Lecture 5: Dimensionality Reduction and Data Visualization

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Recap

- The basic concept in machine learning
- Linear regression, nonlinear regression, kernel regression
- Neural networks, deep learning
- Representations of molecules

Outline

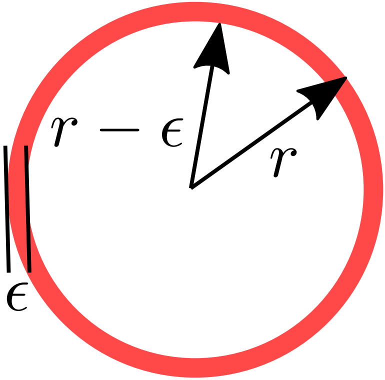
- Curse of the dimensionality
- blessing of non-uniformity
- Prerequisite in Statistics and Mathematics
- Principal component analysis (PCA)
- Non-linear dimensionality reduction methods

Curse of the dimensionality

Volume of a d dimensional sphere of radius r:

$$V(r) = \frac{2\pi^{d/2} r^d}{d\Gamma(d/2)}$$

where $\Gamma()$ is the gamma function.



Question:
What is the fraction of volume contained in the outermost shell of thickness ϵ?

Curse of the dimensionality

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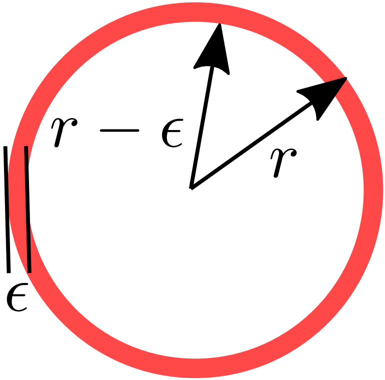

Answer:

$$f_d = \frac{V_d(r) - V_d(r-\epsilon)}{V_d(r)} = 1 - (1 - \frac{\epsilon}{r})^d$$

Curse of the dimensionality

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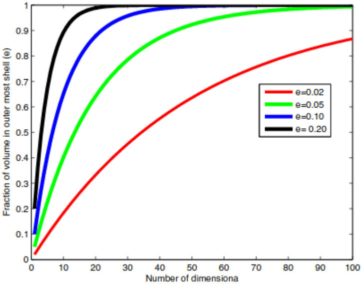
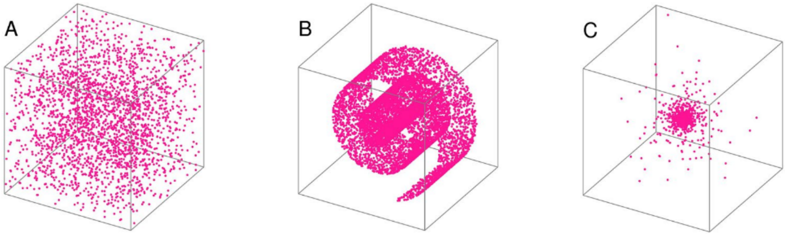


This means that in high dimensional spaces most of the data are on the surface.

Blessing of non-uniformity



Question:
How to reduce the dimensionality of the three data sets here?

Motivation

Why dimensionality reduction?

- Visualization, interpretation
- Cheap to train a model
- Missing data, extrapolation
- Remove redundency in the data set

Prerequisite in Statistics and Mathematics

- Variance σ^2 of 1D data:

