Manifold Learning

ml essentials
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Workshop resources

Notebooks

https://github.com/cc-skuehn/Workshop_Manifold_Learning

Run Notebooks on

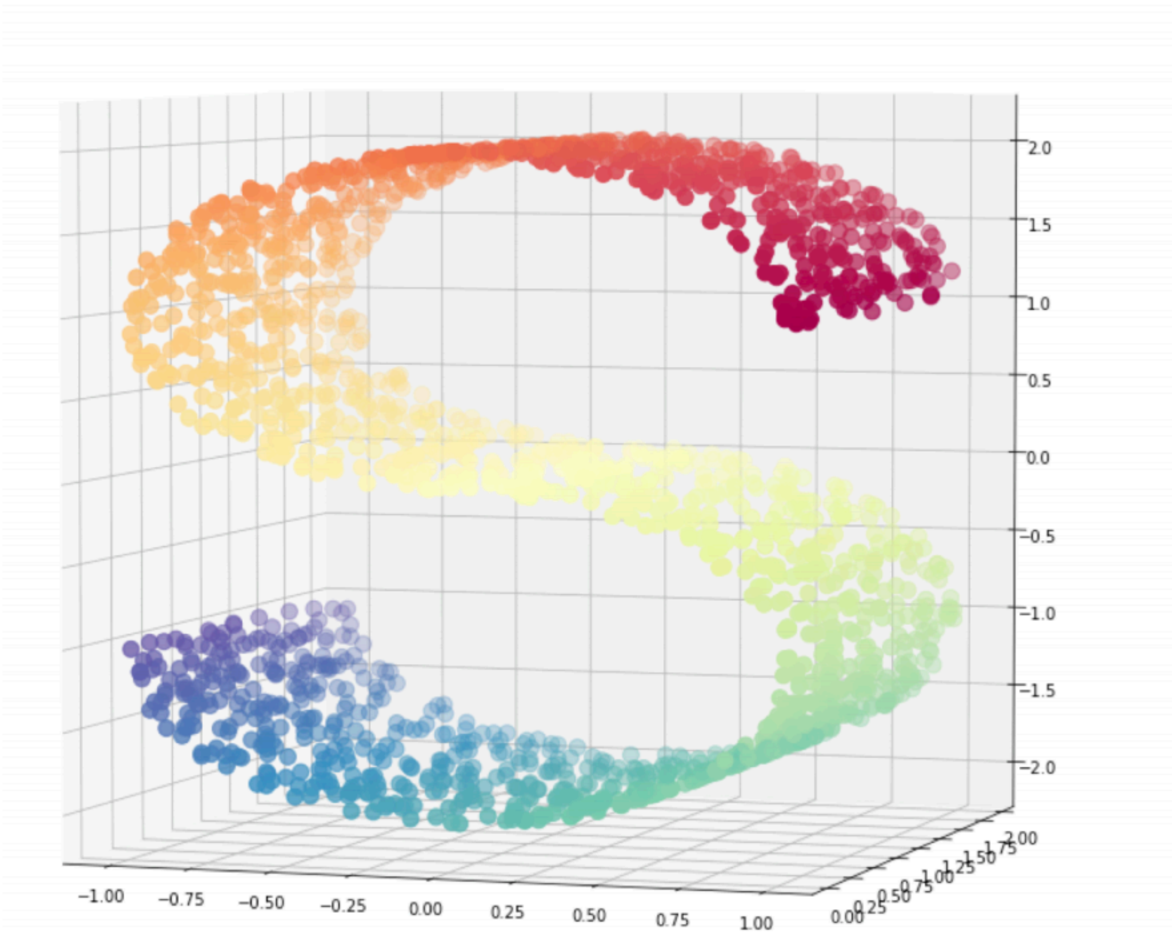
https://colab.research.google.com/

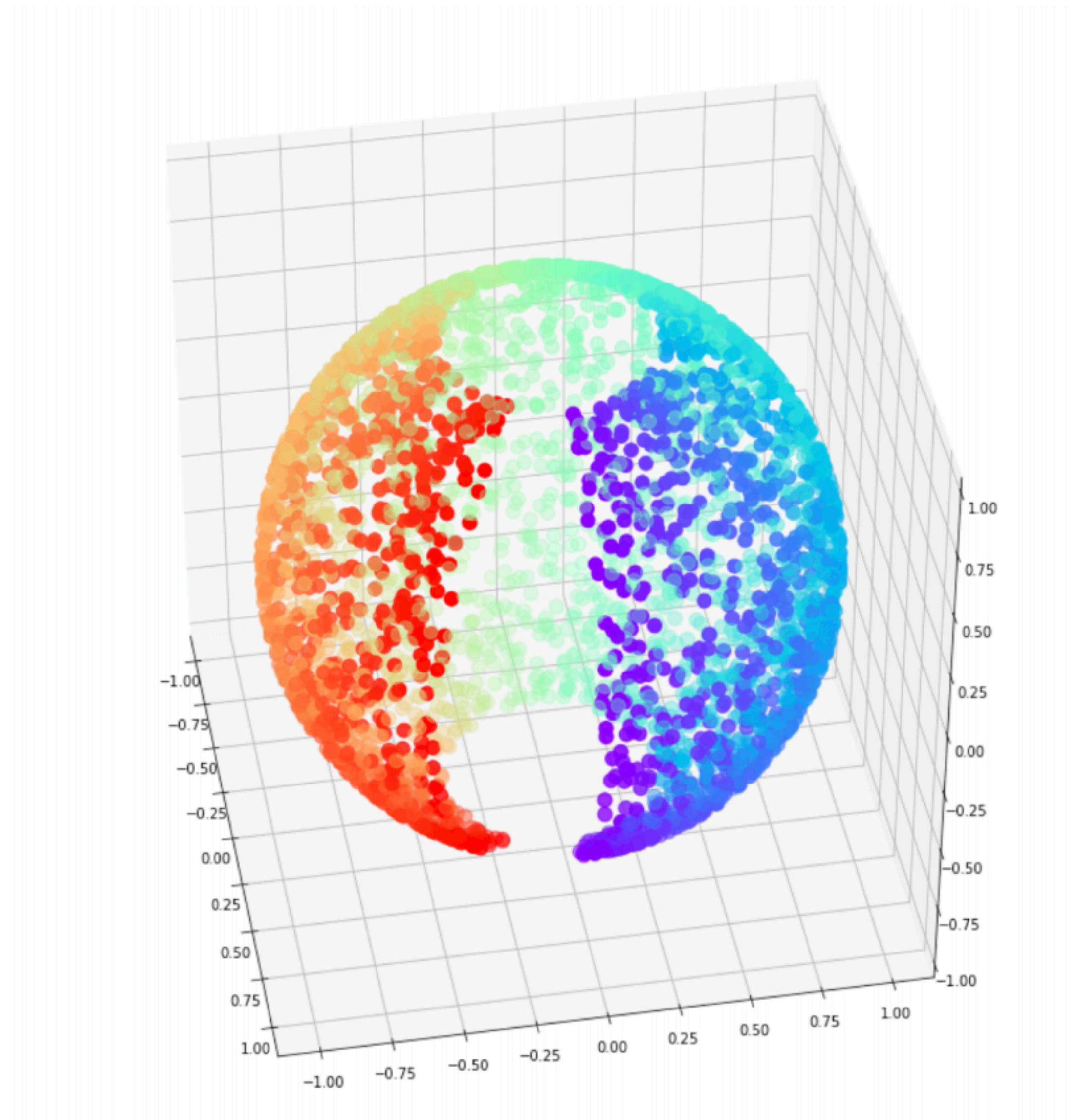
Slides about Manifold Learning

Manifold Learning at MCubed 2018

What is a manifold?

Mathematical concept from Differential Geometry





Why is it a useful concept?

Relativity theory, black holes, and the Poincaré conjecture

- A Manifold locally resembles Euclidean Space
- Allows to generalize useful concepts like Calculus
- Allows to describe geometric properties by means of Calculus
- Einstein’s general theory of relativity
- Gravitational lensing and black holes
- Perelman and the proof of the Poincaré conjecture

Ok, that’s Differential geometry, but where is Machine Learning?

What are properties of a manifold?

