Comparing Dimensionality Reduction Methods using Data Descriptor Landscapes

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HGS MathComp

IWR

In an ideal world

Example workflow in data science

Multivariate data + Dimensionality reduction + Embedding = Insight

Disclaimer: This is *not* a definition but rather based on observing the machine learning colleagues down the hall…

An idealized metaphor

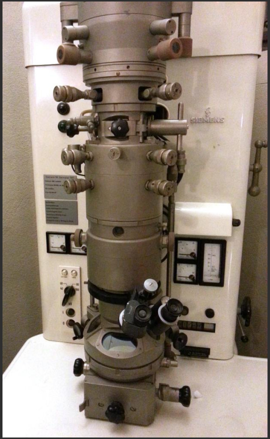

Image source: flickr user “Georg Holderied”

In practice

Opening the toolbox

Image source: flickr user “OZinOH”

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Locally linear embedding (LLE)

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Local tangent space alignment (LTSA)

Image source: flickr user "OZinOH"

In practice

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Challenges

1. Choose a suitable tool.

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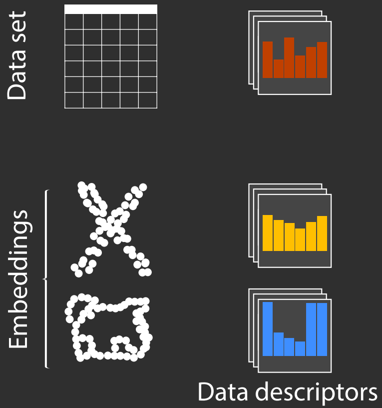
How can visualization help?

Our proposed approach



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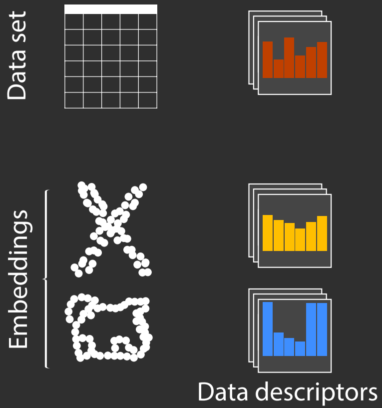

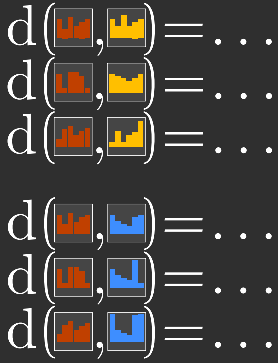

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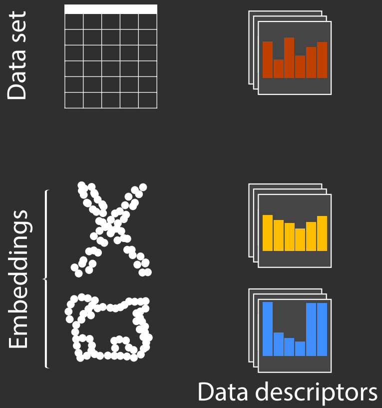

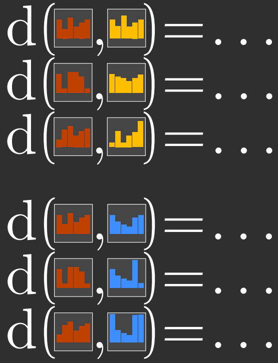

Idea: If data descriptors are *close*, the properties they measure are retained.

