# Persistent homology for multivariate data visualization

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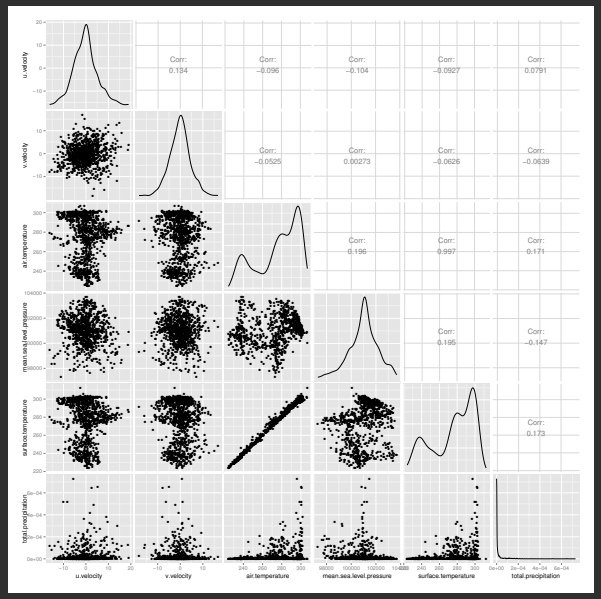
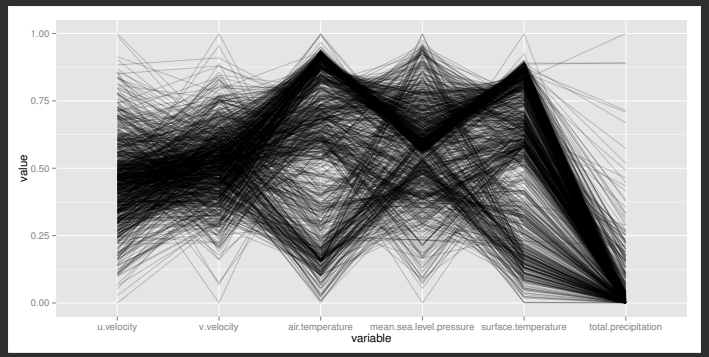
# Motivation

## Understanding the ‘shape’ of data


Unstructured data




Scatterplot matrix




Parallel coordinates

# Agenda

1. Theory: Algebraic topology
2. Theory: Persistent homology
3. Applications

# Part I

# Theory: Algebraic topology

# Algebraic topology

*Algebraic topology is the branch of mathematics that uses tools from abstract algebra to study manifolds. The basic goal is to find algebraic invariants that classify topological spaces up to homeomorphism.*

Adapted from `https://en.wikipedia.org/wiki/Algebraic_topology`.

# Manifolds

A $d$-dimensional Riemannian manifold $\mathbb{M}$ in some $\mathbb{R}^n$, with $d \ll n$, is a space where every point $p \in \mathbb{M}$ has a neighbourhood that 'locally looks' like $\mathbb{R}^d$.

A 2-dimensional manifold

# Homeomorphisms

A homeomorphism between two spaces $X$ and $Y$ is a continuous function $f\colon X \to Y$ whose inverse $f^{-1}\colon Y \to X$ exists and is continuous as well.

Intuitively, we may *stretch*, *bend*—but not *tear* and *glue* the two spaces.

# Algebraic invariants

An invariant is a property of an object that remains unchanged upon transformations such as scaling or rotations.

## Example

*Dimension* is a simple invariant: $\mathbb{R}^2 \neq \mathbb{R}^3$ because $2 \neq 3$.

## In general

Let $\mathcal{M}$ be the family of manifolds. An invariant permits us to define a function $f\colon \mathcal{M} \times \mathcal{M} \to \{0, 1\}$ that tells us whether two manifolds are different or 'equal' (with respect to that invariant).

No invariant is *perfect*—there will be objects that have the same invariant even though they are different.

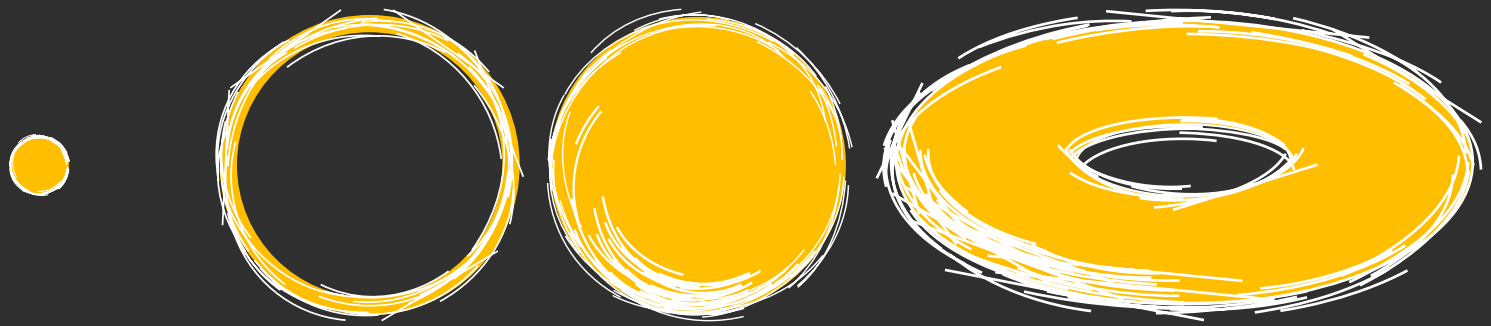
# Betti numbers

A useful topological invariant

Informally, they count the number of holes in different dimensions that occur in a data set.

| | |
|---|---|
| $\beta_0$ | Connected components |
| $\beta_1$ | Tunnels |
| $\beta_2$ | Voids |
| ⋮ | ⋮ |

| Space | $\beta_0$ | $\beta_1$ | $\beta_2$ |
|---|---|---|---|
| Point | 1 | 0 | 0 |
| Circle | 1 | 1 | 0 |
| Sphere | 1 | 0 | 1 |
| Torus | 1 | 2 | 1 |



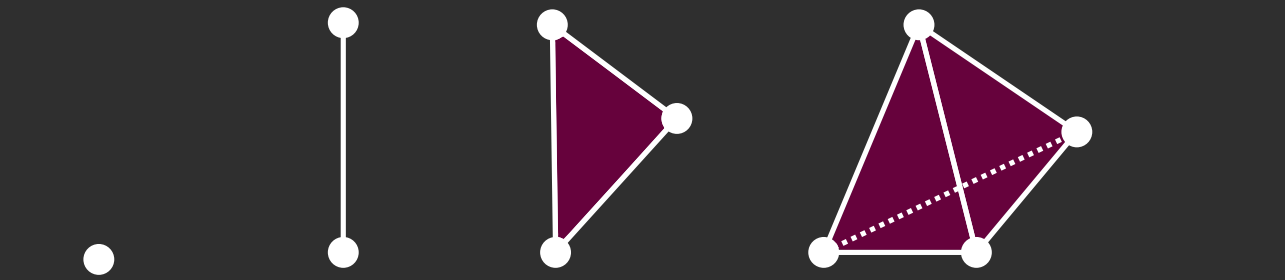
# Signature property

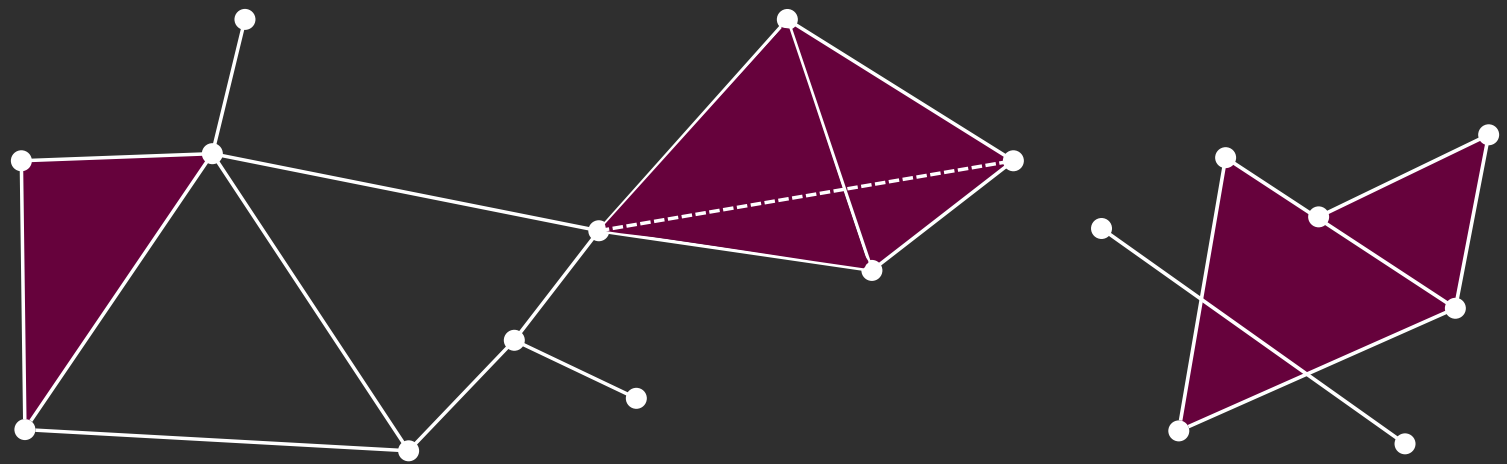
If $\beta_i^X \neq \beta_i^Y$, we know that $X \ncong Y$. The converse is *not* true, unfortunately:


| Space | $\beta_0$ | $\beta_1$ |
|---|---|---|
| X | 1 | 1 |
| Y | 1 | 1 |

We have $\beta_0 = 1$ and $\beta_1 = 1$ for X and Y, but still $X \ncong Y$.

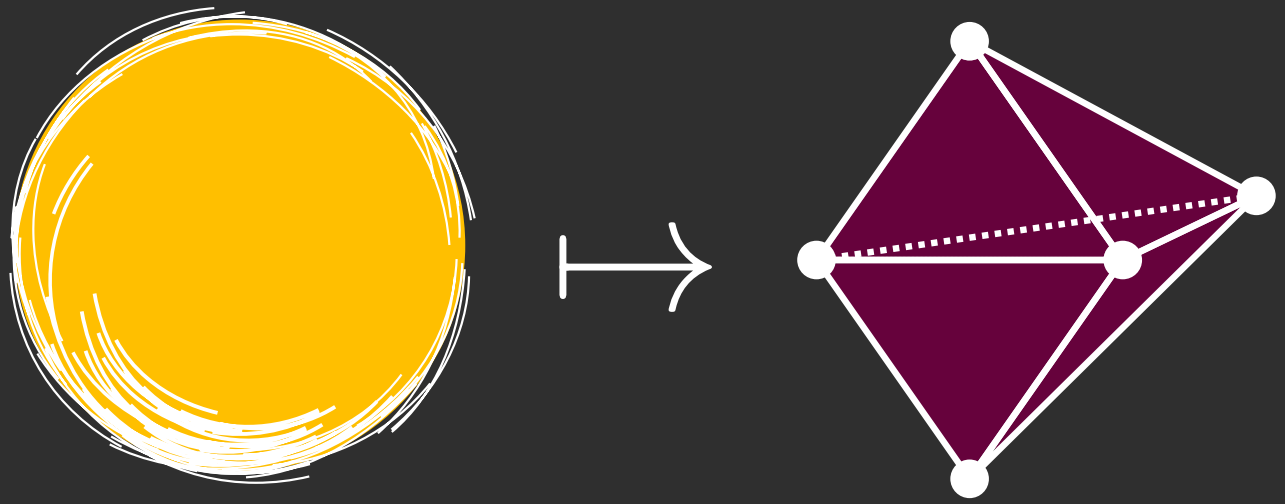
# Simplicial complexes



# Simplicial complexes

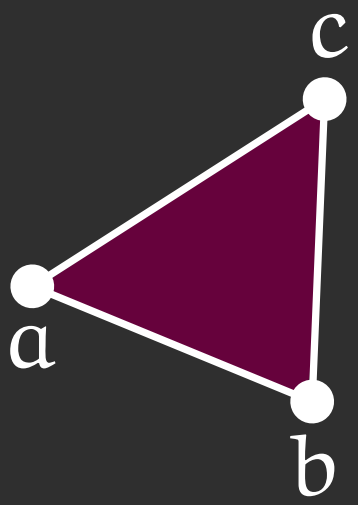
## Example



The simplicial complex representation is compact and permits the calculation of the Betti numbers using an efficient matrix reduction scheme.

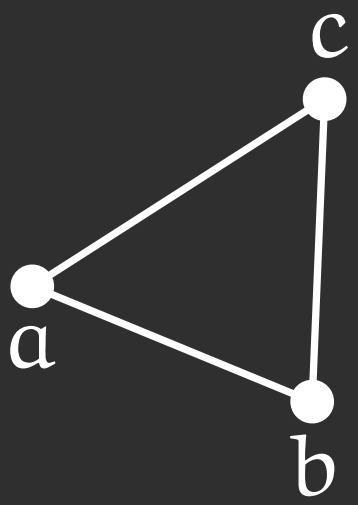
# Basic idea

## Calculating boundaries




The boundary of the triangle is:

$$\partial_2\{a, b, c\} = \{b, c\} + \{a, c\} + \{a, b\}$$




The set of edges does *not* have boundary:

$$\begin{aligned}\partial_1 &(\{b, c\} + \{a, c\} + \{a, b\}) \\ &= \{c\} + \{b\} + \{c\} + \{a\} + \{b\} + \{a\} \\ &= 0\end{aligned}$$

# Fundamental lemma

For all $\mathrm{p}$, we have $\partial_{\mathrm{p}-1} \circ \partial_{\mathrm{p}} = 0$: *Boundaries do not have a boundary themselves*.

This permits us to calculate Betti numbers of simplicial complexes by reducing a *boundary matrix* to its *Smith Normal Form* using Gaussian elimination.

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# Part II

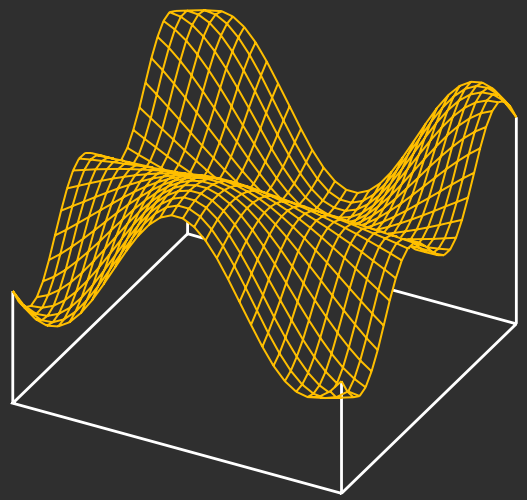
# Theory: Persistent homology

# Real-world multivariate data

- Unstructured point clouds
- $\mathrm{n}$ items with $\mathrm{D}$ attributes; $\mathrm{n} \times \mathrm{D}$ matrix
- Non-random sample from $\mathbb{R}^{\mathrm{D}}$

## Manifold hypothesis

There is an unknown $\mathrm{d}$-dimensional manifold $\mathbb{M} \subseteq \mathbb{R}^{\mathrm{D}}$, with $\mathrm{d} \ll \mathrm{D}$, from which our data have been sampled.



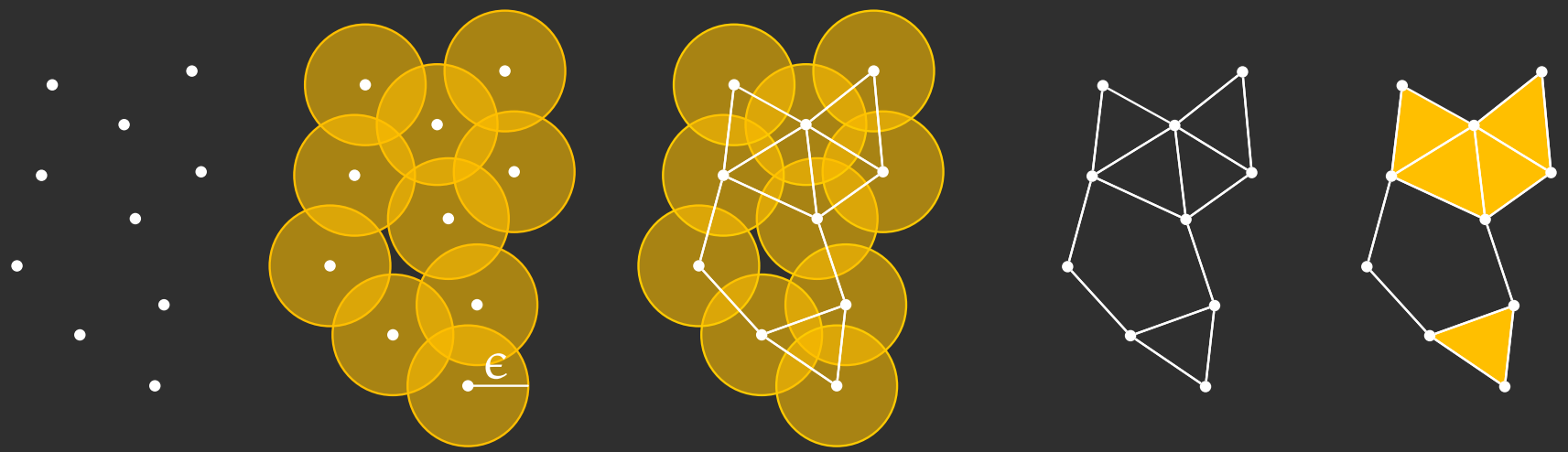
2-manifold in $\mathbb{R}^3$

# Agenda

1. Convert our input data into a simplicial complex $K$.
2. Calculate the Betti numbers of $K$.
3. Use the Betti numbers to compare data sets.

