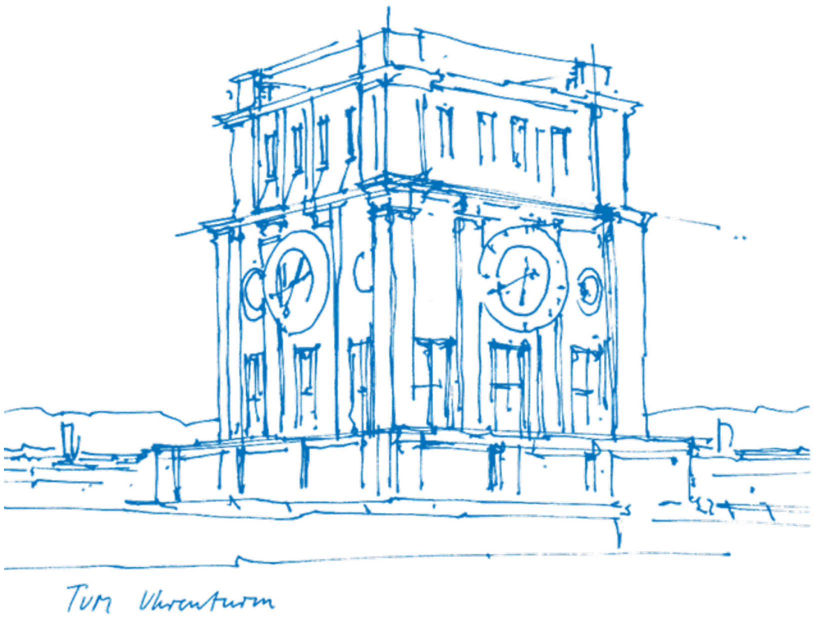
# Representation of data: Manifold learning with Diffusion Maps

Felix Dietrich



# Today: Manifold Learning

## Representation of data with Diffusion Maps

1. Definition: manifold
2. Topology and geometry
3. Manifold learning
4. Laplace-Beltrami operator
5. Diffusion Maps algorithm

# Representation of data

## High-dimensional data with low-dimensional structure - general idea

1. Given input: data matrix $X \in \mathbb{R}^{N \times n}$ with $N$ data points in $n$-dimensional space.
2. ...algorithm...
3. Output: new representation of the data, e.g. as another coordinate matrix $U \in \mathbb{R}^{N \times p}$.

Ideally: $p \ll n$, so that the dimension of the data is reduced (manifold learning, compression).
For visualization, $p = 2, 3, (4)$ is necessary.
Example for a low-dimensional structure: $U \in \mathbb{R}^{1000 \times 3}$ with rows $u_i \in \mathbb{R}^3$, $\|u_i\| = 1$:

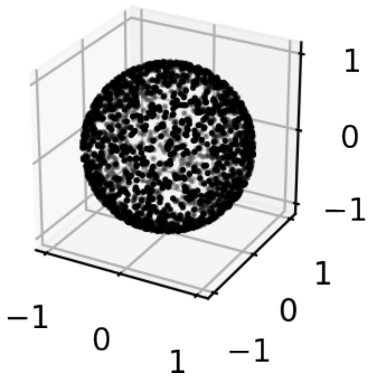



Figure: Data set where the points $u_i$ (black) are distributed on a sphere.

# Representation of data

## High-dimensional data with low-dimensional structure - manifolds

*[Manifolds are] generalizations of curves and surfaces to arbitrarily many dimensions [and] provide the mathematical context for understanding "space" in all of its manifestations.* [Lee, 2012]