$$\sigma^2 = \frac{\sum_i (x_i - \bar{x})^2}{N-1}$$

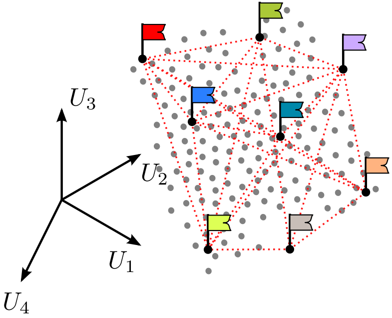
- Covariance

$$C_{jj'} = \frac{\sum_i (X_i^j - \bar{X^j})(X_i^{j'} - \bar{X^{j'}})}{N-1}$$

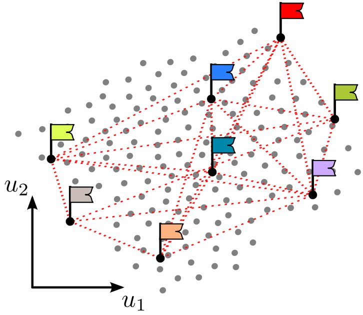
- Eigenvalues and eigenvectors

$$\mathbf{C}\mathbf{v}^j = \lambda^j \mathbf{v}^j$$

Dimension reduction



$\{\mathbf{X}_i\}^D$

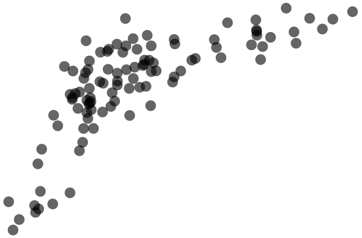


$\{\mathbf{x}_i\}^d$

Question:

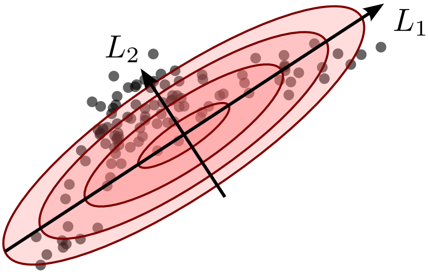
What do you want to preserve?

Principal component analysis



Question:
What is preserved during PCA?

Principal component analysis



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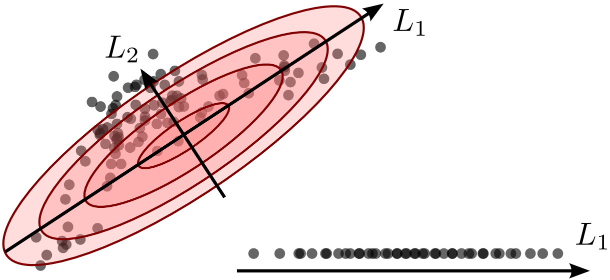

Question:
What is preserved during PCA?

Principal component analysis

PCA identifies the axis that accounts for the largest amount of variance in the data set.

- $\{\mathbf{X}_i\}^D$: data in the D-dimensional space
- $\{\mathbf{x}_i\}^d$: linear projection in the low d dimensional space
- $\mathbf{c}$: normalized projection matrix

$$\mathbf{x}_i = \mathbf{X}_i\mathbf{c}$$

- Covariance of the data: $\mathbf{C} = \mathbf{X}^T\mathbf{X}$
- Covariance of the projected data: $\mathbf{x}^T\mathbf{x}$

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Given d , how to reserve the largest amount of variance?

Principal component analysis

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Keep the first d eigenvectors of the covariance matrix $\mathbf{C} = \mathbf{X}^T\mathbf{X}$

Principal component analysis

- The covariance matrix $\mathbf{C} = \mathbf{X}^T\mathbf{X}$: $D \times D$ form.
- Eigenvalues $\{\lambda^j\}$
- Corresponding eigenvectors $\{\mathbf{v}^j\}$ of the matrix

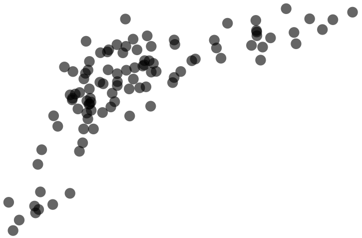
Eigenvalues and eigenvectors fulfills

$$\mathbf{C}\mathbf{v}^j = \lambda^j \mathbf{v}^j$$

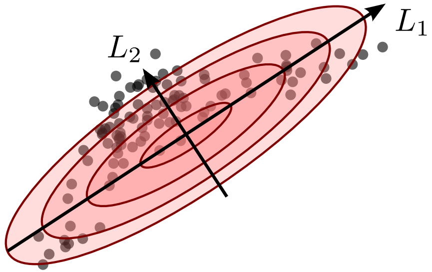
for $j = 1 \dots D$.
One can find the eigenvalues $\{\lambda^j\}$ by solving

$$det(\mathbf{C} - \lambda \mathbf{I}) = 0$$

Principal component analysis



Principal component analysis



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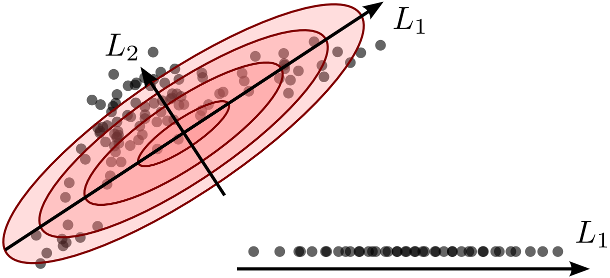

