Introduction to Machine Learning

Lecture 7 Representation and Clustering - Nonlinear Dimensionality Reduction

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Outline

Review

- **Curse of dimensionality**
- **Principal component analysis:** principle, implementation, and statistical ML viewpoint
- **Other linear dimensionality reduction method:** RPCA, NMF, Subspace clustering, compressive sensing

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- **Curse of dimensionality**
- **Principal component analysis:** principle, implementation, and statistical ML viewpoint
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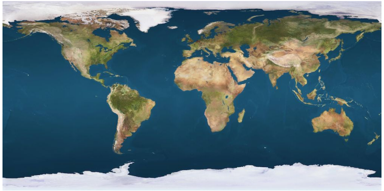
Today

- Manifold learning (MDS, ISOMAP, LLE, Diffusion Map, ...)
- Large-scale manifold learning (t-SNE)
- Kernel method (Kernel PCA)
- Autoencoders

Linear and Nonlinear Dimensionality Reduction

3D data

Linear map to 2D space



Nonlinear map to 2D space.

Recall The Desired Properties of Dimensionality Reduction

- **Minimizing reconstruction error**

$$\exists g : \mathcal{Z} \mapsto \mathcal{X},\ \boldsymbol{x} \approx g(f(\boldsymbol{x})). \tag{1}$$

- (Equivalently,) **Maximizing mutual information** (or minimizing information loss)

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- (Equivalently,) **Maximizing mutual information** (or minimizing information loss)
- **(Nearly) Isometry:**

$$d_{\mathcal{Z}}(f(\boldsymbol{x}), f(\boldsymbol{x}')) \approx d_{\mathcal{X}}(\boldsymbol{x}, \boldsymbol{x}'). \tag{2}$$

The Properties of Various Linear DR Methods

Method	(R)PCA	NMF	Compressive Sensing

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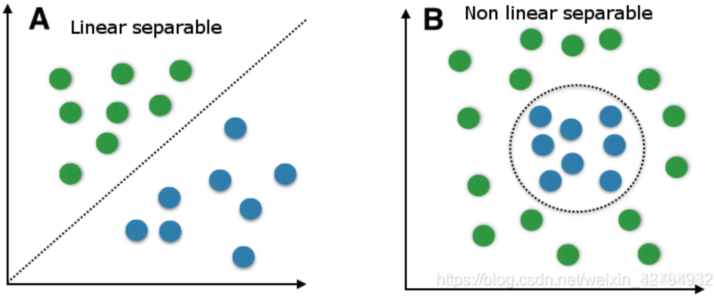
- The conditions of compressive sensing is based on the “sparse representation” assumption of data and the restricted isometric property (RIP) of random projection.

A Typical Case Breaking Isometry Seriously

Linear inseparable data



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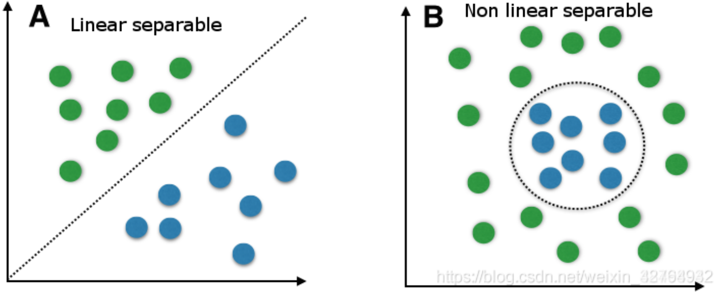

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- **Q: Can we obtain better isometry? If yes, how to do it?**

Typical Nonlinear Dimensionality Reduction Methods

(Classic) Manifold Learning (1995 - 2010)

- Multi-dimensional Scaling (MDS)
- ISOMAP
- Locally Linear Embedding (LLE)
- Eigenmap (Next lecture)
- Local Tangent Space Alignment (LTSA)

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Autoencoding (also can be viewed as manifold learning)

- Various autoencoders

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Principle:

- Given a set of data $\{\boldsymbol{x}_n\}_{n=1}^N$, we can compute a distance matrix:

$$\boldsymbol{D} = [d_{ij}] \in \mathbb{R}^{N\times N}, \quad d_{ij} = d(\boldsymbol{x}_i, \boldsymbol{x}_j). \tag{3}$$

  where $d(\cdot,\cdot)$ can be any valid metric of the sample space.