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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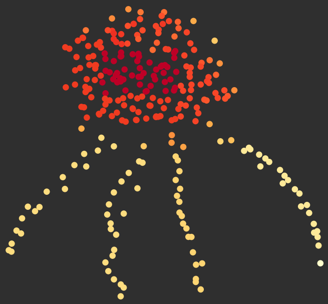

Density

Data descriptors

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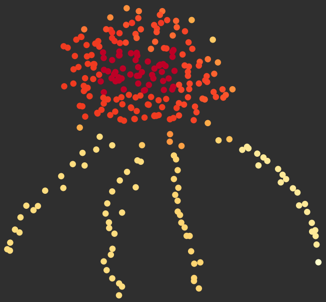
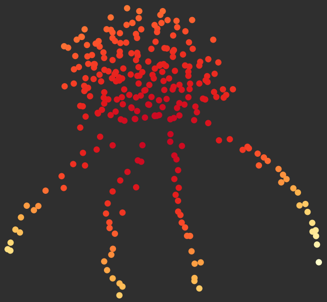


Density



Eccentricity

Low  High

Data descriptors

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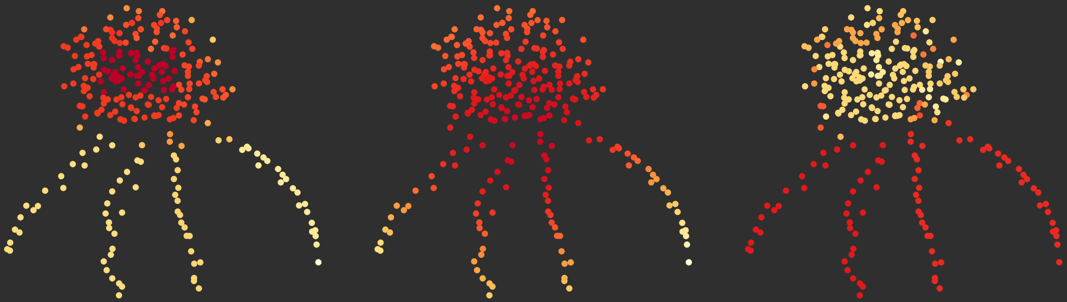

Density Eccentricity Local linearity

How to calculate data descriptor distances?

$\mathrm{d}($, $) := ?$

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Persistent homology, because…

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   Original data $\mathbb{R}^n$
   Embedding $\mathbb{R}^d$ $(d \ll n)$

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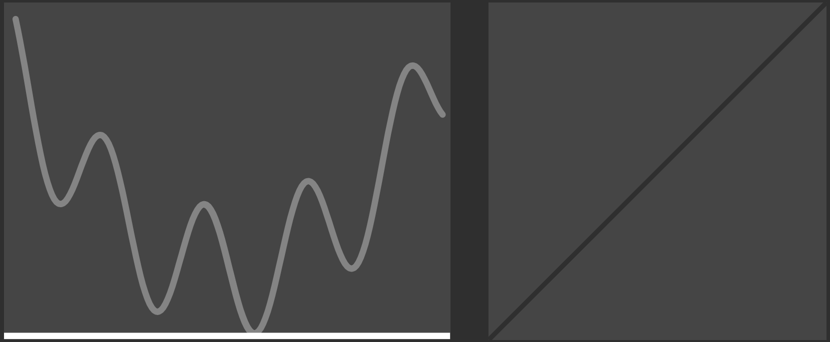
Persistent homology, because…

1. Calculation between different domains:
   Original data $\mathbb{R}^n$
   Embedding $\mathbb{R}^d$ $(d \ll n)$
2. Invariance to some transformations.
3. Robust against noise.

Persistent homology & persistence diagrams

One-dimensional example



Persistent homology & persistence diagrams

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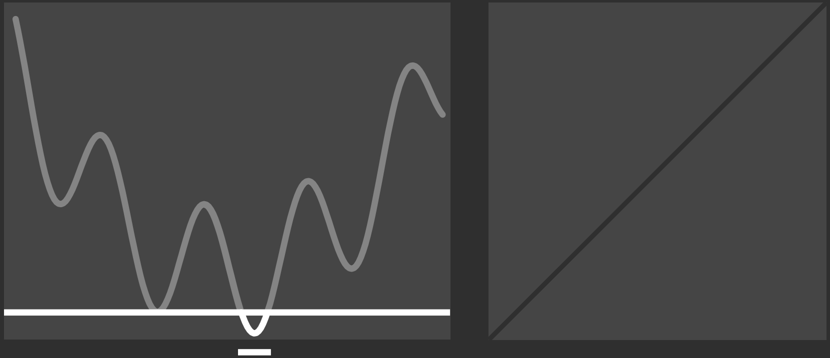

