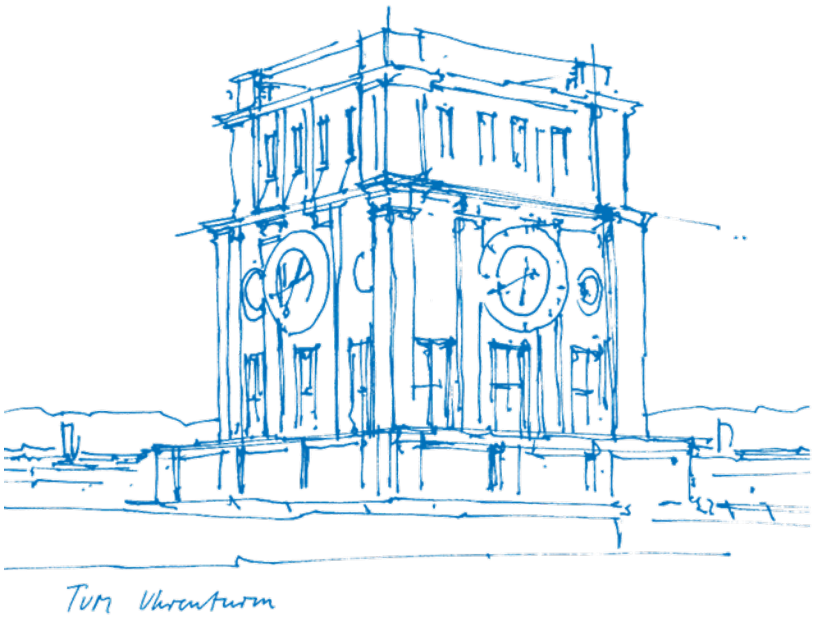
Representation of data:
Manifold learning with Diffusion Maps

Dr. 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 $u_i \in \mathbb{R}^3$, $\|u_i\| = 1$:

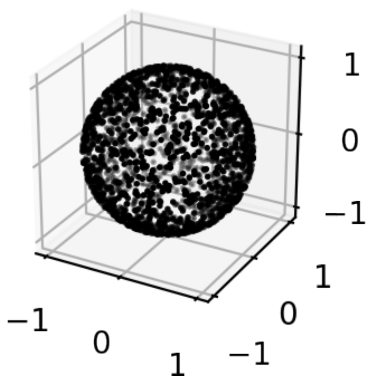


Figure: Data set where the points u_i (black) are distributed on a sphere.

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]

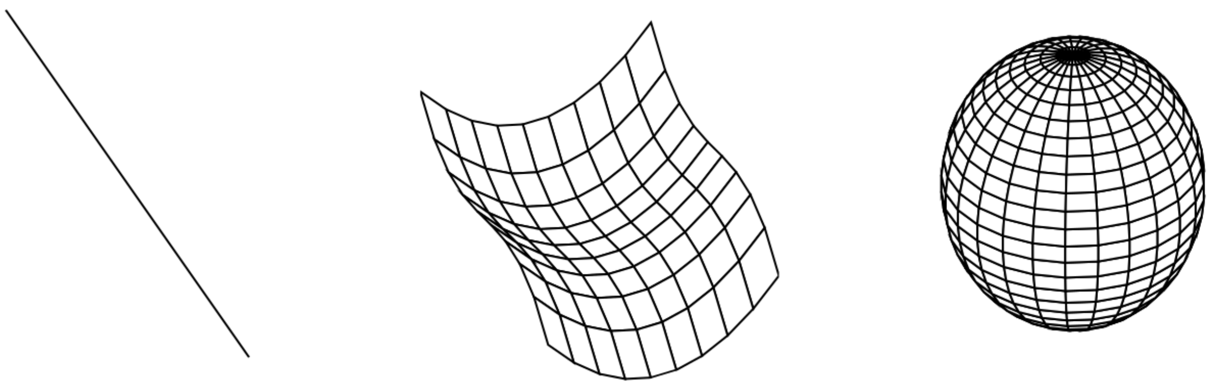


Figure: From [Dietrich, 2017]: Examples for manifolds with different geometries and intrinsic dimensions. The line segment is of intrinsic dimension one, the center surface is a two-dimensional manifold, curved and embedded in three-dimensional space. The sphere has intrinsic dimension two, but cannot 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.]