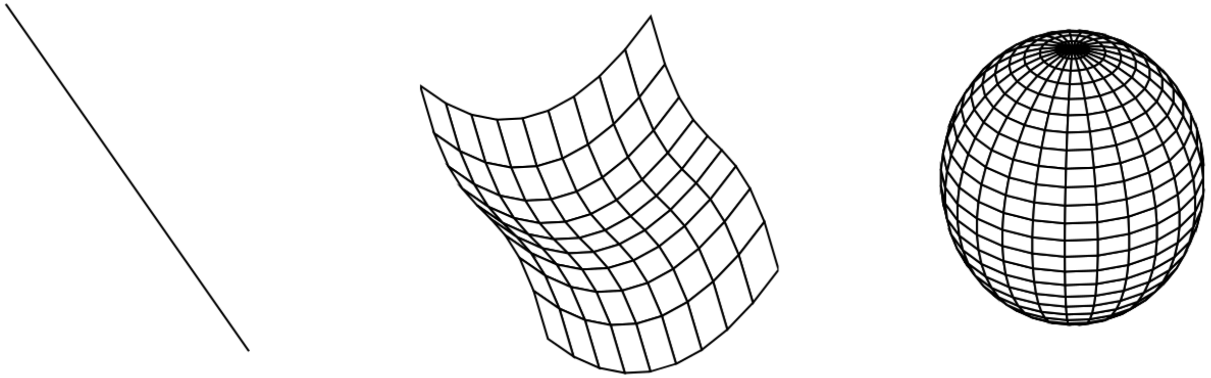


Figure: From [Dietrich, 2017]: Examples for manifolds with different geometries and intrinsic dimensions. The line segment is of intrinsic dimension one, the center surface is a two-dimensional manifold, curved and embedded in three-dimensional space. The sphere has intrinsic dimension two, but cannot be deformed through any homeomorphism into the surface in the center. Remark regarding last lecture: there are also geometric bifurcations!

# Representation of data

## High-dimensional data with low-dimensional structure - manifolds

**Definition: Manifold, shortened.** A topological space $M$ is a topological manifold of dimension $d$ if $M$ is locally Euclidean: each point of $M$ has a neighborhood that is homeomorphic to an open subset of $R^d$. [Lee, 2012]
[To be precise: $M$ has to be Hausdorff and second-countable, too.]

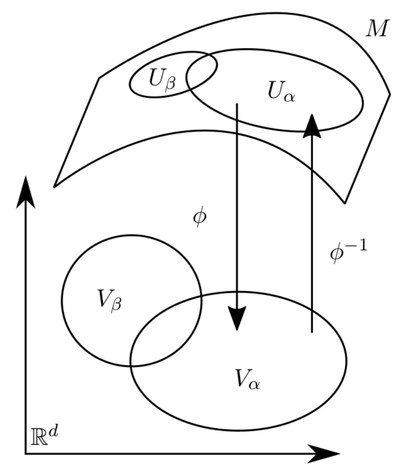
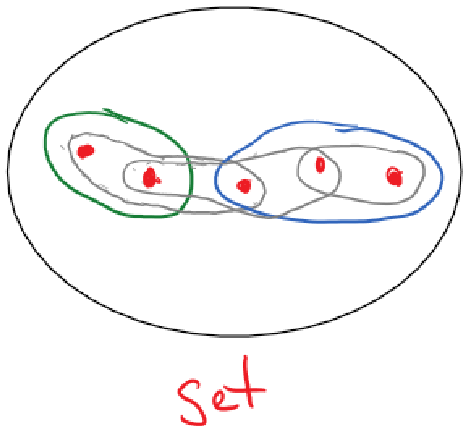
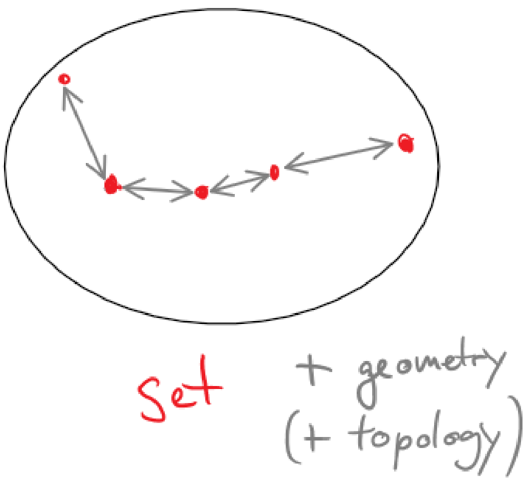



Figure: Visualization of a manifold $M$. The subsets $U_\alpha, U_\beta \subset M$ and $V_\alpha, V_\beta \subset \mathbb{R}^d$ are open sets, $\phi$ is a homeomorphism.

