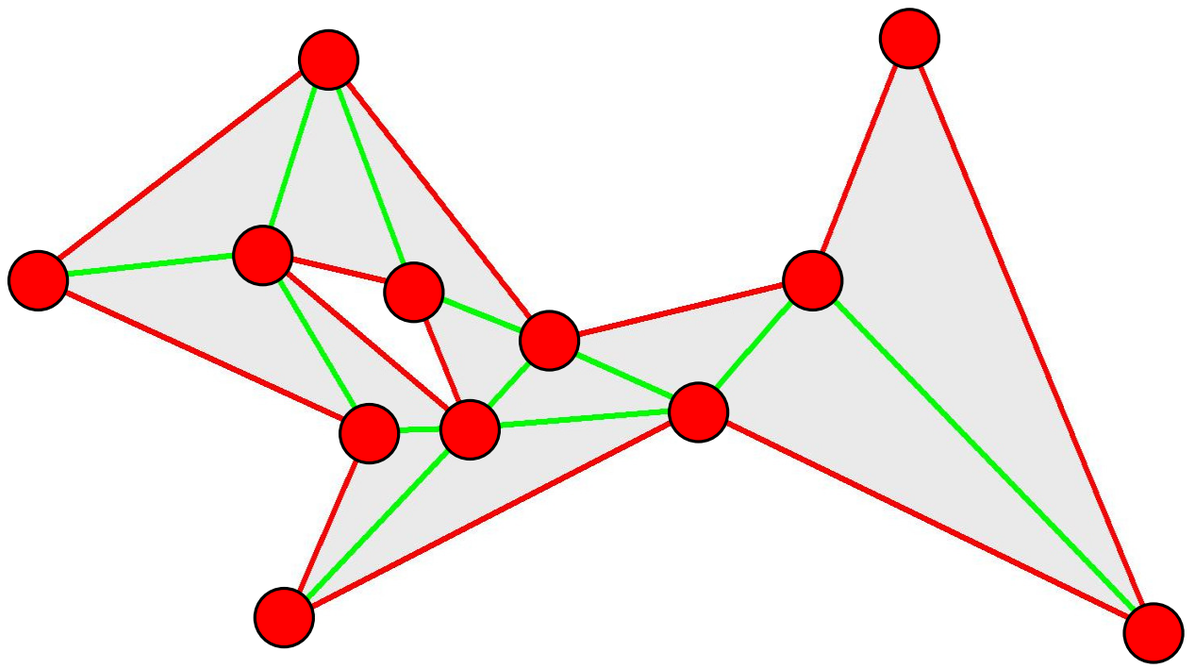

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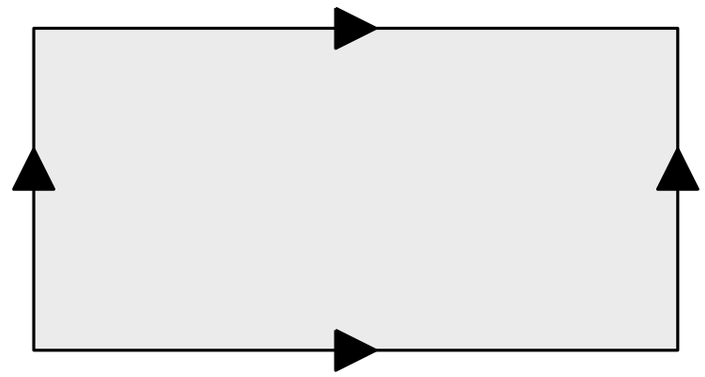
Q: Triangulate

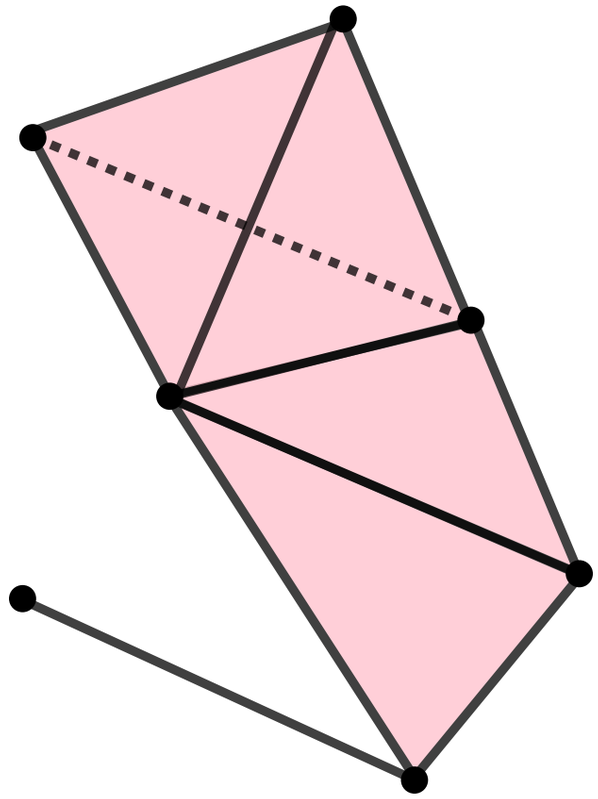


Abstract simplex and simplicial complex

Def: Let $P = \{p_1, \cdots, p_n\}$ be a (finite) set. An abstract simplicial complex K with vertex set P is a set of subsets of P satisfying the two conditions:

- *(i)* the elements of P belong to K,
- *(ii)* if $\tau \in K$ and $\sigma \subseteq \tau$, then $\sigma \in K$.