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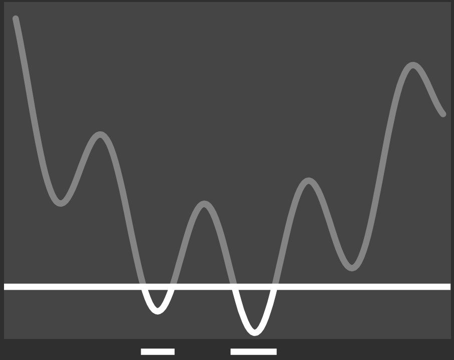

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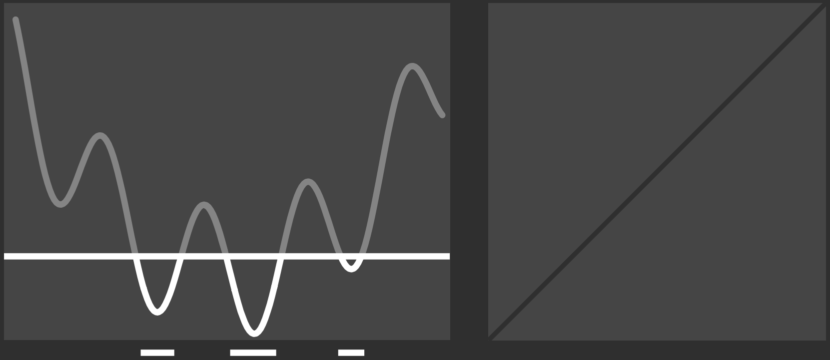

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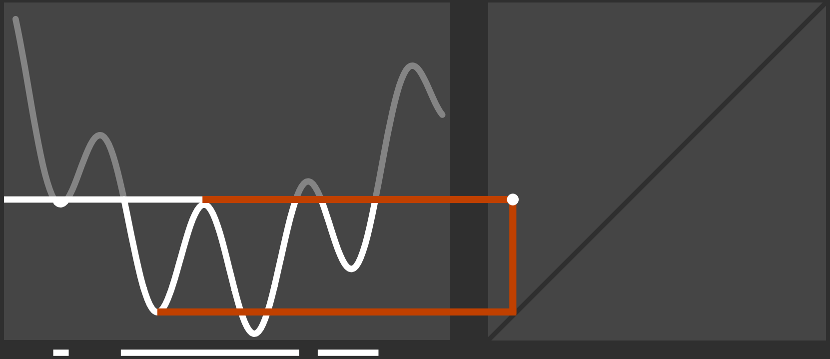

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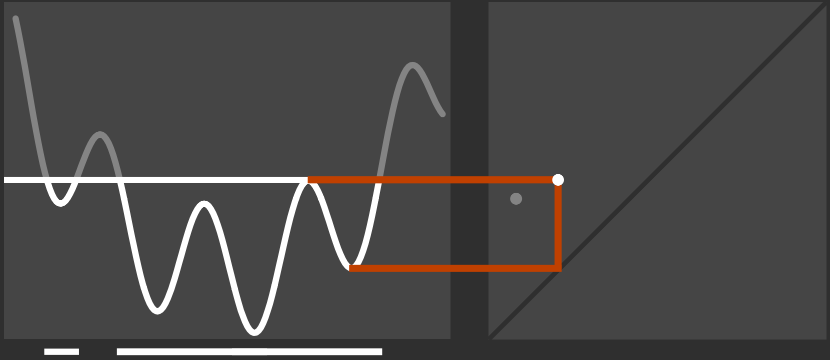