# Representation of data

## Topology versus geometry




Let $X$ be a set. A ***topology on*** $X$ is a collection $\mathcal{T}$ of subsets of $X$, called ***open subsets***, satisfying

(i) $X$ and $\varnothing$ are open.
(ii) The union of any family of open subsets is open.
(iii) The intersection of any finite family of open subsets is open.

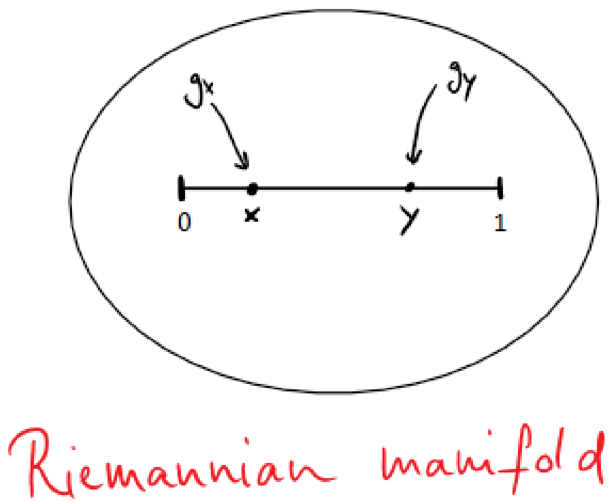
A pair $(X, \mathcal{T})$ consisting of a set $X$ together with a topology $\mathcal{T}$ on $X$ is called a ***topological space***.

A ***metric space*** is a set $M$ endowed with a ***distance function*** (also called a ***metric***) $d : M \times M \to \mathbb{R}$ satisfying the following properties for all $x, y, z \in M$:

(i) POSITIVITY: $d(x, y) \geq 0$, with equality if and only if $x = y$.
(ii) SYMMETRY: $d(x, y) = d(y, x)$.
(iii) TRIANGLE INEQUALITY: $d(x, z) \leq d(x, y) + d(y, z)$.

# Representation of data

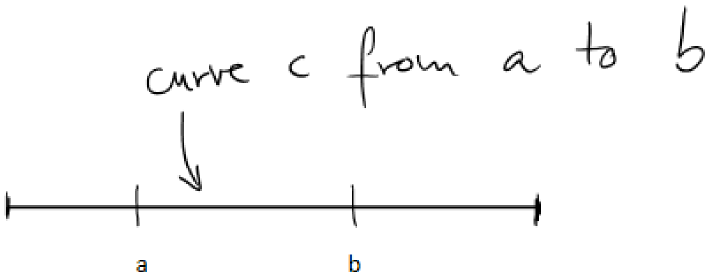
## Riemannian manifolds

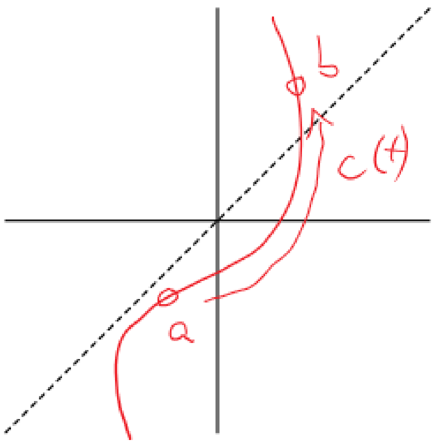



A ***Riemannian metric on*** $M$ is a smooth symmetric covariant 2-tensor field on $M$ that is positive definite at each point. A ***Riemannian manifold*** is a pair $(M, g)$, where $M$ is a smooth manifold and $g$ is a Riemannian metric on $M$. One sometimes simply says "$M$ is a Riemannian manifold" if $M$ is understood to be endowed with a specific Riemannian metric.