The elements of K are the simplices.



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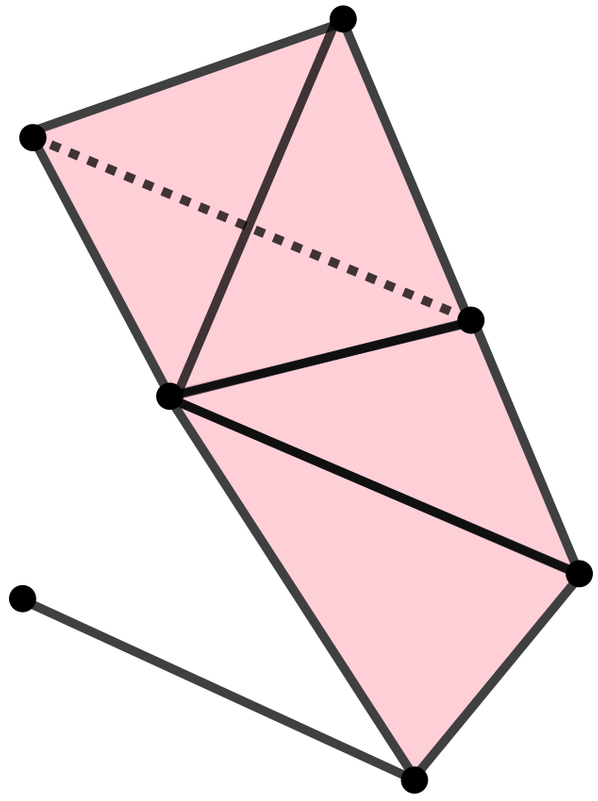

IMPORTANT

Simplicial complexes can be seen at the same time as geometric/topological spaces (good for topological/geometrical inference) and as combinatorial objects (abstract simplicial complexes, good for computations).

Abstract simplex and simplicial complex

Def: A realization of an abstract simplicial complex K is a geometric simplicial complex K' who is isomorphic to K, i.e., there exists a bijection

$$f : \mathrm{vert}(K) \to \mathrm{vert}(K'),$$

such that $\sigma \in K \iff f(\sigma) \in K'$.

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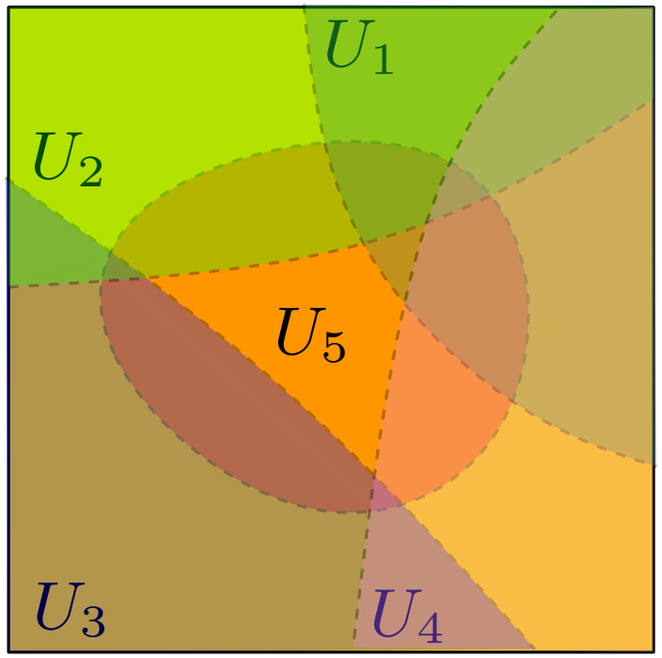
Abstract simplicial complexes and their realizations are *homeomorphic*.

Nerve complex

Def: An open cover of a topological space X is a collection $\mathcal{U} = (U_i)_{i \in I}$ of open subsets $U_i \subseteq X$, $i \in I$ where I is a set, such that $X \subseteq \cup_{i \in I} U_i$.

Nerve complex



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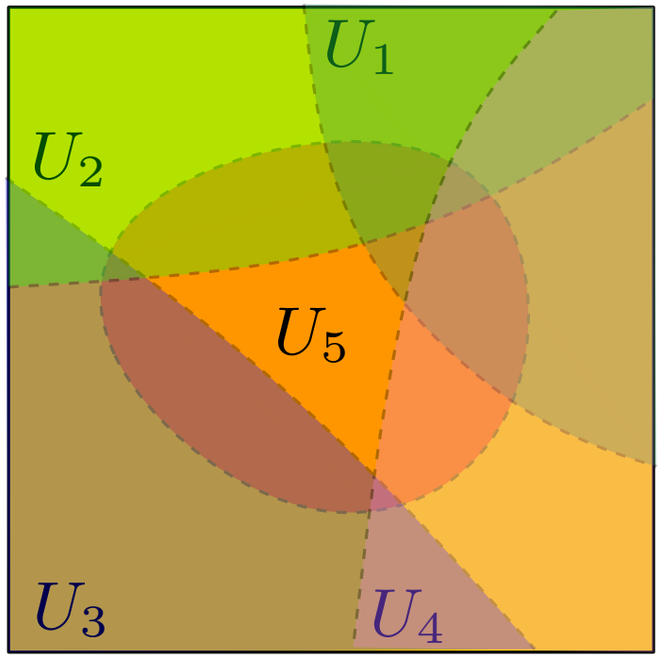

