Introduction to Machine Learning

Lecture 6 Representation and Clustering - (Linear) Dimensionality Reduction

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Outline

Review

- **Non-linear regression:** parametric or nonparametric
- **Kernel** regression, RKHS, and representer theorem
- **Gaussian process:** Definition and basic formulation

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Today

- Curse of dimensionality
- Principal component analysis (PCA)
- Linear projection and factorization model

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- Pros and Cons?
  - Nonlinear mechansims, powerful models
  - Risk of over-fitting
  - Sensitivity to noise
  - High computational complexity

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- **Phenomenon:** When the dimensionality increases, the volume of the space increases so fast that the available data become sparse.
- Typically, the amount of required data often grows exponentially with the dimensionality.

Curse of Dimensionality: Examples

Combinatorial explosion (discrete examples)

- The number of different d-dimensional binary vectors is 2^d.
- Each additional dimension doubles the effort needed to try all combinations, e.g., the increase of search space of Chess/Go

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- For a d-dimensional unit hypercube with a lattice that has a spacing of 10^{-1} between adjacency points would require 10^d sample points.
- Sampling N samples randomly from a d-dimensional sample space, based on a distribution with identity covariance matrix:

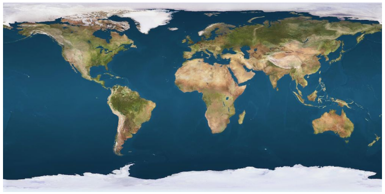
$$\lim_{d \to \infty} \mathbb{E}\left[\frac{D_{\max}(d) - D_{\min}(d)}{D_{\min}(d)}\right] \to 0. \tag{1}$$

Distance functions are losing their usefulness in high dimensions.

How to Suppress This Issue? Dimensionality Reduction

3D data

Linear map to 2D space


Nonlinear map to 2D space.

Linear Dimensionality Reduction

- Original high-dimensional sample space, i.e., $\boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^D$.
- We would like to find a linear projection $f : \mathcal{X} \mapsto \mathcal{Z} \subset \mathbb{R}^L$, where $L \ll D$.
- Generally, $\boldsymbol{z} = f(\boldsymbol{x}) = \boldsymbol{U}^T \boldsymbol{x}$, where $\boldsymbol{U} \in \mathbb{R}^{D \times L}$.

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- **(Nearly) Isometry:**

$$d_{\mathcal{Z}}(f(\boldsymbol{x}), f(\boldsymbol{x}')) \approx d_{\mathcal{X}}(\boldsymbol{x}, \boldsymbol{x}'). \tag{3}$$

Dimensionality Reduction by The Methods We Learned

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Lasso-based Supervised Feature Selection

- Solve the following problem:

$$\min_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 + \lambda\|\boldsymbol{w}\|_1. \tag{4}$$

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How to deal with the case without supervised signal $\boldsymbol{y}$?

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- **Principals components of a collection of data points:**
  - L orthonormal vectors (an orthonormal basis) in the sample space $\mathcal{X} \subset \mathbb{R}^D$

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- **Principle of PCA:** Use some significant principal components to project data into a new coordinate system (equivalently, a represent the projected data via the orthonormal basis of the new space).

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Motivation:

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2. For $\ell = 1, ..., L$:
   - 2.1 Find the ℓ-th principal component:

$$\boldsymbol{v}_\ell = \arg\max_v \|\boldsymbol{R}^{(\ell-1)}\boldsymbol{v}\|_2^2, \qquad s.t. \|\boldsymbol{v}\|_2 = 1, \quad \boldsymbol{v}_i^T\boldsymbol{v} = 0, \forall \boldsymbol{i} = 1, ..., \ell - 1. \tag{7}$$