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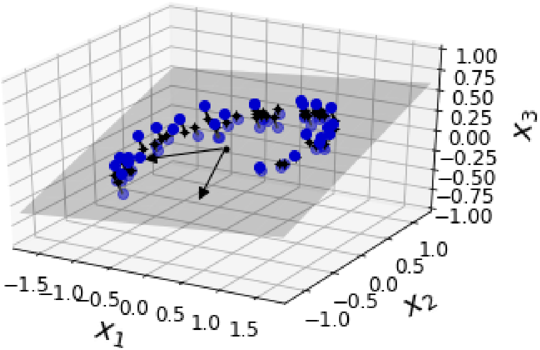

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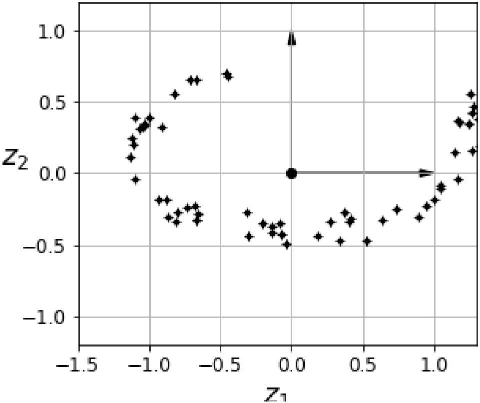
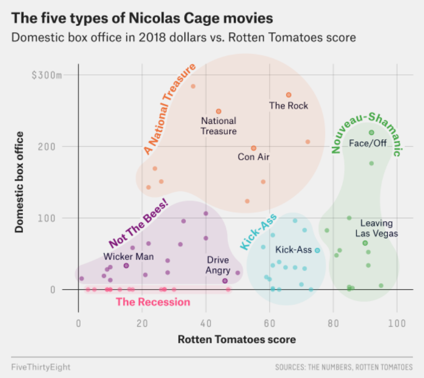


PCA, step by step

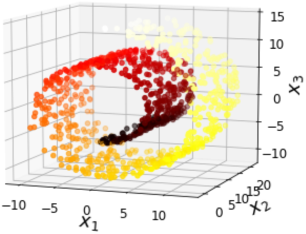
1. Scale and center the data. (How/whether to scale?)
2. Calculate the covariance matrix.
3. Choosing principal components
4. Visualize and validate.



what if we change the units of the axes?

Criticism of PCA

- No universal way of scaling.
- Interesing features of the data may be hiding in "small" dimensions.
- Do not handle complex topology well.



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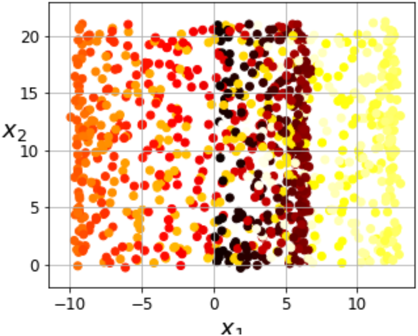
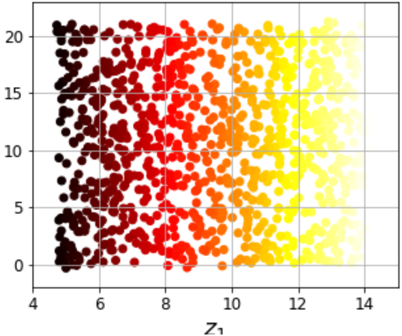


What you get with PCA



What you want

Multidimensional scaling (MDS)

A literal implementation of the general idea of dimensionality reduction

- Define a $N \times N$ matrix $\mathbf{D}$ of pairwise distances between N points
- Find a low d projection $\{\mathbf{x}_i\}$ that maximally preserves $\mathbf{D}$

$$\|\mathbf{x}_i - \mathbf{x}_j\| \approx D_{ij}.$$

which means to minimize the "stress" (distortion)

$$\text{Stress} \sim \left\| \mathbf{D} - \|\mathbf{x}_i - \mathbf{x}_j\| \right\|^2.$$

- Usually the optimization is done iteratively.