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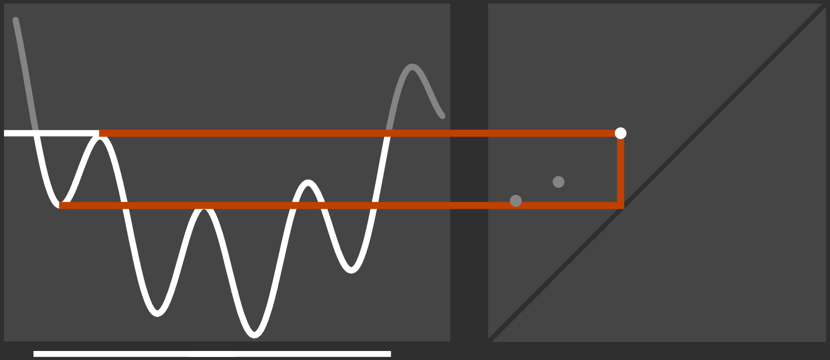

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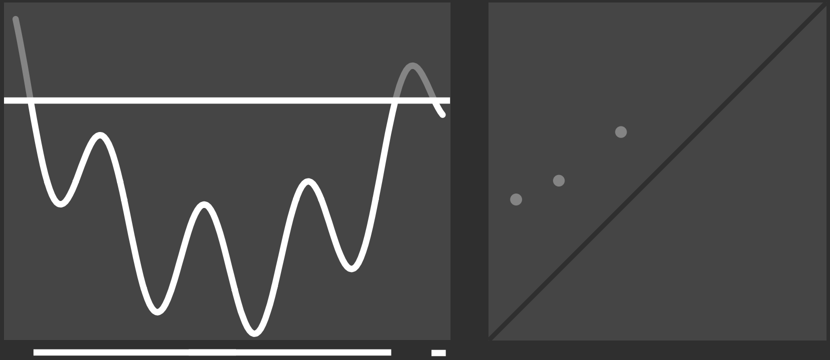

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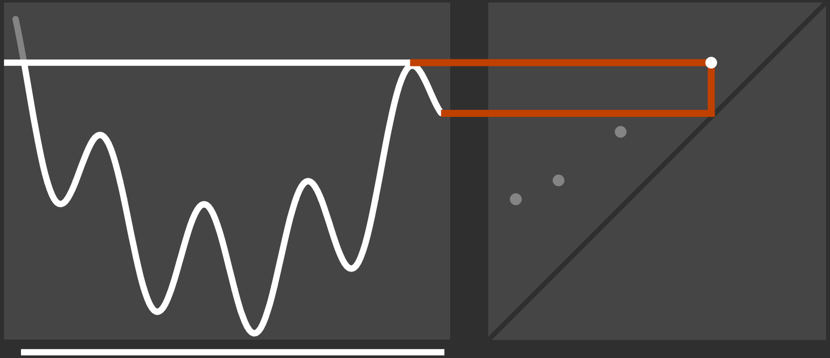