Important Properties – Topology and more

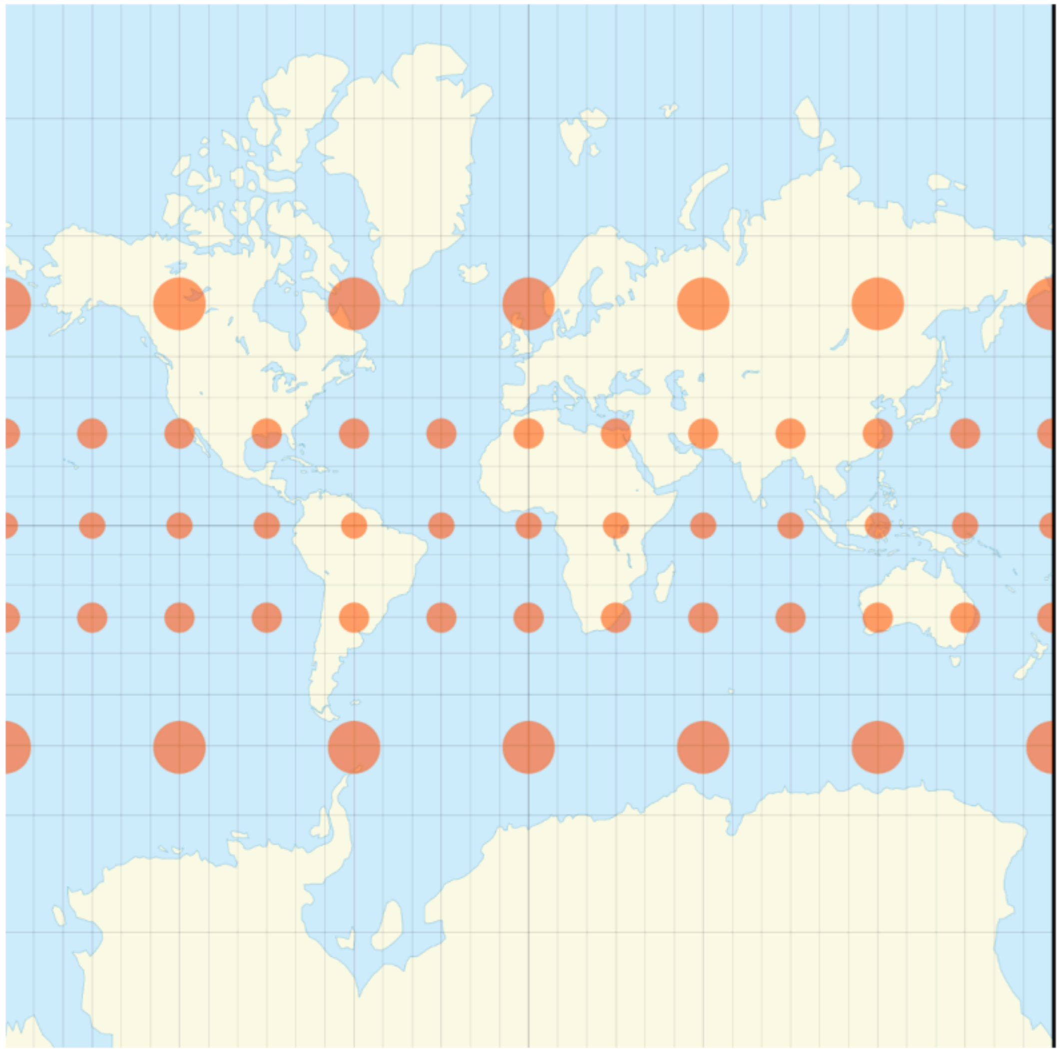
- Number of Connected Components
- Holes
- Curvature
- Smoothness
- Dimensionality
- ...you_name_it...

What are properties of a good visualization?

