Machine Learning 机器学习

Lecture 11: Dimension reduction & Feature selection 降维和特征选择

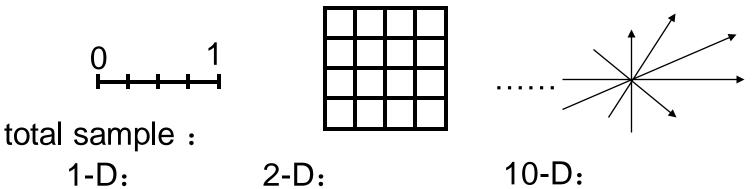
李洁 nijanice@163.com

- Many explored domains have hundreds to tens of thousands of variables/features with many irrelevant and redundant ones!
- In domains with many features the underlying probability distribution can be very complex and very hard to estimate (e.g. dependencies between variables)!
- Irrelevant and redundant features can confuse learners!

- Limited training data!
- Limited computational resources!
- Curse of dimensionality!

- Spatial sampling

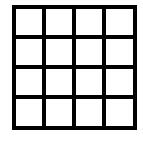
4 units for each dimension, 10 samples per unit

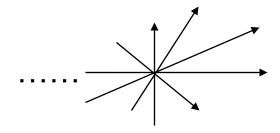


- Spatial sampling

4 units for each dimension, 10 samples per unit







total sample:

1-D: 4

2-D: 4*4=16

10-D: 4^10=1048576

~40

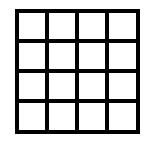
~160

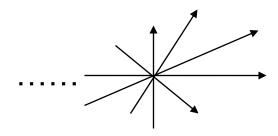
~10M

Spatial sampling

4 units for each dimension, 10 samples per unit







total sample:

1-D: 4 2-D: 4*4=16

10-D: 4^10=1048576

~40

~160

~10M

Sample sparsity

total sample: 1000

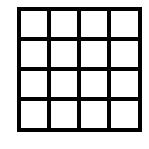
partition of each dimension: 4

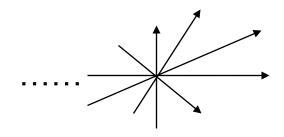
Samples per unit:

- Spatial sampling

4 units for each dimension, 10 samples per unit







total sample:

~40

~160

~10M

- Sample sparsity

total sample: 1000

partition of each dimension: 4

Samples per unit : 1D: 1000/4 = 250

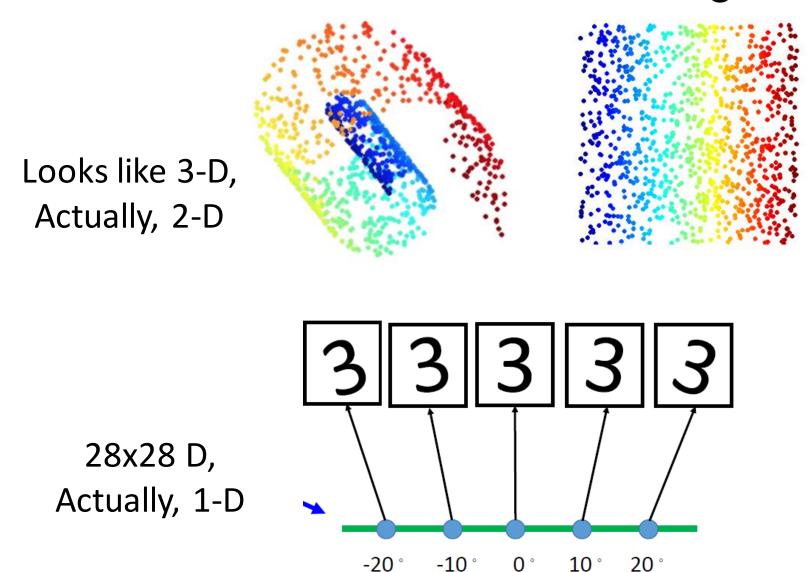
2D: 1000/(4*4) = 62.5

10D: $1000/(4^10) = 0.001$

噪声影响 Noise influence

- Feature space: 101D
- The distance between the positive and negative samples at the first dimension: 1
- The noise of the sample in its residual dimension: 10%
- "Noise distance": $\sqrt{100 \times 0.1^2} = 1$
- Even if the noise is only 10%, the noise distance in high dimensional space is enough to mask the essential difference between positive and negative samples.

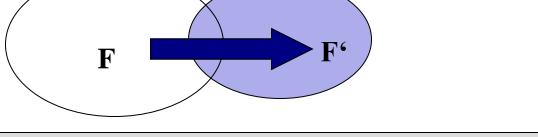
低维嵌入 Low dimensional embedding



降维与特征选择

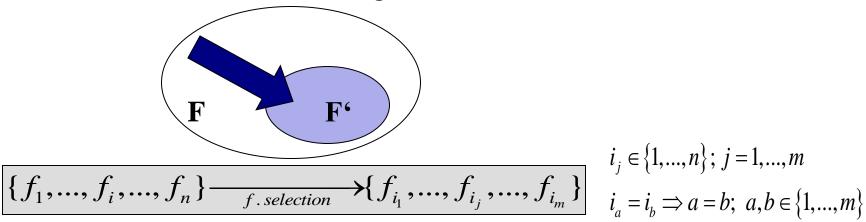
Dmensionality reduction & Feature selection

Dimensionality reduction: creating a subset of new features by combinations of the existing features



$$\{f_1,...,f_i,...,f_n\} \xrightarrow{f.extraction} \{g_1(f_1,...,f_n),...,g_j(f_1,...,f_n),...,g_m(f_1,...,f_n)\}$$

Feature Selection: choosing a subset of all the features



$$i_j \in \{1,...,n\}; j = 1,...,m$$

 $i_a = i_b \Rightarrow a = b; a,b \in \{1,...,m\}$

Machine Learning Problems

Supervised Learning U

Unsupervised Learning

classification or categorization

clustering

regression

dimensionality reduction

Discrete

Continuous

降维方法 Dmensionality reduction Method

- Principal Component Analysis (PCA)
- Multidimensional Scaling (MDS)
- Locally Linear Embedding (LLE)
- Laplacian Eigenmaps (LE)
- Isometric Mapping(Isomap)
- T-distributed Stochastic Neighbor Embedding (t-SNE)
- Auto-encoders
- Non-negative Matrix Factorization(NMF)
- Canonical Correlation Analysis(CCA)
- Independent Component Analysis (ICA)
- Probabilistic PCA
- Kernel PCA
- (Linear Discriminant Analysis(LDA)-supervised)

— ...

- Given 53 blood and urine samples (features) from 65 people.
- How can we visualize the measurements?

Matrix format (65x53)

	H-WBC	H-RBC	H-Hgb	H-Hct	H-MCV	H-MCH	H-MCHC
A1	8.0000	4.8200	14.1000	41.0000	85.0000	29.0000	34.0000
A2	7.3000	5.0200	14.7000	43.0000	86.0000	29.0000	34.0000
A3	4.3000	4.4800	14.1000	41.0000	91.0000	32.0000	35.0000
A4	7.5000	4.4700	14.9000	45.0000	101.0000	33.0000	33.0000
A5	7.3000	5.5200	15.4000	46.0000	84.0000	28.0000	33.0000
A6	6.9000	4.8600	16.0000	47.0000	97.0000	33.0000	34.0000
A7	7.8000	4.6800	14.7000	43.0000	92.0000	31.0000	34.0000
A8	8.6000	4.8200	15.8000	42.0000	88.0000	33.0000	37.0000
A9	5.1000	4.7100	14.0000	43.0000	92.0000	30.0000	32.0000

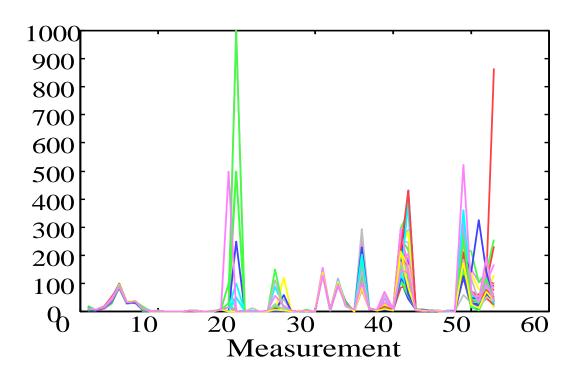
Features

Difficult to see the correlations between the features...

