Dimension Reduction and Principle Component Analysis

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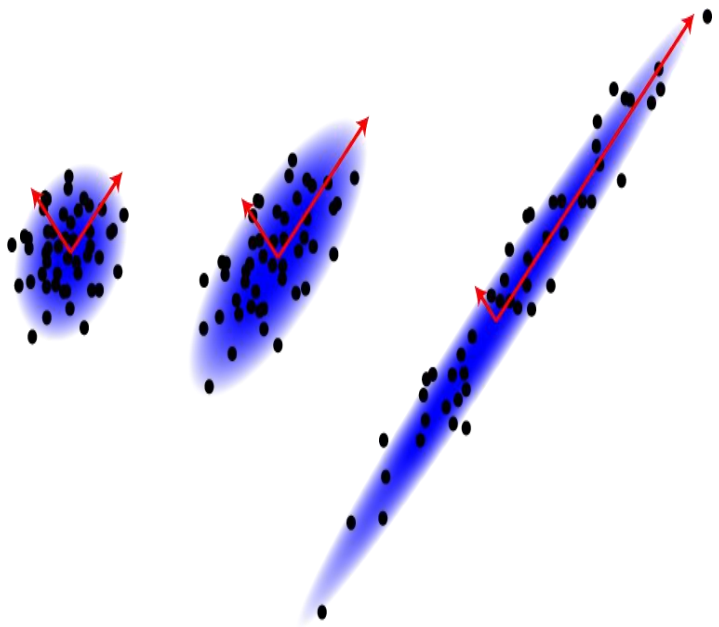
Motivation: Curse of Dimensionality

- Data may contain very similar or even the same columns

Highly Correlated Data!

Curse of Dimensionality for Big Data!

A	B	C	D	E	F	G	H
线性代数	数学分析1	数学分析2	概率论	机器学习	人工智能	离散数学	计算机网络
91	91	89	88	88	84	86	76
73	89	90	66	80	82	90	82
71	62	60	71	60	84	66	63
85	93	85	72	82	83	80	89
78	66	94	69	80	81	86	65
69	73	73	64	90	80	87	90
83	97	96	70	86	85	87	77
95	100	100	97	88	84	88	76
69	68	60	72	76	78	73	79
78	68	84	62	76	80	80	63
84	87	79	73	86	83	81	71
80	91	88	80	81	79	87	72
85	92	87	85	92	86	83	81
71	65	100	75	86	80	86	85
68	79	66	60	71	83	60	84
82	92	81	78	89	81	95	94
96	88	89	76	80	74	87	64
85	82	94	71	88	85	83	82
81	78	91	70	78	79	85	80



Motivation: Data Visualization

- We are interested in the intrinsic information of data
- People can only understand 2D or 3D data

A	B	C	D	E	F	G	H
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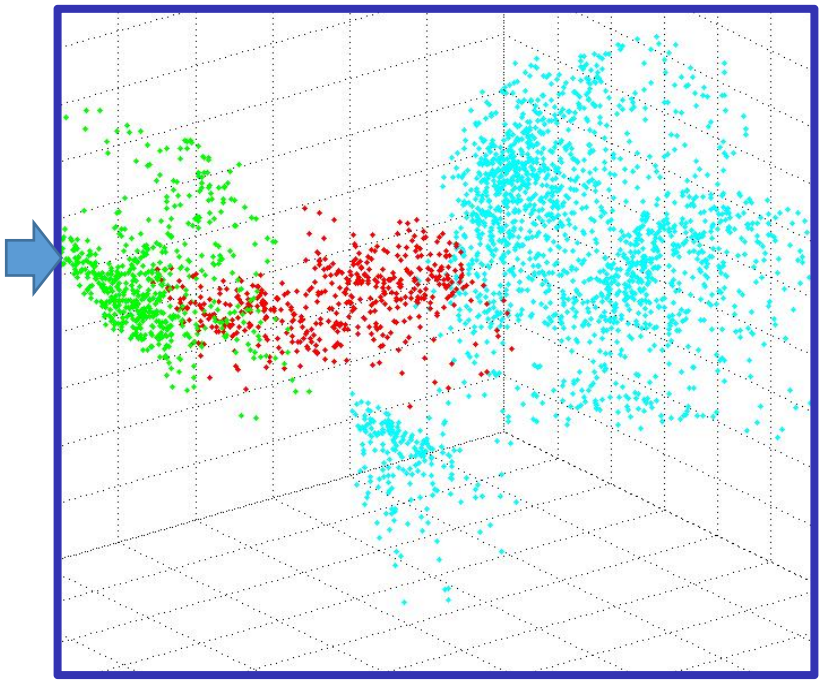
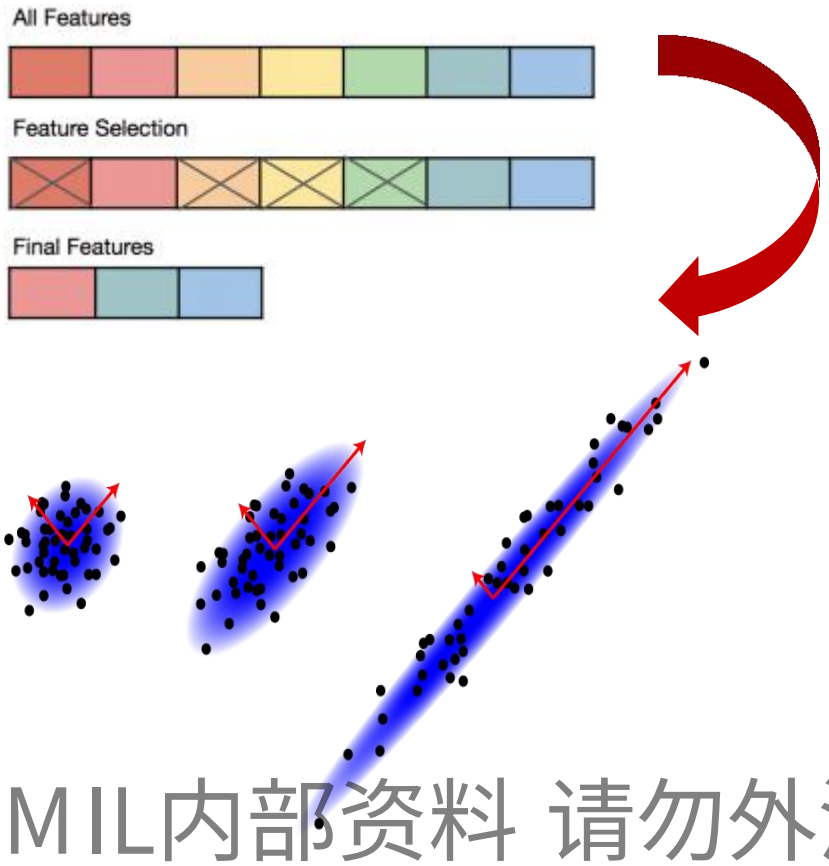