(Fair warning: It won't be so simple)

# Converting unstructured data into a simplicial complex

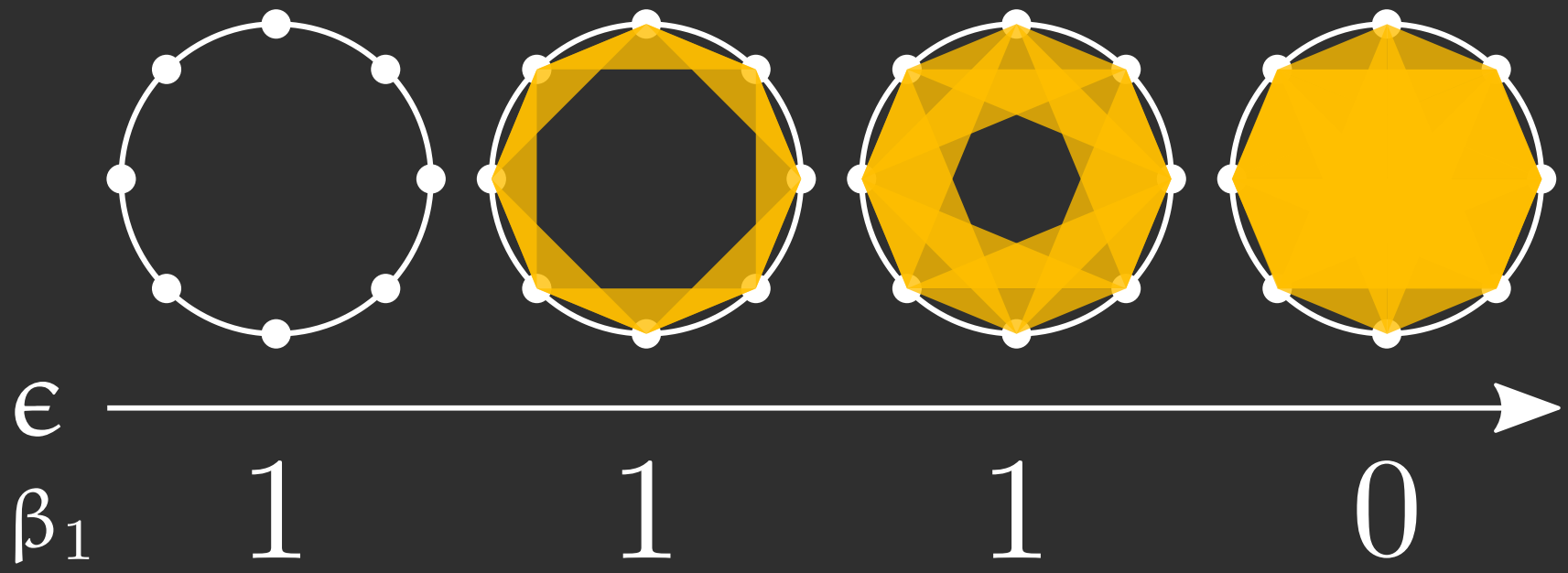



Require: Distance measure (e.g. Euclidean distance), maximum scale threshold $\epsilon$.

Construct the Vietoris–Rips complex $\mathcal{V}_\epsilon$ by adding a $k$-simplex whenever all of its $(k-1)$-dimensional faces are present.

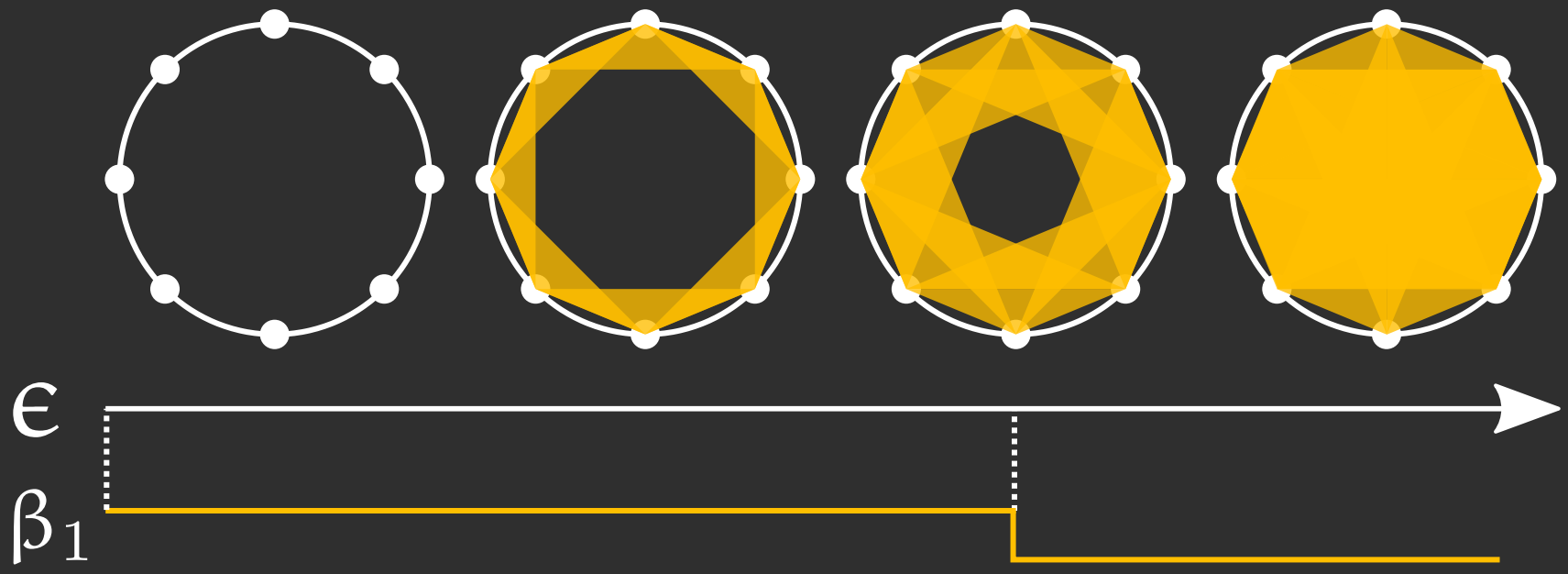
# Calculating Betti numbers directly from $\mathcal{V}_\epsilon$

Unstable behaviour



# Calculating *persistent* Betti numbers

## Persistent homology



# How does this work in practice?

## An example for $\beta_0$

- Have a function $f\colon \mathcal{V}_\epsilon \to \mathbb{R}$ on the *vertices* of the Vietoris–Rips complex.

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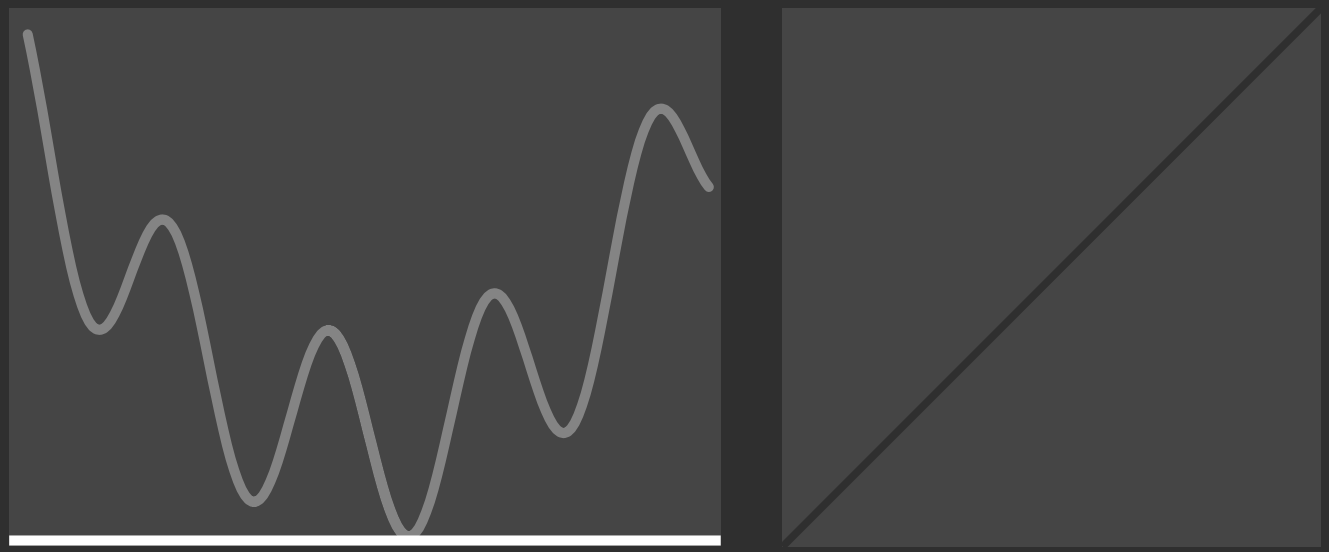
- This can be done by traversing the values of $f$ in increasing order and stopping at 'critical points'.

# Persistent homology & persistence diagrams

## One-dimensional example



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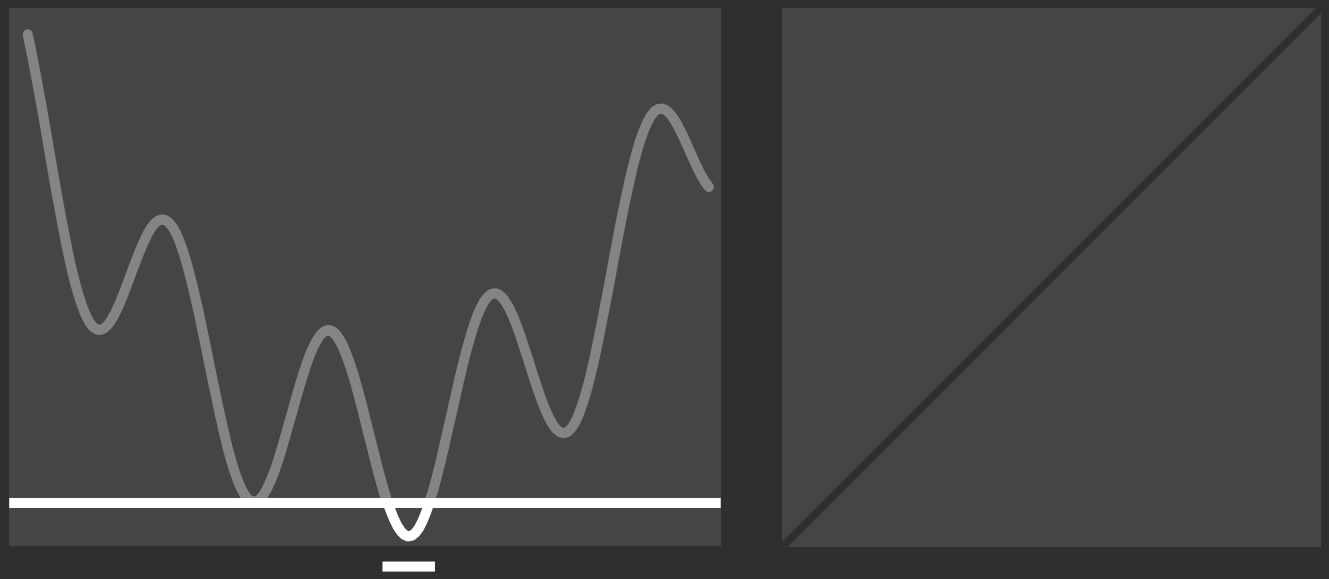

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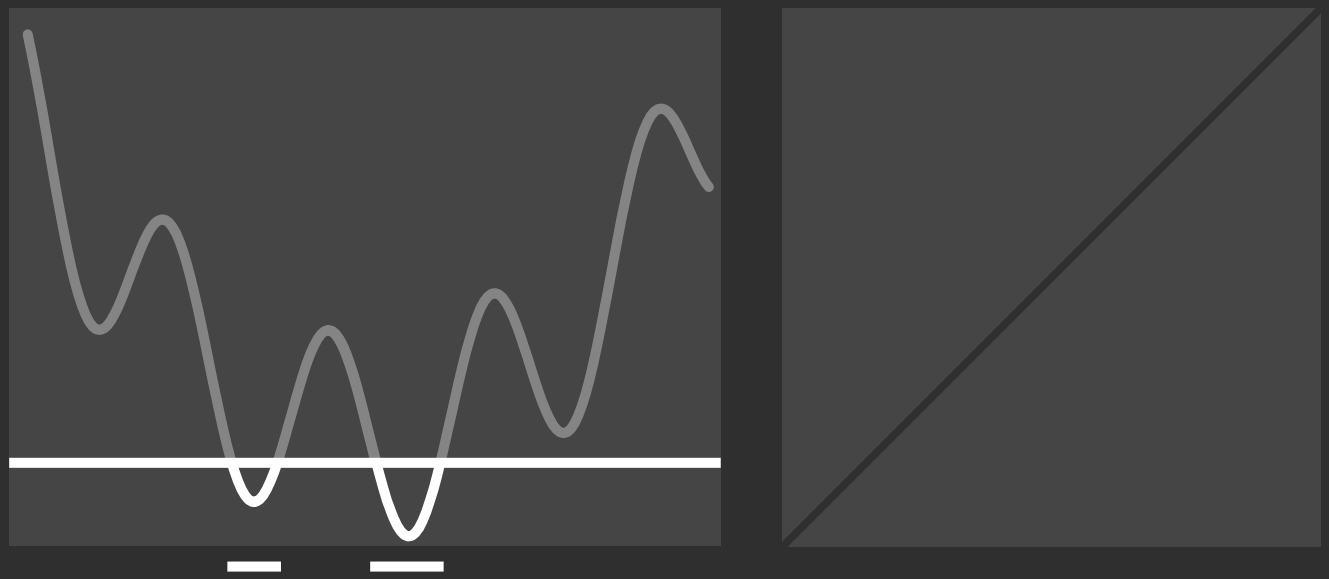

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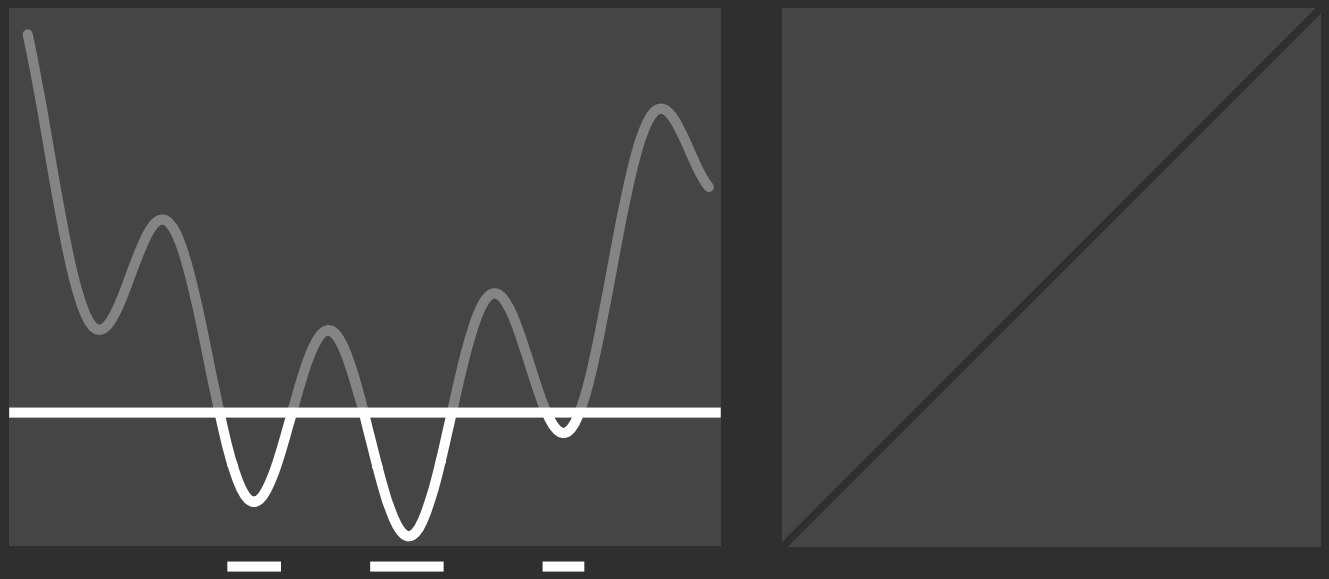