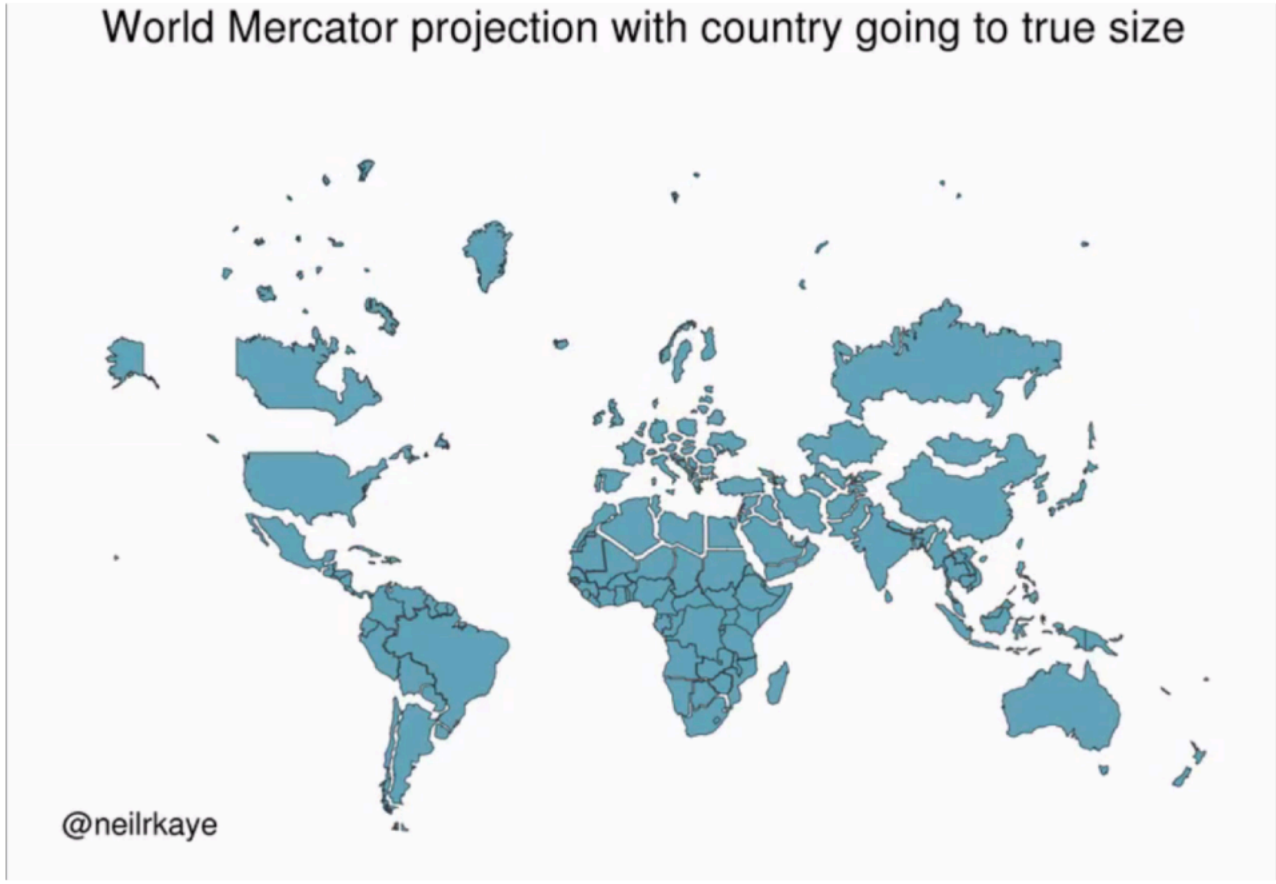
Preserve important properties

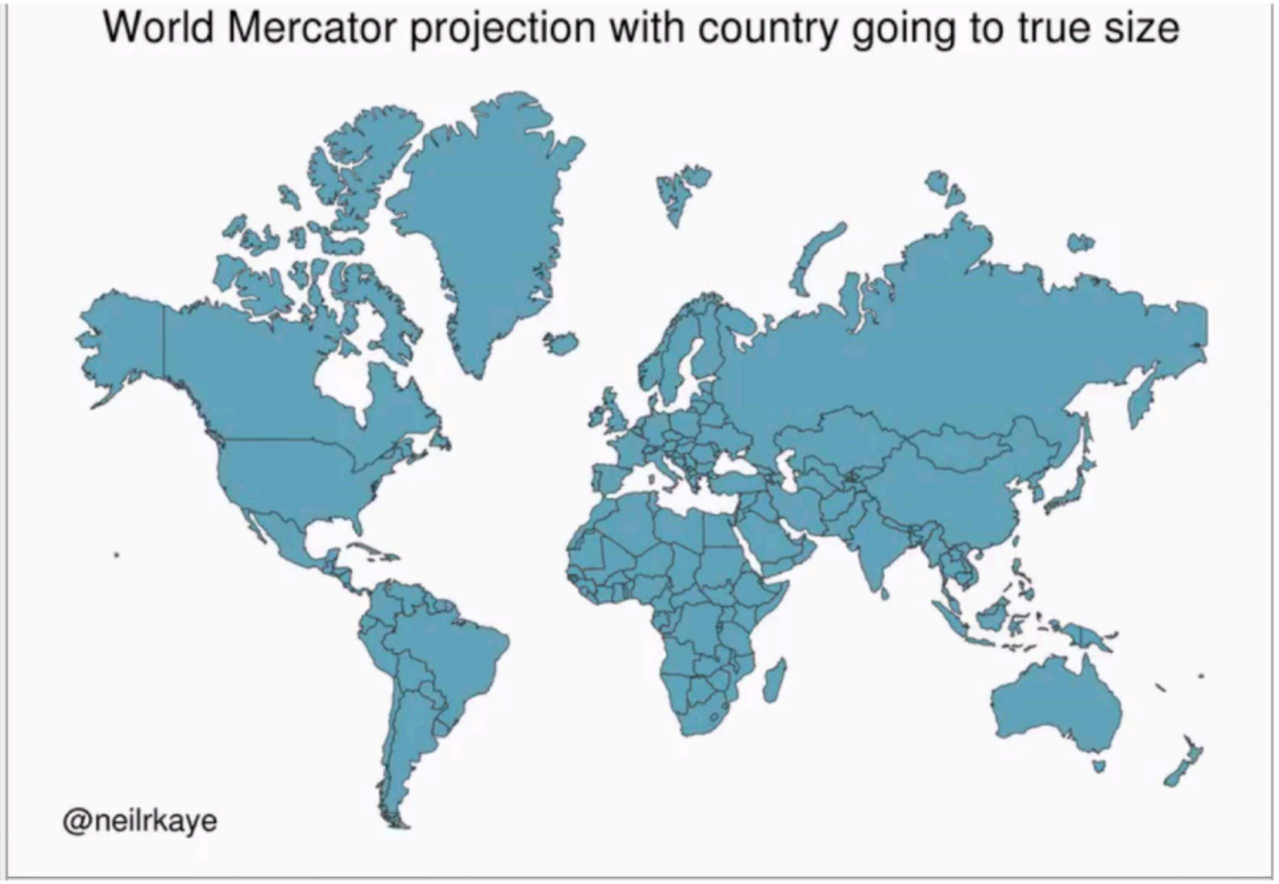
- Number of connected components?
- Holes?
- Curvature?
- Smoothness?
- Dimensionality?
- Distances between points?
- Angles, orientations?
- Local versus global properties?