Motivation: Feature Selection

High dimension vector x

Low dimension vector z



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69	73	73	64	90	80	87	90
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84	87	79	73	86	83	81	71
80	91	88	80	81	79	87	72
85	92	87	85	92	86	83	81
71	65	100	75	86	80	86	85
68	79	66	60	71	83	60	84
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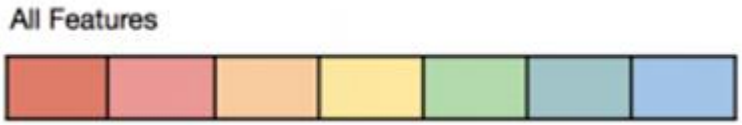
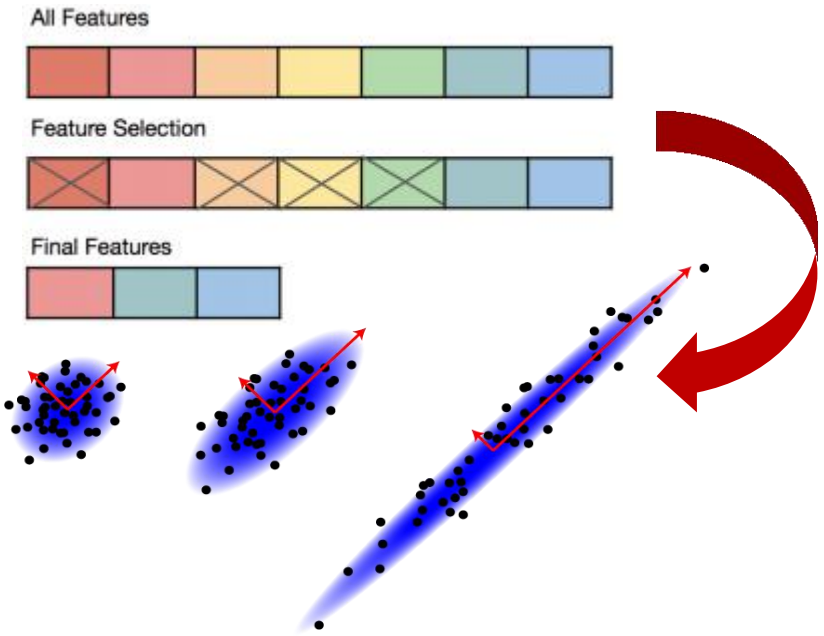
Motivation: Feature Selection

High dimension vector x

Low dimension vector z





4. Feature Selection

- 4.1 Filter Method
  - Variance [guide] [demo]
  - Correlation [guide] [demo]
  - Chi-Square [guide] [demo]
  - Mutual Information Filter [guide] [demo]
  - Information Value (IV) [guide]
- 4.2 Wrapper Method
  - Forward Selection [guide] [demo]
  - Backward Elimination [guide] [demo]
  - Exhaustive Feature Selection [guide] [demo]
  - Genetic Algorithm [guide]
- 4.3 Embedded Method
  - Lasso (L1) [guide] [demo]
  - Random Forest Importance [guide] [demo]
  - Gradient Boosted Trees Importance [guide] [demo]
- 4.4 Feature Shuffling
  - Random Shuffling [guide] [demo]
- 4.5 Hybrid Method
  - Recursive Feature Selection [guide] [demo]
  - Recursive Feature Addition [guide] [demo]

https://github.com/Yimeng-Zhang/feature-engineering-and-feature-selection

Motivation: Feature Projection

High dimension vector x

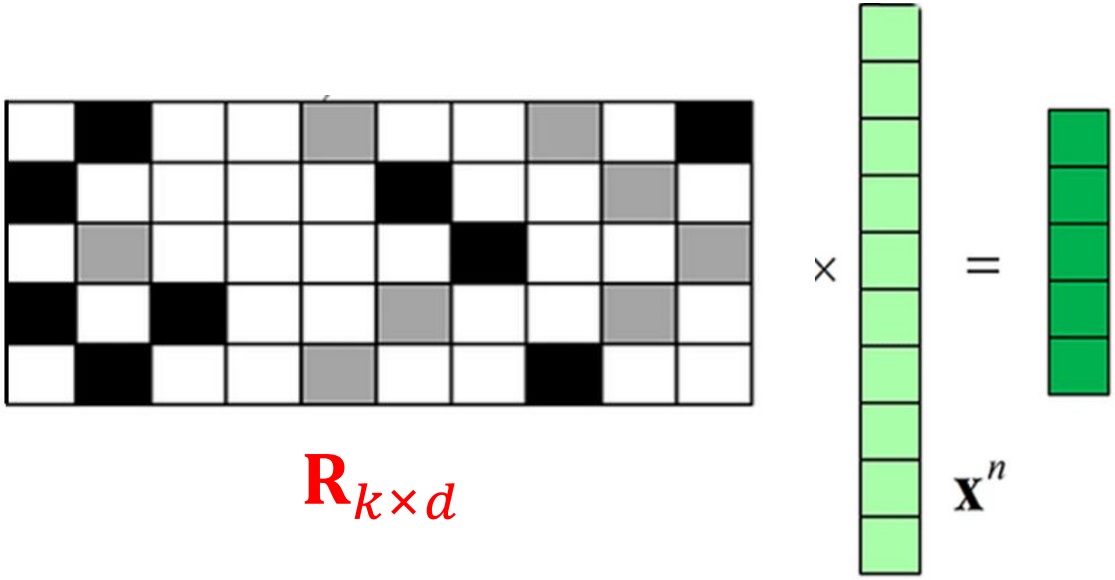
Low dimension vector z

Intrinsic Dimension *k*

Rand(m,d), k = d

现实情况： $k << d$

可学习的样本量： $N > k$



$\mathbf{R}_{k\times d}$ $\mathbf{x}^n$

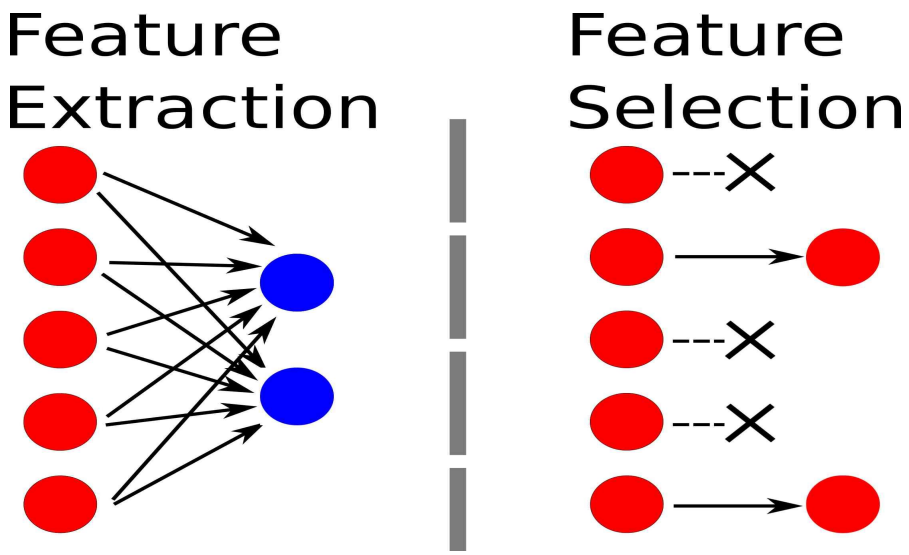
$$\mathbf{z}^k = \mathbf{R}_{k\times d}\mathbf{x}_{d\times 1} = \mathbf{z}_{k\times 1}$$

If $d >> k$, then the dimension is highly reduced

For example: $k = 2$

Feature Selection VS Feature Projection

Feature Projection is also called **Feature Extraction**



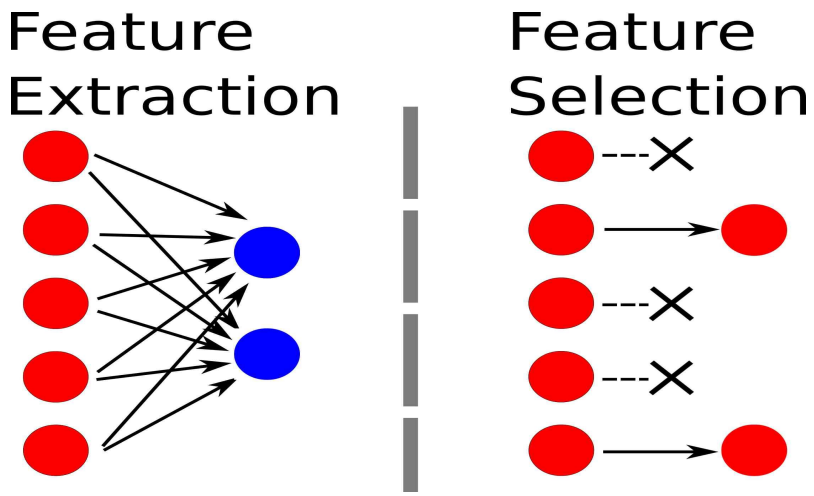
Contents [hide]

$$\mathbf{z}^k = \mathbf{R}_{k\times d}\mathbf{x}_{d\times 1} = \boldsymbol{z}_{k\times 1}$$