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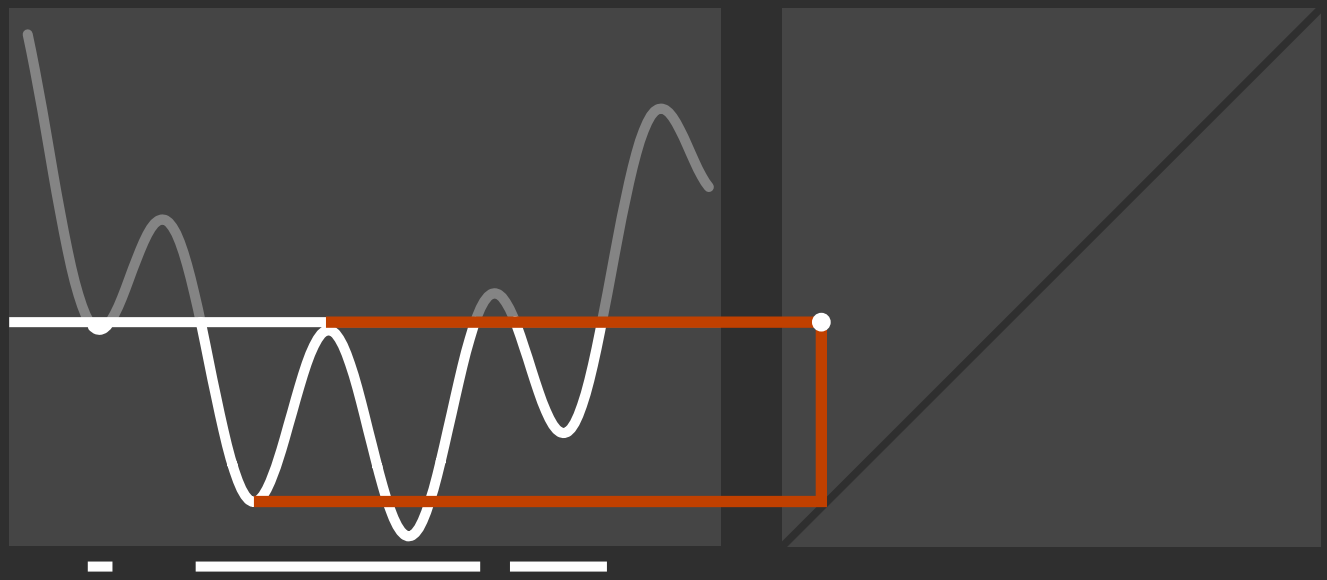

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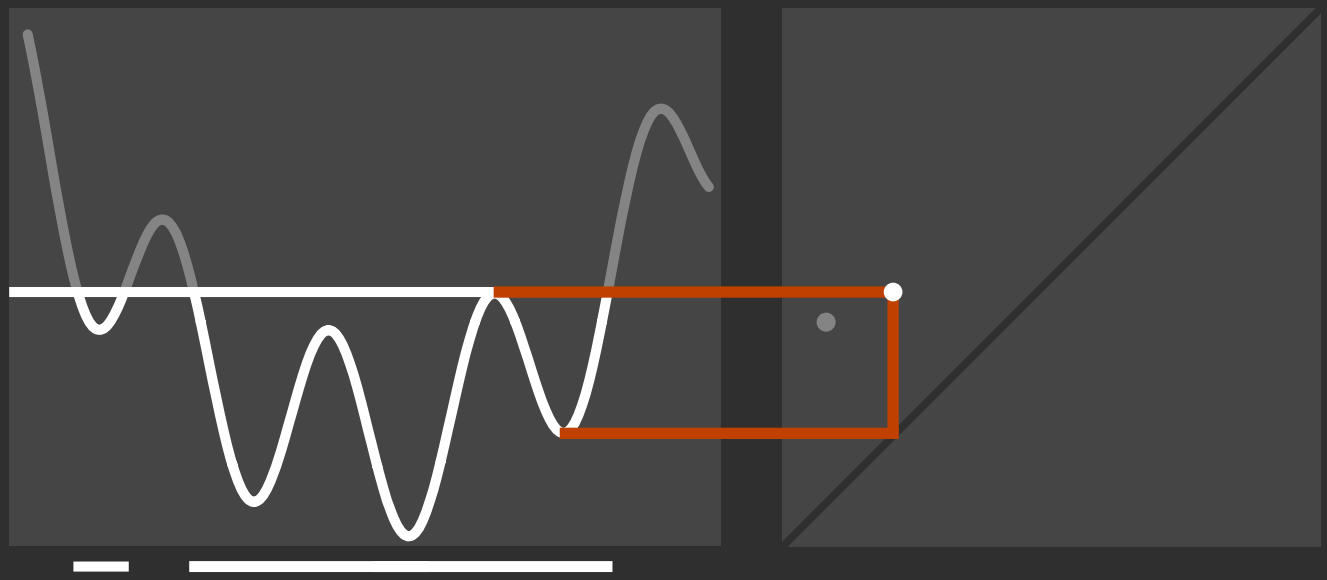

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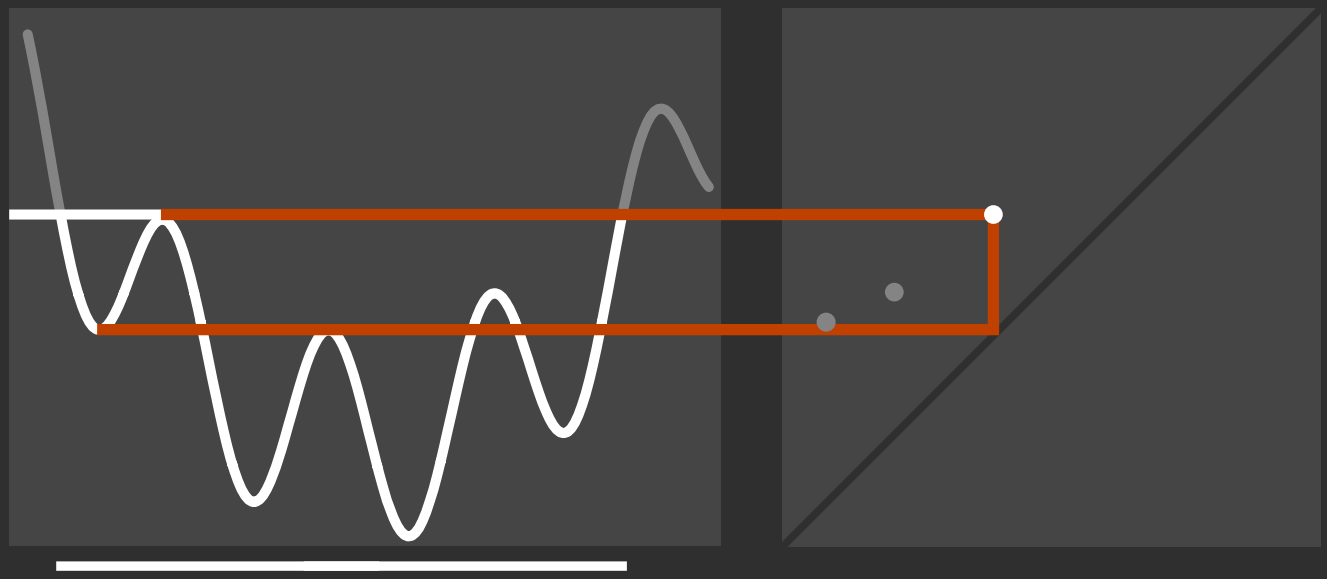

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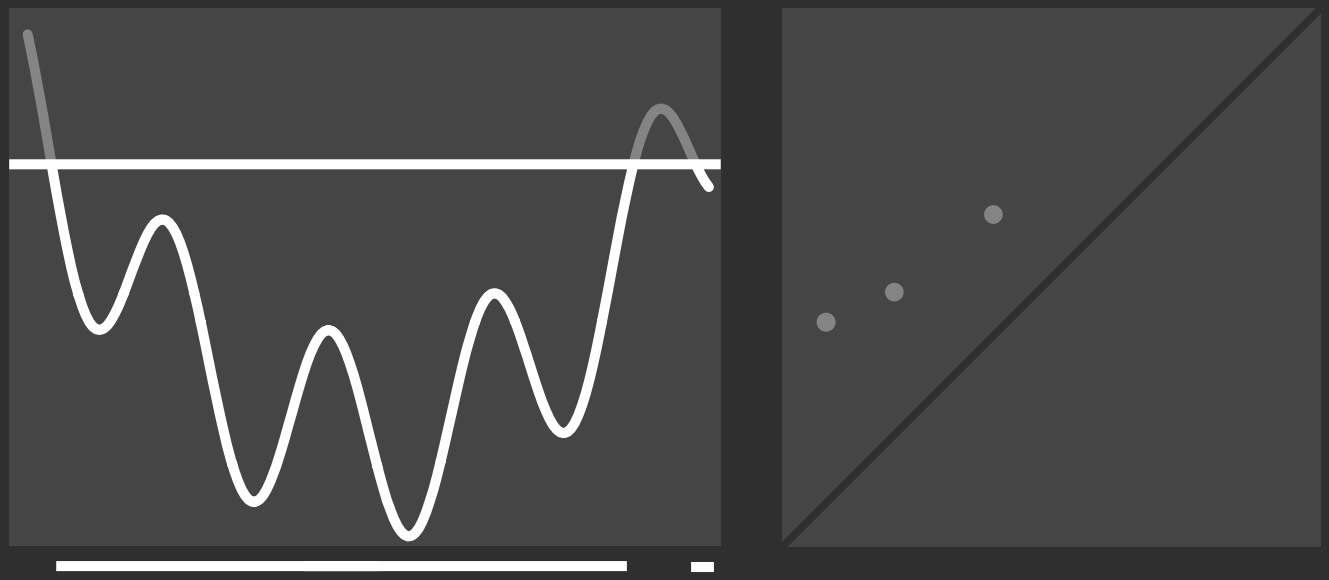

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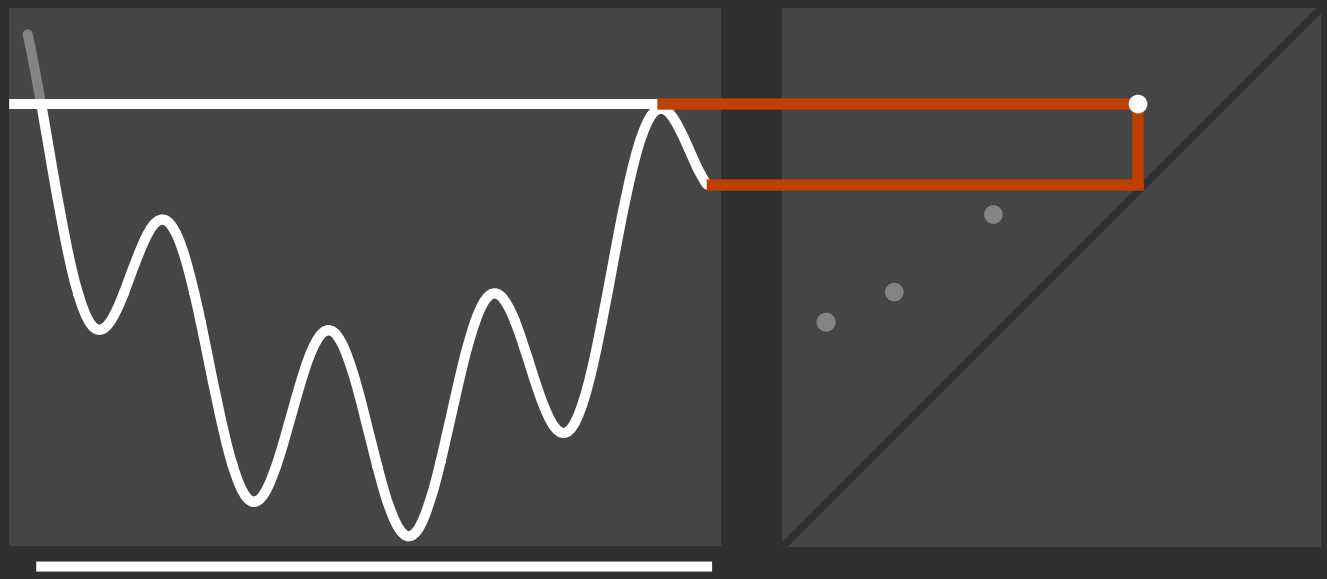

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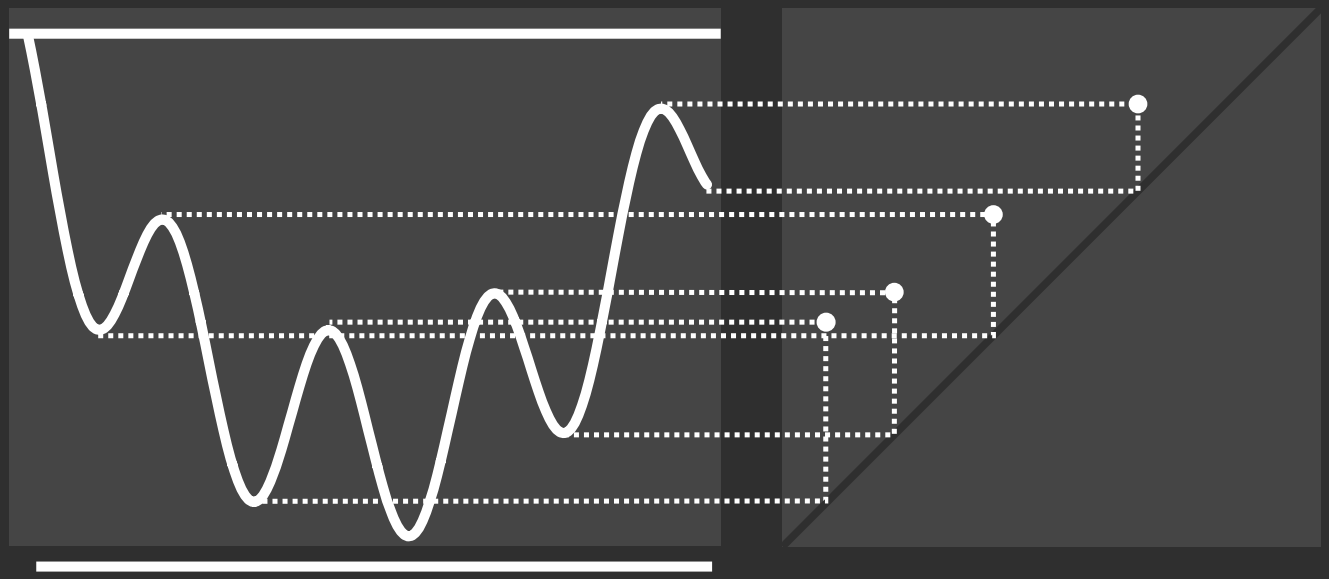

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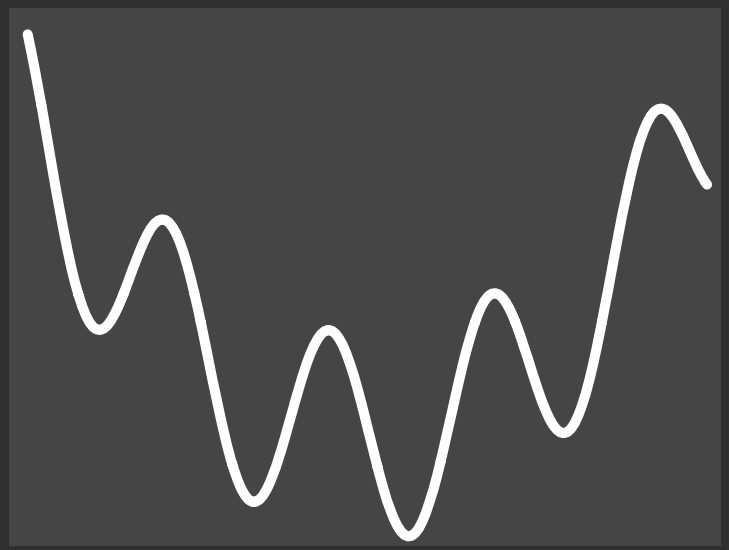
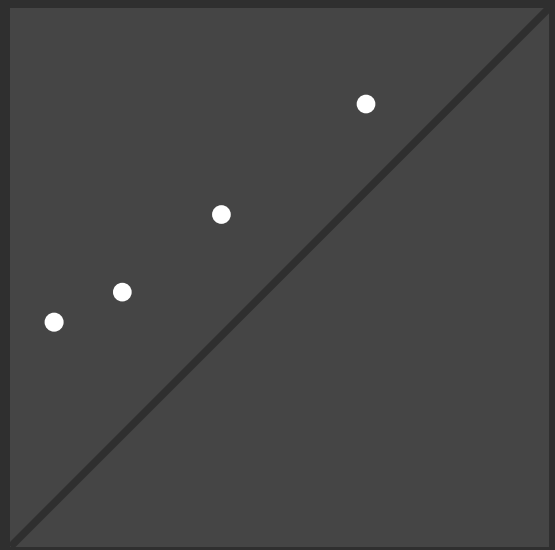


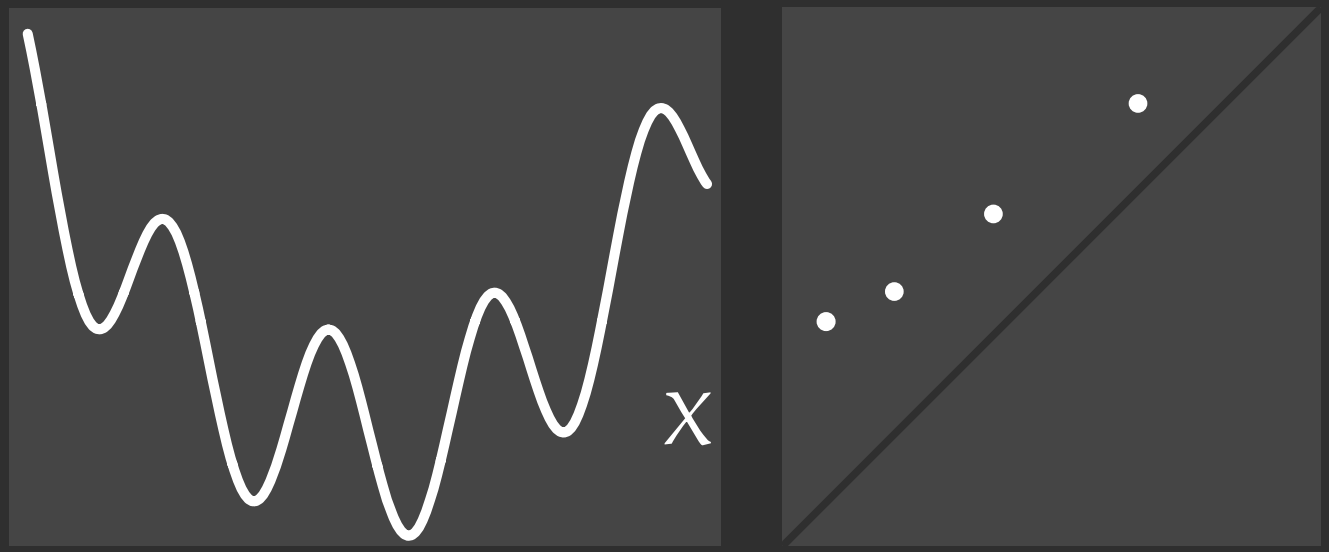


# Uses for persistence diagrams

A persistence diagram is a multi-scale summary of topological activity in a data set. But the diagrams go well and beyond a simple comparison of Betti numbers!