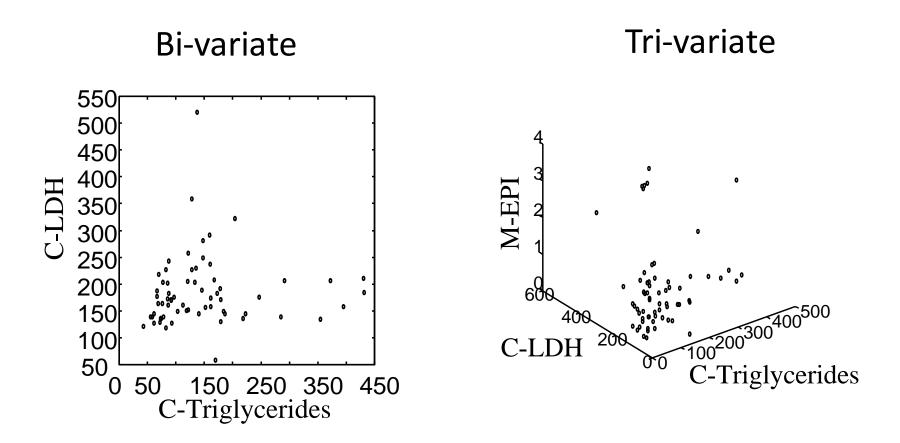
nstances

- Given 53 blood and urine samples (features) from 65 people.
- How can we visualize the measurements?

Matrix format (65x53)



Difficult to compare the different patients...

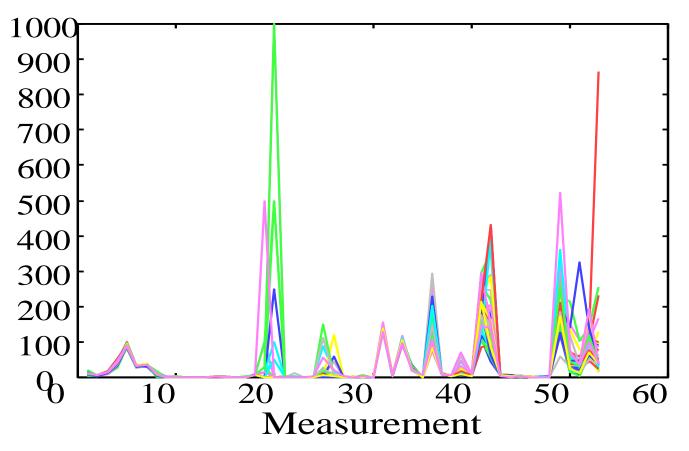


How can we visualize the other variables??? ... difficult to see in 4 or higher dimensional spaces...

- Is there a representation better than the coordinate axes?
- Is it really necessary to show all the 53 dimensions?

- Is there a representation better than the coordinate axes?
- Is it really necessary to show all the 53 dimensions?
 - discard low significance dimensions
 - Get compact description (what if there are strong correlations between the features?)

Spectral format (65 pictures, one for each person)

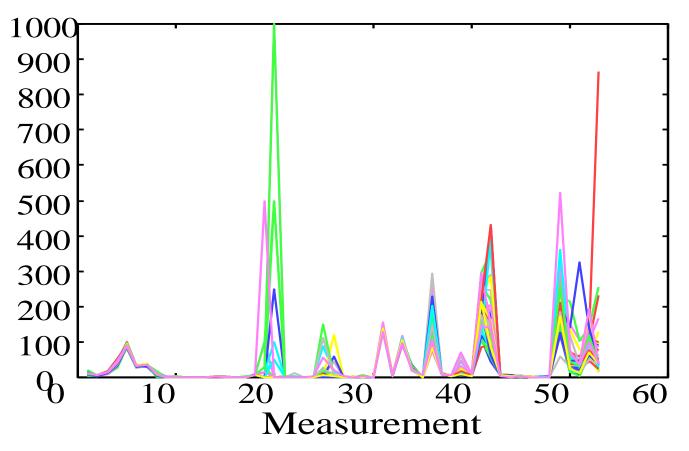


Difficult to compare the different subjects...

- Is there a representation better than the coordinate axes?
- Is it really necessary to show all the 53 dimensions?
 - discard low significance dimensions
 - Get compact description (what if there are strong correlations between the features?)
- How could we find the smallest subspace of the 53-D space that keeps the most information about the original data?

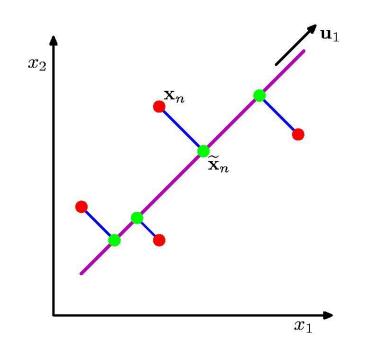
- Is there a representation better than the coordinate axes?
- Is it really necessary to show all the 53 dimensions?
 - discard low significance dimensions
 - Get compact description (what if there are strong correlations between the features?)
- How could we find the smallest subspace of the 53-D space that keeps the most information about the original data?
- A solution: Principal Component Analysis

Spectral format (65 pictures, one for each person)



Difficult to compare the different subjects...

主成分分析 Principle Component Analysis



PCA:

- Orthogonal projection of data onto lower-dimension linear space that...
 - maximizes variance of projected data (purple line)
 - minimizes mean squared distance between data point and projections (sum of blue lines)

主成分分析 Principle Component Analysis

Data Preparation:

 Standardize the data if the features have different units or scales. (centering, scaling)

Compute and Select Principal Components:

- Iterative Algorithms(For very large datasets, can find the main components without computing the full covariance matrix)
- Covariance Matrix (data dimensions are not excessively high)
- Singular Value Decomposition (can handle matrices of any size)

Transform the Original Dataset:

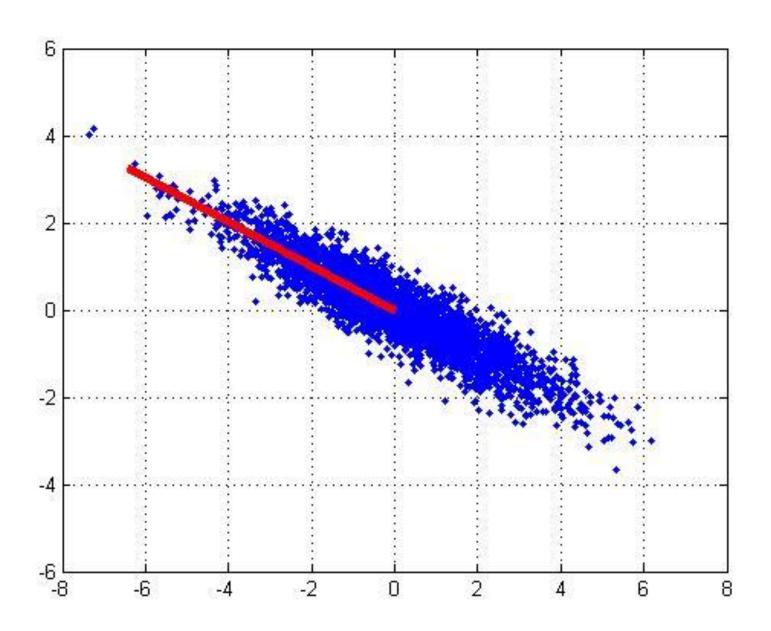
 Project the original dataset into the new space formed by the selected principal components to obtain the reduced-dimensionality data representation.