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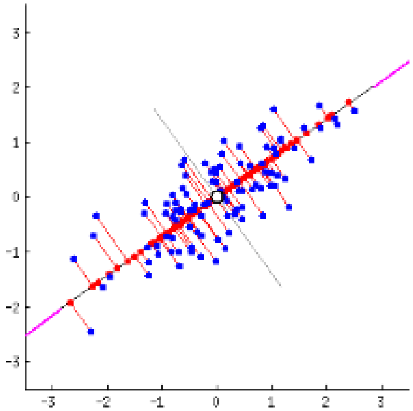
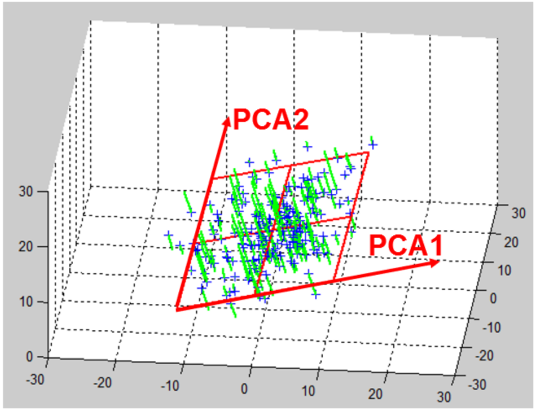
Illustration of PCA





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- $\boldsymbol{U}_L\boldsymbol{\Sigma}_L = \boldsymbol{X}\boldsymbol{V}_L \in \mathbb{R}^{N\times L}$: The new representation of the data (The projections obtained by PCs).

Revisit Data Whitening through PCA

Data Whitening of Data Matrix $\boldsymbol{X} \in \mathbb{R}^{N \times D}$

- Estimate expectation $\hat{\mu}_d = \frac{1}{N} \sum_{n=1}^{N} x_{nd}$ for $d = 1, \ldots, D$.
- Estimate covariance matrix

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- **Consider all PCs:** Data Whitening $\simeq$ Shifting + PCA + Scaling

$$(N-1) \tilde{\boldsymbol{X}} \widehat{\boldsymbol{\Gamma}}^{-\frac{1}{2}} = \tilde{\boldsymbol{X}} \boldsymbol{V} \boldsymbol{\Lambda}^{-\frac{1}{2}} \boldsymbol{V}^T = (\tilde{\boldsymbol{X}} \boldsymbol{V} \boldsymbol{\Lambda}^{-\frac{1}{2}}) \boldsymbol{V}^T \simeq \tilde{\boldsymbol{X}} \boldsymbol{V} \boldsymbol{\Lambda}^{-\frac{1}{2}} \tag{13}$$

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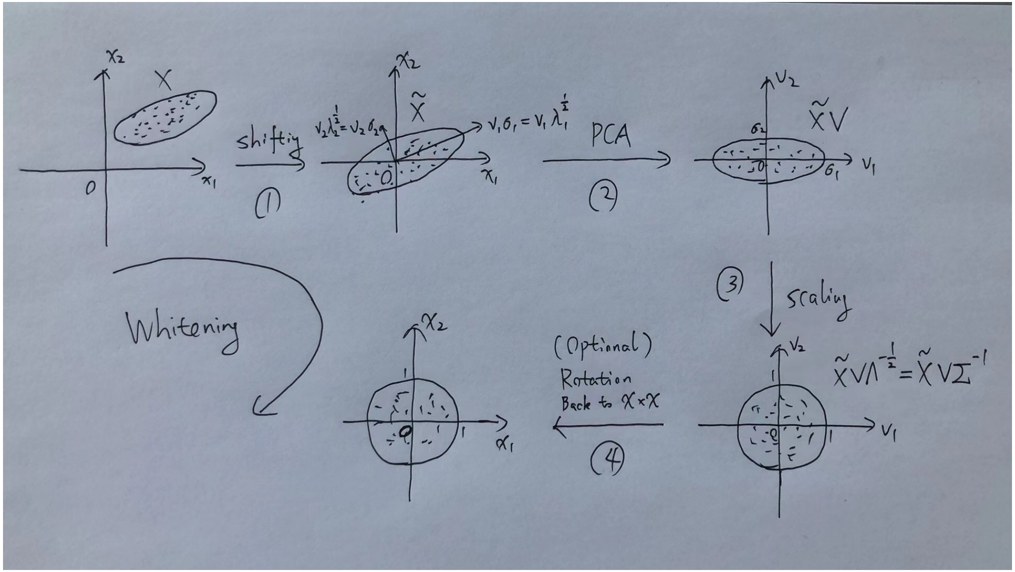