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Def: Given a cover of a topological space X, $\mathcal{U} = (U_i)_{i \in I}$, its nerve is the abstract simplicial complex $C(\mathcal{U})$ whose vertex set is $\mathcal{U}$ and s.t.

$$\sigma = [U_{i_0}, U_{i_1}, \ldots, U_{i_k}] \in C(\mathcal{U}) \text{ if and only if } \cap_{j=0}^{k} U_{i_j} \neq \emptyset.$$

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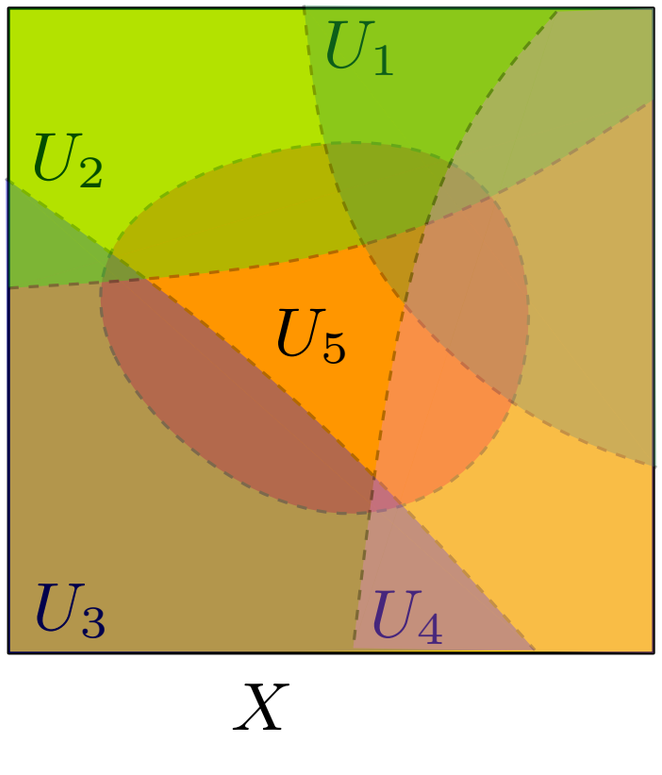