主成分分析算法一(顺序求解) PCA algorithm I (sequential)

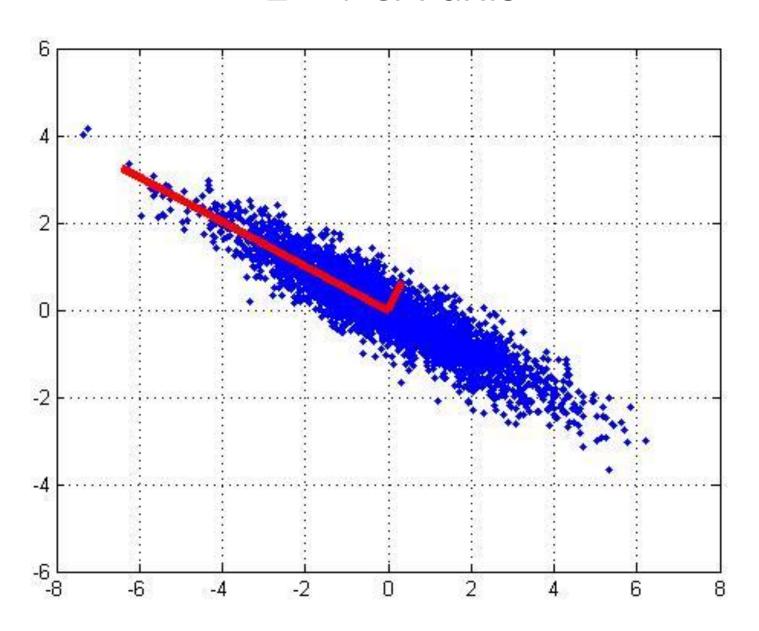
Vectors originating from the center of mass

- Principal component #1 points in the direction of the largest variance.
- Each subsequent principal component...
 - is orthogonal to the previous ones, and
 - points in the directions of the largest
 variance of the residual subspace

1st PCA axis



2nd PCA axis



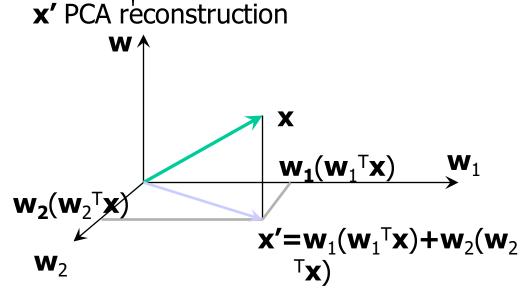
主成分分析算法一(顺序求解) PCA algorithm I (sequential)

Given the **centered** data $\{\mathbf{x}_1, ..., \mathbf{x}_m\}$, compute the principal vectors:

$$\mathbf{w}_{1} = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m} \sum_{i=1}^{m} \{(\mathbf{w}^{T} \mathbf{x}_{i})^{2}\} \qquad 1^{\text{st}} \text{ PCA vector} \qquad \text{can be obtained by gradient}$$

$$\mathbf{w}_{k} = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m} \sum_{i=1}^{m} \{[\mathbf{w}^{T} (\mathbf{x}_{i} - \sum_{j=1}^{k-1} \mathbf{w}_{j} \mathbf{w}_{j}^{T} \mathbf{x}_{i})]^{2}\} \qquad \text{$kth PCA vector}$$

We maximize the variance of the projection in the residual subspace



主成分分析算法二(特征值分解) PCA algorithm II(sample covariance matrix)

• Given data $\{x_1, ..., x_m\}$, compute covariance matrix Σ

$$\Sigma = \frac{1}{m} \sum_{i=1}^{m} (\mathbf{x}_{i} - \overline{\mathbf{x}}) (\mathbf{x} - \overline{\mathbf{x}})^{T}$$
 where
$$\overline{\mathbf{x}} = \frac{1}{m} \sum_{i=1}^{m} \mathbf{x}_{i}$$
 (Optional) Standardization

- Eigenvalue decomposition $\Sigma = U \wedge U^T$
- PCA basis vectors = the eigenvectors of Σ

Larger eigenvalues ⇒ more important eigenvectors

主成分分析算法二(特征值分解) PCA algorithm II(sample covariance matrix)

PCA algorithm(**X**, *k*): top *k* eigenvalues/eigenvectors

```
% \mathbf{X} = \mathbf{N} \times \mathbf{m} data matrix, each data point \mathbf{x}_i = \text{column vector}, i=1..m
```

- $X \leftarrow$ subtract mean \overline{X} from each column vector \mathbf{x}_i in X
- $\Sigma \leftarrow XX^T$...compute covariance matrix of X
- $\{\lambda_i, \mathbf{u}_i\}_{i=1..N}$ = eigenvectors/eigenvalues of Σ ... Sort the eigenvalues in descending order $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{N'}$
- Return { λ_i, **u**_i }_{i=1..k}
 % top *k* principle components

主成分分析算法三(奇异值分解) PCA algorithm III (SVD of the data matrix)

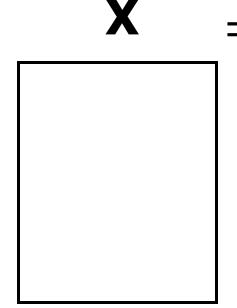
Singular Value Decomposition of the **centered** data matrix **X**.

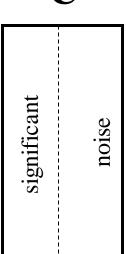
$$\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_m] \in \mathbb{R}^{N \times m}$$
,

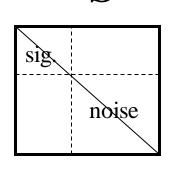
m: number of instances,

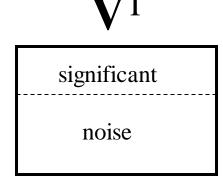
N: dimension

$$X_{N \times m} = U_{N \times N} S_{N \times m} V_{m \times m}^T \approx U_{N \times k} S_{k \times k} V_{k \times m}^T$$









主成分分析算法三(奇异值分解) PCA algorithm III (SVD of the data matrix)

Columns of U

- the principal vectors, $\{ \mathbf{u}^{(1)}, \dots, \mathbf{u}^{(k)} \}$
- orthogonal and has unit norm so $U^{T}U = I$
- Can reconstruct the data using linear combinations of { u⁽¹⁾, ..., u^(k) }

Matrix S

- Diagonal
- Shows importance of each eigenvector

Columns of V^T

The coefficients for reconstructing the samples

主成分个数 How many PCA components

Problem: How many to keep?

Many criteria.

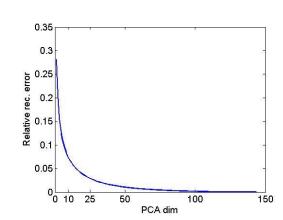
e.g. % total data variance:

 $\max(m) \ni \frac{\sum_{i=(m+1):n}^{l}}{\sum_{i} \lambda_{i}} < \varepsilon$

	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

L₂ error and PCA dim

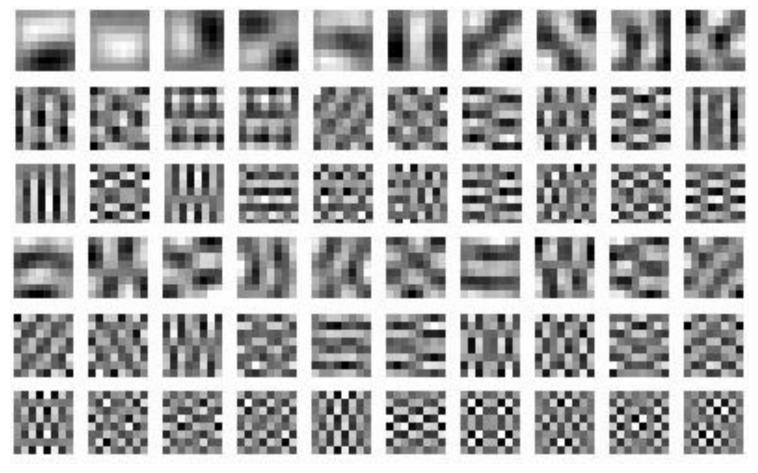


Original Image



- Divide the original 372x492 image into patches:
 - Each patch is an instance that contains 12x12 pixels on a grid
- View each as a 144-D vector.