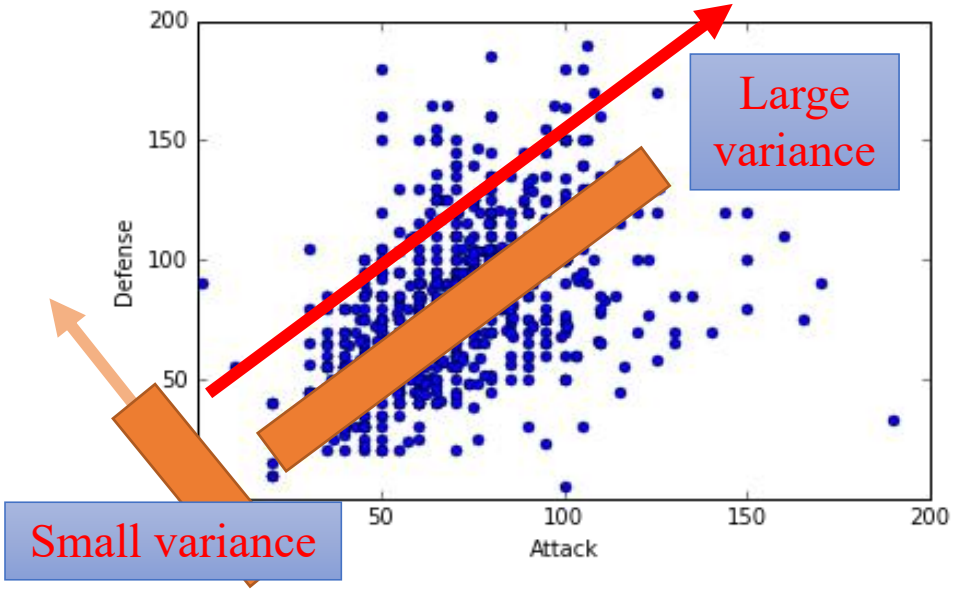
- How to find a good **projection matrix R**?
- How to measure the goodness? PCA, NMF, LDA, GDA.

Contents

Feature Extraction and PCA



$$\mathbf{z}^k = \mathbf{R}_{k\times d}\mathbf{x}_{d\times 1} = \boldsymbol{z}_{k\times 1}$$



Project data $\mathbf{x}$ onto $\mathbf{w}_1$, and obtain $\mathbf{z}_1$

- How to find a good **projection matrix R**?
- How to measure the goodness? PCA, NMF, LDA, GDA.
- PCA is the simplest one: Maximize the data variance!

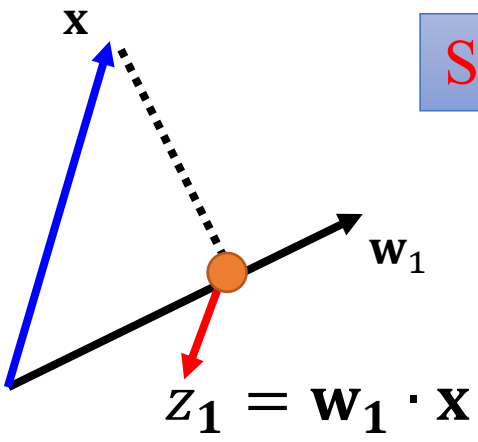
Maximum **Variance** Formulation

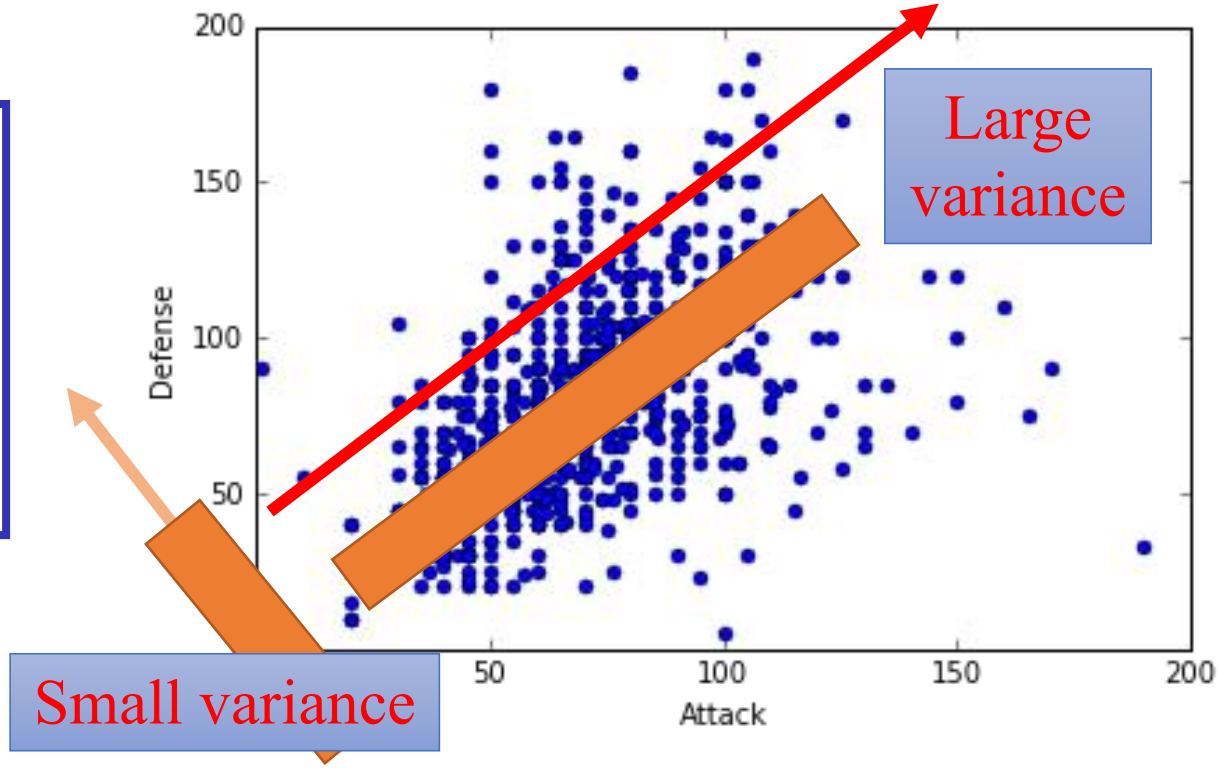
$$\mathbf{y} = \mathbf{wx}$$

$\mathbf{z} = \mathbf{Wx}$

Reduce to 1-D:

$z_1 = \mathbf{w_1} \cdot \mathbf{x}$





Project data $\mathbf{x}$ onto $\mathbf{w}_1$, and obtain $\mathbf{z}_1$

We want the variance of $\mathbf{z}_1$ as large as possible

$$\underset{\mathbf{w_1}}{\text{argmax}}\, var(z_1) = \frac{1}{N}\sum (z_1 - \bar{z}_1)^2$$

$$s.t.\ \ \|\mathbf{w}_1\|_2 = 1$$

Where N is the number of samples

Maximum Variance Formulation

$\mathbf{z} = \mathbf{W}\mathbf{x}$

Reduce to 1-D:

$z_1 = \mathbf{w}_1 \cdot \mathbf{x}$

$z_2 = \mathbf{w}_2 \cdot \mathbf{x}$

$$\mathbf{W} = \begin{bmatrix} (\mathbf{w}_1)^{\mathrm{T}} \\ (\mathbf{w}_2)^{\mathrm{T}} \\ \vdots \end{bmatrix}$$

Orthogonal matrix

Project data $\mathbf{x}$ onto $\mathbf{w}_1$ and obtain z_1

We want the variance of z_1 as large as possible

$$\underset{\mathbf{w_1}}{\operatorname{argmax}}\, var(z_1) = \frac{1}{N}\sum (z_1 - \bar{z}_1)^2$$

$$s.t.\ \ \|\mathbf{w}_1\|_2 = 1$$

Project data $\mathbf{x}$ onto $\mathbf{w}_2$ and obtain z_2

We want the variance of z_2 as large as possible

$$\underset{\mathbf{w_2}}{\operatorname{argmax}}\, var(z_2) = \frac{1}{N}\sum (z_2 - \bar{z}_2)^2$$

$$s.t.\ \ \|\mathbf{w}_2\|_2 = 1\ \ \mathbf{w}_1 \cdot \mathbf{w}_2 = 0$$

Formula Derivation

$$Var(\mathbf{Z}_1) = \frac{1}{N}\sum (z_1 - \bar{z}_1)^2$$

$\mathbf{w}_1 \cdot \mathbf{x}$

$$= \frac{1}{N}\sum (\mathbf{w}_1 \cdot \mathbf{x} - \mathbf{w}_1 \cdot \bar{\mathbf{x}})^2$$

$$= \frac{1}{N}\sum (\mathbf{w}_1 \cdot (\mathbf{x} - \bar{\mathbf{x}}))^2$$

$$= \frac{1}{N}\sum ((\mathbf{w}_1)^{\mathrm{T}}(\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^{\mathrm{T}}\mathbf{w}_1)$$

$$= (\mathbf{w}_1)^{\mathrm{T}}\frac{1}{N}\sum ((\mathbf{x} - \bar{\mathbf{x}})(\mathbf{x} - \bar{\mathbf{x}})^{\mathrm{T}})\mathbf{w}_1$$

$$= (\mathbf{w}_1)^{\mathrm{T}}\mathrm{Cov}(\mathbf{X})\,\mathbf{w}_1$$

$$= (\mathbf{w}_1)^{\mathrm{T}}\mathbf{S}\mathbf{w}_1$$

$$\bar{z}_1 = \frac{1}{N}\sum z_1 = \frac{1}{N}\sum \mathbf{w}_1 \cdot \mathbf{x}$$

$$= \mathbf{w}_1 \cdot \frac{1}{N}\sum \mathbf{x} = \mathbf{w}_1 \cdot \bar{\mathbf{x}}$$

Find $\mathbf{w}_1$ maximizing $(\mathbf{w}_1)^{\mathrm{T}}\mathbf{S}\mathbf{w}_1$

where $\|\mathbf{w}_1\|_2^2 = (\mathbf{w}_1)^{\mathrm{T}}\mathbf{w}_1 = 1$

$S = \mathrm{Cov}(\mathbf{X})$

Formula Derivation

$$\underset{\mathbf{w}_1}{\operatorname{argmax}} (\mathbf{w}_1)^{\mathrm{T}}\mathbf{S}\mathbf{w}_1 \qquad s.t. \quad (\mathbf{w}_1)^{\mathrm{T}}\mathbf{w}_1 = 1$$

$\mathbf{S} = Cov(\mathbf{X})$ Symmetric Positive-semidefinite (non-negative eigenvalues)

Using Lagrange multiplier:

$$g(\mathbf{w}_1) = (\mathbf{w}_1)^{\mathrm{T}}\mathbf{S}\mathbf{w}_1 - \alpha((\mathbf{w}_1)^{\mathrm{T}}\mathbf{w}_1 - 1)$$

$\partial g(\mathbf{w}_1)/\partial w_{11}=0$

$\partial g(\mathbf{w}_1)/\partial w_{12}=0$

$\vdots$

$$\mathbf{S}\mathbf{w}_1 - \alpha\mathbf{w}_1 = 0$$

$$\mathbf{S}\mathbf{w}_1 = \alpha\mathbf{w}_1$$

$\mathbf{w}_1$: eigenvector

$$(\mathbf{w}_1)^{\mathrm{T}}\mathbf{S}\mathbf{w}_1 = \alpha(\mathbf{w}_1)^{\mathrm{T}}\mathbf{w}_1 = 0$$

Choose the maximum one

$\mathbf{w}_1$ is the eigenvector of the covariance $\mathbf{S}$ matrix, corresponding to the largest eigenvalue λ_1

Formula Derivation

$$\underset{\mathbf{w_2}}{\operatorname{argmax}} (\mathbf{w}_2)^{\mathrm{T}}\mathbf{S}\mathbf{w}_2 \quad s.t. \quad (\mathbf{w}_2)^{\mathrm{T}}\mathbf{w}_2 = 1 \quad (\mathbf{w}_2)^{\mathrm{T}}\mathbf{w}_1 = \mathbf{0}$$

$$g(\mathbf{w}_2) = (\mathbf{w}_2)^{\mathrm{T}}\mathbf{S}\mathbf{w}_2 - \alpha((\mathbf{w}_2)^{\mathrm{T}}\mathbf{w}_2 - 1) - \beta\,((\mathbf{w}_2)^{\mathrm{T}}\mathbf{w}_1 - 0)$$

$$\partial g(\mathbf{w}_2)/\,\partial w_{21} = 0$$

$$\partial g(\mathbf{w}_2)/\,\partial w_{22} = 0$$

$$\vdots$$

$$\mathbf{S}\mathbf{w}_2 - \alpha\mathbf{w}_2 - \beta\mathbf{w}_1 = 0$$

$$(\mathbf{w}_1)^{\mathrm{T}}\mathbf{S}\mathbf{w}_2 - \alpha(\mathbf{w}_1)^{\mathrm{T}}\mathbf{w}_2 - \beta(\mathbf{w}_1)^{\mathrm{T}}\mathbf{w}_1 = 0$$

$(\mathbf{w}_1)^{\mathrm{T}}\mathbf{S}\mathbf{w}_2$: 0 — $\alpha(\mathbf{w}_1)^{\mathrm{T}}\mathbf{w}_2$: 0 — $\beta(\mathbf{w}_1)^{\mathrm{T}}\mathbf{w}_1$: 1

$$= (\mathbf{w}_1)^{\mathrm{T}}\mathbf{S}\mathbf{w}_2 = (\mathbf{w}_2)^{\mathrm{T}}\mathbf{S}\mathbf{w}_1$$

$$\mathbf{S}\mathbf{w}_1 = \lambda_1\mathbf{w}_1$$

$$= \lambda_1(\mathbf{w}_2)^{\mathrm{T}}\mathbf{w}_1 = 0$$

$$\beta = 0: \Rightarrow \mathbf{S}\mathbf{w}_2 - \alpha\mathbf{w}_2 = 0 \Rightarrow \mathbf{S}\mathbf{w}_2 = \alpha\mathbf{w}_2$$

$\mathbf{w}_2$ is the eigenvector of the covariance matrix $\mathbf{S}$, corresponding to the 2nd largest eigenvalue λ_2

How to Reduce Dimension by PCA?