- Metric MDS aims at finding low-dimensional latent representations $\{\boldsymbol{z}_n\}_{n=1}^N$ via

$$\min_{\{\boldsymbol{z}_n\}_{n=1}^N \in \Omega} \underbrace{\left(\sum_{i\neq j} (d_{ij} - \|\boldsymbol{z}_i - \boldsymbol{z}_j\|_p)^2\right)^{1/2}}_{\mathrm{Stress}_d(\{\boldsymbol{z}_n\}_{n=1}^N)}, \tag{4}$$

  where $p = 1$ or 2 in general.

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$$\min \mathrm{Strain}_d(\{\boldsymbol{z}_n\}_{n=1}^N) = \left(\frac{\sum_{i,j=1}^N (k_{ij} - \boldsymbol{z}_i^T \boldsymbol{z}_j)^2}{\sum_{i,j=1}^N k_{ij}^2} \right)^{1/2},$$

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where

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Could you connect it with PCA or Least-Square Data Denoising?

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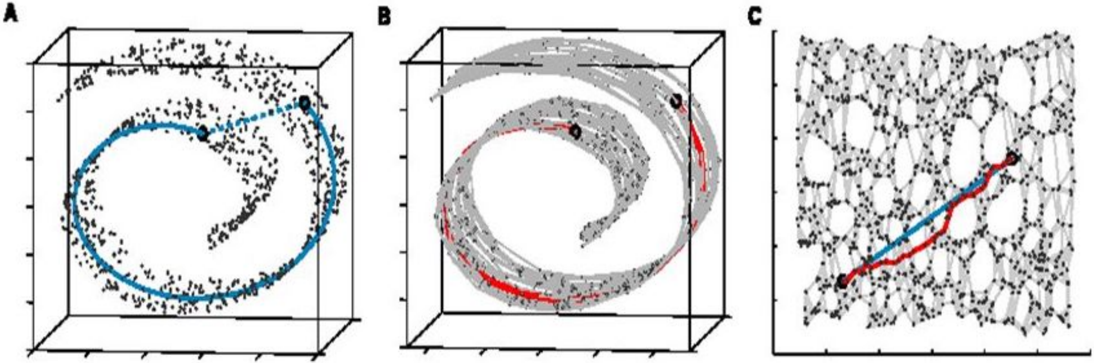
3. Compute low-dimensional embedding by MDS:

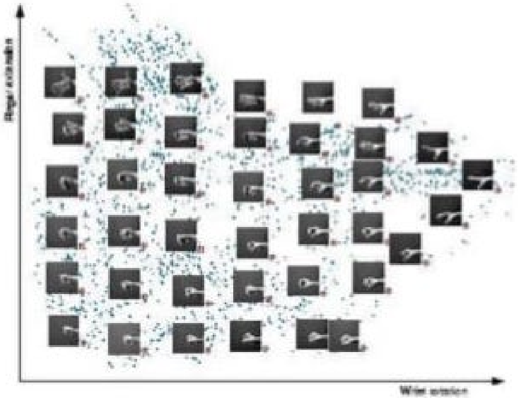
$$\boldsymbol{K} = -\frac{1}{2}\boldsymbol{C}(\boldsymbol{D} \odot \boldsymbol{D})\boldsymbol{C} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T \quad \Rightarrow \quad \boldsymbol{Z} = \boldsymbol{U}_L\boldsymbol{\Lambda}_L^{\frac{1}{2}} \tag{8}$$

ISOMAP v.s. Metric MDS



ISOMAP

Face varying in pose and illumination



Hand varying in finger extension & wrist rotation

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- **Local linear self-representation:** Given a sample $\boldsymbol{x}$ and its K neighbors $\boldsymbol{X} = [\boldsymbol{x}_1, ..., \boldsymbol{x}_K]$, where $d(\boldsymbol{x}, \boldsymbol{x}_k) \leq \tau$ for $k = 1, ..., K$.