60 most important eigenvectors:

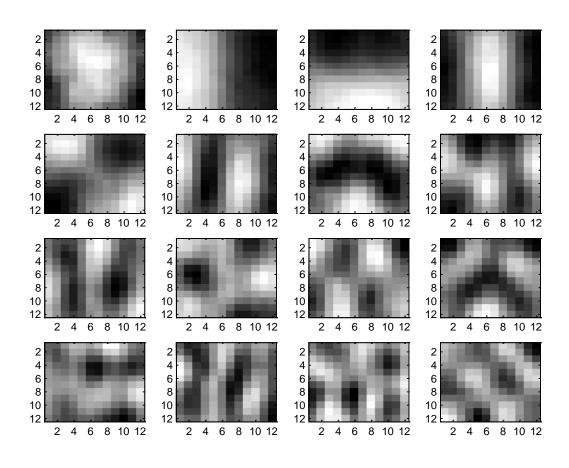


Looks like the discrete cosine bases of JPG!...

PCA compression: 144D) 60D



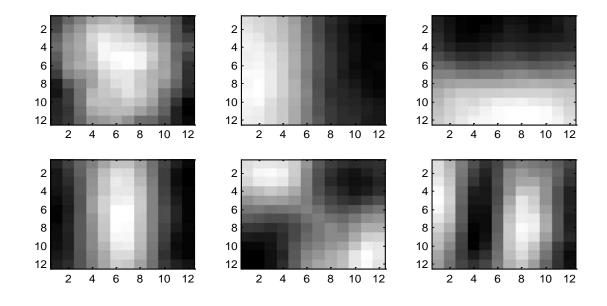
16 most important eigenvectors:



PCA compression: 144D) 16D



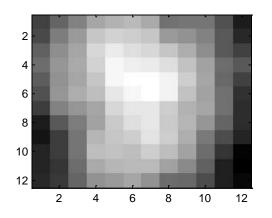
6 most important eigenvectors:

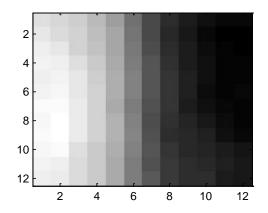


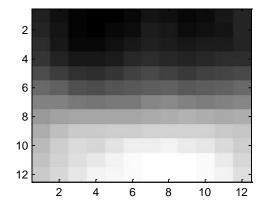
PCA compression: 144D)6D



3 most important eigenvectors:



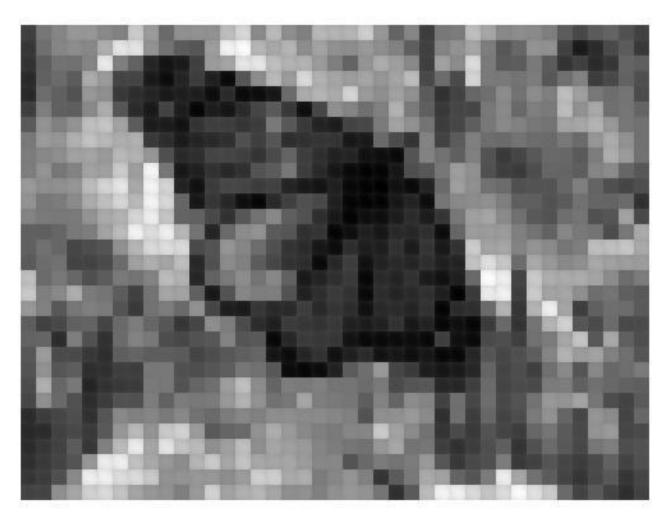




PCA compression: 144D)3D



PCA compression: 144D) 1D



主成分分析用于滤除噪声 PCA application: Noise Filtering



Noisy image

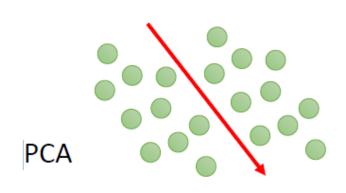
主成分分析用于滤除噪声 PCA application: Noise Filtering

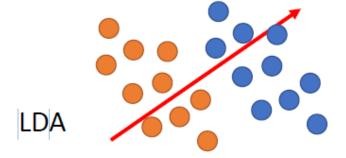


Denoised image using 15 PCA components

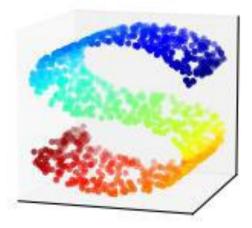
主成分分析弱点 Weakless of PCA

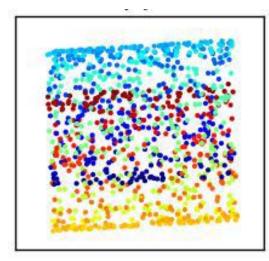
Unsupervised



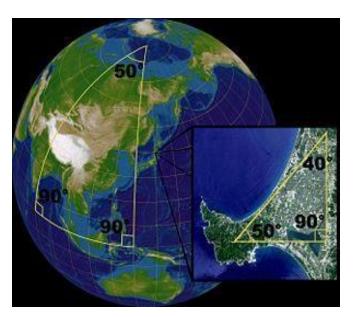


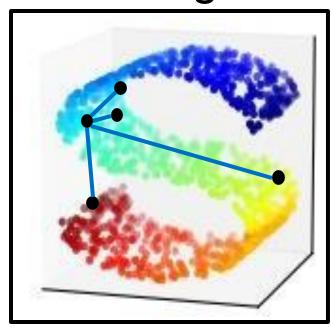
Linear:

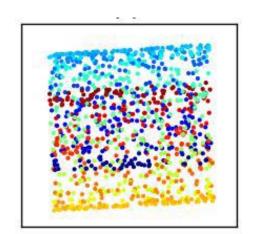


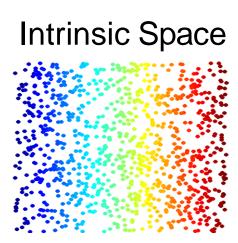


流形学习 Manifold Learning









t-分布领域嵌入算法(t-SNE)

T-distributed Stochastic NeighborEmbedding

Compute similarity between all pairs of x: $S(x^i, x^j)$

$$P(x^{j}|x^{i}) = \frac{S(x^{i}, x^{j})}{\sum_{k \neq i} S(x^{i}, x^{k})}$$

Compute similarity between all pairs of z: $S'(z^i, z^j)$

$$Q(z^{j}|z^{i}) = \frac{S'(z^{i}, z^{j})}{\sum_{k \neq i} S'(z^{i}, z^{k})}$$

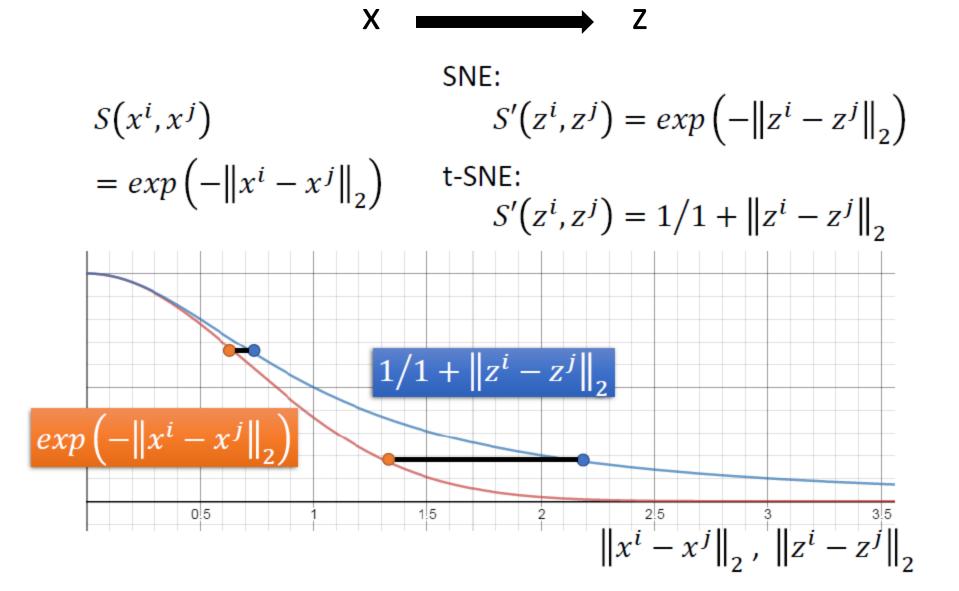
Find a set of z making the two distributions as close as possible