To reduce dimension of data $\mathbf{X}$ from d to k ($k < d$), we perform:

- **Step 1:** Calculate the covariance matrix $\mathbf{S} = Cov(\mathbf{X})$
- **Step 2: Do Eigen-decomposition: $\mathbf{S} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{-1}$:**

$$[\mathbf{Q}, \boldsymbol{\Lambda}] = \mathbf{eigs(S)}$$

- **Step 3: Select the first k orthonormal eigenvectors from Q to form the projection matrix $\mathbf{W}^{\mathrm{T}} = \mathbf{Q}(:, 1{:}k)$,** corresponding to the k largest eigenvalues
- **Step 4:** Reduce the dimension to k-dimension by :

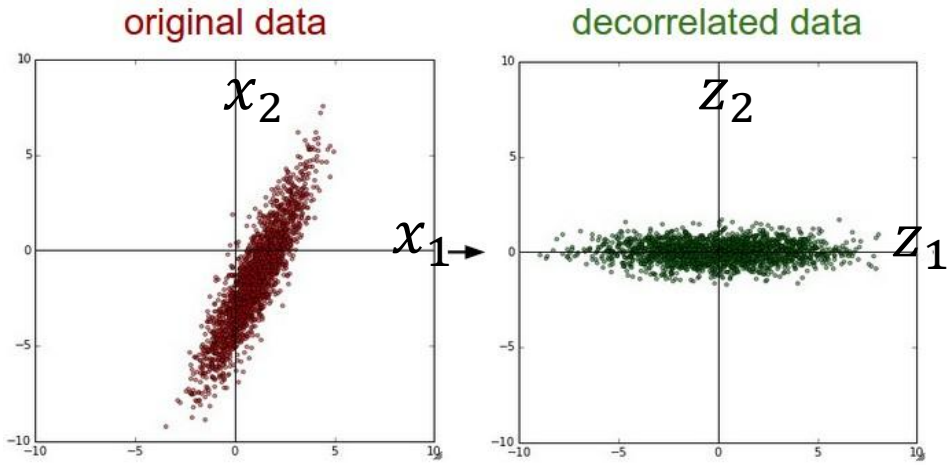
$$\mathbf{z} = \mathbf{W}\mathbf{x} = \begin{bmatrix} (\mathbf{w}_1)^{\mathrm{T}} \\ (\mathbf{w}_2)^{\mathrm{T}} \\ \vdots \\ (\mathbf{w}_k)^{\mathrm{T}} \end{bmatrix} \mathbf{x}$$

Example: Decorrelation

$$\mathbf{Z} = \mathbf{WX}$$

$$Cov(\mathbf{Z}) = \boldsymbol{D}$$ 对角化

Diagonal matrix



$$Cov(\mathbf{Z}) = \frac{1}{n}\sum(\mathbf{z}-\bar{\mathbf{z}})(\mathbf{z}-\bar{\mathbf{z}})^{\mathrm{T}} = \mathbf{WSW}^{\mathrm{T}}$$

$Cov(\mathbf{X})$

$$= \mathbf{W}[\mathbf{Sw}_1 \cdots \mathbf{Sw}_k]$$

$$= \mathbf{W}[\lambda_1\mathbf{Sw}_1 \cdots \lambda_k\mathbf{Sw}_k]$$

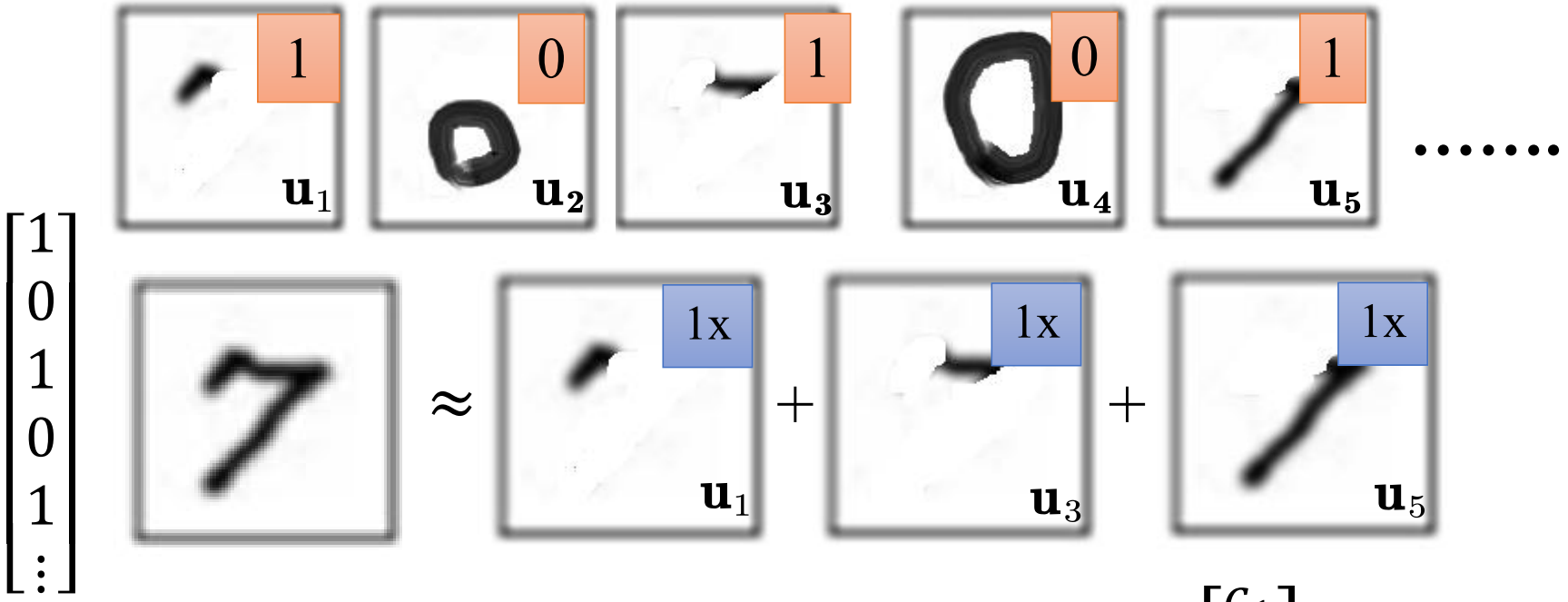
$$= [\lambda_1\mathbf{e}_1 \cdots \lambda_k\mathbf{e}_k] = \boldsymbol{D}$$ → Diagonal matrix

特征值分解性质：

$$\mathbf{S} = \mathbf{Q\Lambda Q}^{-1}, \quad \mathbf{Q} = \mathbf{Q}^{-1}$$

Minimum Error Formulation

Basic Component:



$$\mathbf{x} \approx c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + \cdots + c_k\mathbf{u}_k + \tilde{\mathbf{x}}$$