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- **LLE (Locally Linear Embedding):** Given $\boldsymbol{X} = [\boldsymbol{x}_1, ..., \boldsymbol{x}_N]$, find low-dimensional representations $\boldsymbol{Z} = [\boldsymbol{z}_1, ..., \boldsymbol{z}_N]$ that inherit the local linear self-representation relations.

Locally Linear Embedding (LLE)

Solution:

1. Compute the linear coefficients

$$\min_{\boldsymbol{W}} \sum_{i=1}^{N} \|\boldsymbol{x}_i - \boldsymbol{X}_i \boldsymbol{w}_i\|_2^2, \;\; s.t. \; \sum_{k=1}^{K} w_{ik_i} = 1, \text{ and } \{k_i\}_{k=1}^{K} = \text{neighbors' index} \quad (10)$$

where $\boldsymbol{W} = [w_{ij}] \in \mathbb{R}^{N \times N}$, and $\forall \boldsymbol{i} \in \{1, ..., N\}$

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$$\min_{\boldsymbol{Z}} \sum_{i=1}^{N} \|\boldsymbol{z}_i - \boldsymbol{Z}_i \boldsymbol{w}_i\|_2^2 = \min_{\boldsymbol{Z}} \operatorname{tr}(\boldsymbol{Z\Phi Z}^T), \quad s.t. \; \boldsymbol{ZZ}^T = \boldsymbol{I}_L, \boldsymbol{Z}\boldsymbol{1}_L = \boldsymbol{0}. \tag{12}$$

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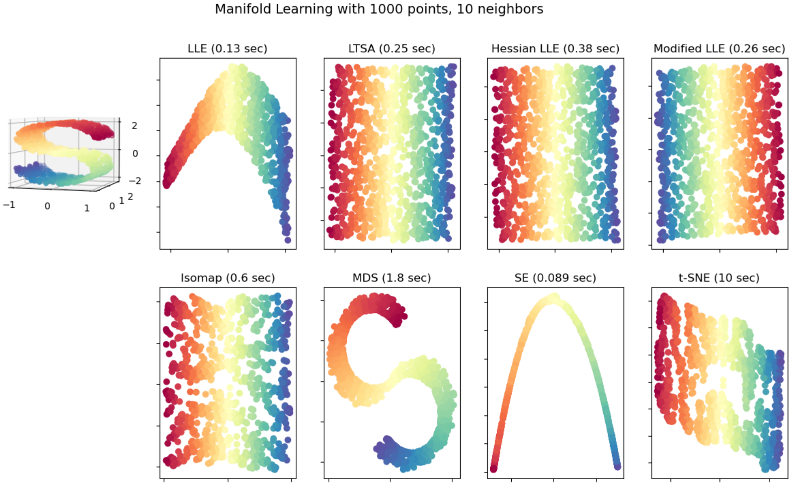
3. $\boldsymbol{\Phi} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$, $\lambda_1 \geq ... \geq \lambda_N$, and $\boldsymbol{Z} = \boldsymbol{U}_{N-L+1:N}$.

Classic Manifold Learning Methods



Most of them require construct a KNN graph first.

Nonlinear DR Methods: Kernel PCA

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(Linear) PCA:

- Consider the covariance matrix of zero-mean samples: $\boldsymbol{C} = \boldsymbol{X}^T\boldsymbol{X} \in \mathbb{R}^{D\times D}$.
- Apply Eigenvalue Decomposition $\boldsymbol{C} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$
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SVD-based Implementation:

- Apply SVD $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$.
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- The Gram matrix of linear kernel $\boldsymbol{K} = \boldsymbol{X}\boldsymbol{X}^T \in \mathbb{R}^{N\times N}$.

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Replacing the linear kernel to arbitrary kernel, you obtain the Kernel PCA:)

- $K(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{x}^T\boldsymbol{y}+1)^2$, $\exp(-\|\boldsymbol{x}-\boldsymbol{y}\|^2/h)$, ...