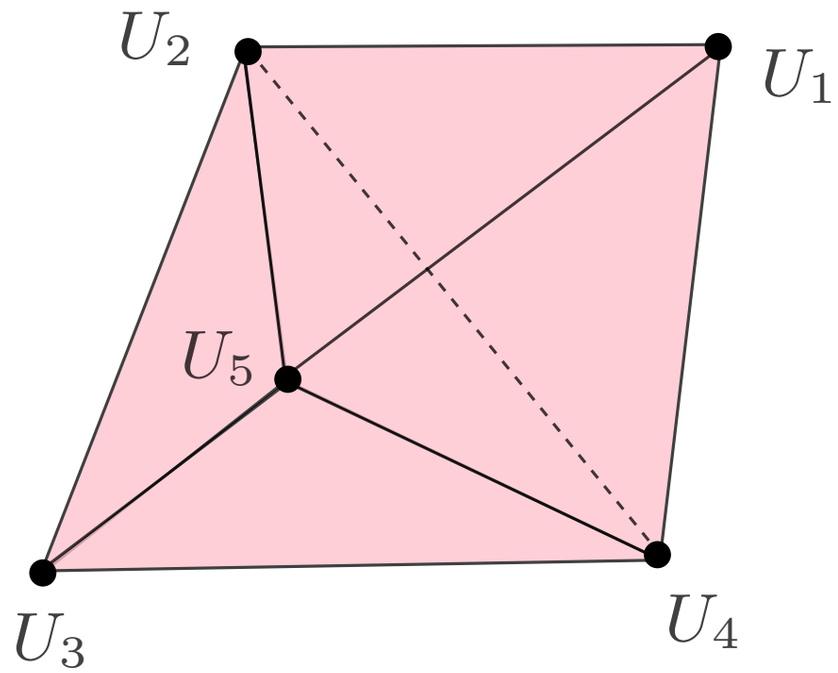

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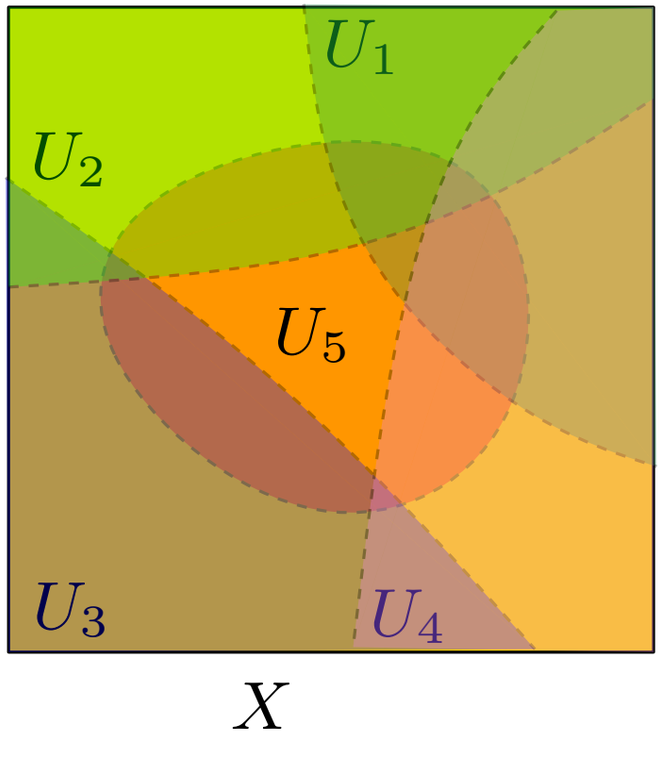
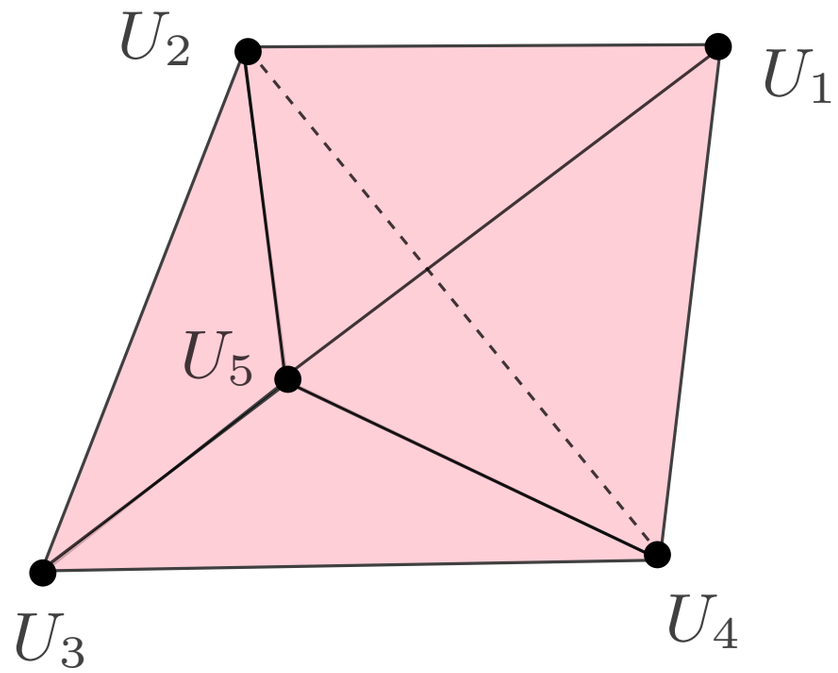
Nerve complex

[*On the imbedding of systems of compacta in simplicial complexes*, Borsuk, Fund. Math., 1948]





The Nerve Theorem: Let $\mathcal{U} = (U_i)_{i \in I}$ be a finite open cover of a subset X of $\mathbb{R}^d$ such that any intersection of the U_i's is either empty or contractible. Then X and $C(\mathcal{U})$ are homotopy equivalent.

In particular, every convex set is contractible.

Čech and (Vietoris)-Rips complexes

Def: Given a point cloud $P = \{P_1, \ldots, P_n\} \subset \mathbb{R}^d$, its Čech complex of radius $r > 0$ is the abstract simplicial complex $C(P, r)$ s.t. $\mathrm{vert}(C(P, r)) = P$ and

$$\sigma = [P_{i_0}, P_{i_1}, \ldots, P_{i_k}] \in C(P, r) \quad \text{iif} \quad \cap_{j=0}^{k} B(P_{i_j}, r) \neq \emptyset.$$