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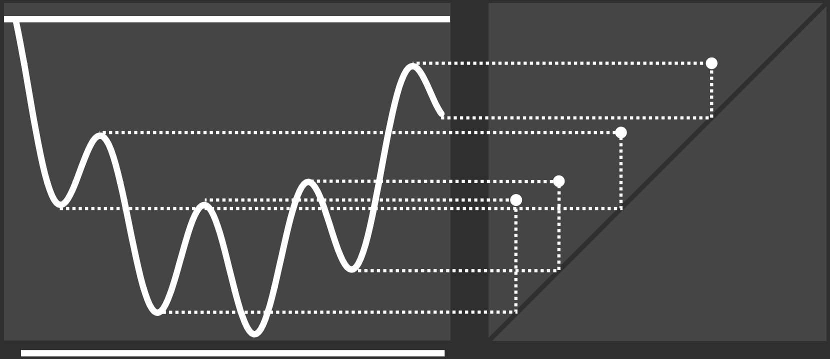
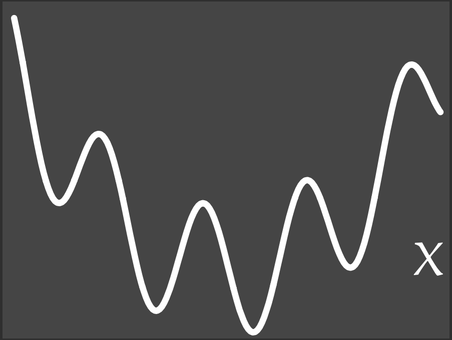
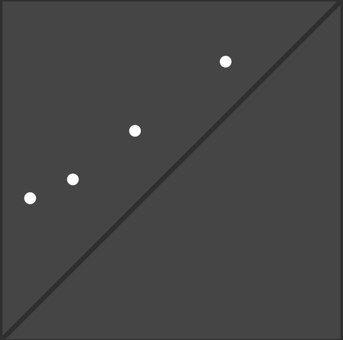


Persistent homology & persistence diagrams

Distance calculations





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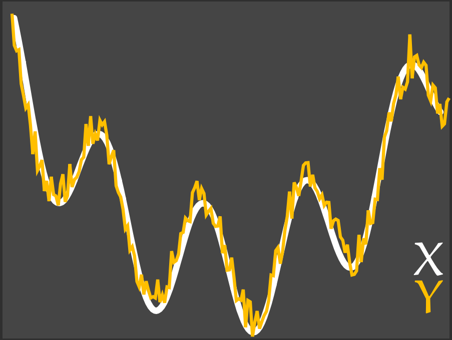

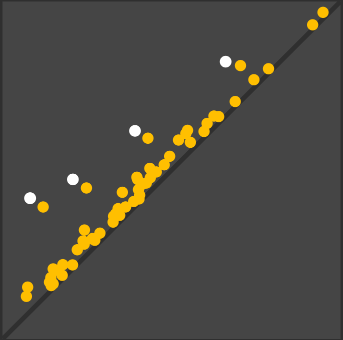

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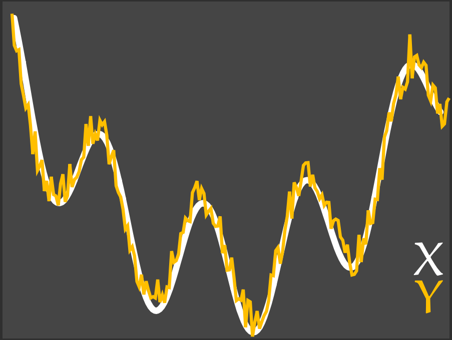
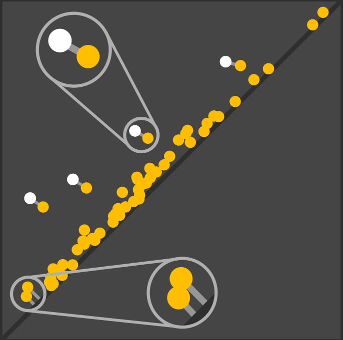
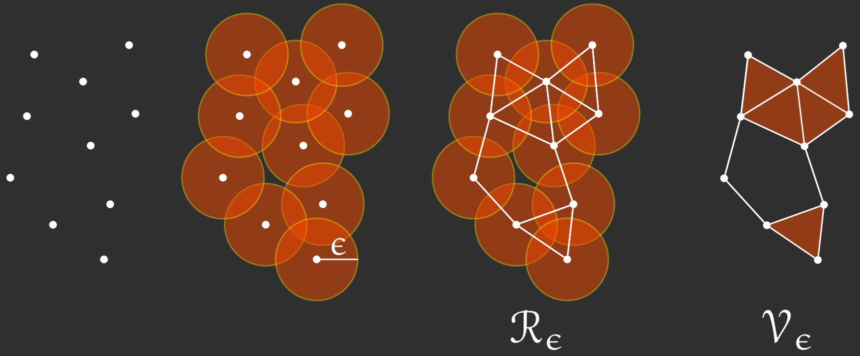




$$W_2(X, Y) = \sqrt{\inf_{\eta\colon X \to Y} \sum_{x \in X} \|x - \eta(x)\|_\infty^2}$$