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- An i.i.d. Gaussian noise model for observed data $\boldsymbol{X}$

$$\boldsymbol{X}_{noisy} = \boldsymbol{X}_{clean} + \boldsymbol{E}, \quad \forall \epsilon_{nd} \in \boldsymbol{E} \sim \mathcal{N}(0, \sigma^2)$$

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- When the feasible domain corresponds to a low-rank constraint

$$\Omega := \{\boldsymbol{X} \in \mathbb{R}^{N \times D} \mid \text{rank}(\boldsymbol{X}) \leq L\}. \tag{16}$$

We have

$$\widehat{\boldsymbol{X}} = \arg\min_{\boldsymbol{X} \in \Omega} \|\boldsymbol{X}_{noisy} - \boldsymbol{X}\|_F^2 = \boldsymbol{U}_L \boldsymbol{\Sigma}_L \boldsymbol{V}_L^T, \quad \text{where } \boldsymbol{X}_{noisy} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T. \tag{17}$$

(It is natural – recall the sequential minimization of residual.)

Extend PCA to More Generalized Data Denoising Model

Robust PCA: Consider sparse noise

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Solving these problems requires iterative low-rank factorization/SVD and factor updating.

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Subspace Clustering:

- Recall the supervised feature selection:

$$\min_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 + \gamma\|\boldsymbol{w}\|_1 .$$

Extend PCA to More Generalized Data Denoising Model

Subspace Clustering:

- Recall the supervised feature selection:

$$\min_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 + \gamma\|\boldsymbol{w}\|_1. \tag{20}$$

- When the supervised signal $\boldsymbol{y}$ is the data itself:

$$\min_{\boldsymbol{W}\in\mathbb{R}^{D\times D}} \|\boldsymbol{X} - \boldsymbol{X}\boldsymbol{W}\|_F^2 + \gamma_1\|\boldsymbol{W}\|_1 + \gamma_2\|\boldsymbol{W}\|_*.$$

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Dictionary Learning:

$$\boldsymbol{\Psi}, \boldsymbol{A} = \arg\min_{\boldsymbol{\Psi},\boldsymbol{A}} \|\boldsymbol{X} - \boldsymbol{\Psi}\boldsymbol{A}\|_F^2 + \gamma\|\boldsymbol{A}\|_1 \tag{22}$$

Do We Have To Learn The Projection? — Compressive Sensing

For $\boldsymbol{x} \in \mathbb{R}^N$, if the following condition holds:

$$\exists \boldsymbol{\Psi}, \quad \boldsymbol{x} \approx \boldsymbol{\Psi}\boldsymbol{\alpha} \quad \text{and} \quad \|\boldsymbol{\alpha}\|_0 \leq S. \tag{23}$$

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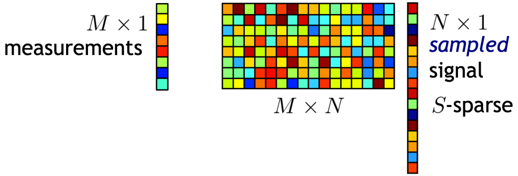
- $\boldsymbol{y} = \boldsymbol{\Phi}\boldsymbol{x}$.
- $\boldsymbol{\Phi}$ is a **random** matrix.