> *L'algèbre est généreuse, elle donne souvent plus qu'on lui demande.*
>
> —D'Alembert

# Distance calculations



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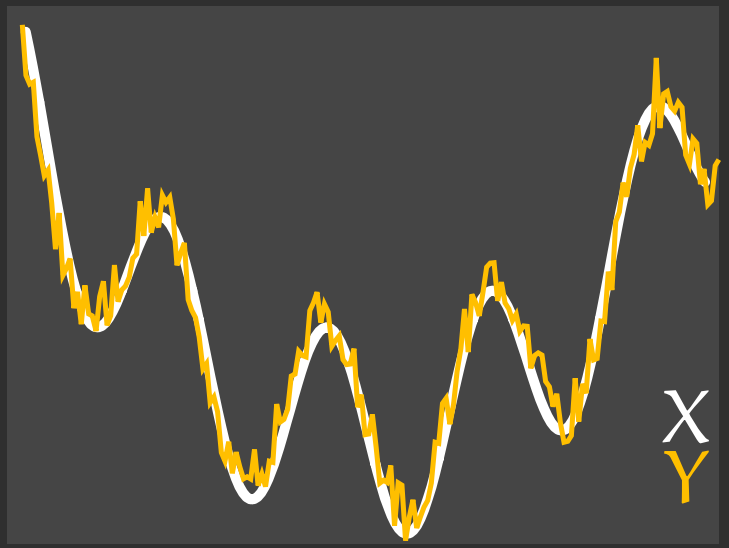


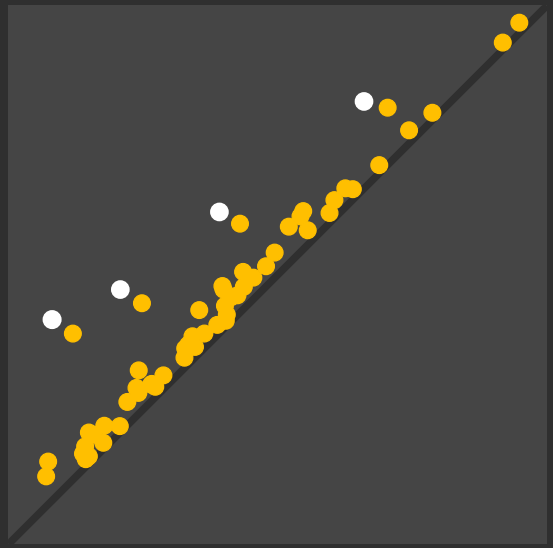

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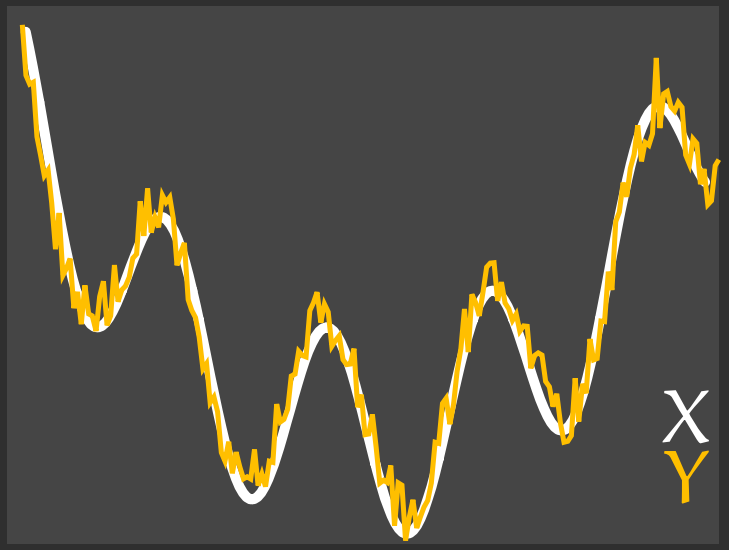
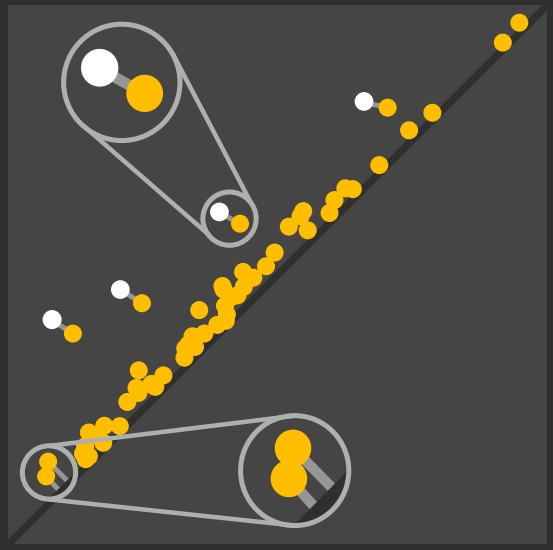
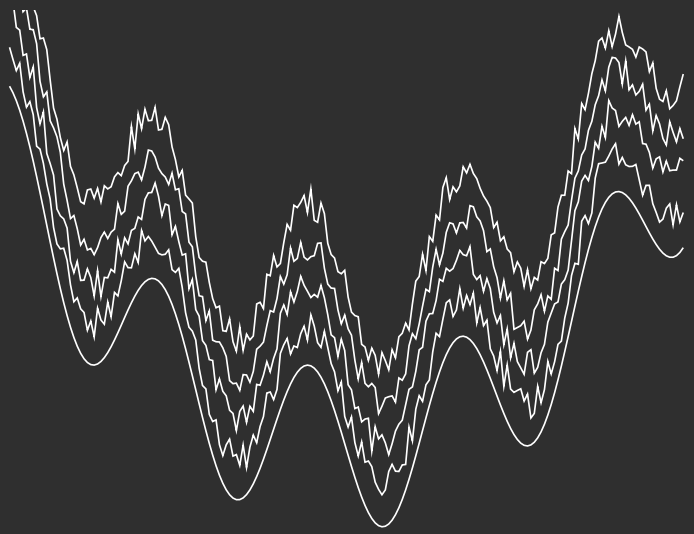


$$W_2(X, Y) = \sqrt{\inf_{\eta:\, X \to Y} \sum_{x \in X} \|x - \eta(x)\|_\infty^2}$$

# Sensitivity of distances

## Wasserstein versus function space distances



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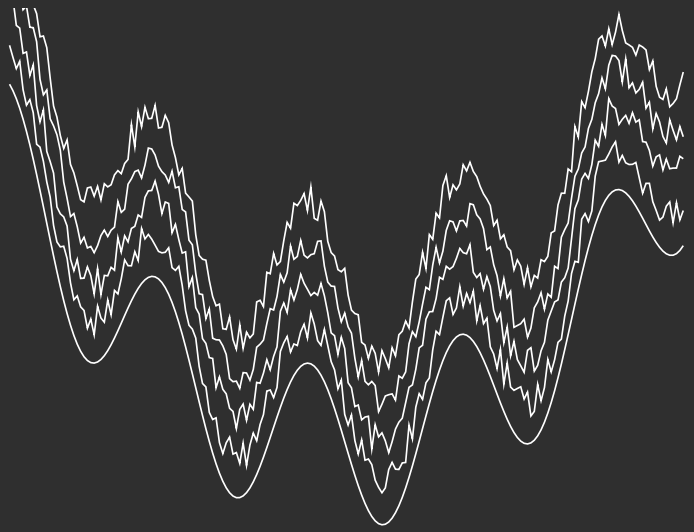
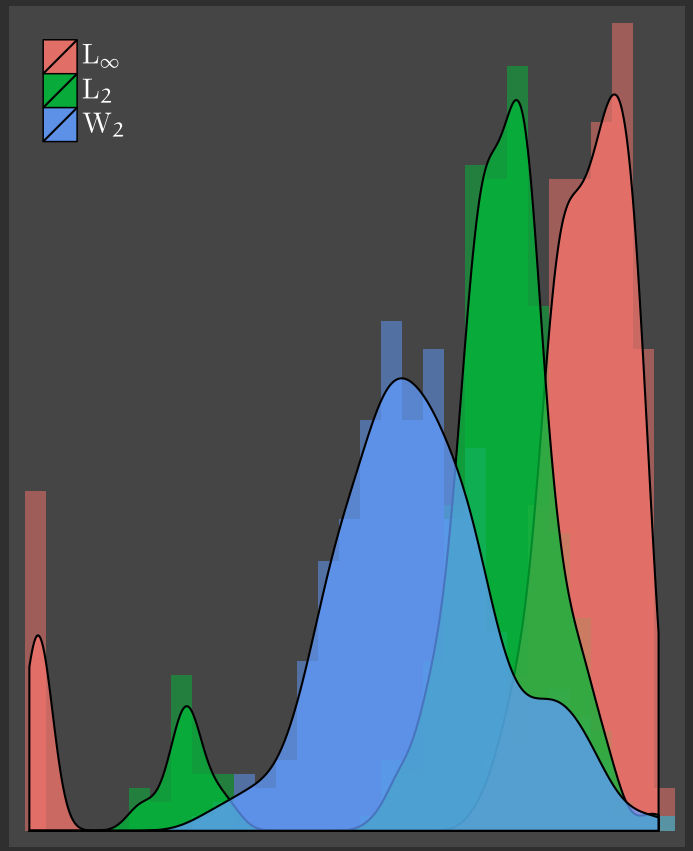


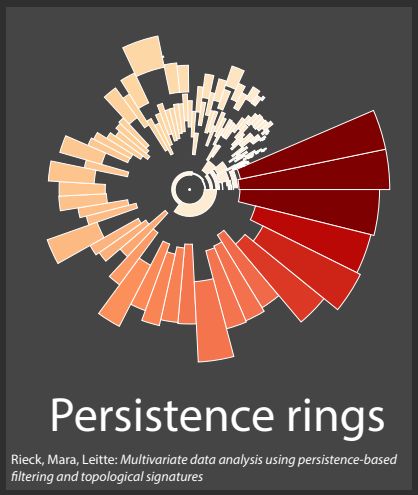



Only the Wasserstein distance does not distort the ‘shape’ of noise in the data.

# Part III

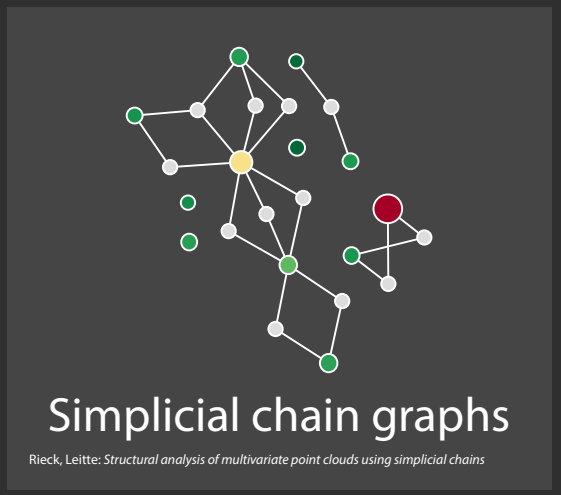
# Applications

# Published projects



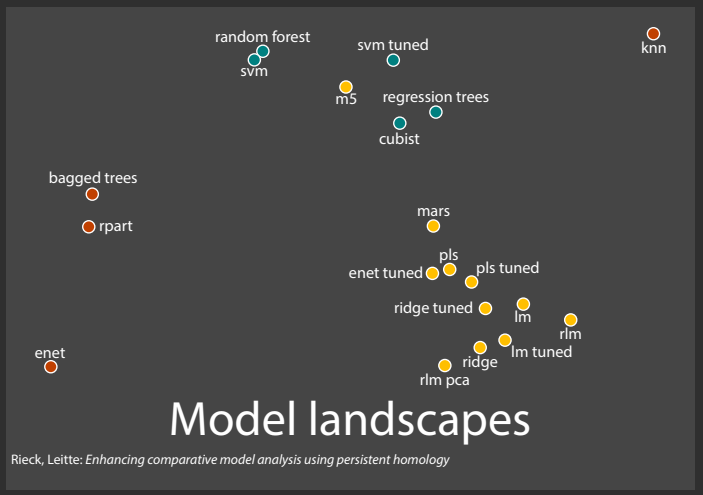
## Persistence rings

Rieck, Mara, Leitte: *Multivariate data analysis using persistence-based filtering and topological signatures*



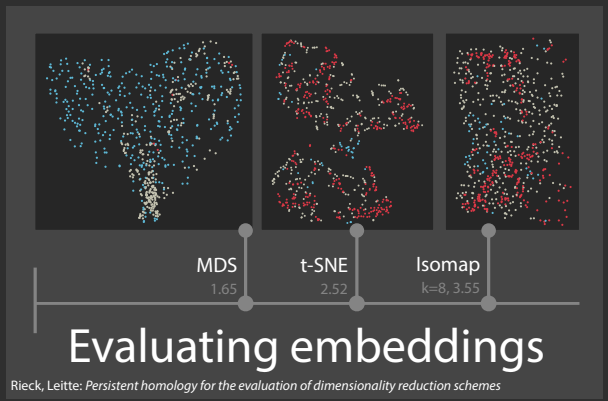
## Simplicial chain graphs

Rieck, Leitte: *Structural analysis of multivariate point clouds using simplicial chains*



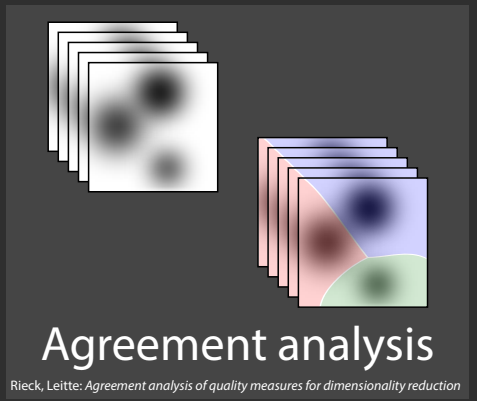

## Model landscapes

Rieck, Leitte: *Enhancing comparative model analysis using persistent homology*



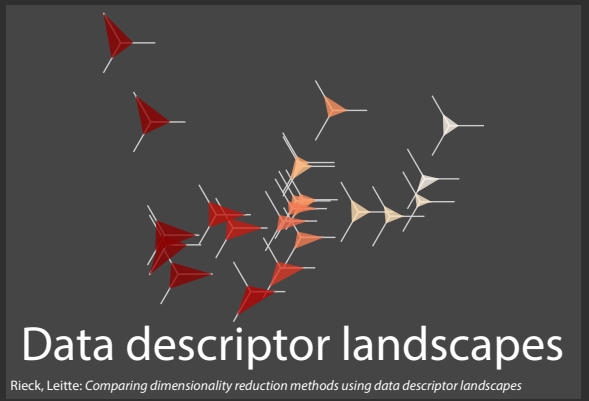

## Evaluating embeddings

Rieck, Leitte: *Persistent homology for the evaluation of dimensionality reduction schemes*



## Agreement analysis

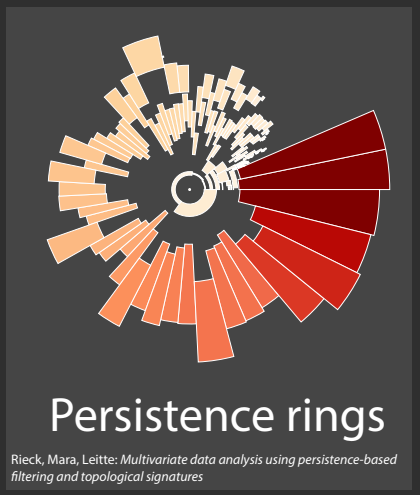
Rieck, Leitte: *Agreement analysis of quality measures for dimensionality reduction*



## Data descriptor landscapes

Rieck, Leitte: *Comparing dimensionality reduction methods using data descriptor landscapes*