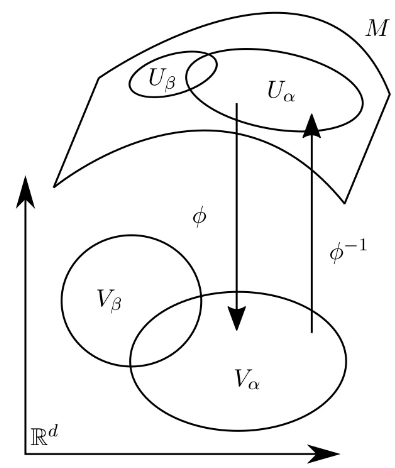
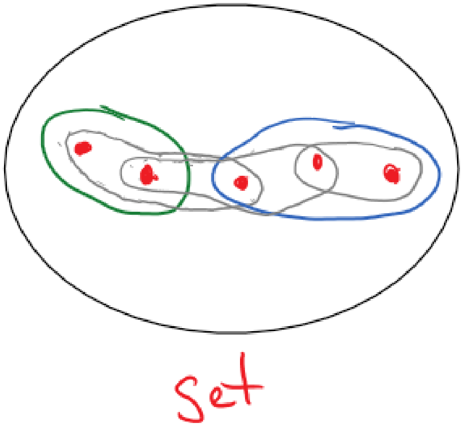
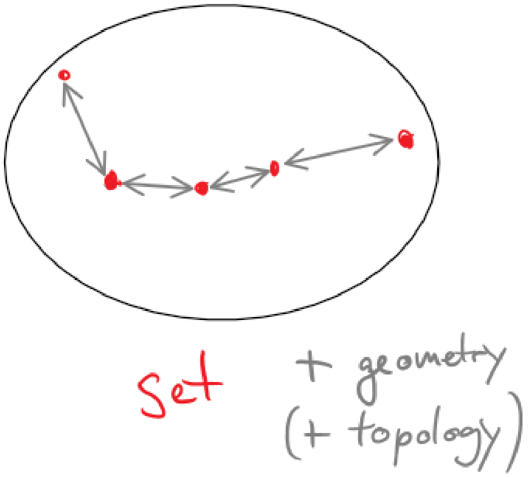


Figure: Visualization of a manifold M. The subsets $U_\alpha, U_\beta \subset M$ and $V_\alpha, V_\beta \subset \mathbb{R}^d$ are open sets, ϕ is a homeomorphism.