You cannot have it all!



Which one is correct?





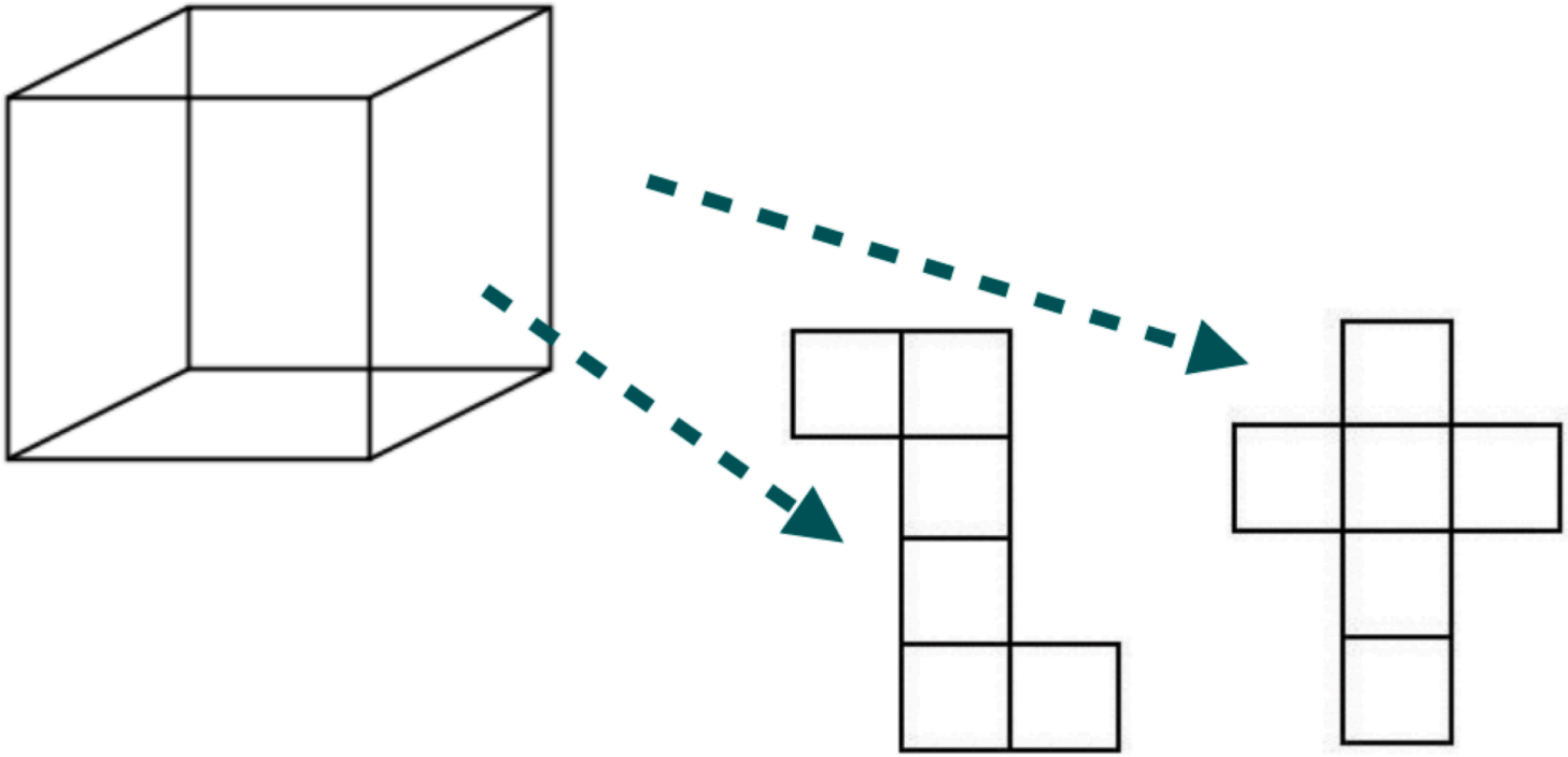
What does „Learning“ mean in Manifold Learning?