# Published projects



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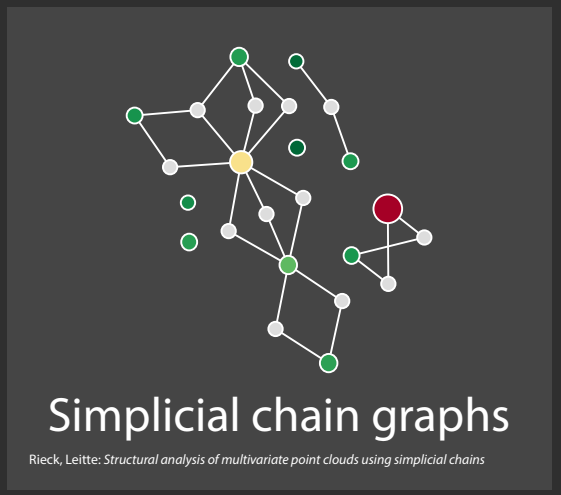

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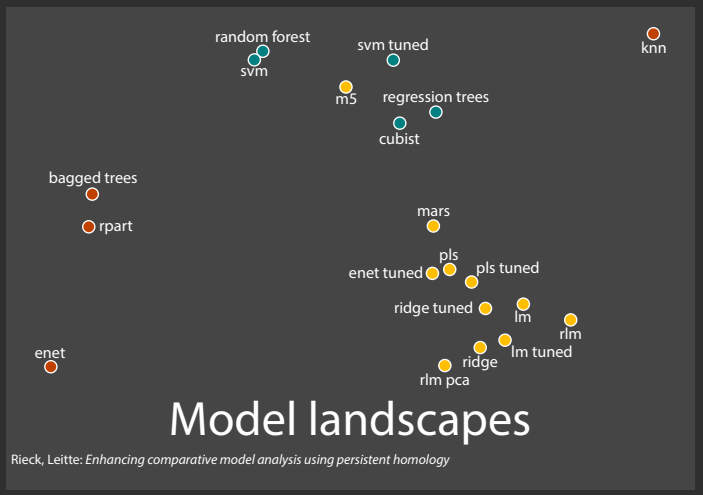
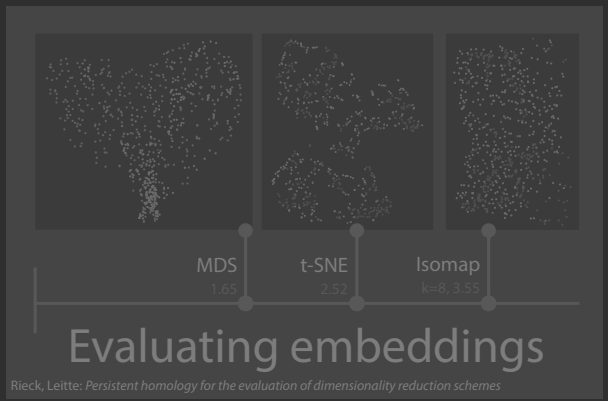


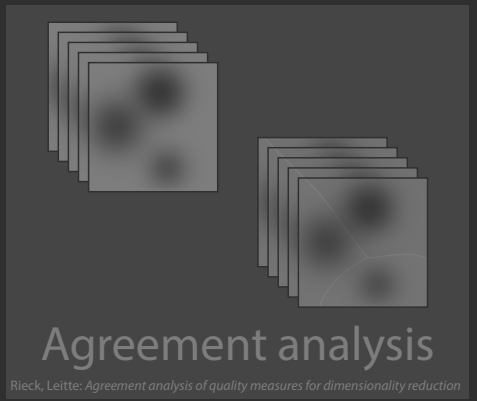

## Model landscapes

Rieck, Leitte: *Enhancing comparative model analysis using persistent homology*




## Evaluating embeddings

Rieck, Leitte: *Persistent homology for the evaluation of dimensionality reduction schemes*



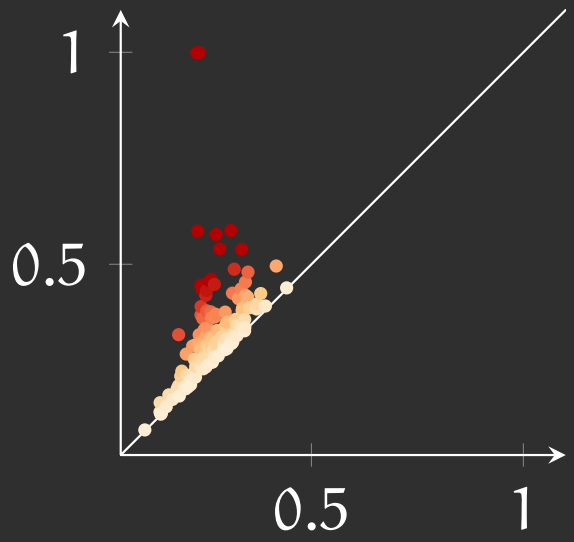
## Agreement analysis

Rieck, Leitte: *Agreement analysis of quality measures for dimensionality reduction*

## Data descriptor landscapes

Rieck, Leitte: *Comparing dimensionality reduction methods using data descriptor landscapes*

# Qualitative visualizations: Persistence rings



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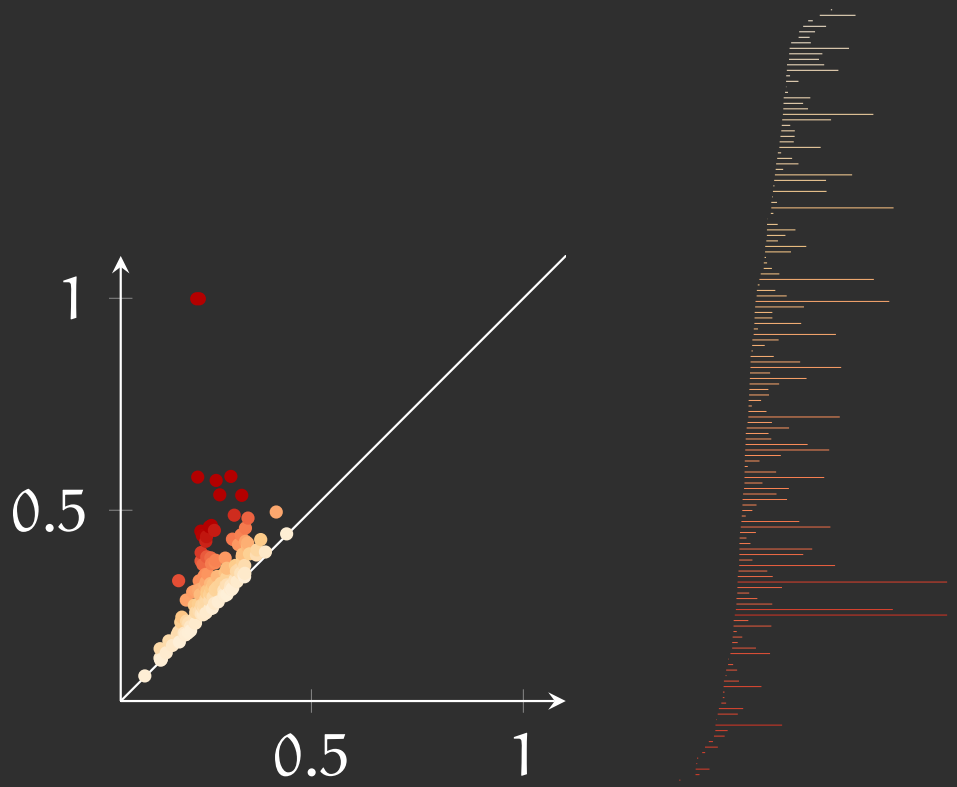

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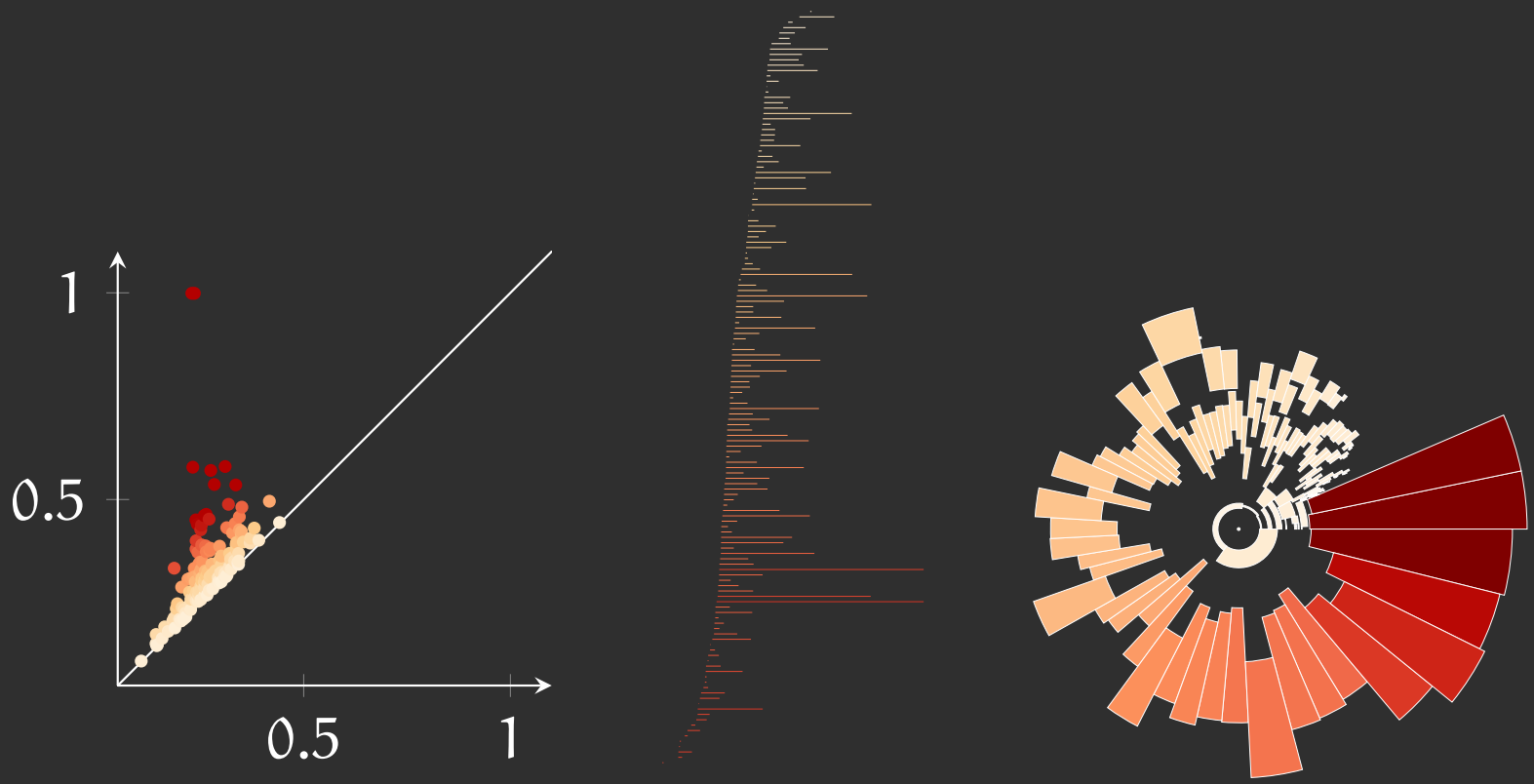


# Qualitative visualizations: Simplicial chain graphs

## Motivation

Analyse the connectivity of topological features for *ensembles* of data sets: Different runs of an experiment, different times at which measurements are being taken…

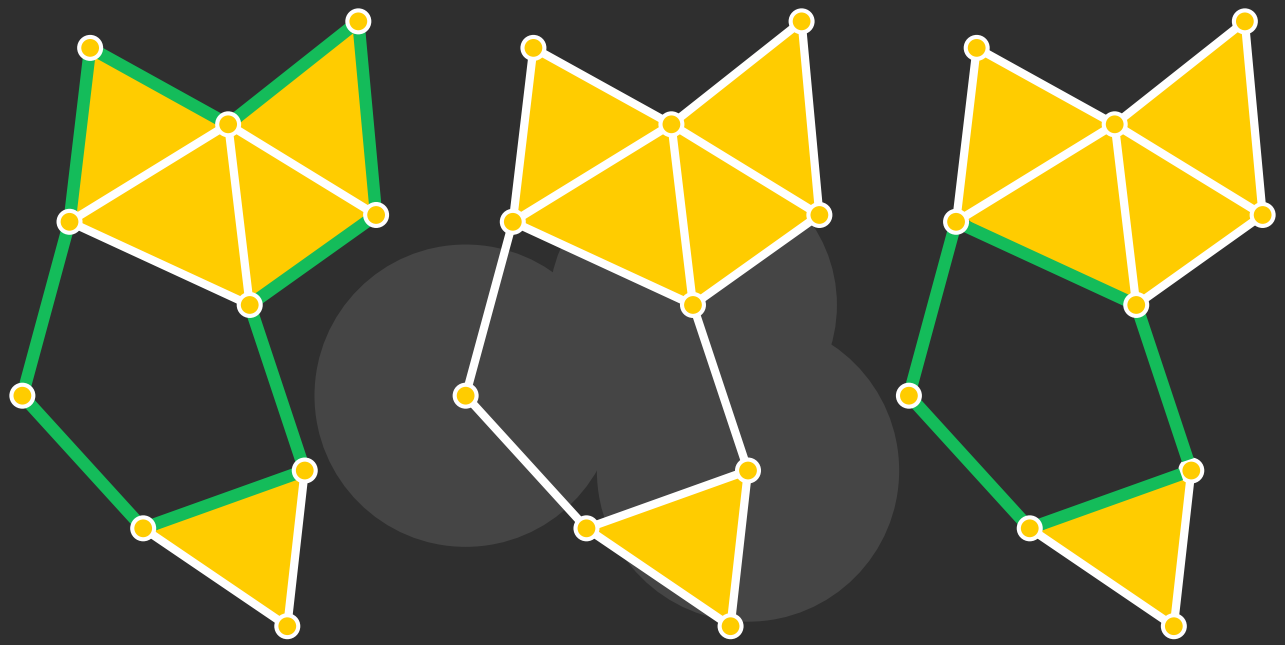
# Central idea

Obtain geometrical descriptions of topological features (‘holes’) while calculating persistent homology.

This is known as the ‘localization problem’ in persistent homology.

# Solving the localization problem

1. Define a *geodesic ball* in a simplicial complex.
2. Solve all-pairs-shortest-paths problem to find possible sites.
3. Branch-and-bound strategy to improve performance.



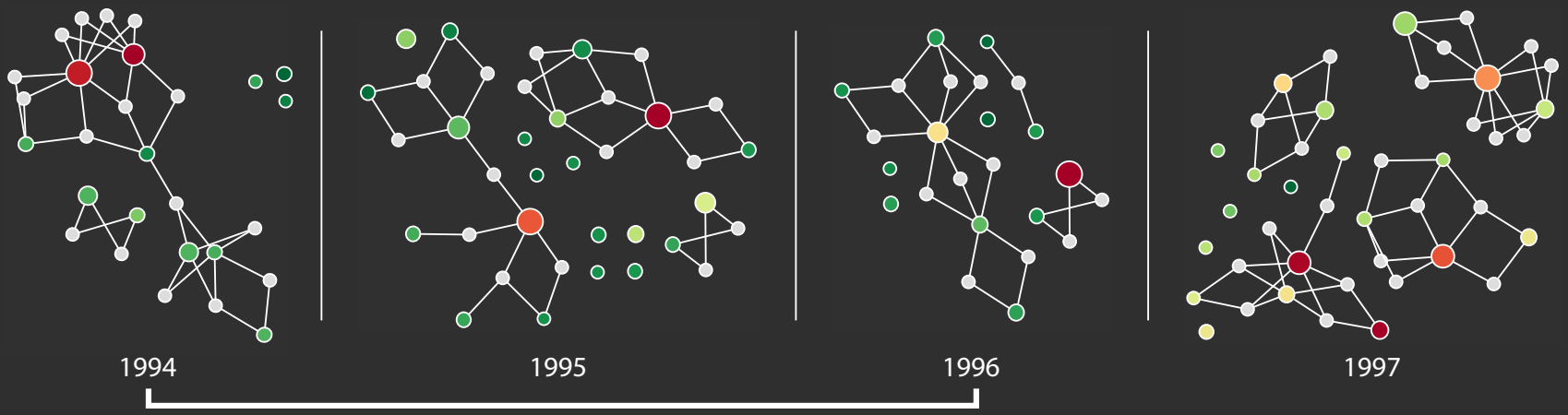
# Simplicial chain graph

## Basic example

Advantage: The space in which we localize the features usually has a high dimensions, but the graph will always be drawn in $\mathbb{R}^2$.

# Results

Data: Tropical Atmosphere Ocean Array



# Lessons learned

1. We can obtain features via persistent homology that permit a comparative analysis.
2. Visualizing these features becomes abstract very quickly.
3. Need more ‘quantitative’ topological visualizations.