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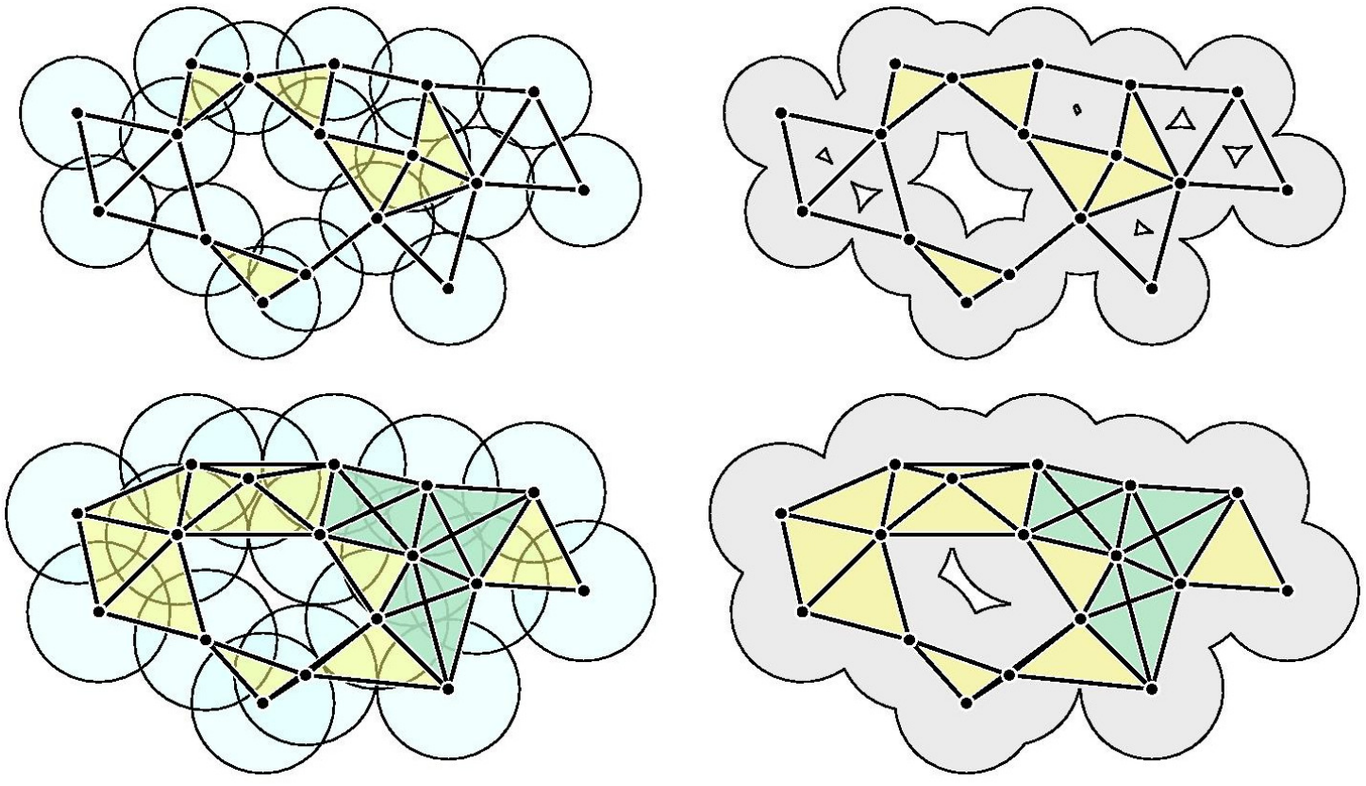
Q: Does the Nerve Theorem apply to Čech complexes?



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$$\sigma = [P_{i_0}, P_{i_1}, \ldots, P_{i_k}] \in R(P, r) \text{ iif } \|P_{i_j} - P_{i_{j'}}\| \leq 2r, \forall 1 \leq j, j' \leq k.$$

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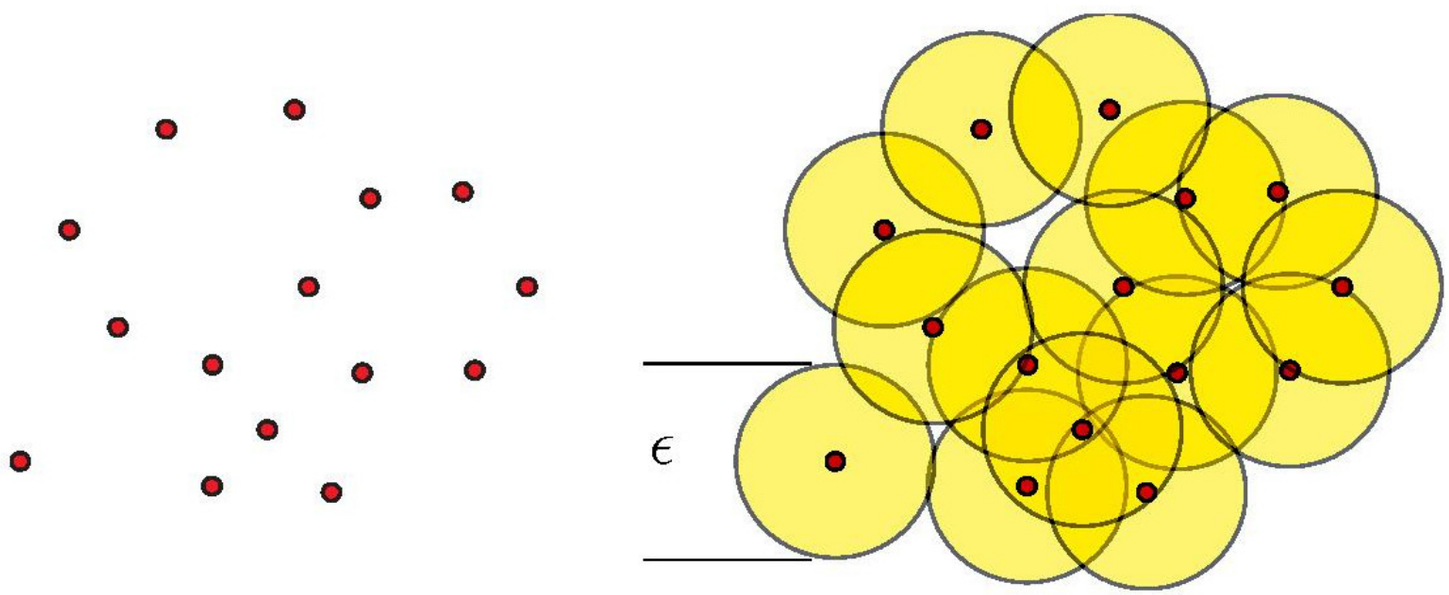
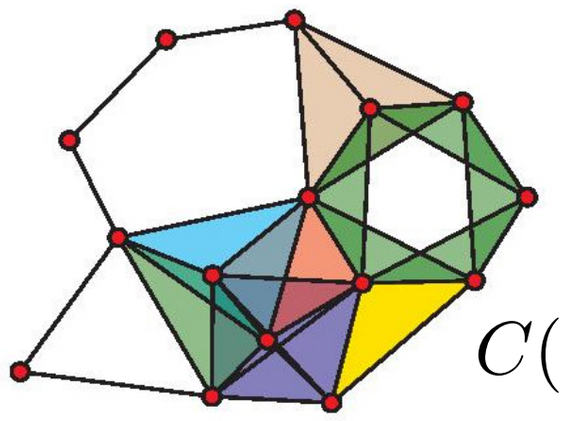
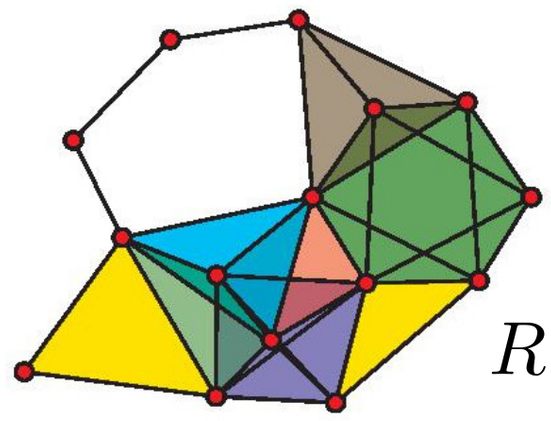