# Representation of data

## Curves on Riemannian manifolds




$$L_a^b(c) := \int_a^b \sqrt{g(c'(t), c'(t))}\,\mathrm{d}t = \int_a^b \|c'(t)\|\,\mathrm{d}t.$$

# Representation of data

## Topology versus geometry

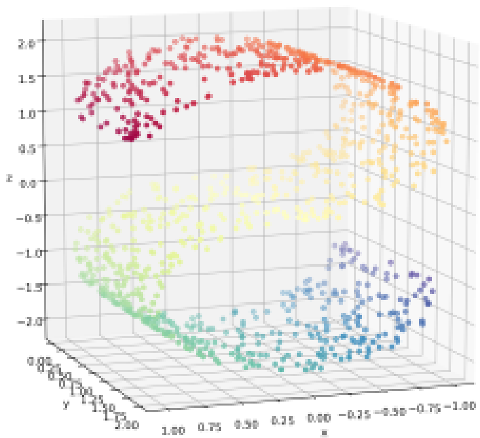
SAME topology

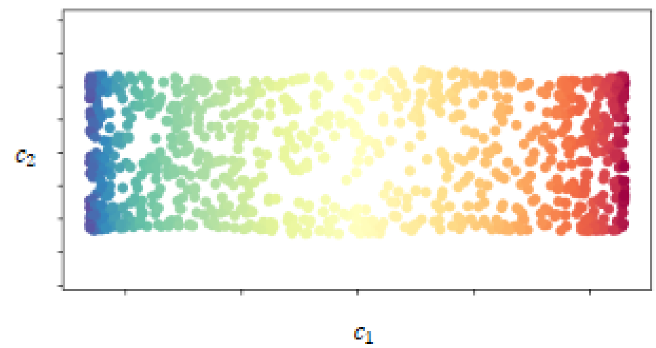
DIFFERENT geometry

https://upload.wikimedia.org/wikipedia/commons/2/26/Mug_and_Torus_morph.gif
Author: Lucas Vieira

# Representation of data

## Manifold learning - in general




| | A | B | C | D | E |
|---|---|---|---|---|---|
| 1 | x | y | z | | |
| 2 | 0.579699 | 0.418081 | 0.049091 | | |
| 3 | 0.918333 | 0.819384 | 0.889048 | | |
| 4 | 0.641222 | 0.453401 | 0.587756 | | |
| 5 | 0.827659 | 0.808729 | 0.108997 | | |
| 6 | 0.320323 | 0.698129 | 0.04561 | | |
| 7 | 0.223276 | 0.876384 | 0.149571 | | |
| 8 | 0.01184 | 0.972112 | 0.989366 | | |
| 9 | 0.087981 | 0.895696 | 0.379578 | | |
| 10 | 0.491548 | 0.171433 | 0.018083 | | |
| 11 | 0.453172 | 0.083112 | 0.907416 | | |
| 12 | 0.797321 | 0.076609 | 0.912459 | | |

| | A | B | C | D |
|---|---|---|---|---|
| 1 | c1 | c2 | | |
| 2 | 0.008613 | 0.964437 | | |
| 3 | 0.4912 | 0.477741 | | |
| 4 | 0.912283 | 0.650359 | | |
| 5 | 0.964879 | 0.159634 | | |
| 6 | 0.254983 | 0.316284 | | |
| 7 | 0.241464 | 0.989014 | | |
| 8 | 0.892201 | 0.011716 | | |
| 9 | 0.682857 | 0.478074 | | |
| 10 | 0.973667 | 0.323248 | | |
| 11 | 0.357255 | 0.258019 | | |
| 12 | 0.181788 | 0.141262 | | |
| 13 | 0.882955 | 0.9977 | | |

# Representation of data

## Nonlinear manifold learning: Diffusion Maps

1. Basic idea: eigenfunctions of the diffusion operator $\Delta$ embed the manifold with data $X$ [Coifman et al., 2005, Coifman and Lafon, 2006].
2. Algorithm: compute a few eigenfunctions evaluated on the data, use them as new coordinates $U$ [Nadler et al., 2006, Berry et al., 2013].
3. Challenge: how to define a diffusion operator on a point cloud $X$?