Pixels in a digit image

component

$\begin{bmatrix}c_1\\c_2\\\vdots\\c_k\end{bmatrix}$ Represent a digit image

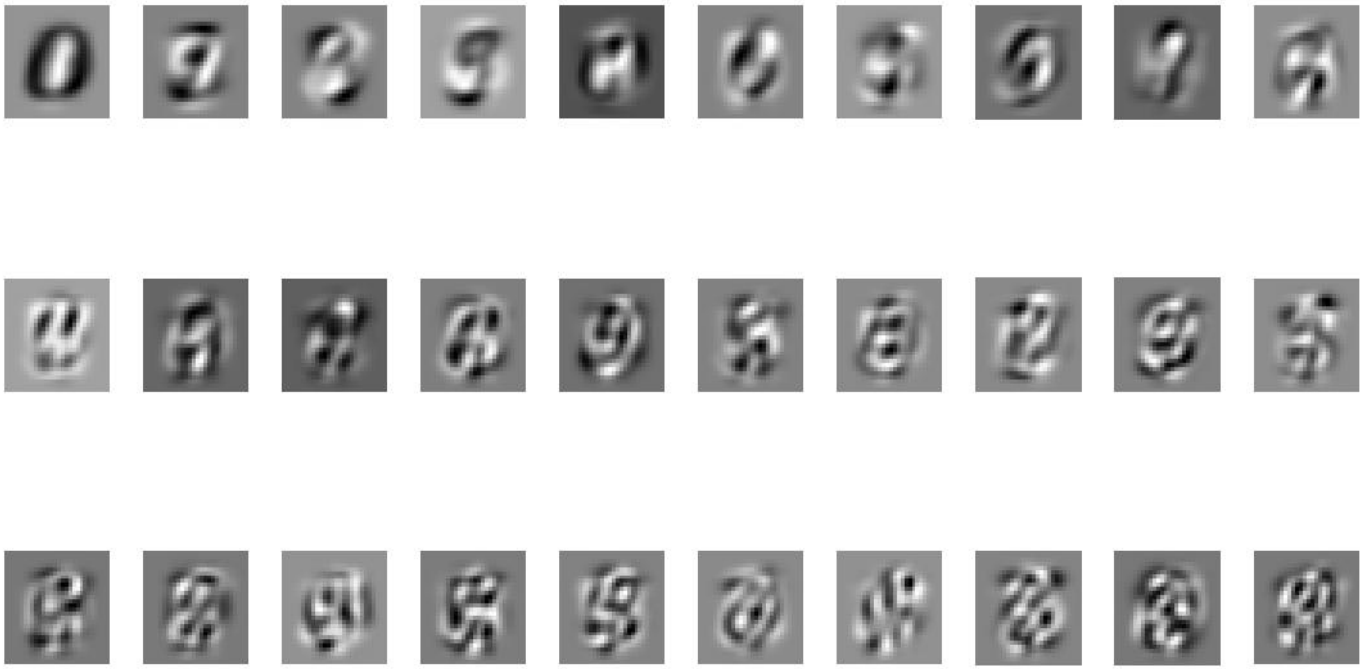
Example: MNIST

$$= \mathbf{a}_1 \mathbf{w}_1 + \mathbf{a}_2 \mathbf{w}_2 + \cdots$$

x

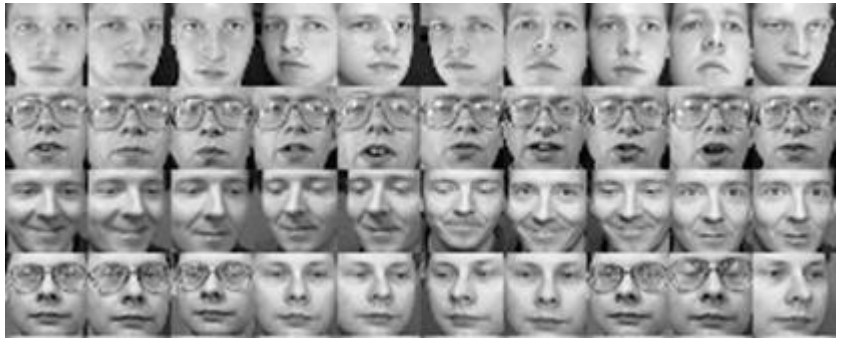
images

30 components:



Example: Face

Eigen-face



30 components:

http://www.cs.unc.edu/~lazebnik/research/spring08/assignment3.html

Minimum Error Formulation

$$\mathbf{x} - \tilde{\mathbf{x}} \approx c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + \cdots + c_k\mathbf{u}_k = \hat{\mathbf{x}}$$

Find $\{\mathbf{u}_1, ..., \mathbf{u}_k\}$ to minimize the following reconstruction error:

$$\boldsymbol{L} = \underset{\{\mathbf{u}_1,\mathbf{u}_2,\cdots,\mathbf{u}_k\}}{\operatorname{argmax}} \left\| (\mathbf{x} - \tilde{\mathbf{x}}) - \underbrace{\sum_{k=1}^{K} c_k\mathbf{u}_k}_{\hat{\mathbf{x}}} \right\|_2$$

PCA: $\mathbf{z} = \mathbf{W}\mathbf{x}$

$$\mathbf{z} = \begin{bmatrix} (\mathbf{w}_1)^{\mathrm{T}} \\ (\mathbf{w}_2)^{\mathrm{T}} \\ \vdots \\ (\mathbf{w}_k)^{\mathrm{T}} \end{bmatrix} \mathbf{x}$$

$\{\mathbf{w}_1, \mathbf{w}_2, \cdots, \mathbf{w}_k\}$ (from PCA) is the component $\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_k\}$ (minimizing $\boldsymbol{L}$)

Proof in [Bishop, Chapter 12.1.2]

Minimum Error Formulation

$$\mathbf{x} - \tilde{\mathbf{x}} \approx c_1\mathbf{u}_1 + c_2\mathbf{u}_2 + \cdots + c_k\mathbf{u}_k = \hat{\mathbf{x}}$$

Find $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$ to minimize the following reconstruction error:

$$\|(\mathbf{x} - \tilde{\mathbf{x}}) - \hat{\mathbf{x}}\|_2$$

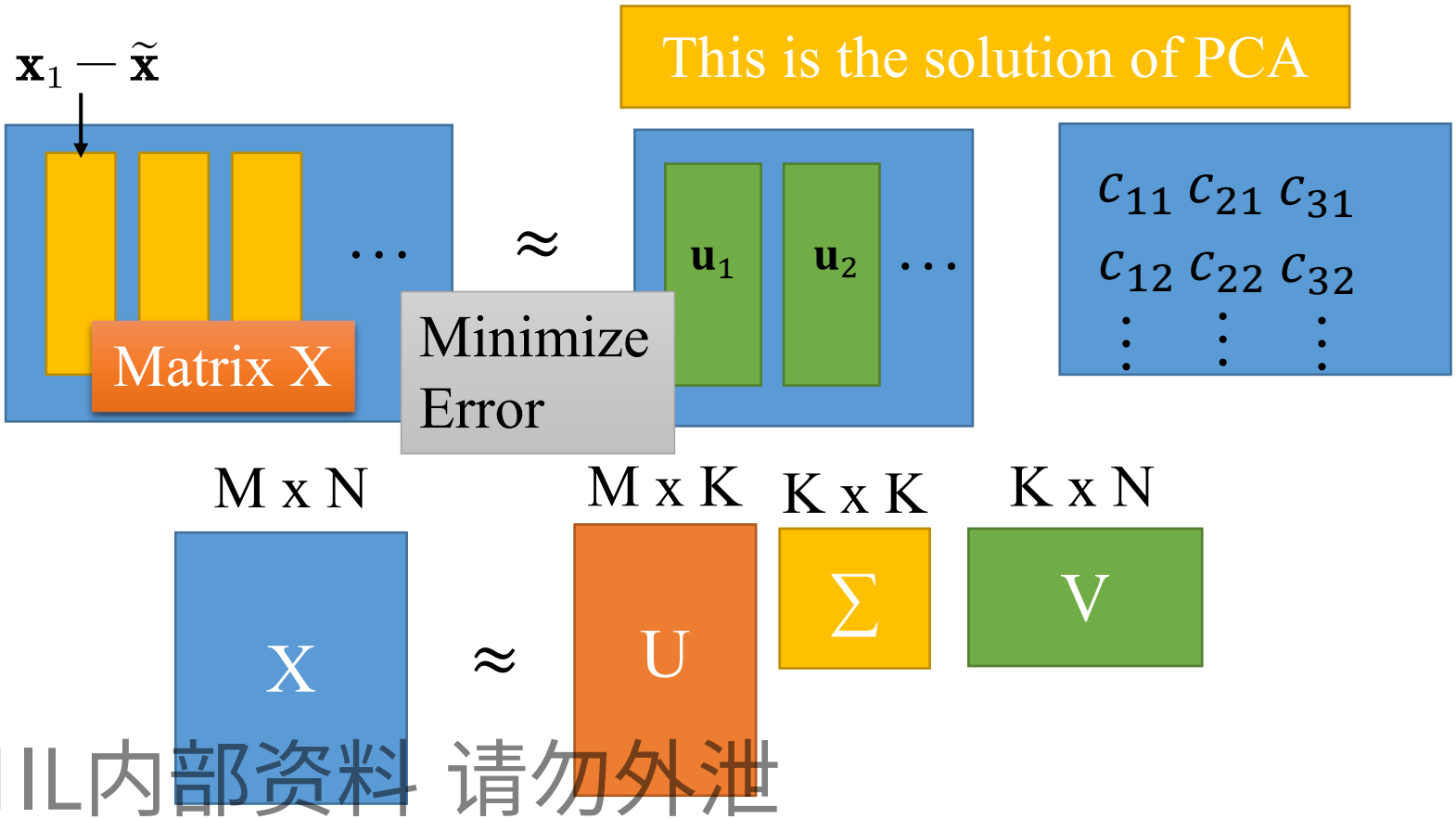
$$\mathbf{x}_1 - \tilde{\mathbf{x}} \approx c_{11}\mathbf{u}_1 + c_{12}\mathbf{u}_2 + \cdots$$
$$\mathbf{x}_2 - \tilde{\mathbf{x}} \approx c_{21}\mathbf{u}_1 + c_{22}\mathbf{u}_2 + \cdots$$
$$\mathbf{x}_3 - \tilde{\mathbf{x}} \approx c_{31}\mathbf{u}_1 + c_{32}\mathbf{u}_2 + \cdots$$
$$\vdots \quad \vdots$$