$C(P, \epsilon)$



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Good news is that Rips and Čech complexes are related:

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Prop: $R(P, r/2) \subseteq C(P, r) \subseteq R(P, r)$.

Q: Prove it.

Storing simplicial complexes

[*The Simplex Tree: An Efficient Data Structure for General Simplicial Complexes*, Boissonnat, Maria, Algorithmica, 2014]

We want to store simplicial complexes with a data structure that allows to perform standard operations (insertion of a simplex, checking if a simplex is present, etc) in a fast and easy way.

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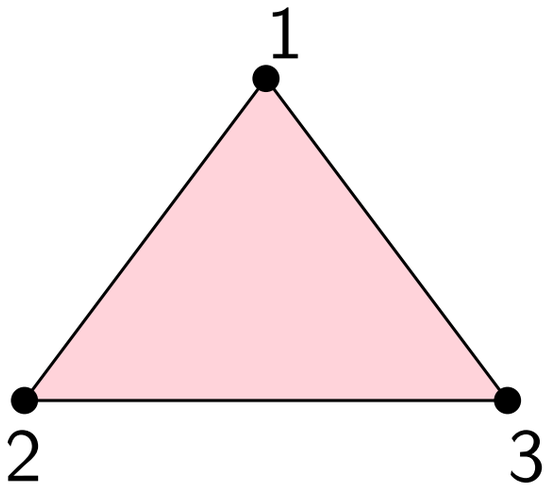
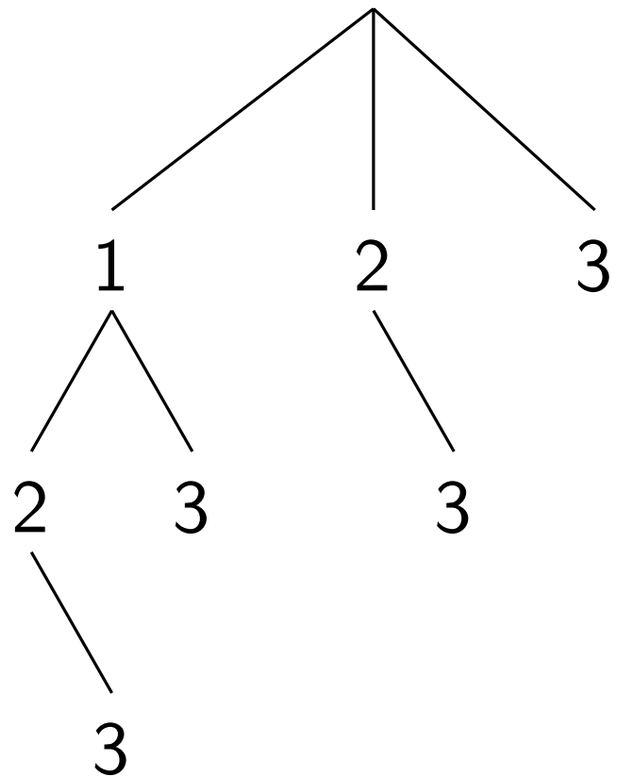
Idea: store sorted simplices in a prefix tree (also called *trie)*.