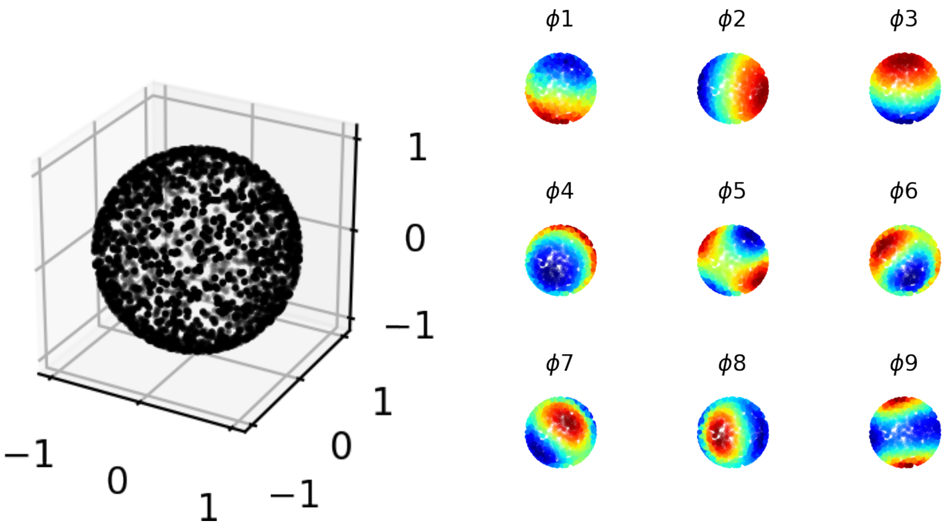



Figure: Spherical data set and eigenfunctions of the Laplace-Beltrami (Diffusion) operator.

# Representation of data

## Nonlinear manifold learning: Diffusion Maps

**Challenge**: how to define a diffusion operator on a point cloud $X$?

**Diffusion equation**: find a function $f : T \times M \to \mathbb{R}$, with specified initial data $f(0,x) = g(x)$, solve

$$\frac{\partial}{\partial t} f = \Delta f. \tag{1}$$

**Note**: if $M = \mathbb{R}$, the real line, $\Delta = \frac{\partial^2}{\partial x^2}$.

# Representation of data

## Nonlinear manifold learning: Diffusion Maps

**Challenge**: how to define a diffusion operator on a point cloud $X$?
**Diffusion equation**: find a function $f : T \times M \to \mathbb{R}$, with specified initial data $f(0,x) = g(x)$, solve

$$\frac{\partial}{\partial t} f = \Delta f. \tag{1}$$

**Note**: if $M = \mathbb{R}$, the real line, $\Delta = \frac{\partial^2}{\partial x^2}$.
**Main idea**: the solution of equation (1) with initial condition $f(0,x) = \delta_x$ is

$$f(t,x) = \exp(t\Delta)\delta_x. \tag{2}$$

Locally and for small $t$, that solution is a "bump function" centered at $x$, of the form

$$k(t,y) = \exp(-\|x-y\|^2/t) \tag{3}$$

where $x$ is the center point and $y$ is another point in the neighborhood of $x$.

# Representation of data

## Nonlinear manifold learning: Diffusion Maps

**Challenge**: how to define a diffusion operator on a point cloud $X$?

**Diffusion equation**: find a function $f : T \times M \to \mathbb{R}$, with specified initial data $f(0, x) = g(x)$, solve

$$\frac{\partial}{\partial t} f = \Delta f. \tag{1}$$

**Note**: if $M = \mathbb{R}$, the real line, $\Delta = \frac{\partial^2}{\partial x^2}$.

**Main idea**: the solution of equation (1) with initial condition $f(0, x) = \delta_x$ is

$$f(t, x) = \exp(t\Delta)\delta_x. \tag{2}$$

Locally and for small $t$, that solution is a “bump function” centered at $x$, of the form