- **Learning the high-dimensional manifold**
  - Somewhat independent from low-dim approximation
  - Mathematical theories can be complex
  - Local versus global properties, distance vs. density etc.
- **Learning the low-dimensional approximation (or embedding)**
  - Depends on properties to be preserved
  - Depends on choice of similarity/distance measure
- **Learning the mapping from high-dim to low-dim**
  - Depends on everything above
- **Learning the structure without assumptions?**
  - **No.** *All methods make use of explicit and / or implicit assumptions. Sometimes it’s hard to figure these out but they determine what you get / see in the end.*

Manifold Learning Methods in sklearn

- **Locally Linear Embedding**
  - Neighborhood-preserving
- **Isomap**
  - Quasi-isometric
- **Multi-Dimensional Scaling (MDS)**
  - Quasi-isometric
- **Spectral Embedding**
  - Spectral clustering based on similarity (Laplacian Eigenmaps)
- **Local Tangent Space Alignment (LTSA)**

Local Tangent Space Alignment



Dimensionality Reduction Methods

- **PCA**
  - Preserves variance
  - Best approximation by linear subspace
  - Comes with quantitative estimation of loss
  - Solves multiple approximations at once
- **Gaussian Random Projections**
  - Preserves distances
  - Based on Johnson-Lindenstrauss lemma
  - Simple and reliable
  - Generates a random projection matrix using a Gaussian
- **Sparse Random Projections**
  - Preserves distances and enforces sparsity
  - Uses a much simpler probability distribution

„Advanced“ Methods – Advanced Math

- **tSNE** ***or t-Distributed Stochastic Neighbor Embedding***
  - Transforms Euclidean distances between points into conditional probabilities for similarity
  - Idea is to find a 2D/3D probability distribution that is similar to he high-dim distribution
  - Learns a mapping that preserves these probabilities
  - Minimizes Kullback-Leibler divergence (somehow)
- **UMAP** ***or Uniform Manifold Approximation and Projection***
  - Based on Differential Geometry and Algebraic Topology
  - Preserves important structural properties
  - If you really want to know more:
    - *Category Theory*
    - *Functors*
    - *Fuzzy Topological Representation*

Demo Time

Sometimes, words are insufficient...

In mathematics, a **manifold** is a topological space that locally resembles Euclidean space near each point. More precisely,

One-dimensional manifolds include lines and circles, but not figure eights (because they have *crossing points* that are not l
self-intersections) in three dimensional real space, but also the Klein bottle and real projective plane, which will always self-

So let’s use code!

```
print(__doc__)

from time import time

import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from matplotlib.ticker import NullFormatter
%matplotlib inline
from sklearn import manifold, datasets
```

Google Colab

- https://colab.research.google.com/notebooks/welcome.ipynb
- Sign in with your Google Account
- Load first Jupiter Notebook from GitHub repo:
    - File -> Open Notebook -> Github -> Enter Github URL
        - cc-skuehn -> Workshop_Manifold_Learning
        - Manifold_S_Dataset.ipynb

Backup - Experiments

- https://distill.pub/2016/misread-tsne/