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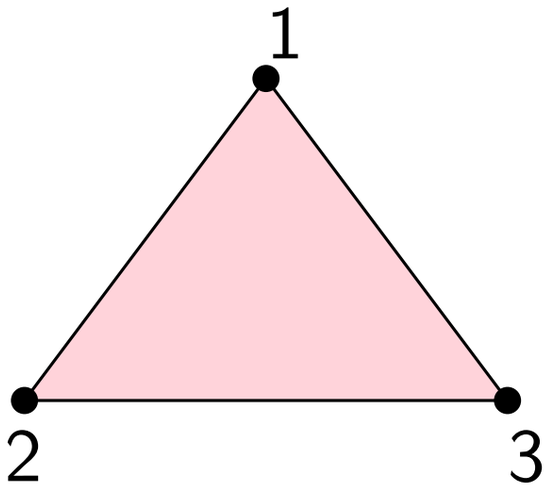

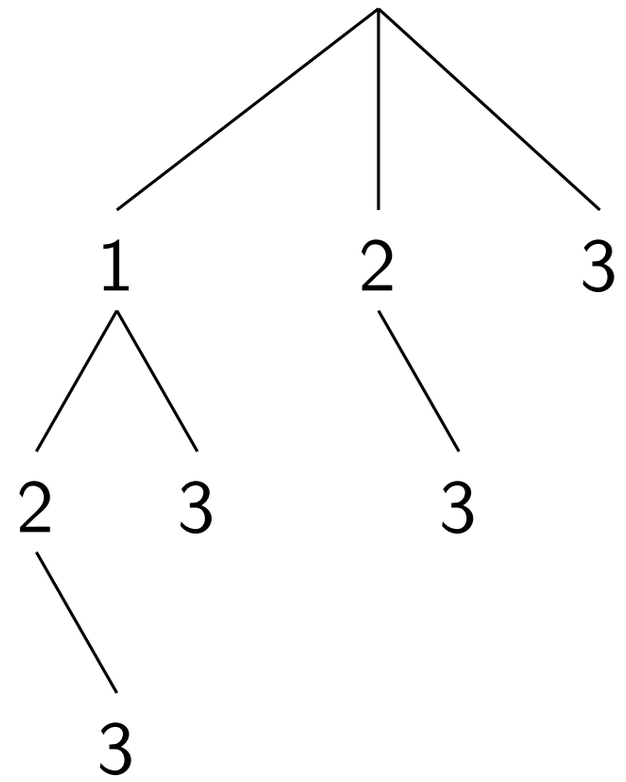

This is called the *simplex tree*.

It allows to store all simplices explicitly without storing all adjacency relations, while maintaining low complexity for basic operations.

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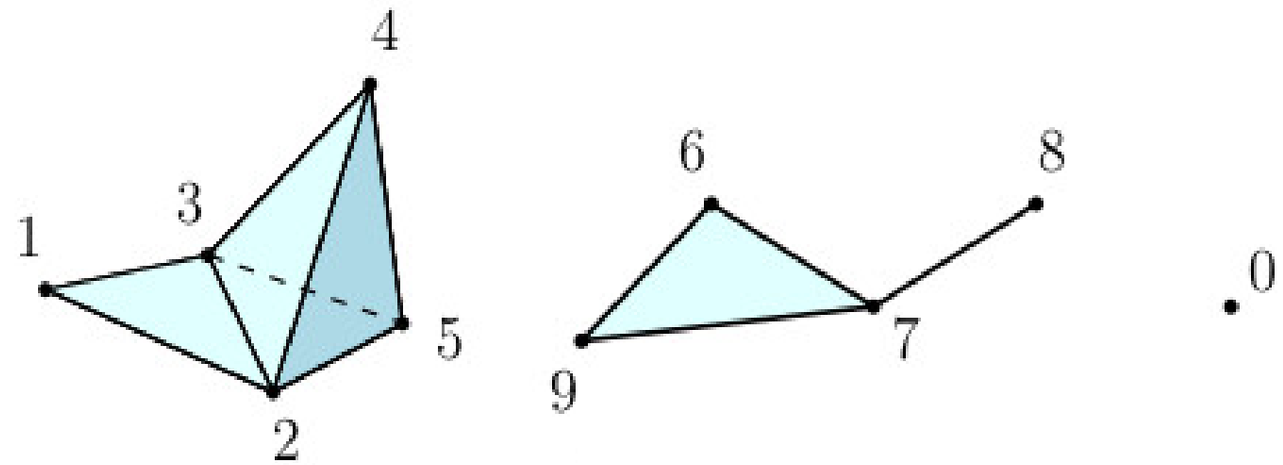