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

Topology versus geometry

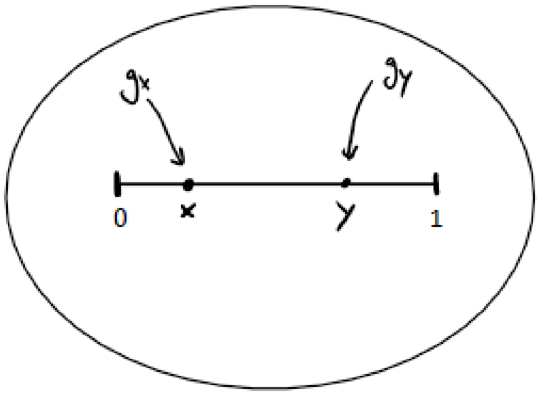
SAME topology

DIFFERENT geometry

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

Representation of data

Riemannian manifolds

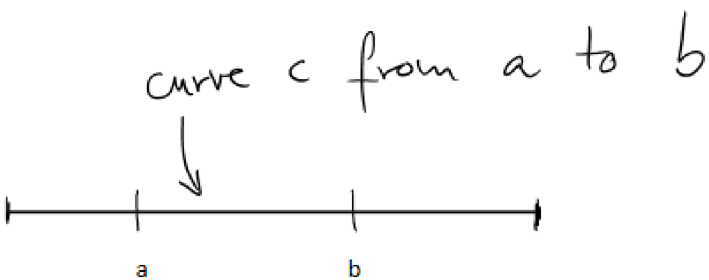


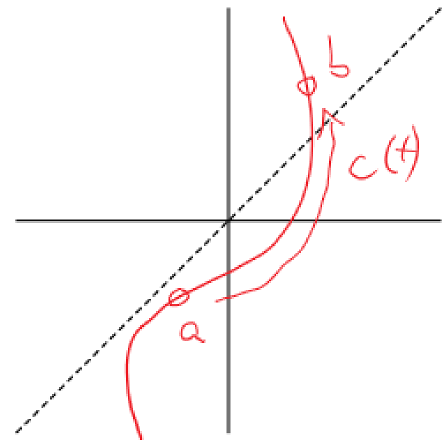
Riemannian manifold

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

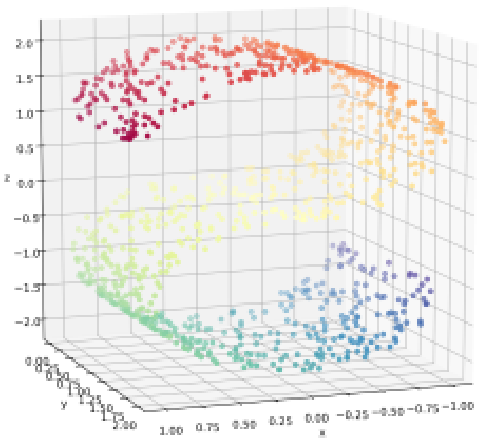


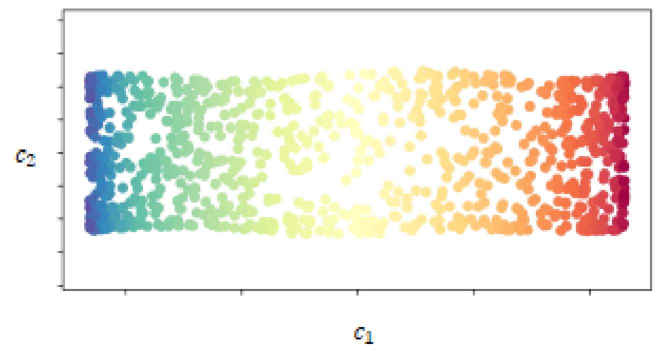


$$L_a^b(c) := \int_a^b \sqrt{g(c'(t), c'(t))}\,\mathrm{d}t = \int_a^b \|c'(t)\|\,\mathrm{d}t.$$

Representation of data

Manifold learning - in general





	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	

	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 Δ 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?