$$k(t, y) = \exp(-\|x - y\|^2 / t) \tag{3}$$

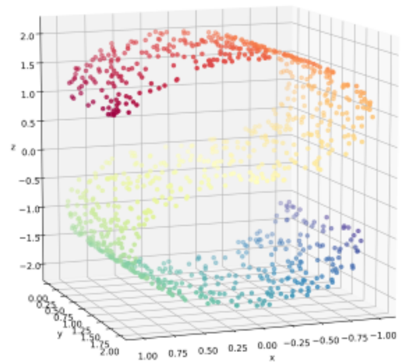
where $x$ is the center point and $y$ is another point in the neighborhood of $x$.

**Algorithm**: compute $k$ for all pairs of $N$ points in the data set, with a small value of $t$. This results in a “kernel matrix” $K \in \mathbb{R}^{N \times N} \approx \exp(t\Delta)$. Then, solve the eigenproblem

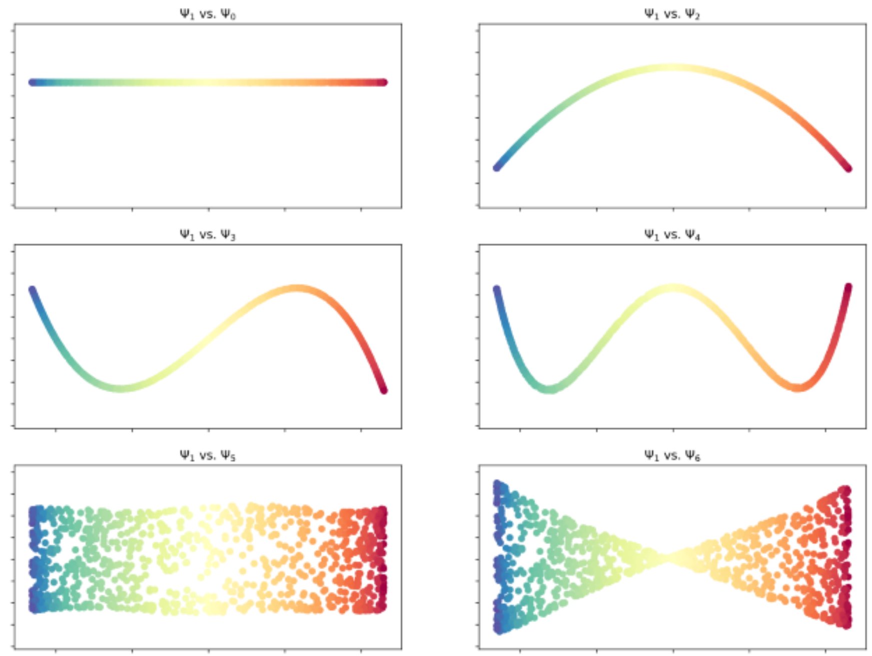
$$\exp(t\Delta)\phi_l = \lambda_l \phi_l. \tag{4}$$

# Representation of data

## Manifold learning - S-curve with Diffusion Maps




| | A | B | C | D |
|---|---|---|---|---|
| 1 | x | y | z | |
| 2 | 0.579699 | 0.418081 | 0.049091 | |
| 3 | 0.918333 | 0.819384 | 0.889048 | |
| 4 | 0.641222 | 0.453401 | 0.587756 | |
| 5 | 0.827659 | 0.808729 | 0.108997 | |
| 6 | 0.320323 | 0.698129 | 0.04561 | |
| 7 | 0.223276 | 0.876384 | 0.149571 | |
| 8 | 0.01184 | 0.972112 | 0.989366 | |
| 9 | 0.087981 | 0.895696 | 0.379578 | |
| 10 | 0.491548 | 0.171433 | 0.018083 | |
| 11 | 0.453172 | 0.083112 | 0.907416 | |
| 12 | 0.797321 | 0.076609 | 0.912459 | |




Also see here: `https://datafold-dev.gitlab.io/datafold/tutorial_basic_dmap_scurve.html`