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- Because we are never working directly in the (implicit) feature space.
- The kernel PCA does not compute the principal components directly, but the projections of data onto the top-L components.

Kernel PCA

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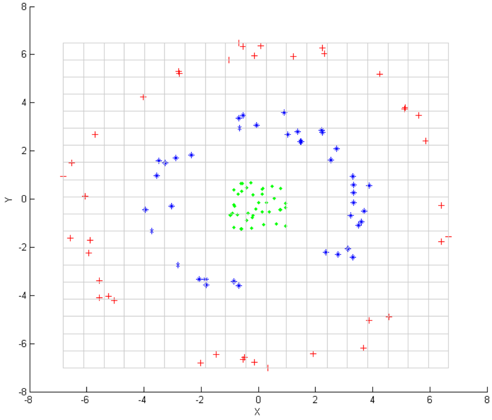
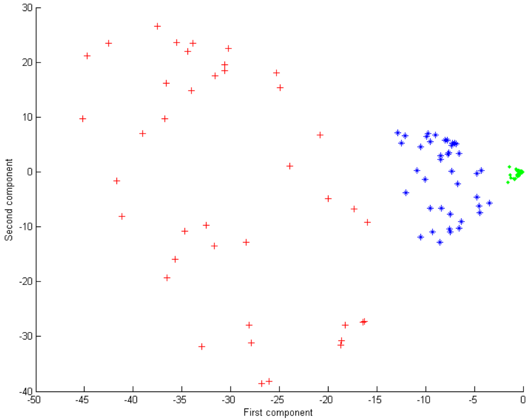
- Kernel PCA = Linear PCA in the feature space associated with the kernel.

Kernel PCA



8
6
4
2
0
-2
-4
-6
-8
Y
-8
-6
-4
-2
0
2
4
6
8
X



30
20
10
0
-10
-20
-30
-40
Second component
-50
-45
-40
-35
-30
-25
-20
-15
-10
-5
0
First component

Revisit MDS and ISOMAP as Kernel PCA Methods

- MDS (Linear Kernel):

$$\boldsymbol{K} = -\frac{1}{2}\boldsymbol{C}(\boldsymbol{D} \odot \boldsymbol{D})\boldsymbol{C} = \boldsymbol{C}\boldsymbol{X}\boldsymbol{X}^T\boldsymbol{C} = \tilde{\boldsymbol{X}}\tilde{\boldsymbol{X}}^T$$

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- ISOMAP (A positive semi-definite kernel based on doubly centered geodesic distance, a.k.a., Mercer kernel):

$$\boldsymbol{K} = -\frac{1}{2}\boldsymbol{C}(\boldsymbol{D}_{geo} \odot \boldsymbol{D}_{geo})\boldsymbol{C} \tag{15}$$

t-Stochastic Neighborhood Embedding

Motivation:

- Large-scale dimensionality reduction.
- Visualization and clustering of high-dimensional data.

Principle:

- Given $\{\boldsymbol{x}_n\}_{n=1}^N$, define a probability p_{ij} that is proportional to the similarity between $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$:

$$p_{ij} = \frac{p_{j|i} + p_{i|j}}{2N} \quad \text{and} \quad p_{ii} = 0 \tag{16}$$

$$p_{j|i} = \frac{\exp(-\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2 / (2\sigma_i^2))}{\sum_{k \neq i} \exp(-\|\boldsymbol{x}_i - \boldsymbol{x}_k\|^2 / (2\sigma_i^2))}. \tag{17}$$

Nonlinear DR Methods: t-Stochastic Neighborhood Embedding

- t-SNE aims to learn $\{\boldsymbol{z}_n \in \mathbb{R}^K\}_{n=1}^N$ ($K = 2, 3$ typically) by
  1. Define a similarity q_{ij} between $\boldsymbol{z}_i$ and $\boldsymbol{z}_j$ as

$$q_{ij} = \frac{(1 + \|\boldsymbol{z}_i - \boldsymbol{z}_j\|^2)^{-1}}{\sum_k \sum_{k \neq l} (1 + \|\boldsymbol{z}_k - \boldsymbol{z}_l\|^2)^{-1}} \quad \text{and} \quad q_{ii} = 0 \tag{18}$$

where $\{q_{ij}\}$ yield a t-distribution.