Extension to multivariate input data

Rips graphs and Vietoris–Rips complexes



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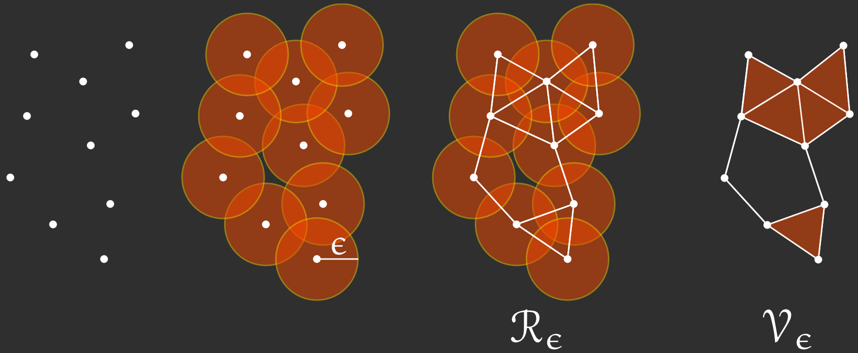

For $\epsilon \leqslant \epsilon'$, we have $\mathcal{R}_\epsilon \subseteq \mathcal{R}_{\epsilon'}$ and $\mathcal{V}_\epsilon \subseteq \mathcal{V}_{\epsilon'}$.

How to combine multiple data descriptors?

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Use feature vectors as input for PCA!

Data descriptor landscapes

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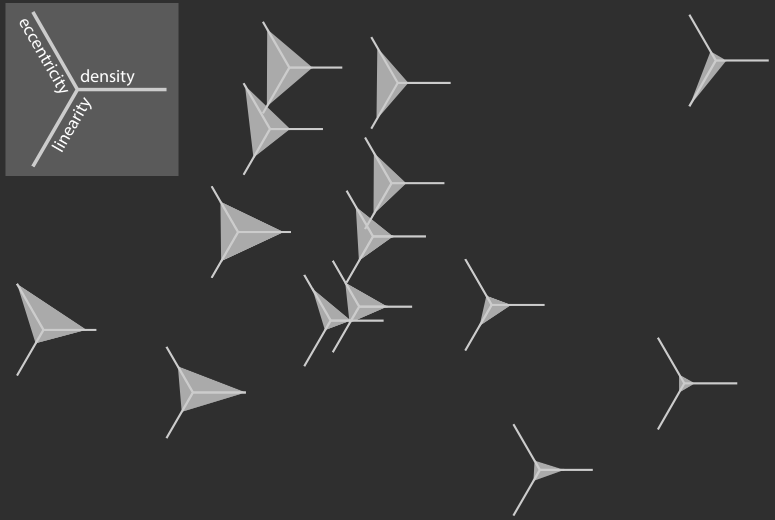