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If $\mathbf{D}$ is the Euclidean norm, classical MDS (use eigenvalues) is the best linear projection preserving the squared distances. It corresponds to PCA, but it is more easily generalized to different dissimilarities.

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What are the other ways of defining $\mathbf{D}$?

Transforming the feature Space

- Design matrix $\mathbf{X}$:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_N \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(d)} \\ x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(d)} \\ \vdots & \vdots & \vdots & \vdots \\ x_N^{(1)} & x_N^{(2)} & \dots & x_N^{(d)} \end{bmatrix}$$

- Take a feature vector and apply non-linear transformation ϕ:

$$\phi : \mathcal{R}^d \rightarrow \mathcal{R}^k$$

- Polynomial basis:

$$\phi(x) = \begin{bmatrix} 1 & x^1 & x^2 & x^3 & x^4 \end{bmatrix}$$

- Others: splines, radial basis functions, ...
- Take the distance $\mathbf{D}$ in the feature space.

Kernel to distance

- Derivation of the kernel trick in the lecture notes.
- $\mathbf{K}$ is the kernel matrix. k_{ij} is the similarities between each pair of data i and j.
- Obtain the distance matrix $\mathbf{D}$ from the kernel matrix $\mathbf{K}$, e.g.

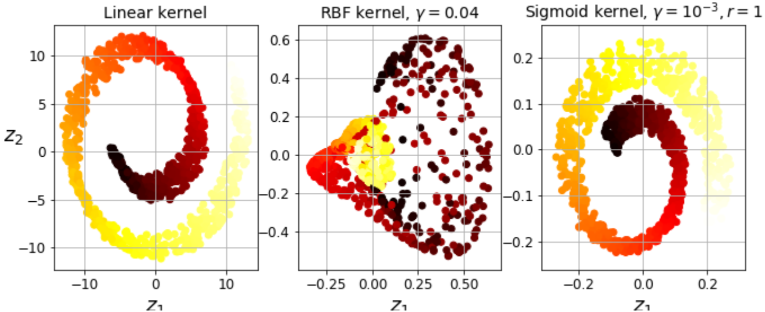
$$d_{ij} = 1 - \frac{k_{ij}}{\sqrt{k_{ii}k_{jj}}}$$

- Cauchy–Schwarz inequality needs to hold for $\mathbf{D}$:

$$d_{ij} + d_{jk} \geq d_{ik}$$

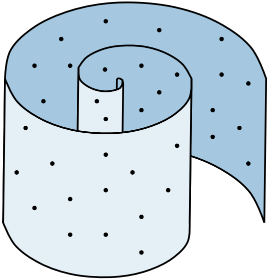
Kernel PCA

- PCA on the kernel matrix



Isometric Mapping (ISOMAP)

- Approximate pairwise geodesic distances.
- A geodesic is the shortest path in manifold between two points x and y. (Approximate geodesics by hopping between neighbours, sensitive to noise).
- Given these pairwise geodesic distances, use MDS to find a d-dimensional embedding that preserves geodesic distances.



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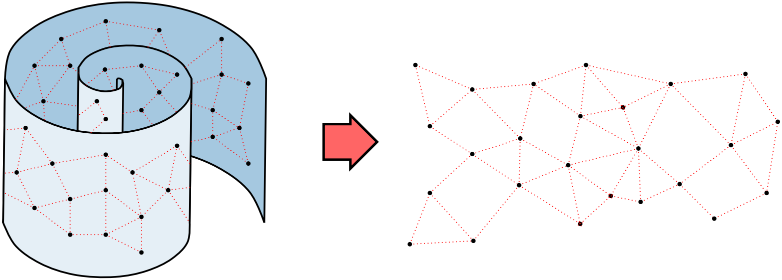

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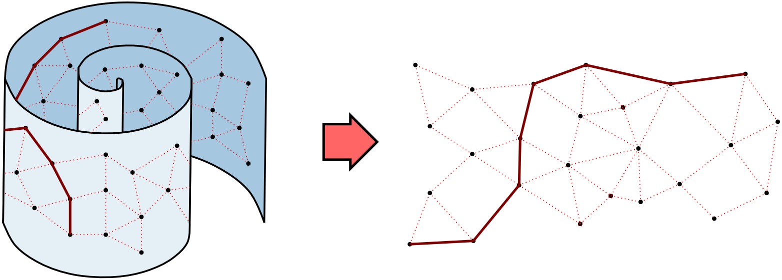