$$L = \sum_{i} KL(P(*|x^{i})||Q(*|z^{i}))$$

$$= \sum_{i} \sum_{j} P(x^{j}|x^{i}) log \frac{P(x^{j}|x^{i})}{Q(z^{j}|z^{i})}$$

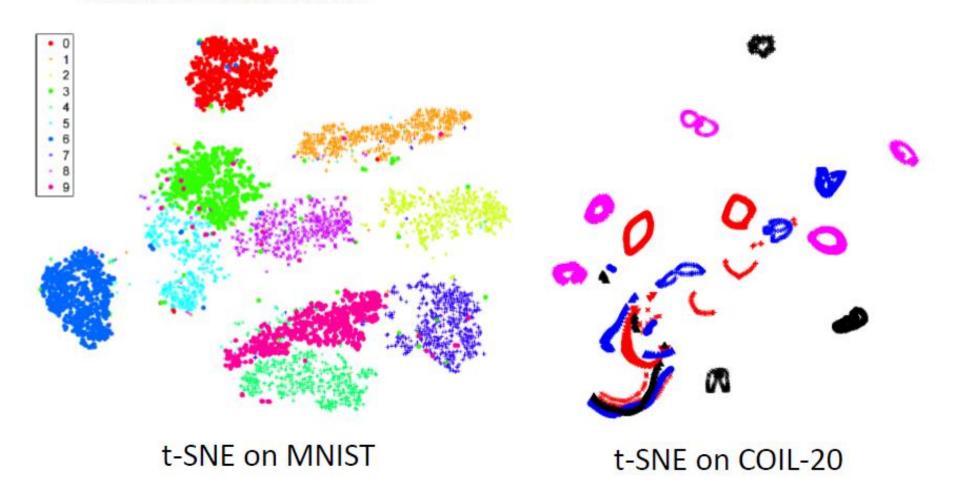
t-分布领域嵌入算法(t-SNE)

T-distributed Stochastic NeighborEmbedding

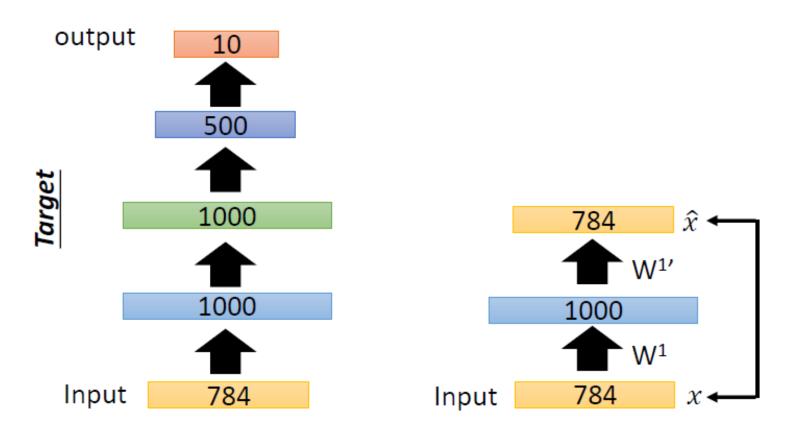


t-分布领域嵌入算法(t-SNE) T-distributed Stochastic NeighborEmbedding

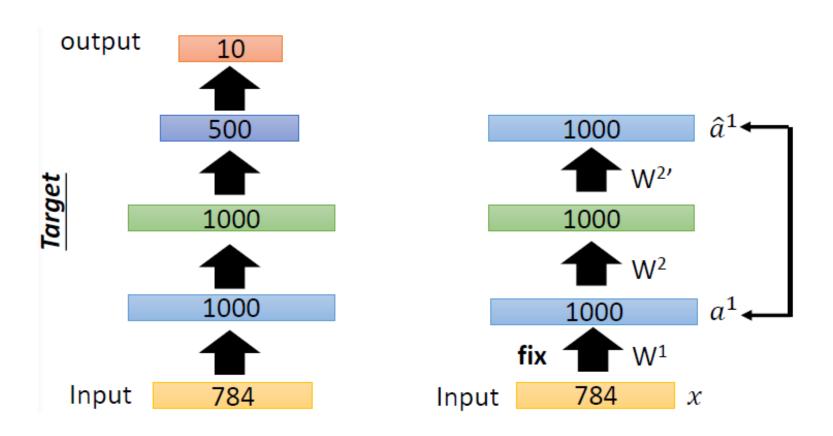
Good at visualization



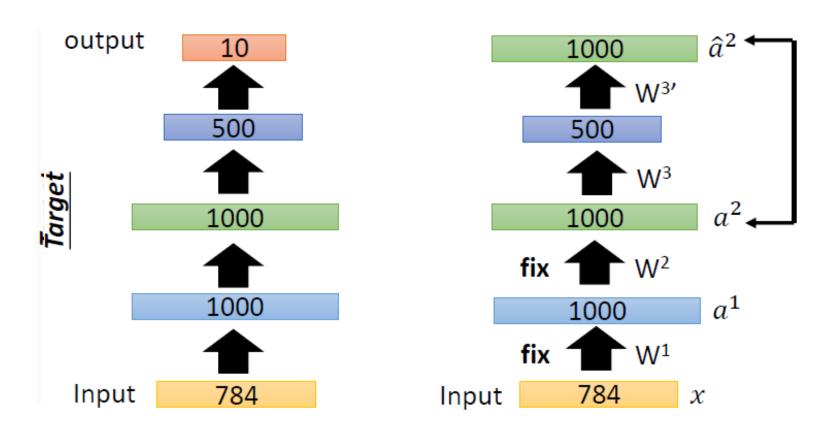
Greedy Layer-wise Pre-training again



Greedy Layer-wise Pre-training again

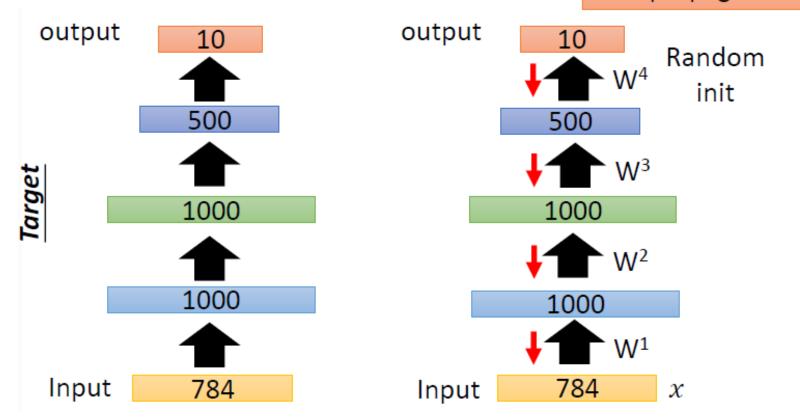


Greedy Layer-wise Pre-training again

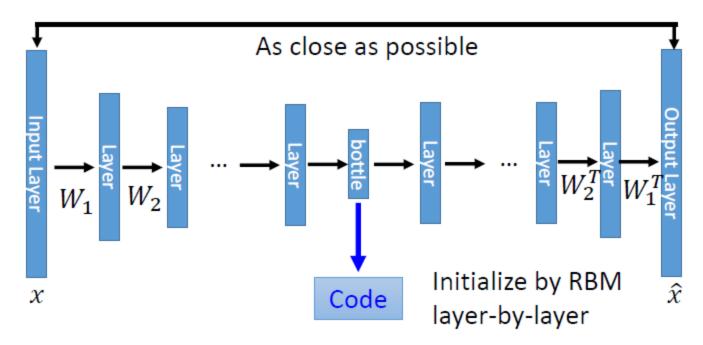


Greedy Layer-wise Pre-training again

Find-tune by backpropagation

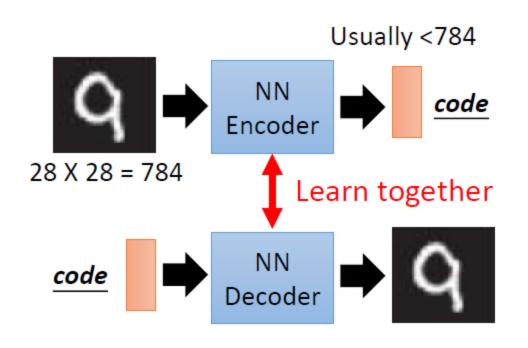


- An auto-encoder is an artificial neural net used for unsupervised learning of efficient codings.
- Greedy Layer-wise Pre-training again