$$\begin{matrix} c_{11} & c_{21} & c_{31} \\ c_{12} & c_{22} & c_{32} \\ \vdots & \vdots & \vdots \end{matrix}$$

Minimum Error Formulation

- **K columns of U:**

a set of orthonormal eigenvectors corresponding to the K largest eigenvalues of $\mathbf{X}\mathbf{X}^{\mathrm{T}}$



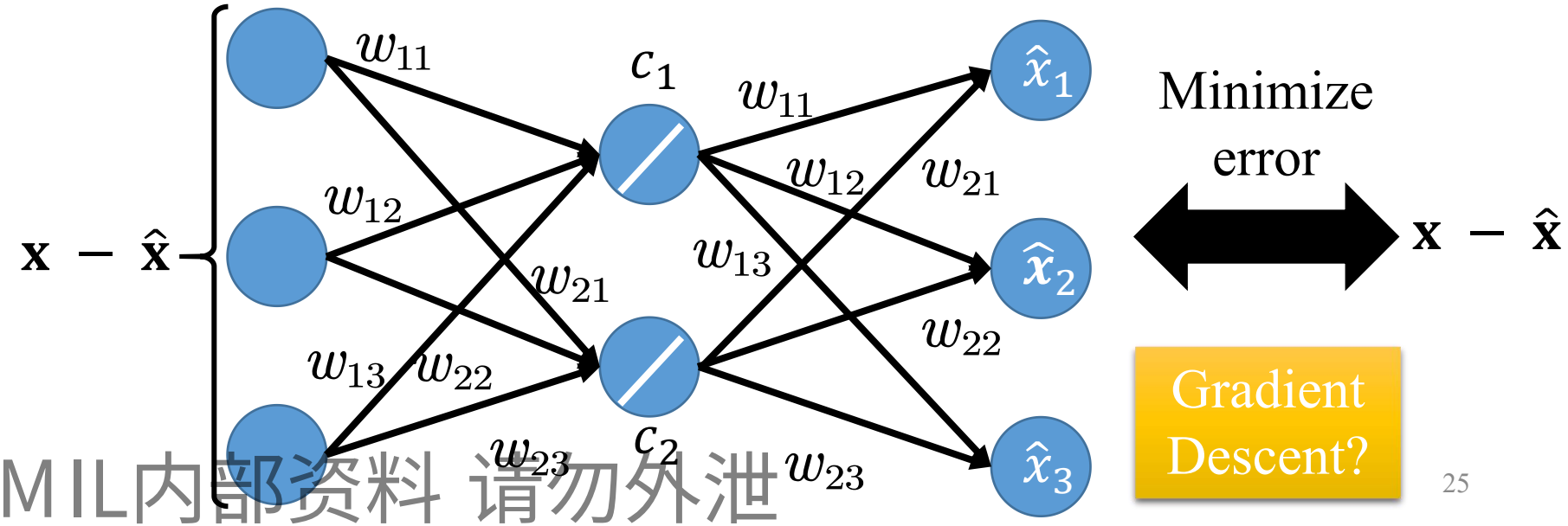
Autoencoder

PCA looks like a neural network with one hidden layer (linear activation function)

If $\{\mathbf{w}_1, \mathbf{w}_2, \cdots, \mathbf{w}_k\}$ is the component $\{\mathbf{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_k\}$, then we have

$$\hat{\mathbf{x}} = \sum_{k=1}^{K} c_k \mathbf{w}_k \quad \Leftrightarrow \quad \mathbf{x} - \hat{\mathbf{x}}$$

For the case where $K = 2$:



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Example: Pokemon

- Inspired from: https://www.kaggle.com/strakul5/d/abcsds/pokemon/principal-component-analysis-of-pokemon-data
- 800 Pokemons with 6 features:

  HP, Atk, Def, Sp Atk, Sp Def, Speed
- How many principle components?

$$\frac{\lambda_i}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6}$$

	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
ratio	0.45	0.18	0.13	0.12	0.07	0.04

Using 4 components is good enough

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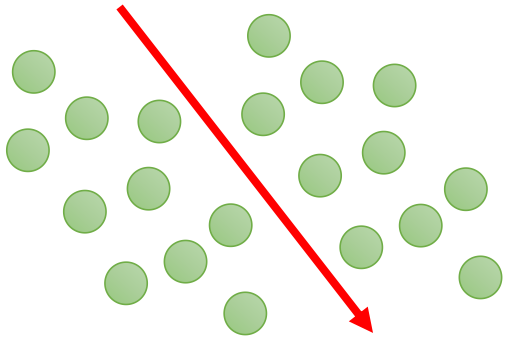
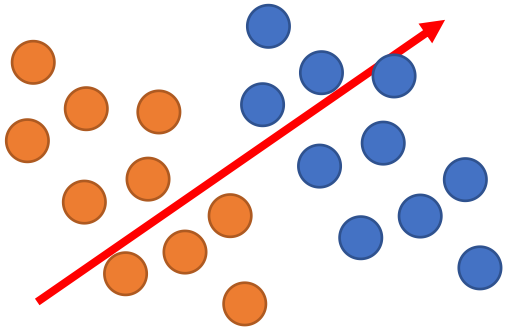
Conclusion