# Representation of data

## Nonlinear manifold learning: Diffusion Maps

Given a data set $\{y_i \in \mathbb{R}^n\}_{i=1}^N$ [Berry et al., 2013]:

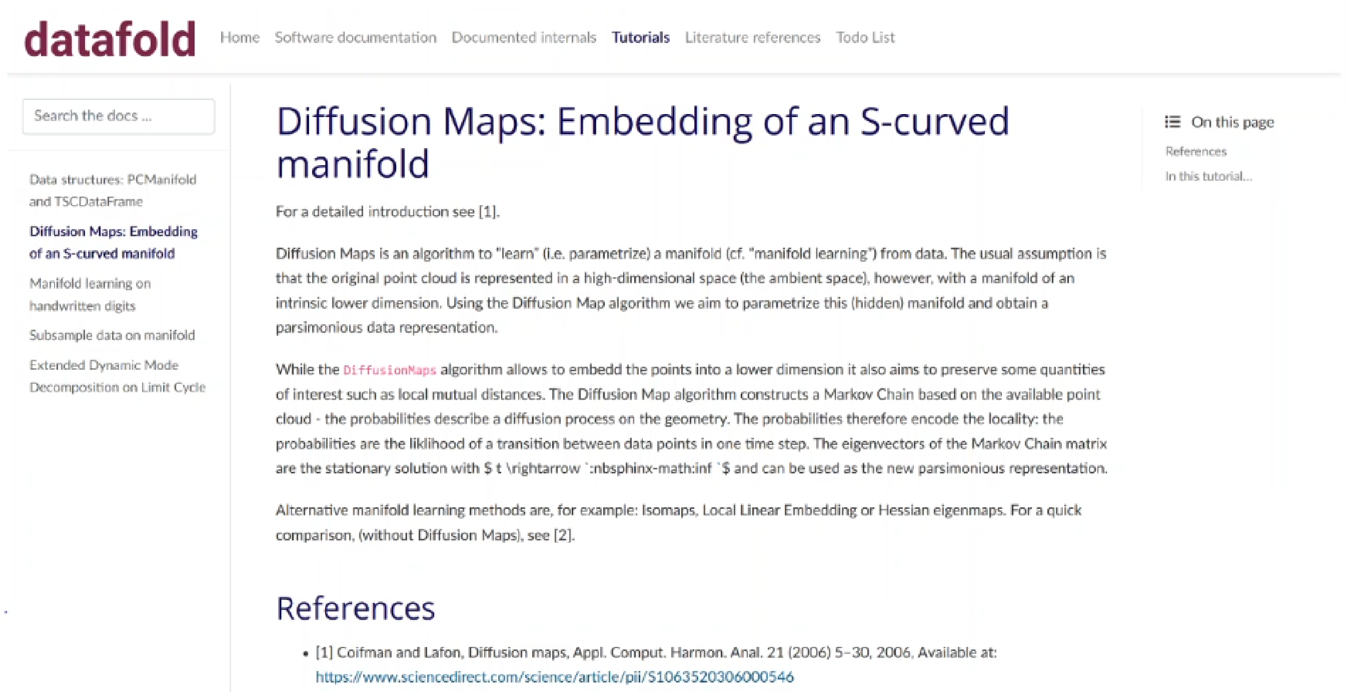
1. Form a distance matrix $D$ with entries
$$D_{ij} = \|y_i - y_j\|,$$
where $i = 1,\dots,N$ are the rows, $j = 1,\dots,N$ are the columns, and $y_i, y_j$ are the data points.
2. Set $\varepsilon$ to 5% of the diameter of the dataset: $\varepsilon = 0.05(\max_{i,j} D_{i,j})$.
3. Form the kernel matrix $W$ with $W_{ij} = \exp\left(-D_{ij}^2/\varepsilon\right)$.
4. Form the diagonal normalization matrix $P_{ii} = \sum_{j=1}^N W_{ij}$.
5. Normalize to form the kernel matrix $K = P^{-1}WP^{-1}$.
6. Form the diagonal normalization matrix $Q_{ii} = \sum_{j=1}^N K_{ij}$.
7. Form the symmetric matrix $\hat{T} = Q^{-1/2}KQ^{-1/2}$.
8. Find the $L+1$ largest eigenvalues $a_l$ and associated eigenvectors $v_l$ of $\hat{T}$.
9. Compute the eigenvalues of $\hat{T}^{1/\varepsilon}$ by $\lambda_l^2 = a_l^{1/\varepsilon}$.
10. Compute the eigenvectors of the matrix $T = Q^{-1}K$ by $\phi_l = Q^{-1/2}v_l$.