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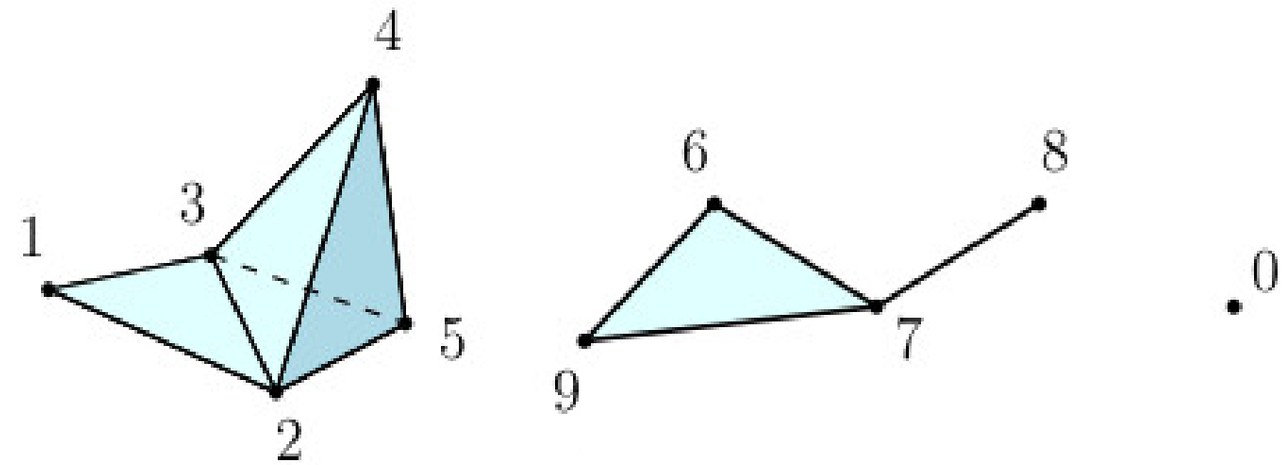

Number of nodes in simplex tree = number of simplices

Depth of simplex tree = 1 + dimension of complex

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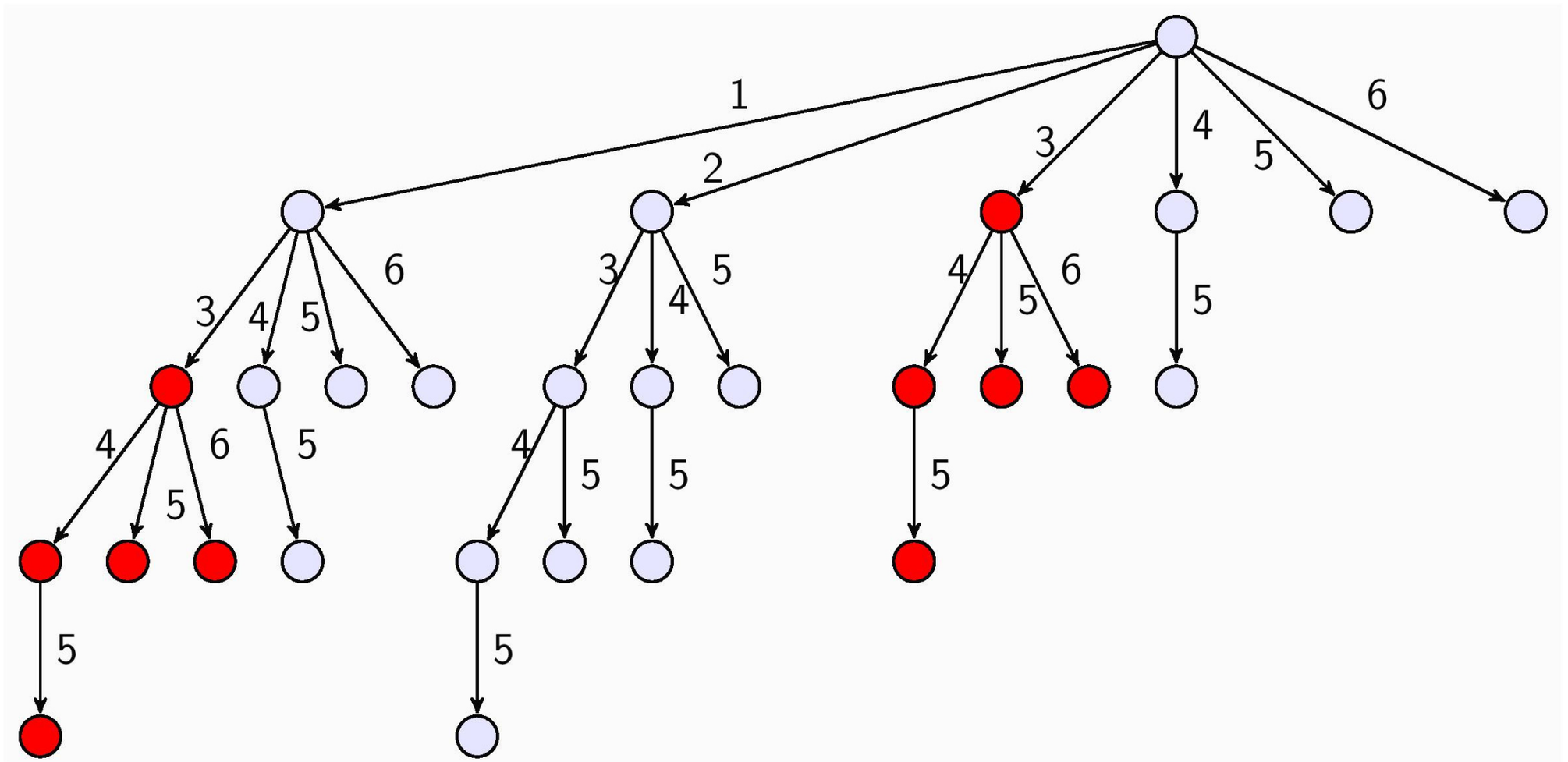

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