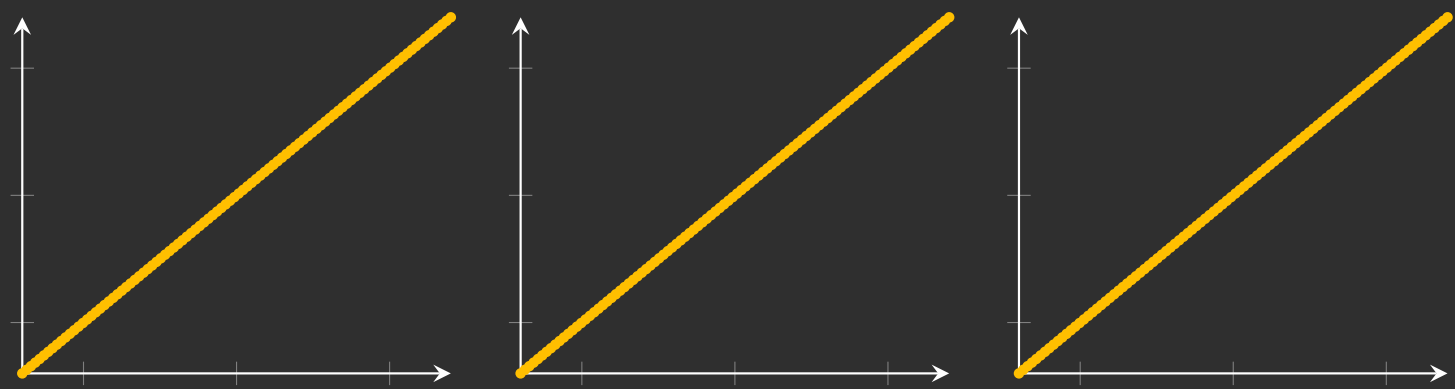
# Quantitative visualizations: Model landscapes

Example: Solubility analysis

- 19 different mathematical models
- 1267 chemical compounds, described by 228-dimensional feature vectors
- Measured ground truth (solubility values)

Each model is a function $f\colon \mathbb{D} \to \mathbb{R}$. How to evaluate similarities & differences between the models?

# State-of-the-art



- Existing measures (RMSE or $R^2$) only focus on *values* of a model.
- The structure/shape is not being used!
- Shortcomings: Sensitivity to noise, 'masking' the influence of outliers…

# Our approach

1. Calculate Vietoris–Rips complex $\mathcal{V}_\epsilon$ on the molecular descriptors.

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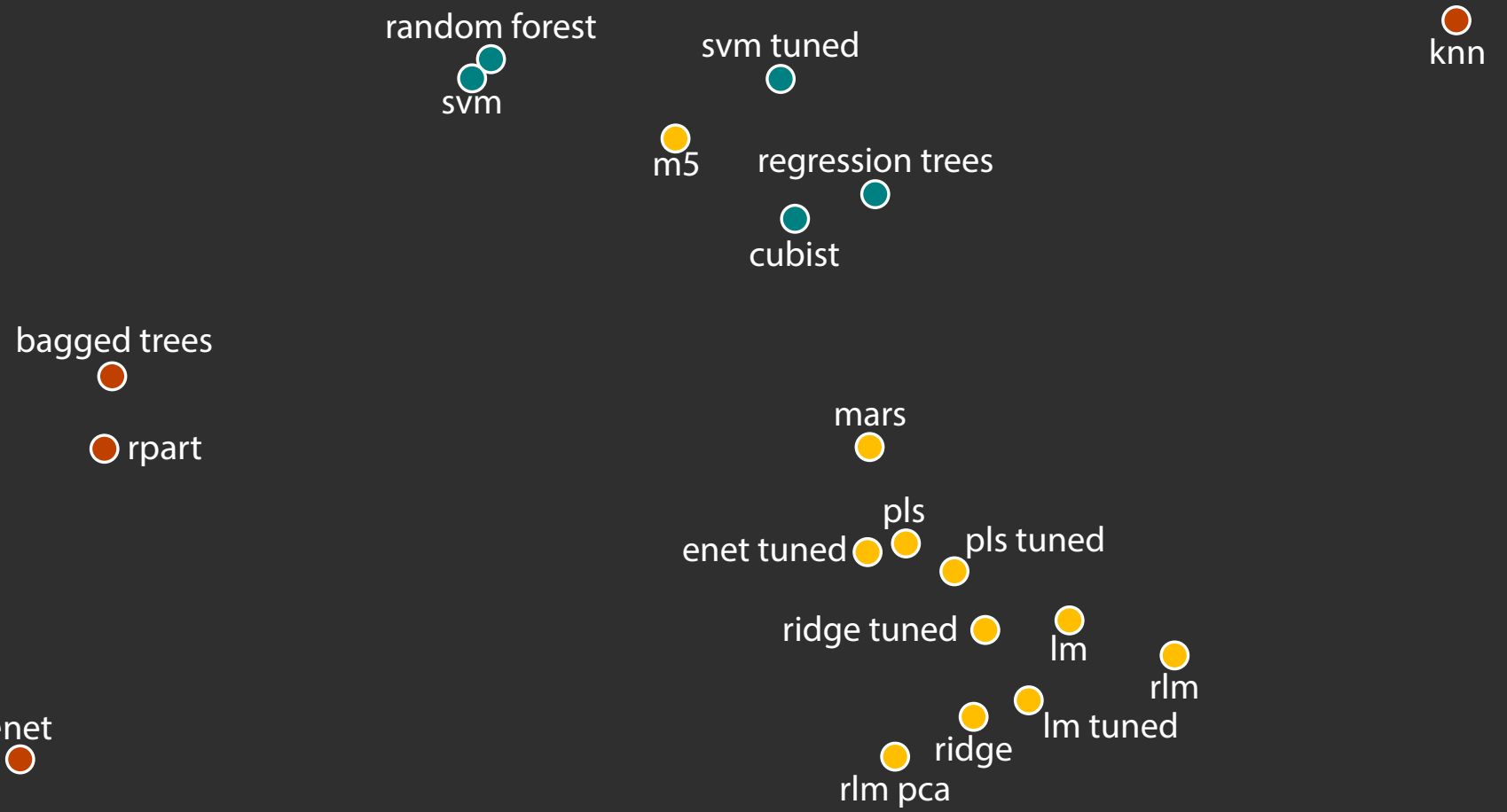
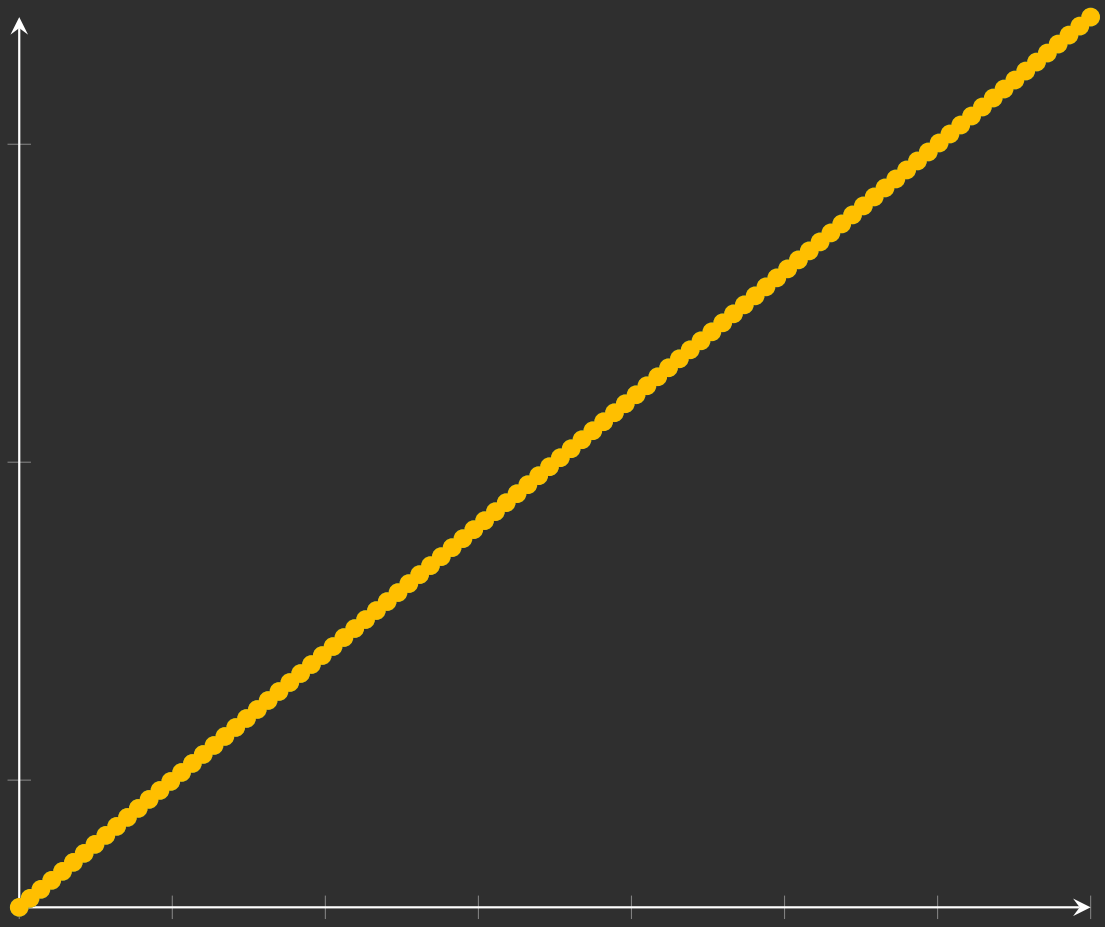
4. Compare diagrams using the Wasserstein distance.
5. *Absolute* comparison with ground truth diagram.
6. *Relative* comparison with all diagrams.

# Visualization of relative model differences



# Why is m5 rated differently?

Comparison with cubist



# Summary

Topological methods yield quantitative and qualitative information about data sets—often, this goes well and beyond the scope of regular geometric approaches.

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Future work

1. Performance improvements: Smaller complexes, other distance measures, …
2. Ensemble data & ‘average’ topological structures
3. Connection to geometric features in data

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Topological methods yield quantitative and qualitative information about data sets—often, this goes well and beyond the scope of regular geometric approaches.

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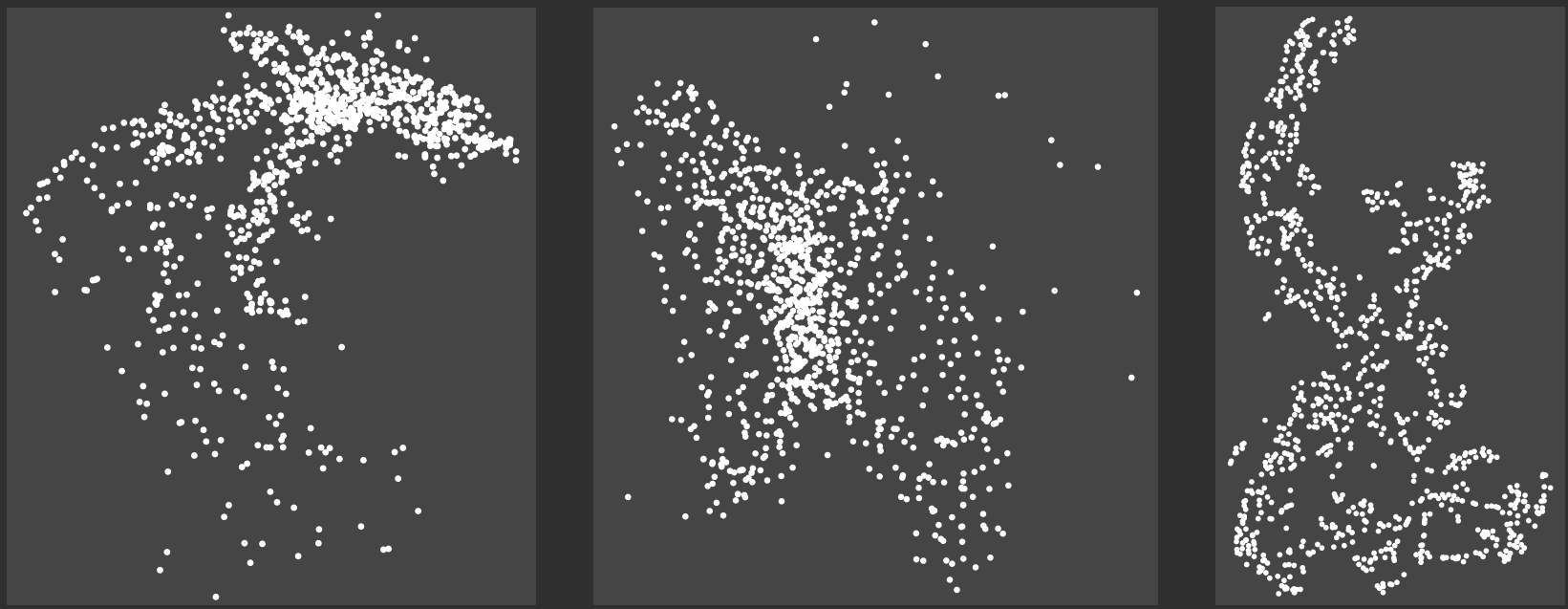
Thank you for your attention!

# Part IV

# Bonus slides

# Quantitative visualizations: Dimensionality reduction



Which of these embeddings are suitable for my data?

# Data descriptors

## Definition & examples

Any function $f\colon \mathbb{D} \subseteq \mathbb{R}^n \to \mathbb{R}$ is an admissible data descriptor. $f$ should measure 'salient properties' of a multivariate data set.

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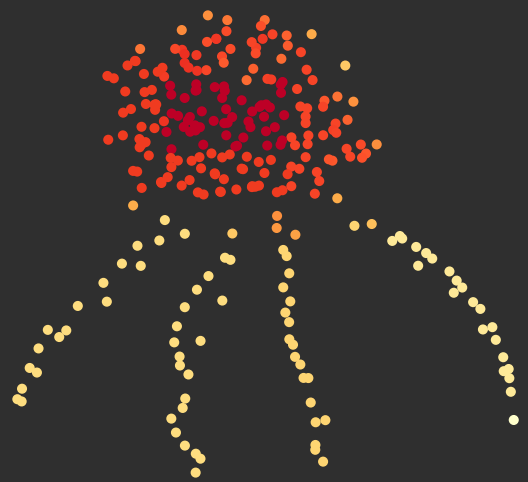

Density

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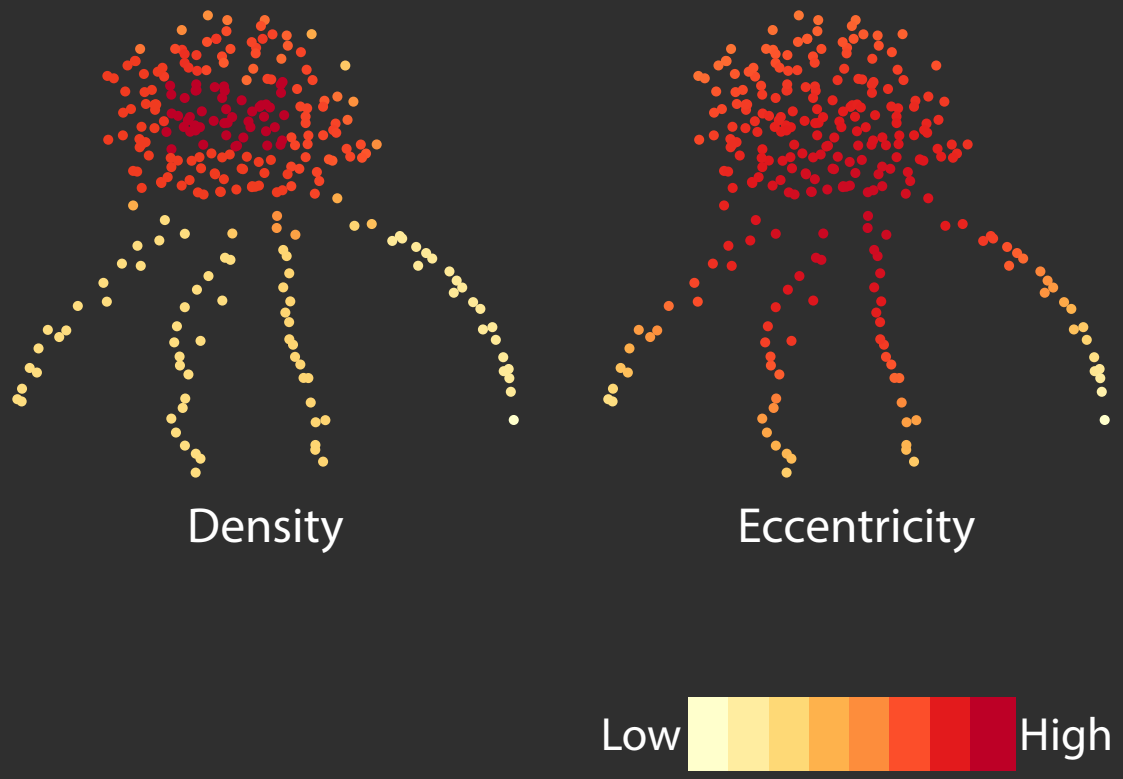