- Unsupervised

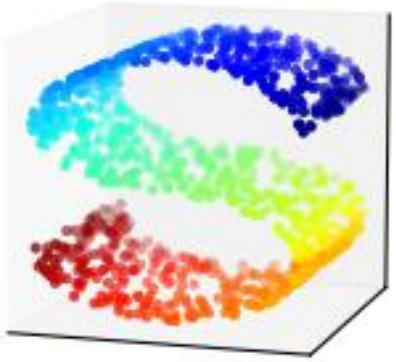


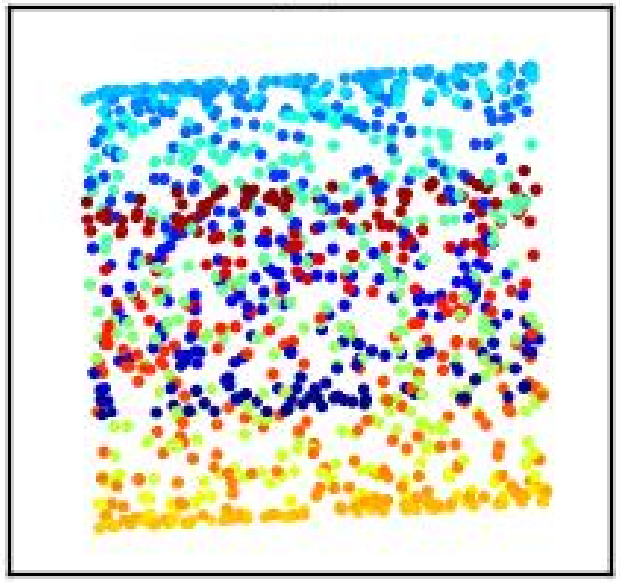
PCA



LDA

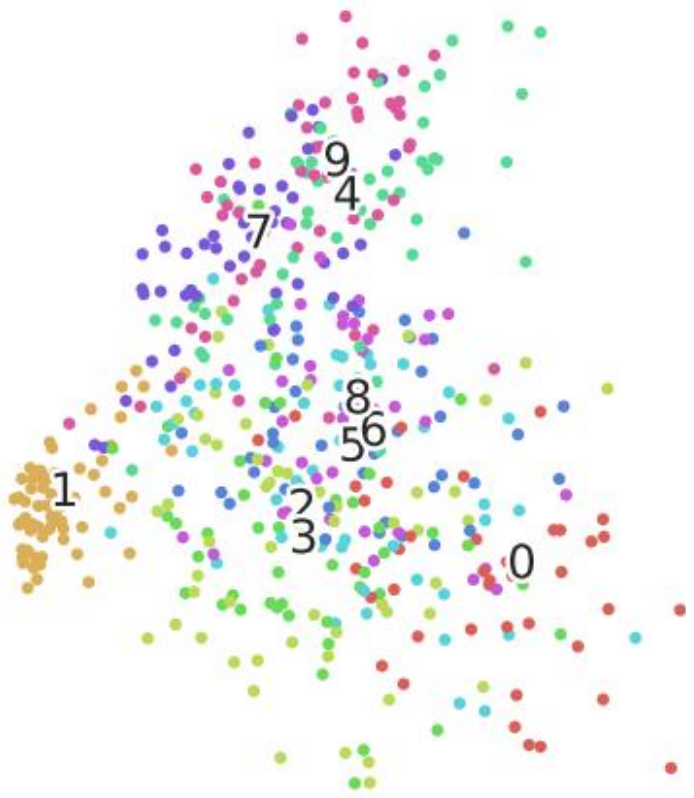
- Linear



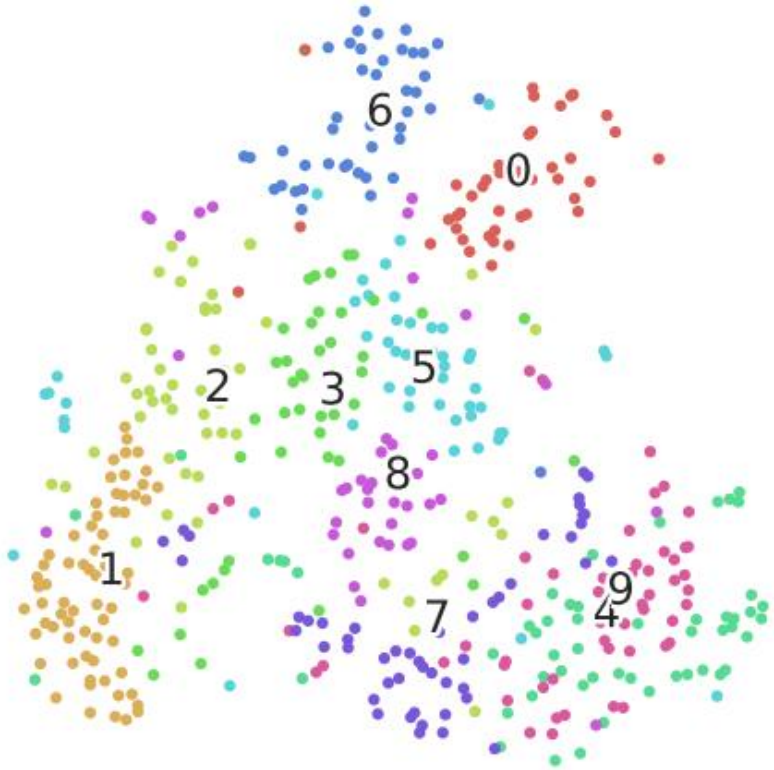


http://www.astroml.org/book_figures/chapter7/fig_S_manifold_PCA.html

Conclusion



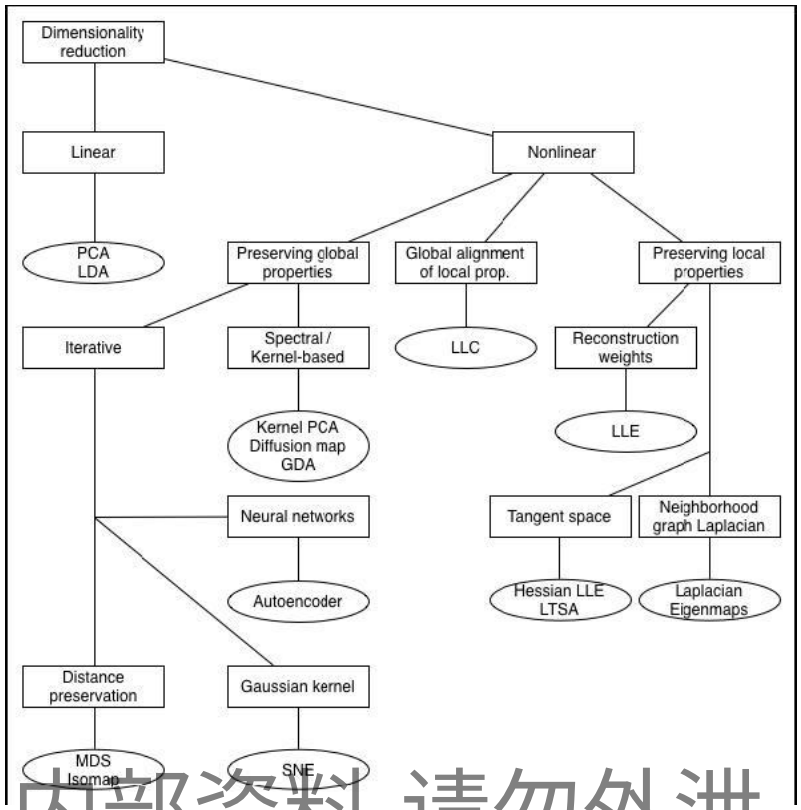
Pixel (28x28) -> PCA (2)



Pixel (28x28) -> tSNE (2)

Appendix

- http://4.bp.blogspot.com/_sHcZHRnxlLE/S9EpFXYjfvI/AAAAAAAABZ0/_oEQiaR3WVM/s640/dimensionality+reduction.jpg
- https://lvdmaaten.github.io/publications/papers/TR_Dimensionality_Reduction_Review_2009.pdf



Thank You