use neural networks to recover the data

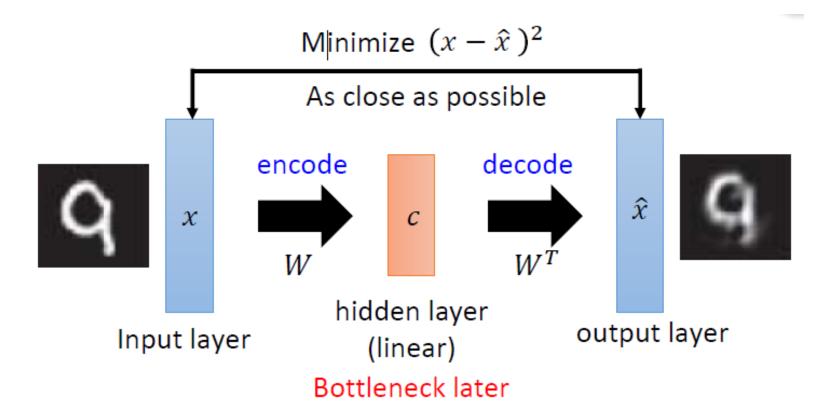
学习自编码器 Learning Auto-encoder



Compact representation of the input object

Can reconstruct the original object

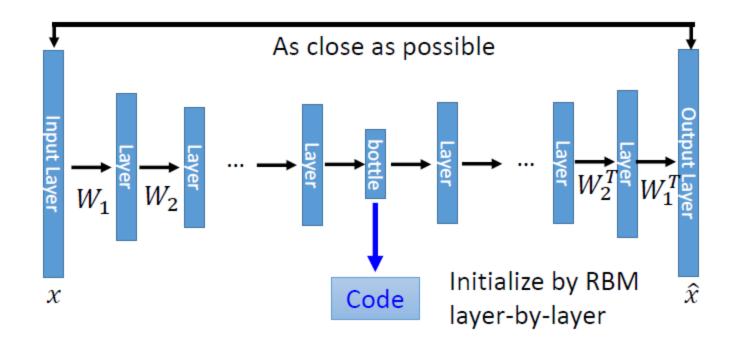
学习PCA Learning PCA



Output of the hidden layer is the code

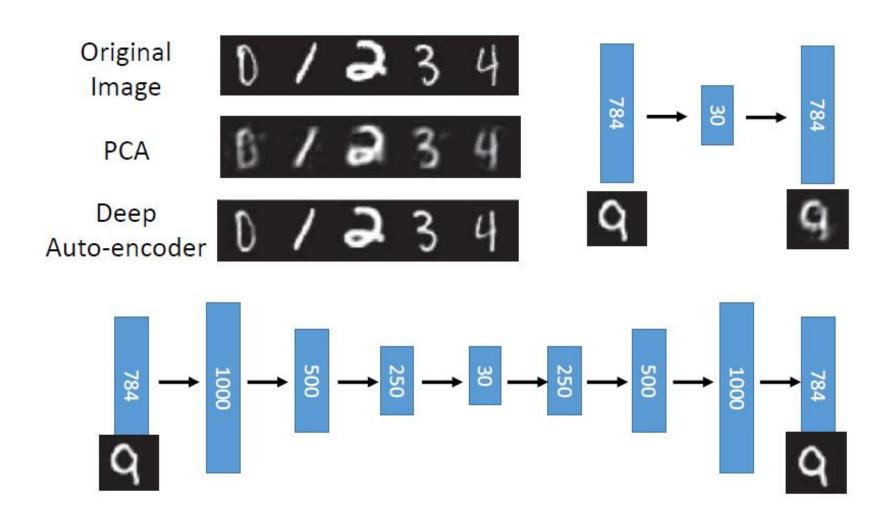
深度自编码器 Deep Auto-encoder

The auto-encoder can be deep

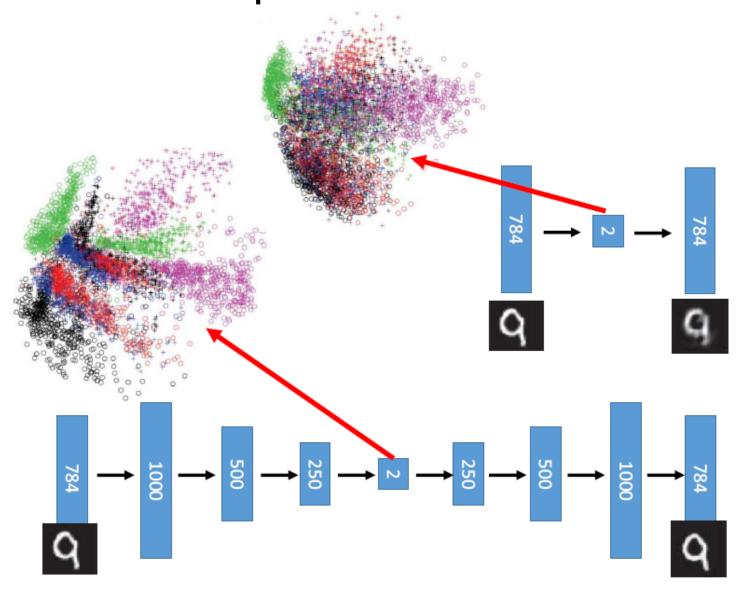


use neural networks to recover the data

深度自编码器 Deep Auto-encoder

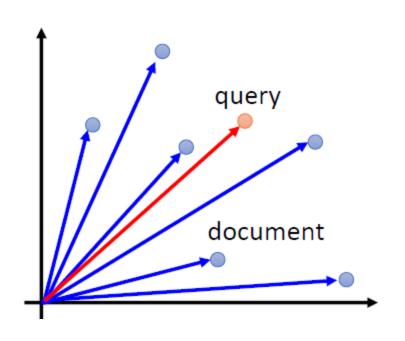


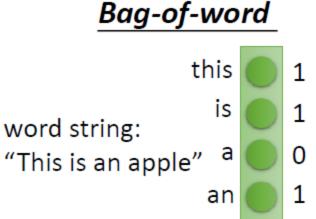
深度自编码器 Deep Auto-encoder



深度自编码器用于文本检索 Auto-encoder for Text Retrieval

Vector Space Model





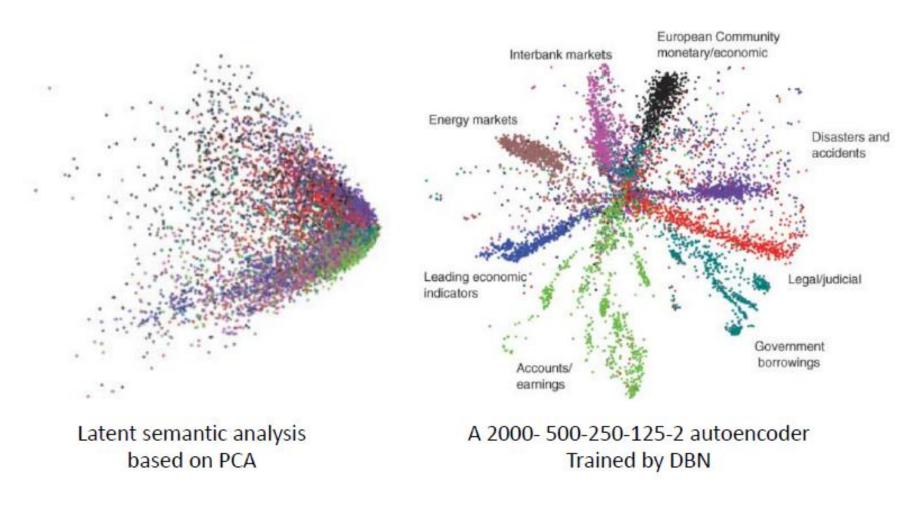
Semantics are not considered

apple

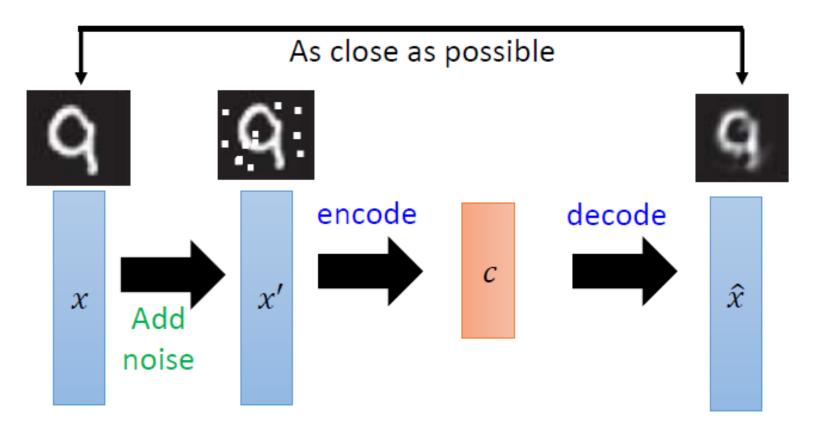
pen

0

深度自编码器用于文本检索 Auto-encoder for Text Retrieval

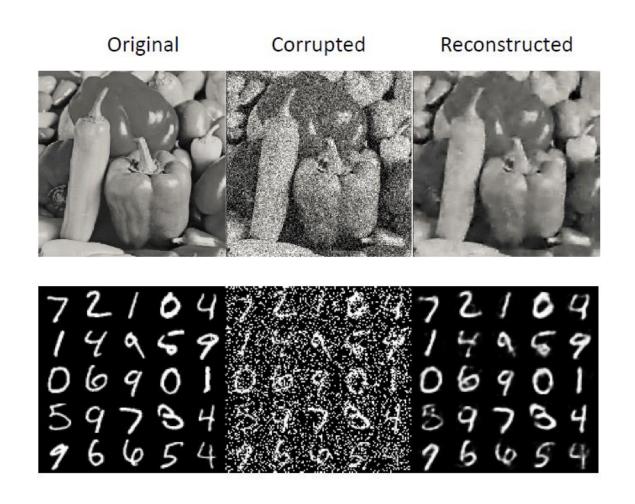


深度自编码器用于去噪声 Denoising Auto-Encoder Examples



Vincent, Pascal, et al. "Extracting and composing robust features with denoising autoencoders." *ICML*, 2008.

深度自编码器用于去噪声 Denoising Auto-Encoder Examples



PCA人脸分析 PCA on Face