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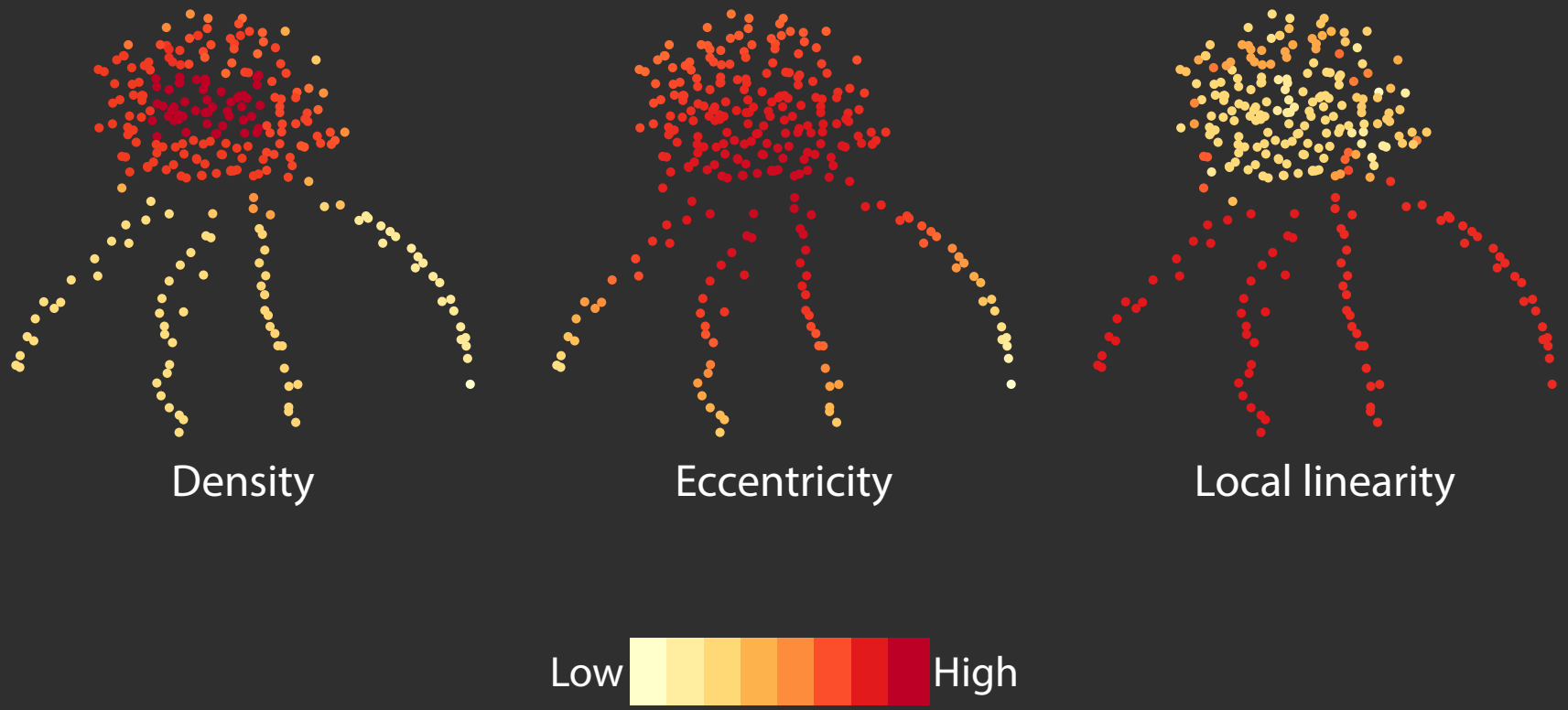
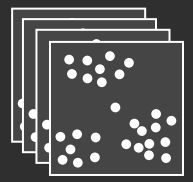


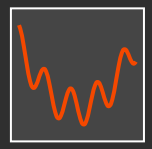
# Workflow

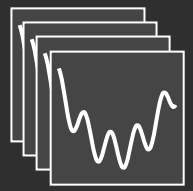
Original data

Embeddings

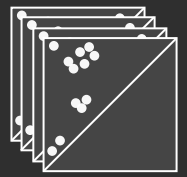


Data descriptors

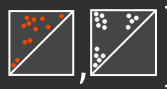




Persistent homology



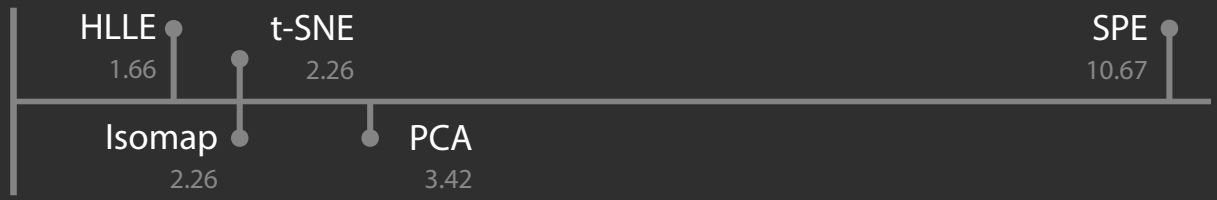
$W_2$(  )

$W_2$(  )

• • •

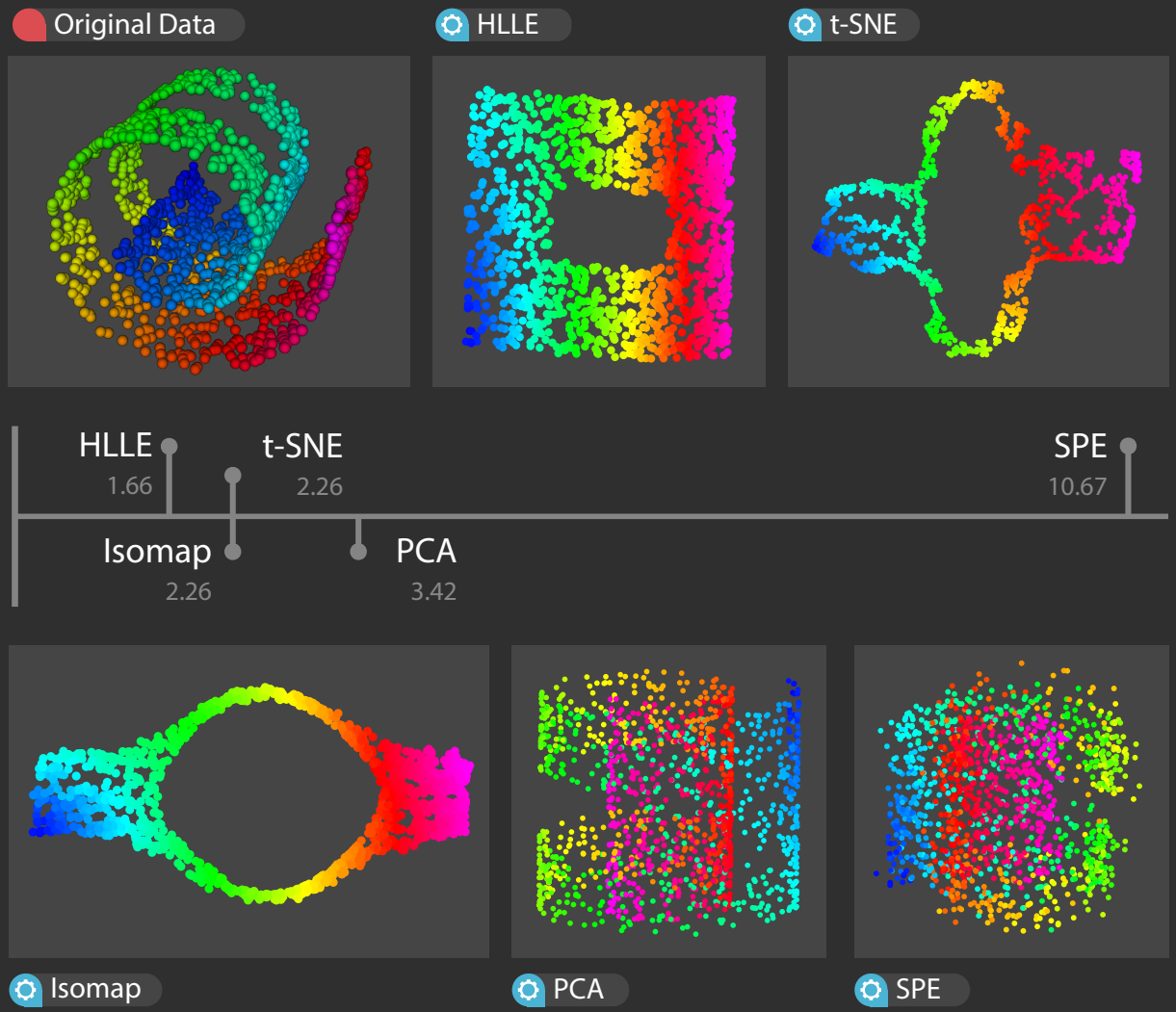
# Visualizing global quality

$$\text{Quality}_{\text{Embedding}} = W_2\left(D_{\text{Original}}, D_{\text{Embedding}}\right)$$

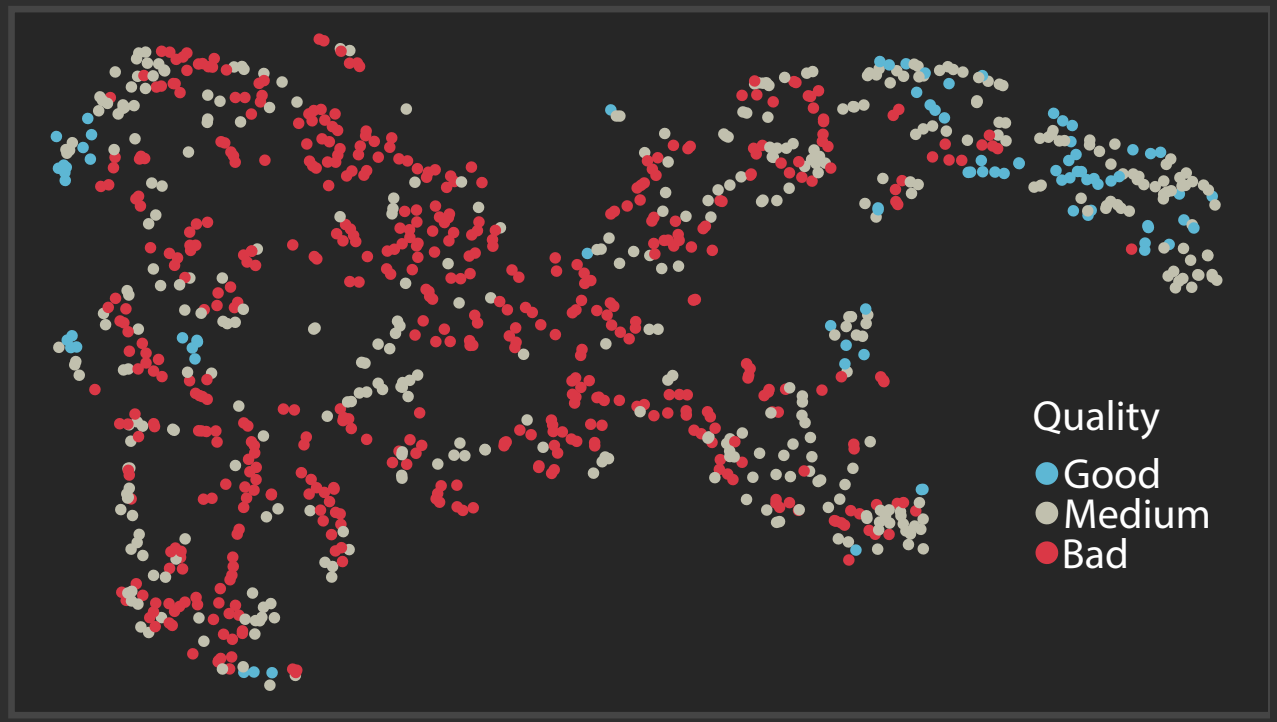


# Correspondence to our intuition

## Global quality information



# Local quality information



# Results

## Isomap faces

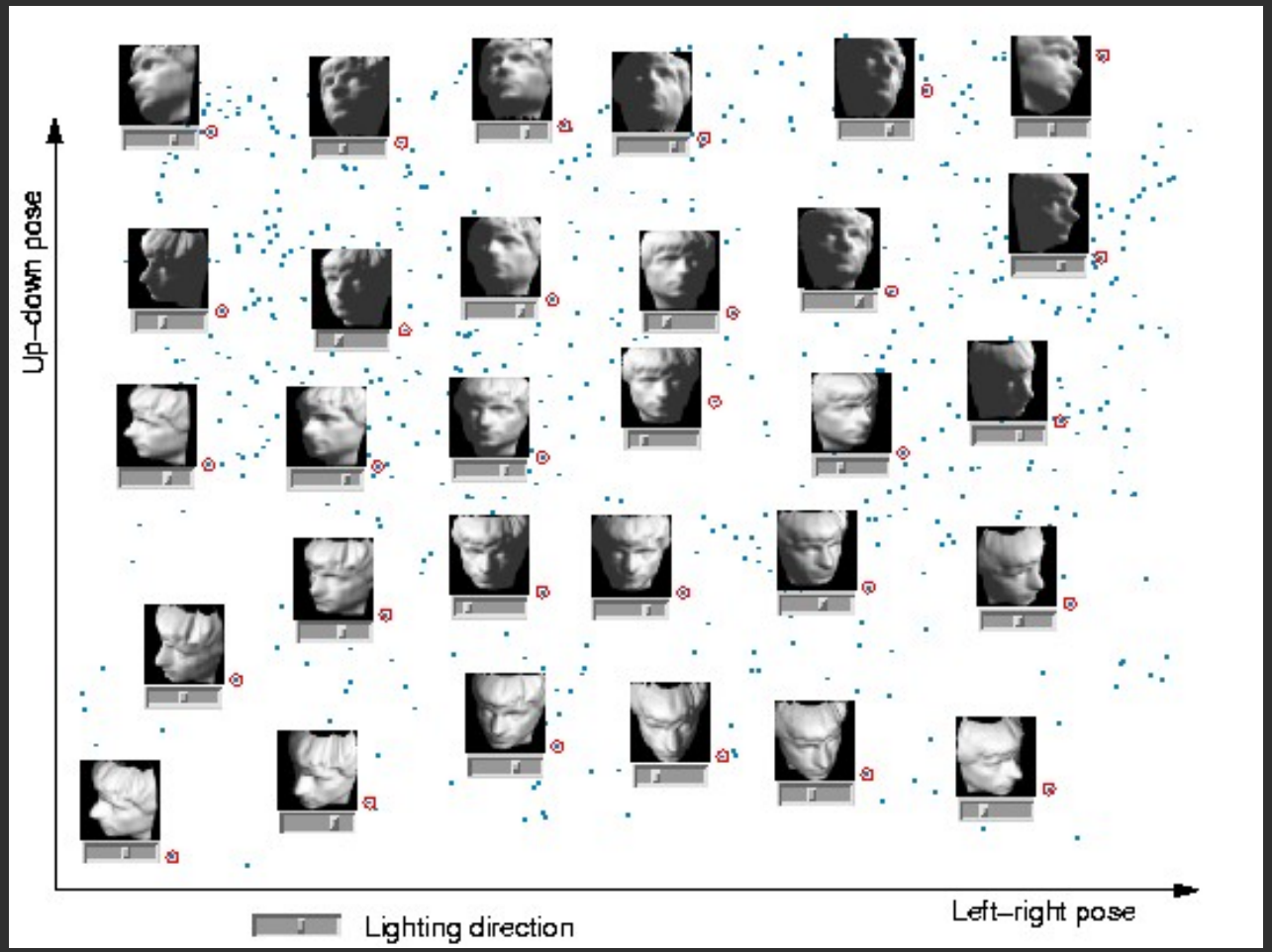
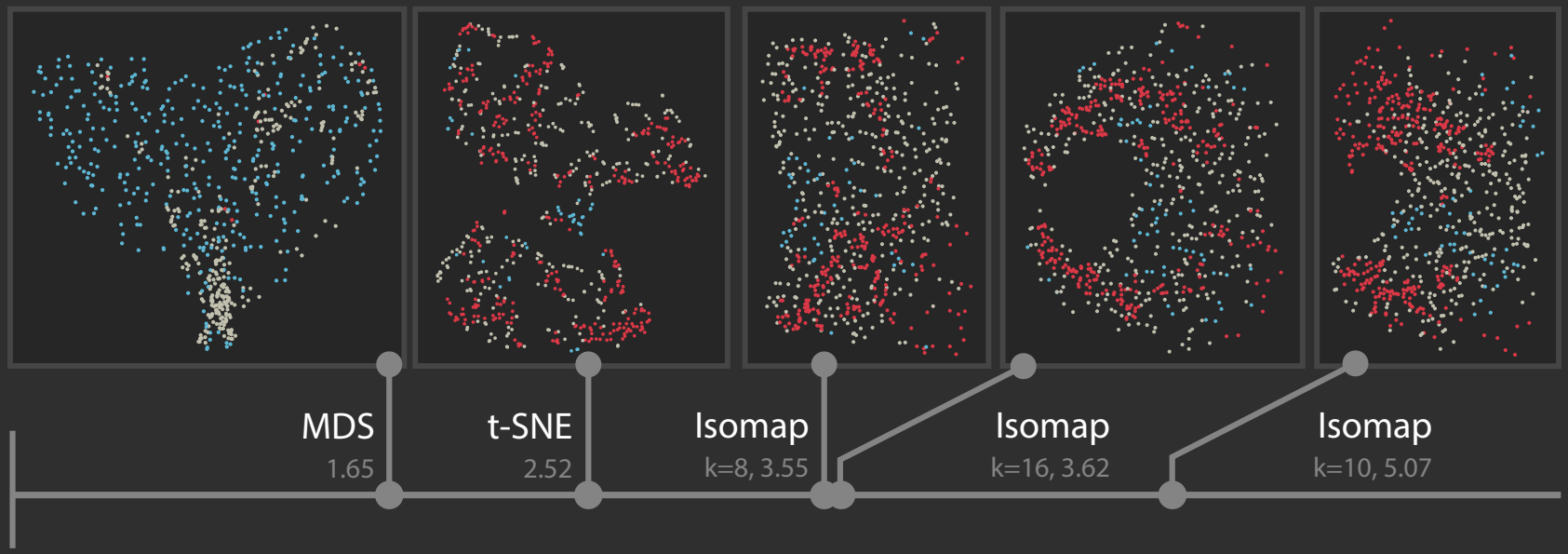