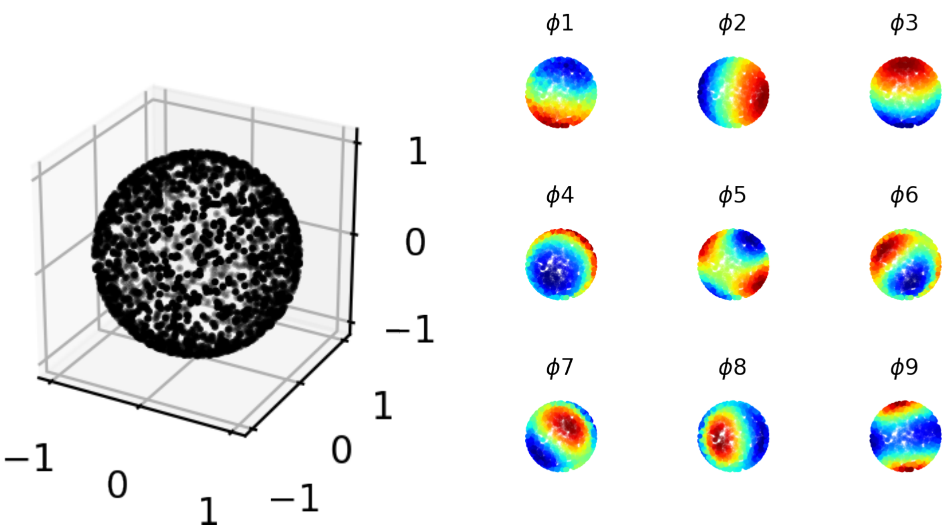


Figure: Spherical data set and eigenfunctions of the Laplace-Beltrami (Diffusion) operator.

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

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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

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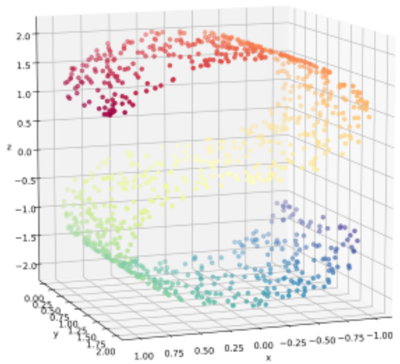
where x is the center point and y is another point in the neighborhood of x.
Algorithm: compute k for all pairs of N points in the data set, with a small value of t. This results in a "kernel matrix" $K \in \mathbb{R}^{N \times N} \approx \exp(t\Delta)$. Then, solve the eigenproblem

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

Representation of data

Manifold learning - S-curve with Diffusion Maps



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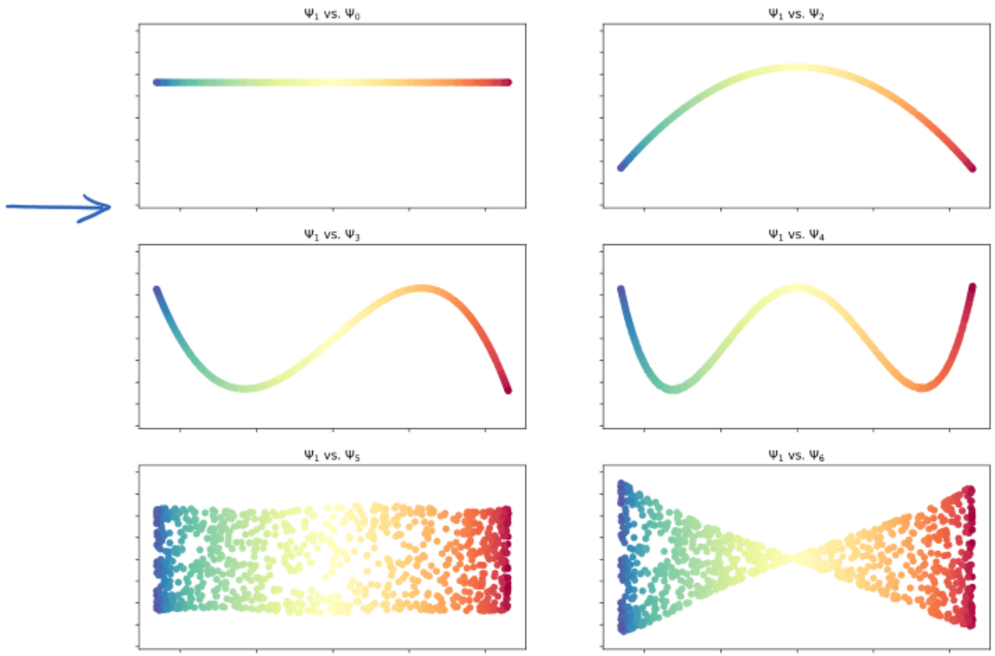


Also see here: https://datafold-dev.gitlab.io/datafold/tutorial_basic_dmap_scurve.html

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]:

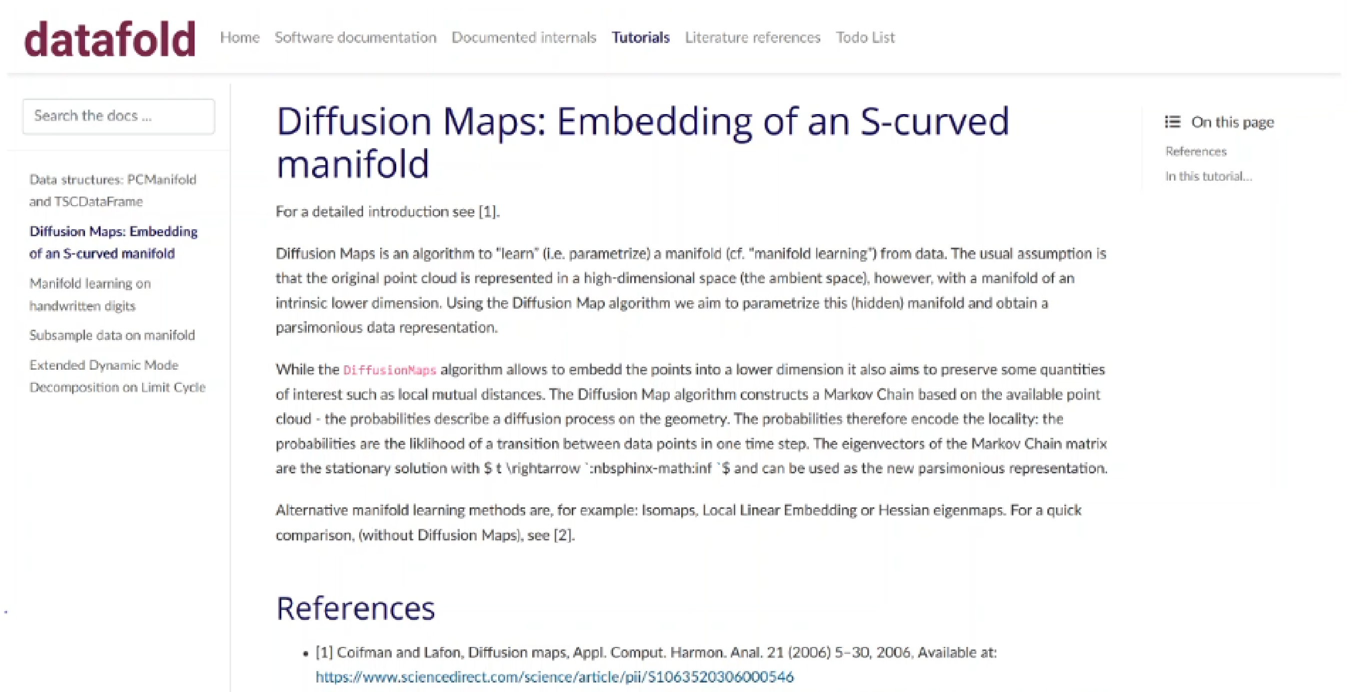
1. Form a distance matrix D with entries
$$D_{ij} = \|y_i - y_j\|,$$
where $i = 1, \ldots, N$ are the rows, $j = 1, \ldots, N$ are the columns, and y_i, y_j are the data points.
2. Set ε to 5% of the diameter of the dataset: $\varepsilon = 0.05(\max_{i,j} D_{i,j})$.
3. Form the kernel matrix W with $W_{ij} = \exp\left(-D_{ij}^2/\varepsilon\right)$.
4. Form the diagonal normalization matrix $P_{ii} = \sum_{j=1}^N W_{ij}$.
5. Normalize to form the kernel matrix $K = P^{-1} W P^{-1}$.
6. Form the diagonal normalization matrix $Q_{ii} = \sum_{j=1}^N K_{ij}$.
7. Form the symmetric matrix $\hat{T} = Q^{-1/2} K Q^{-1/2}$.
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/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Subsample data on manifold
Extended Dynamic Mode Decomposition on Limit Cycle

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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

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

Literature I

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