$$= a_1 \underline{w}^1 + a_2 \underline{w}^2 + \cdots$$

30 components:







Eigen-digits

PCA人脸分析 PCA on Face



30 components:





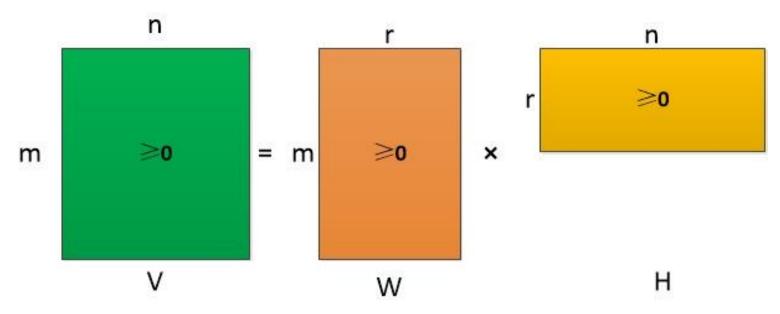


PCA结果 What happens to PCA

$$= \underline{a_1}w^1 + \underline{a_2}w^2 + \cdots$$
Can be any real number

- PCA involves adding up and subtracting some components (images)
 - Then the components may not be "parts of digits"
- Non-negative matrix factorization (NMF)
 - Forcing a_1 , a_2 be non-negative
 - additive combination
 - Forcing w^1 , w^2 be non-negative
 - More like "parts of digits"
- Ref: Daniel D. Lee and H. Sebastian Seung. "Algorithms for non-negative matrix factorization." Advances in neural information processing systems. 2001.

非负矩阵分解(NMF) Non-negative Matrix Factorization

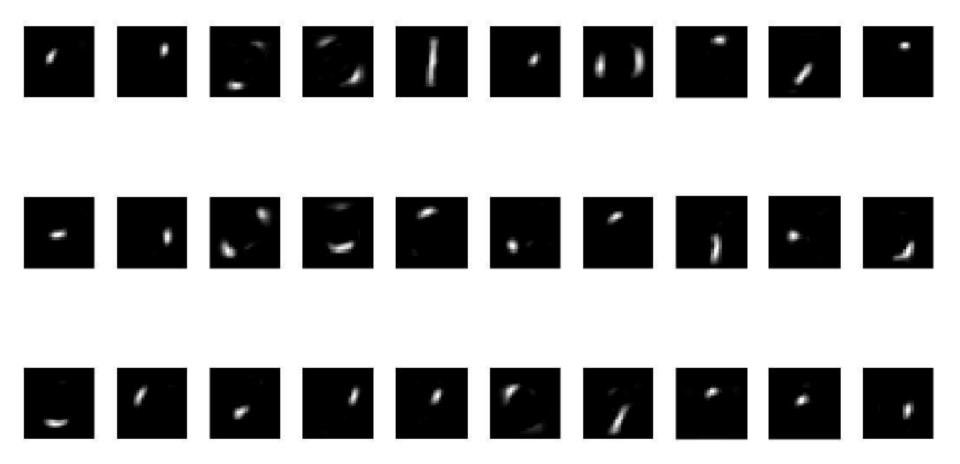


Non-negativity constraint offers physical and real-world interpretability!

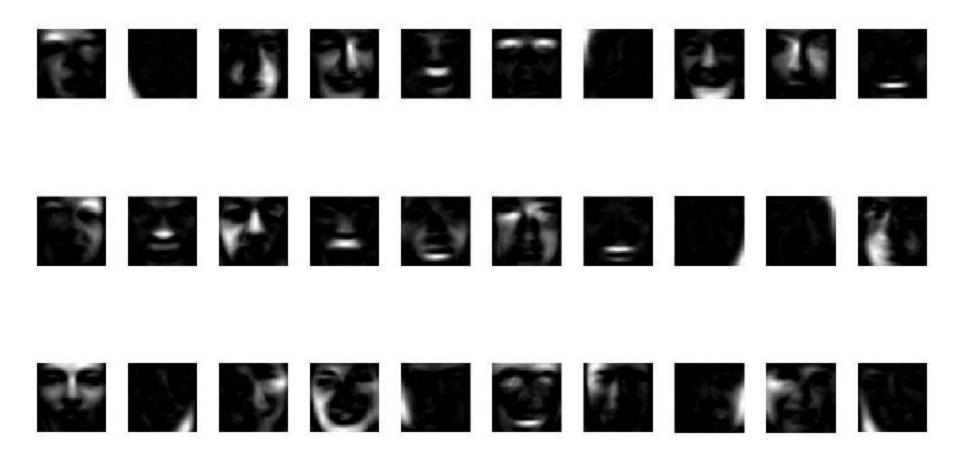
$$argmin\frac{1}{2}||X - WH||^2 = \frac{1}{2}\sum_{ij}(X_{ij} - WH_{ij})^2$$

$$argmin J(W, H) = \sum_{ij} \left(X_{ij} ln \frac{X_{ij}}{WH_{ij}} - X_{ij} + WH_{ij} \right)$$