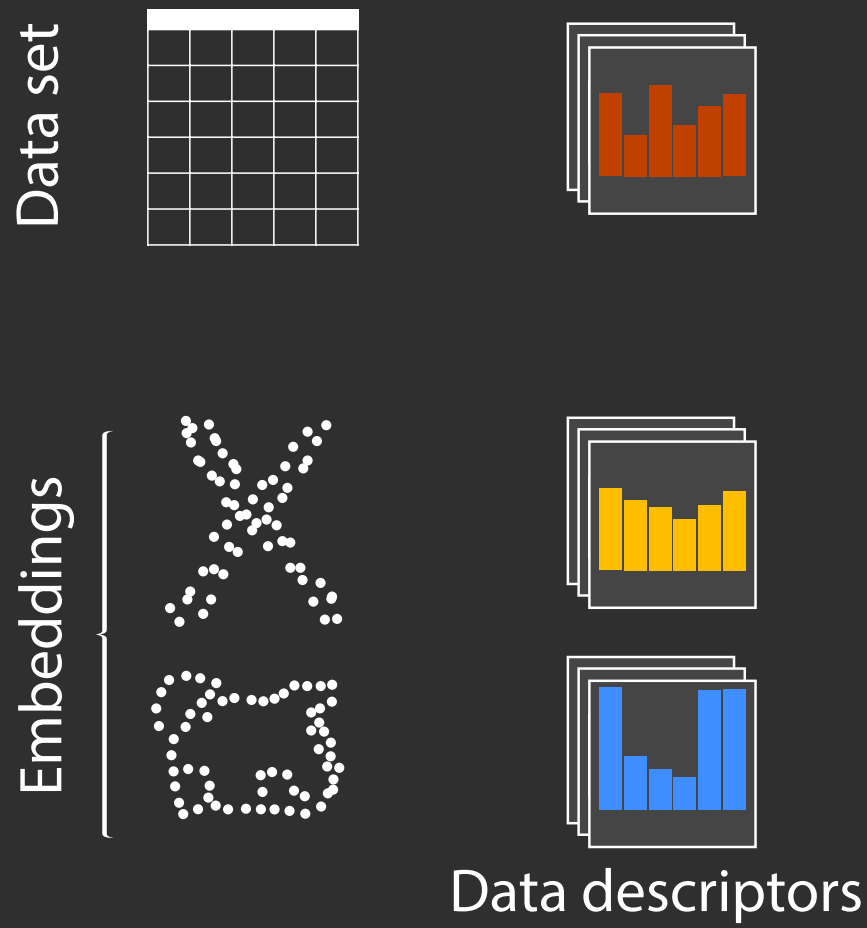

Image source: *A Global Geometric Framework for Nonlinear Dimensionality Reduction* (Joshua B. Tenenbaum, Vin de Silva, John C. Langford), 2000.

# Results

## Isomap faces: Parameter study



# Quantitative visualizations: Multiple data descriptors



# Feature vector approach

# Data descriptor landscapes

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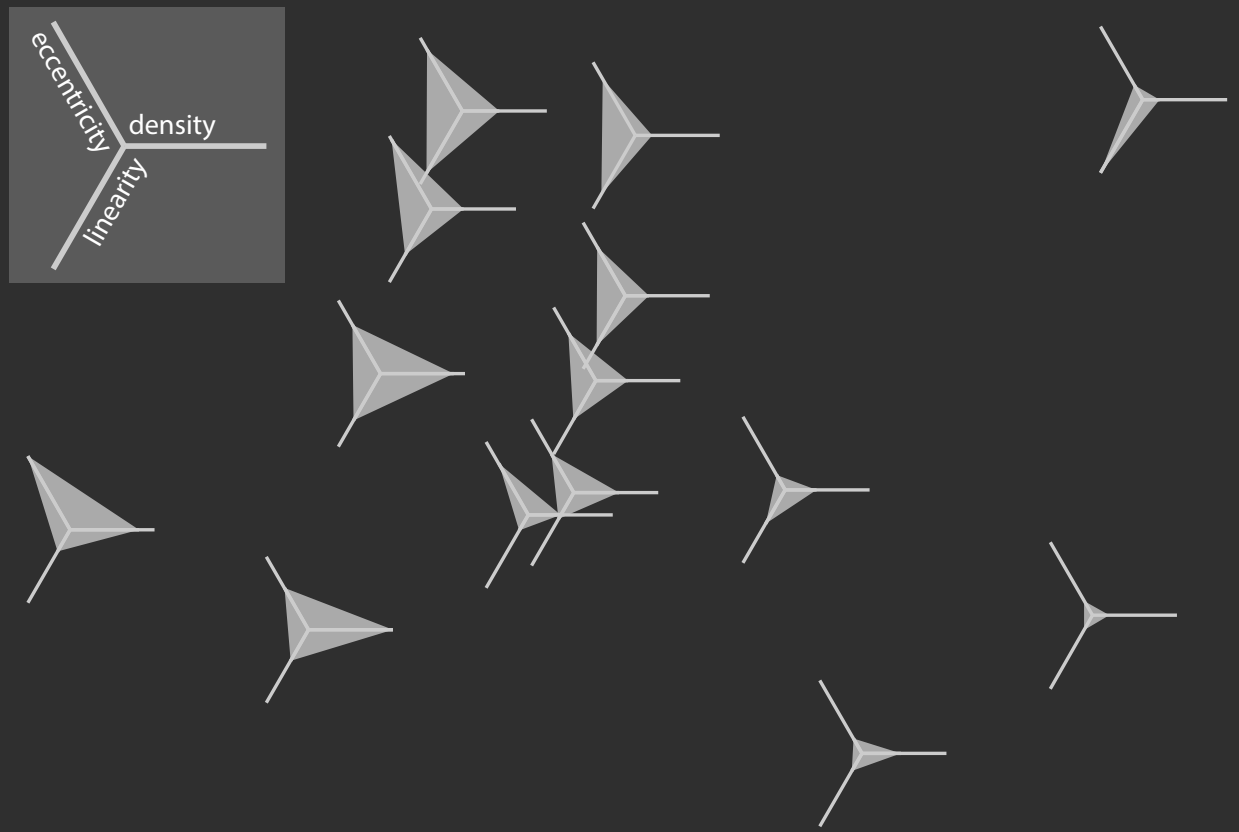

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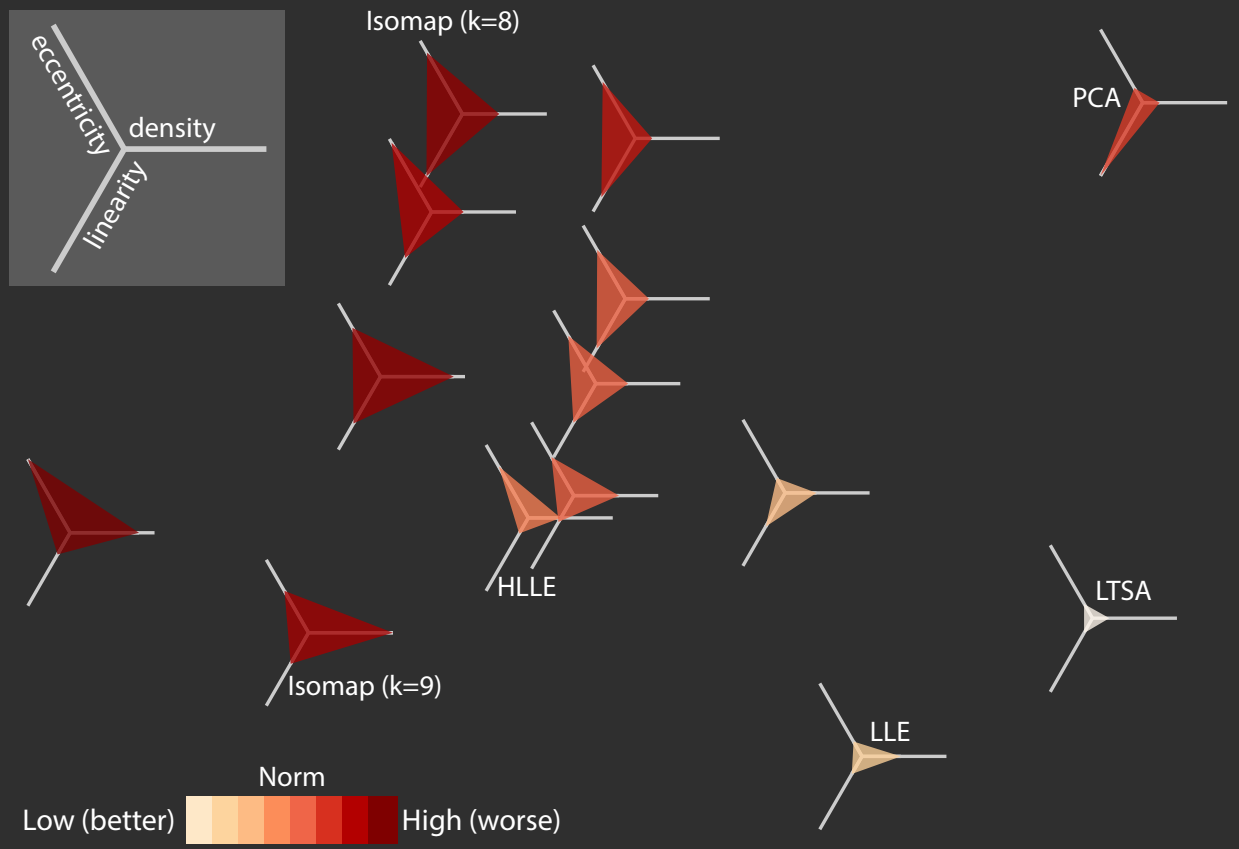

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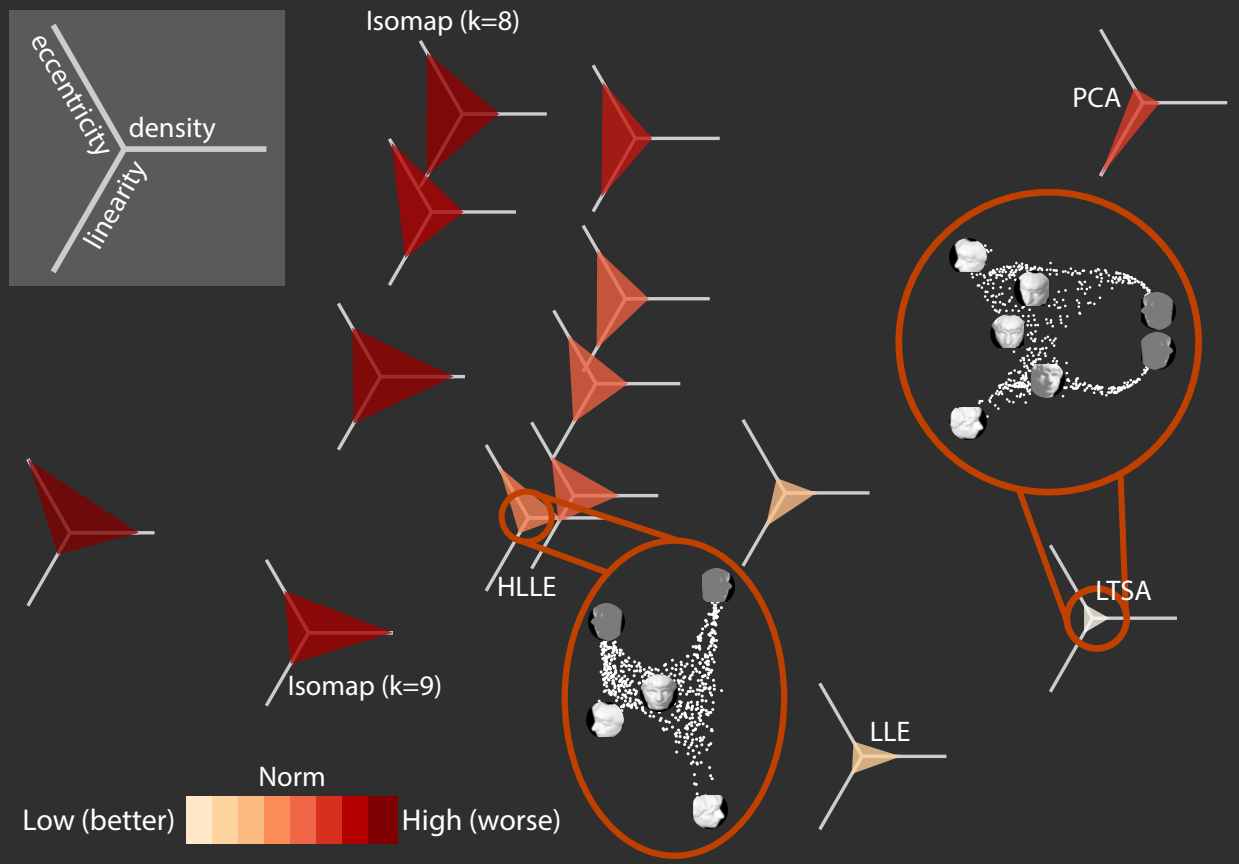
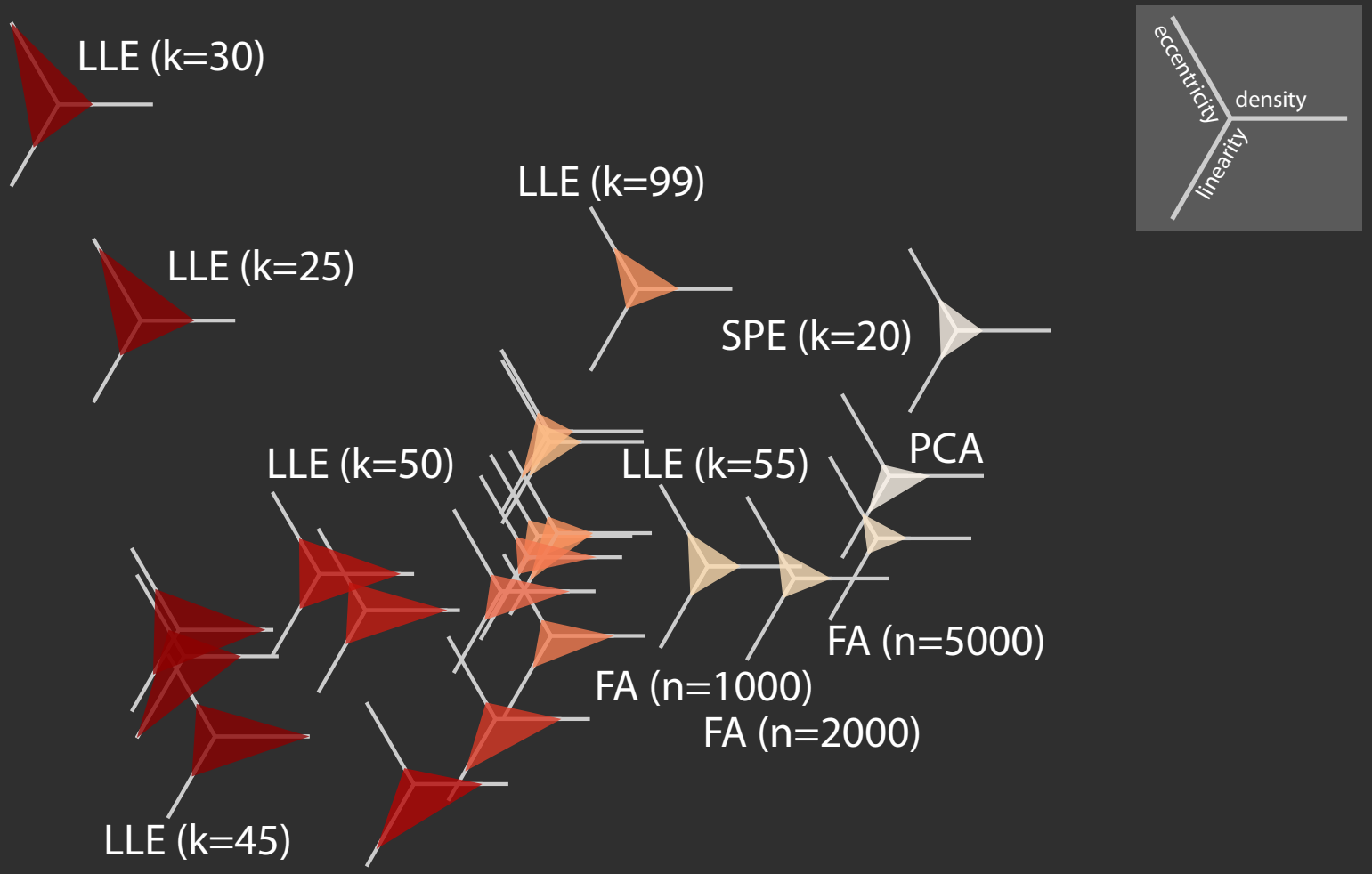


# Data descriptor landscapes

## Grouping behaviour



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