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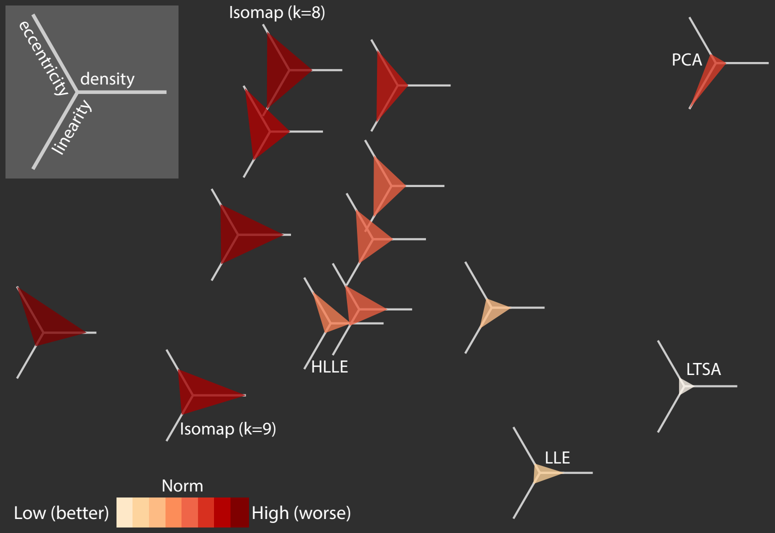

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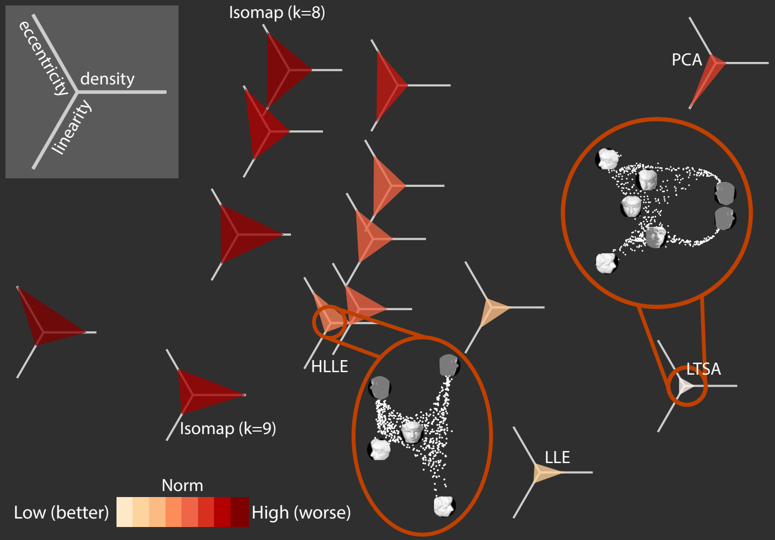


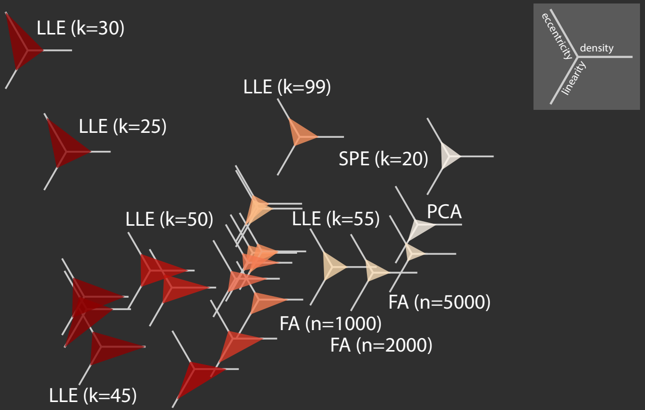
Results

Climate data

- Multivariate simulation data from *German Climate Research Centre* (DKRZ).
- Grid data from 192×96 locations with six continuous attributes over 1460 time steps.
- In total, 18432 vectors from $\mathbb{R}^6$.