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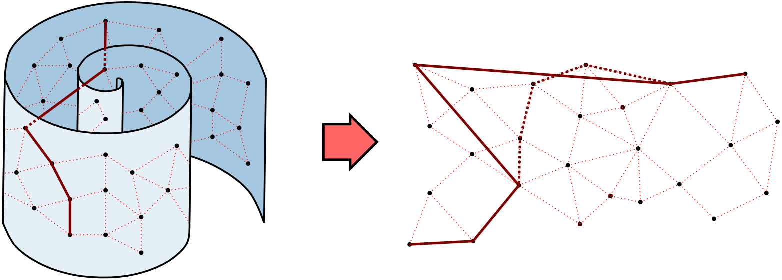
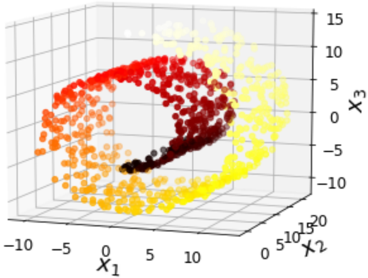


Isometric Mapping (ISOMAP)

Unroll the Swiss roll, with different noise level.



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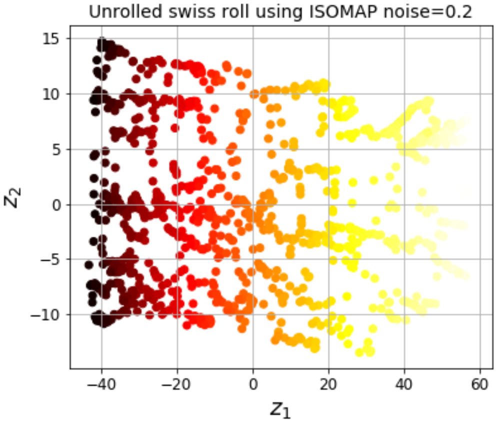

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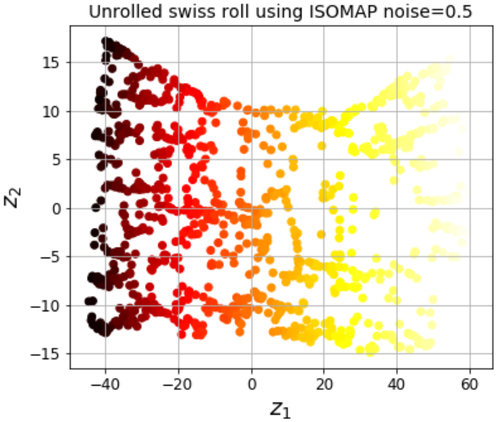

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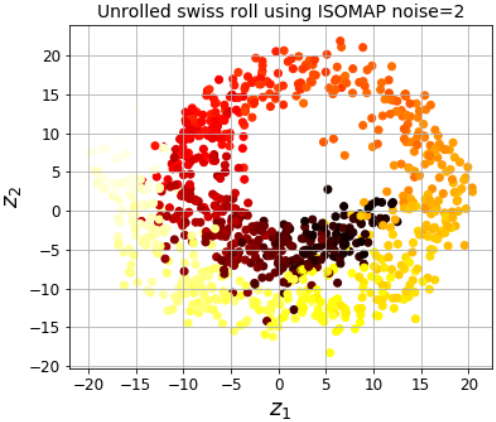
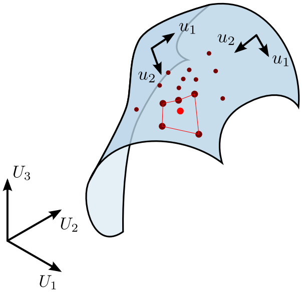


Locally Linear Embedding (LLE)

If the manifold is locally flat each point can be expressed as a combination of its neighbors.

- Find (k-nearest) neighbors for each data point.
- Compute a weight vector $\mathbf{w}_i$ that best reconstructs each $\mathbf{x}_i$ by a linear combination of its k-NN.
- Compute the embedding in $\mathcal{R}^d$ that minimizes reconstruction error using $\mathbf{w}_i$ and its corresponding k-NN.