Steps 1-3 form the ambient kernel, 4-7 normalize it, 8-10 compute the eigenvalues and -vectors.

# Representation of data

## The datafold software

https://pypi.org/project/datafold/


datafold Home Software documentation Documented internals Tutorials Literature references Todo List

Search the docs ...

Data structures: PCManifold and TSCDataFrame

Diffusion Maps: Embedding of an S-curved manifold

Manifold learning on handwritten digits

Subsample data on manifold

Extended Dynamic Mode Decomposition on Limit Cycle

# Diffusion Maps: Embedding of an S-curved manifold

For a detailed introduction see [1].

Diffusion Maps is an algorithm to "learn" (i.e. parametrize) a manifold (cf. "manifold learning") from data. The usual assumption is that the original point cloud is represented in a high-dimensional space (the ambient space), however, with a manifold of an intrinsic lower dimension. Using the Diffusion Map algorithm we aim to parametrize this (hidden) manifold and obtain a parsimonious data representation.

While the `DiffusionMaps` algorithm allows to embedd the points into a lower dimension it also aims to preserve some quantities of interest such as local mutual distances. The Diffusion Map algorithm constructs a Markov Chain based on the available point cloud - the probabilities describe a diffusion process on the geometry. The probabilities therefore encode the locality: the probabilities are the liklihood of a transition between data points in one time step. The eigenvectors of the Markov Chain matrix are the stationary solution with $ t \rightarrow `:nbsphinx-math:inf `$ and can be used as the new parsimonious representation.

Alternative manifold learning methods are, for example: Isomaps, Local Linear Embedding or Hessian eigenmaps. For a quick comparison, (without Diffusion Maps), see [2].

## References

- [1] Coifman and Lafon, Diffusion maps, Appl. Comput. Harmon. Anal. 21 (2006) 5–30, 2006. Available at: https://www.sciencedirect.com/science/article/pii/S1063520306000546

On this page

References

In this tutorial...

See documentation here: `https://datafold-dev.gitlab.io/datafold/index.html`

# Literature I


- Berry, T., Cressman, J. R., Gregurić-Ferenĉek, Z., and Sauer, T. (2013).
  Time-Scale Separation from Diffusion-Mapped Delay Coordinates.
  *SIAM Journal on Applied Dynamical Systems*, 12(2):618–649.
- Coifman, R. R. and Lafon, S. (2006).
  Geometric harmonics: A novel tool for multiscale out-of-sample extension of empirical functions.
  *Applied and Computational Harmonic Analysis*, 21(1):31–52.
- Coifman, R. R., Lafon, S., Lee, A. B., Maggioni, M., Nadler, B., Warner, F., and Zucker, S. W. (2005).
  Geometric diffusions as a tool for harmonic analysis and structure definition of data: Diffusion maps.
  *Proceedings of the National Academy of Sciences of the United States of America*, 102(21):7426–7431.
- Dietrich, F. (2017).
  *Data-Driven Surrogate Models for Dynamical Systems*.
  PhD thesis, Technische Universität München.
- Lee, J. M. (2012).
  *Introduction to Smooth Manifolds*.
  Springer New York.
- Nadler, B., Lafon, S., Coifman, R. R., and Kevrekidis, I. G. (2006).
  Diffusion maps, spectral clustering and reaction coordinates of dynamical systems.
  *Applied and Computational Harmonic Analysis*, 21(1):113–127.