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  2. Learn the $\boldsymbol{z}$'s via

  $$\min_{\boldsymbol{Z}} \mathrm{KL}(P \| Q) := \sum_{i \neq j} p_{ij} \log \frac{p_{ij}}{q_{ij}}. \tag{19}$$

     SGD is applied to solve this problem.

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Rationality:

- Similar $\boldsymbol{x}$'s are modeled by nearby $\boldsymbol{z}$'s and dissimilar $\boldsymbol{x}$'s are modeled by distant $\boldsymbol{z}$'s with high probability.
- Under special settings, approximate a simple form of spectral clustering.

Nonlinear DR Methods: Autoencoders

Drawbacks of the above methods:

- From inductive paradigm to transductive paradigm
- High complexity and inscalable inference
- No reconstruction power

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- High complexity and inscalable inference
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Motivation:

- Achieve (nearly) isometry and reconstruction power jointly.
- Achieve inductive inference
- Reduce complexity of other nonlinear method

Nonlinear DR Methods: Autoencoders

Principle:

- Revisit PCA from a viewpoint of autoencoding.

$$\boldsymbol{X}^* = \arg\,\min_X \|\boldsymbol{X}_{noisy} - \boldsymbol{X}\|_F^2, \quad s.t.\ \mathrm{rank}(\boldsymbol{X}) \le L$$

Nonlinear DR Methods: Autoencoders

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&= \boldsymbol{U}_L \boldsymbol{\Sigma}_L \boldsymbol{V}_L^T \\
&\Rightarrow \text{Encoder: } \boldsymbol{X}_{noisy} \boldsymbol{V}_L = \boldsymbol{U}_L \boldsymbol{\Sigma}_L \\
&\quad\ \ \text{Decoder: } \boldsymbol{X}^* = \boldsymbol{X}_{noisy} \boldsymbol{V}_L \boldsymbol{V}_L^T
\end{aligned} \tag{20}
$$

- $\boldsymbol{V}_K$ and $\boldsymbol{V}_K^T$ work as the encoder and the decoder, respectively.

Nonlinear DR Methods: Autoencoders

- In general, a typical autocoder consists of

$$\text{Encoder: } f : \mathcal{X} \mapsto \mathcal{Z}, \quad \text{Decoder: } g : \mathcal{Z} \mapsto \mathcal{X}$$

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- In general, a typical autocoder consists of

$$\text{Encoder: } f: \mathcal{X} \mapsto \mathcal{Z}, \quad \text{Decoder: } g: \mathcal{Z} \mapsto \mathcal{X} \tag{21}$$

- Given a set of data $\{\boldsymbol{x}_n\}_{n=1}^N$,

$$\min_{f,g} \underbrace{\sum_{n=1}^{N} \text{loss}(\boldsymbol{x}_n, g(f(\boldsymbol{x}_n)))}_{\text{loss}(\boldsymbol{X}, g(f(\boldsymbol{X})))} + \text{reg}(q_{\boldsymbol{Z}|\boldsymbol{X}}, p_{\boldsymbol{Z}}) \tag{22}$$

  where $p_{\boldsymbol{Z}}$ is a predefined prior distribution of latent codes, while $q_{\boldsymbol{Z}|\boldsymbol{X}}$ is the posterior distribution of the latent codes given the corresponding data, which is determined by the encoder f.

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- More details will be given in the following lectures.

In Summary

- Introduce classic manifold learning methods
- Introduce the most widely-used manifold learning method, t-SNE
- Introduce the kernelization of PCA.
- Introduce autoencoders (briefly)

Next...

- Data representation, clustering, and unsupervised learning
- Kmeans and spectral clustering
- Evaluation of clustering method.