Data descriptor landscape for climate data

Linear vs. non-linear methods



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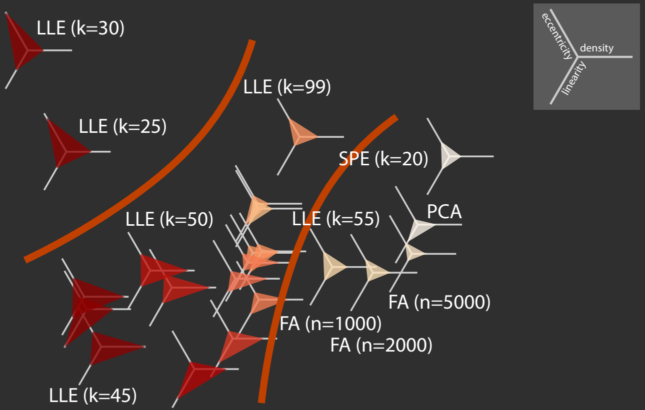
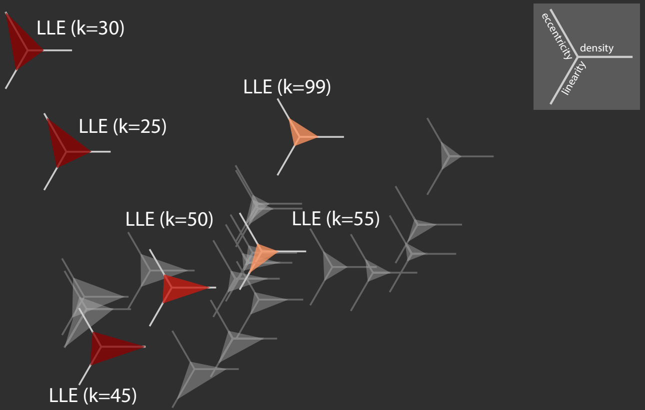


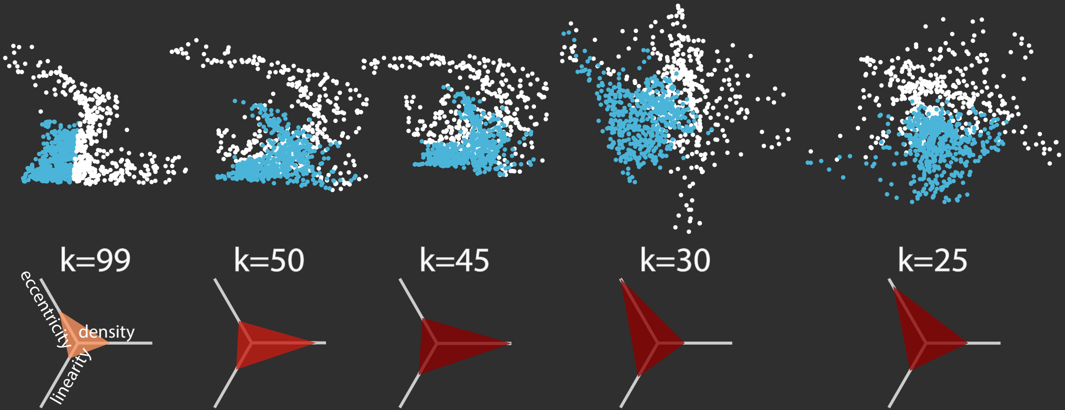
A closer look at LLE

Stability analysis

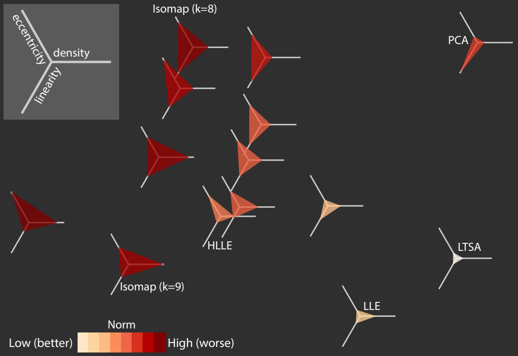


A closer look at LLE

Brushing some embeddings



Conclusion



- *Data descriptor approach*:
  - Functional description of salient properties.
  - Landscapes as a new visual metaphor for comparing multiple dimensionality reduction methods.
- Main applications: Variability and stability analysis of dimensionality reduction methods.
- Future work: Domain-specific data descriptors

Thank you for your attention!