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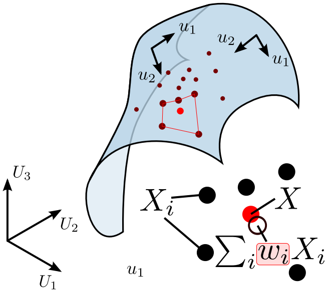

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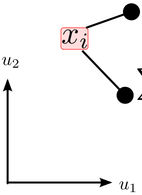
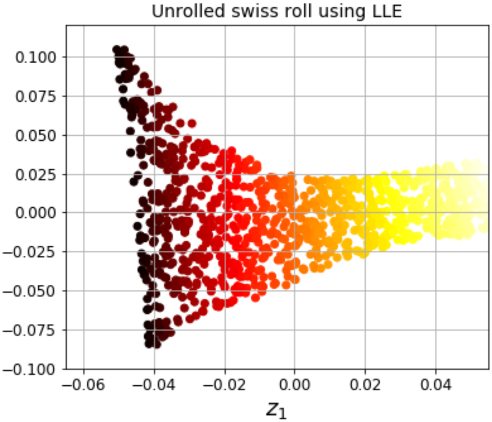
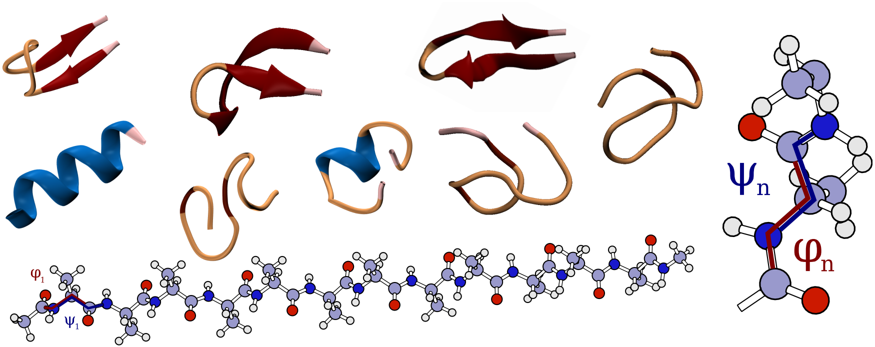


Unroll the Swiss roll, with noise level = 0.2.



Other dimensionality reduction schemes

Dimensionality reduction for chemical data



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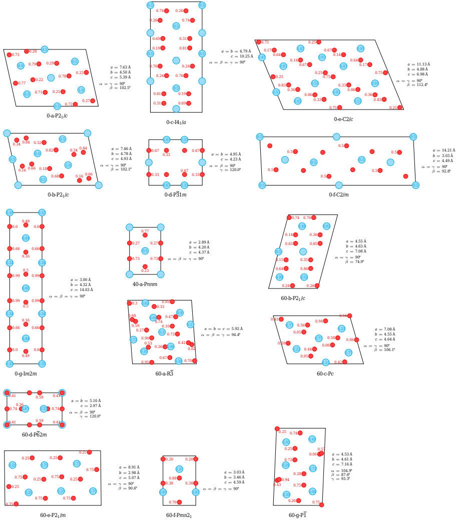

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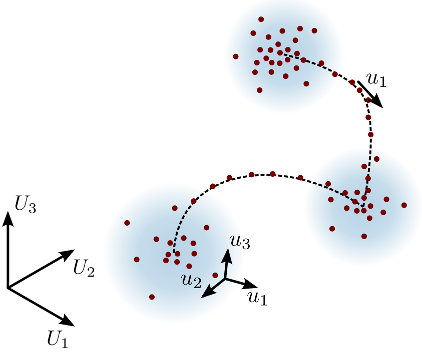

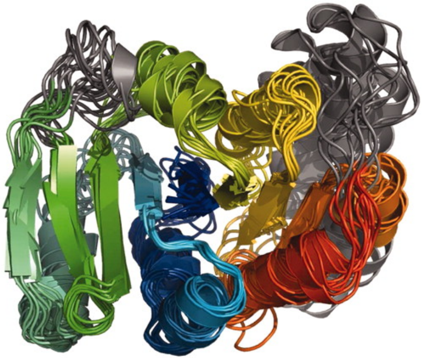

Outline of next lecture

- Representing structual data
- More tricks of the trade
    - Sparsification
    - Clustering

Questions?

Thank you for your attention!