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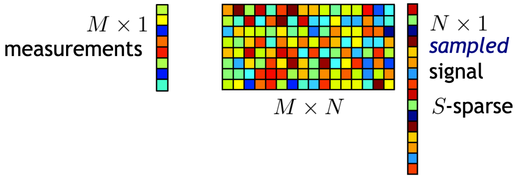
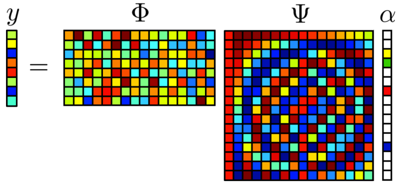


Recovery guarantee of $\boldsymbol{x}$:

1. $\hat{\alpha} = \arg\min \|\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\Psi}\boldsymbol{\alpha}\|_2^2 + \gamma\|\boldsymbol{\alpha}\|_1$.



2. $\tilde{\boldsymbol{x}} = \boldsymbol{\Psi}\hat{\alpha}$.

Compressive Sensing: Main Theorem

When $\mathbf{\Phi}$ satisfies the **Restricted Isometry Property (RIP)**,

$$\forall \boldsymbol{x}_1, \boldsymbol{x}_2 \in \{\boldsymbol{x} \in \mathbb{R}^N \mid \|\boldsymbol{x}\|_0 \leq S\}, \quad \exists \delta < 1 \quad , 1 - \delta \leq \frac{\|\mathbf{\Phi}\boldsymbol{x}_1 - \mathbf{\Phi}\boldsymbol{x}_2\|_2^2}{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|_2^2} \leq 1 + \delta \tag{24}$$

We have

- $M \geq \frac{1}{C} S \log \frac{N}{S}$ leads to an exact reconstruction with a probability $1 - \mathcal{O}(N^{-M})$.
- Solving $\min_{\boldsymbol{y}=\mathbf{\Phi}\boldsymbol{\alpha}} \|\boldsymbol{\alpha}\|_1$ is equivalent to $\min_{\boldsymbol{y}=\mathbf{\Phi}\boldsymbol{\alpha}} \|\boldsymbol{\alpha}\|_0$.

Compressive Sensing: Restricted Isometry Property (RIP)

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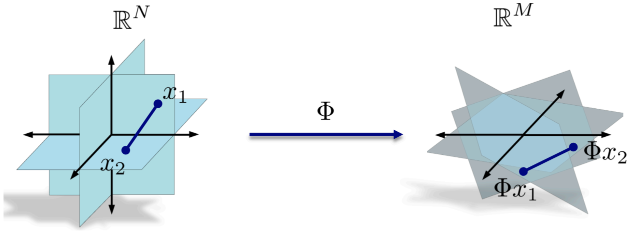

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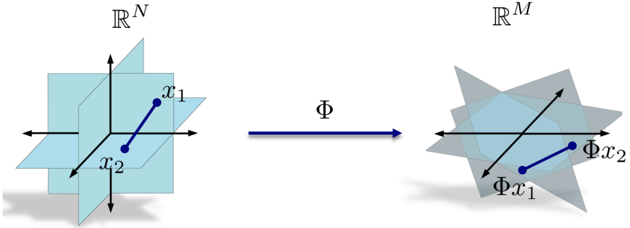

- **Sub-Gaussian matrix:** Gaussian, Bernoulli ($\{0, 1\}$), Rademacher (± 1), Any Bounded Distributions.
- **Random Fourier submatrix:** $\boldsymbol{SFD}$, $\boldsymbol{S} \in \{0,1\}^{M \times N}$, $\boldsymbol{S1}_N = \boldsymbol{1}_M$, $\boldsymbol{D} = \text{diag}(\pm 1)$.

In Summary

- The motivation of dimensionality reduction
- Principle component analysis and its algorithms
- Other projection and factorization models

Next...

- Nonlinear dimensionality reduction (manifold learning, kernel PCA, ...)