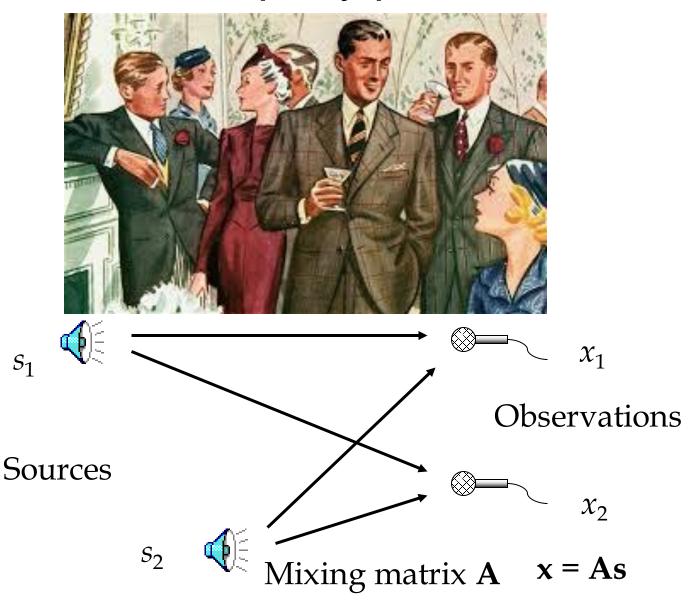
非负矩阵分解应用 NMF on MNIST



非负矩阵分解应用 NMF on Face



鸡尾酒会问题 Cocktail-party problem



鸡尾酒会问题 Cocktail-party problem

$$x_1(t) = a_{11}s_1(t) + a_{12}s_2(t)$$

$$x_2(t) = a_{21}s_1(t) + a_{22}s_2(t)$$

We observe

$$\begin{pmatrix} x_1(1) \\ x_2(1) \end{pmatrix}, \begin{pmatrix} x_1(2) \\ x_2(2) \end{pmatrix}, \dots, \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix}$$

We want

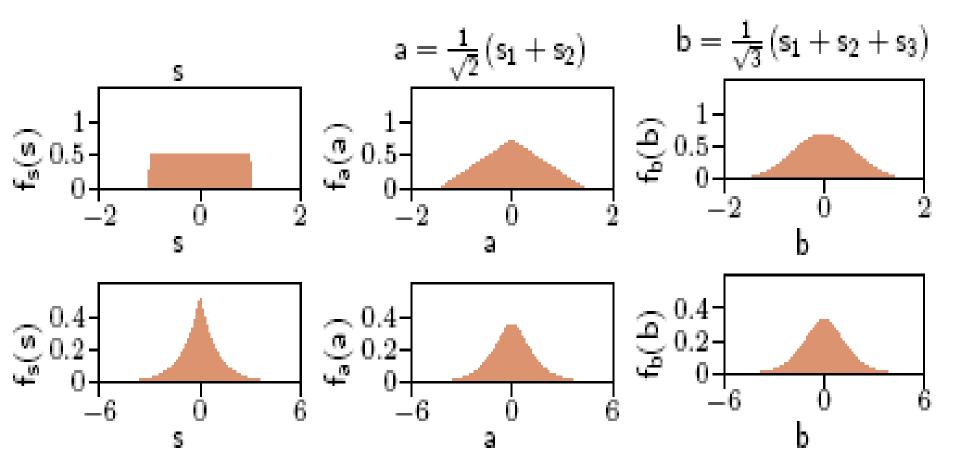
$$\begin{pmatrix} s_1(1) \\ s_2(1) \end{pmatrix}, \begin{pmatrix} s_1(2) \\ s_2(2) \end{pmatrix}, \dots, \begin{pmatrix} s_1(t) \\ s_2(t) \end{pmatrix}$$

But we don't know $\{a_{ij}\}$, nor $\{s_i(t)\}$

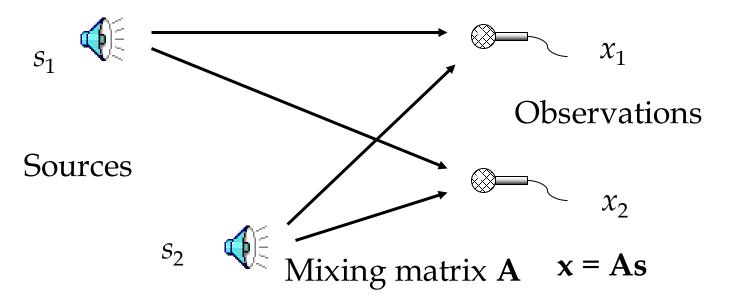
Goal: Estimate $\{s_i(t)\}$, (and also $\{a_{ij}\}$)

中心极限定理 Central Limit Theorem

The sum of independent variables converges to the normal distribution



ICA 假设 ICA Assumptions



- 1. $s_1,...s_K$ statistical Independence
- 2. Nongaussianity (at most one component is Gaussian)
- 3. A is column full-rank

ICA 原则 ICA Principal (Non-Gaussian is Independent)

$$y = w^T x = w^T A s = z^T s$$

- Key to estimating A is non-gaussianity
- y is a linear combination of s_i , with weights given by z_i .
- z^Ts is more gaussian than either of s_i . AND becomes least gaussian when its equal to one of s_i .
- So we could take w as a vector which maximizes the non-gaussianity of w^Tx .
- Such a w would correspond to a z with only one non zero comp. So we get back the s_i

非高斯性衡量

Measures of Non-Gaussianity

• Kurtotis : gauss=0 (sensitive to outliers)

$$kurt(y) = E\{y^4\} - 3(E\{y^2\})^2$$

Entropy : gauss=largest

$$H(y) = -\int f(y)\log f(y)dy$$

• Neg-entropy : gauss = 0 (difficult to estimate)

$$J(y) = H(y_{gauss}) - H(y)$$

Approximations

$$J(y) = \frac{1}{12}E\{y^2\}^2 + \frac{1}{48}kurt(y)^2$$
$$J(y) \approx \left[E\{G(y)\} - E\{G(y)\}\right]^2$$

where v is a standard gaussian random variable and :

$$G(y) = \frac{1}{a} \log \cosh(a.y)$$

$$G(y) = -\exp(-a.u^2/2)$$

FastICA算法 FastICA Algorithm

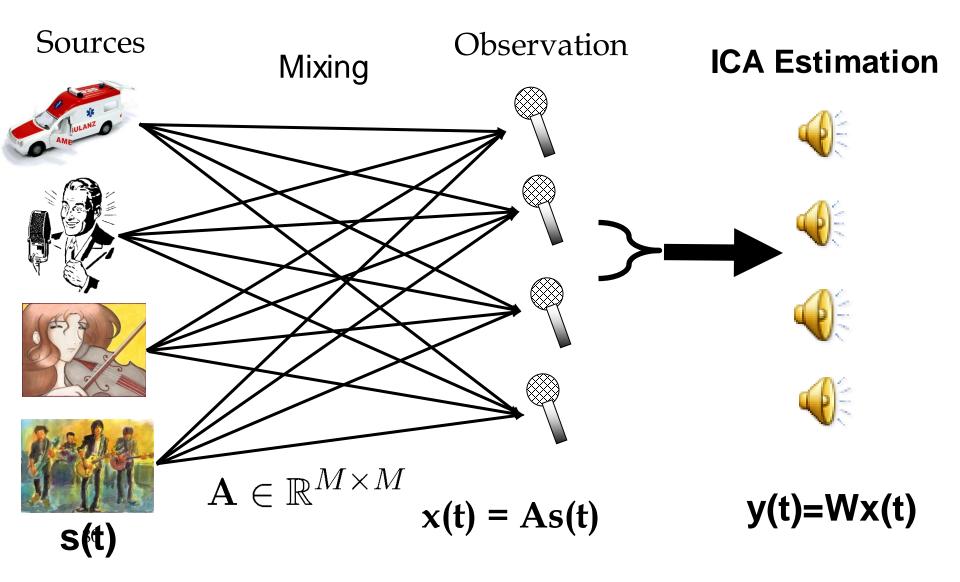
- Based on: W
- Basic form: $J(y) \approx [E\{G(y)\} E\{G(v)\}]^2$
 - Choose an initial (e.g. Random) weight vector

 - Let $w^+ = E\{xg(w^Tx)\} E\{g'(w^Tx)\}w$
 - If not converged, go back to step 2
- For several units: decorrelation

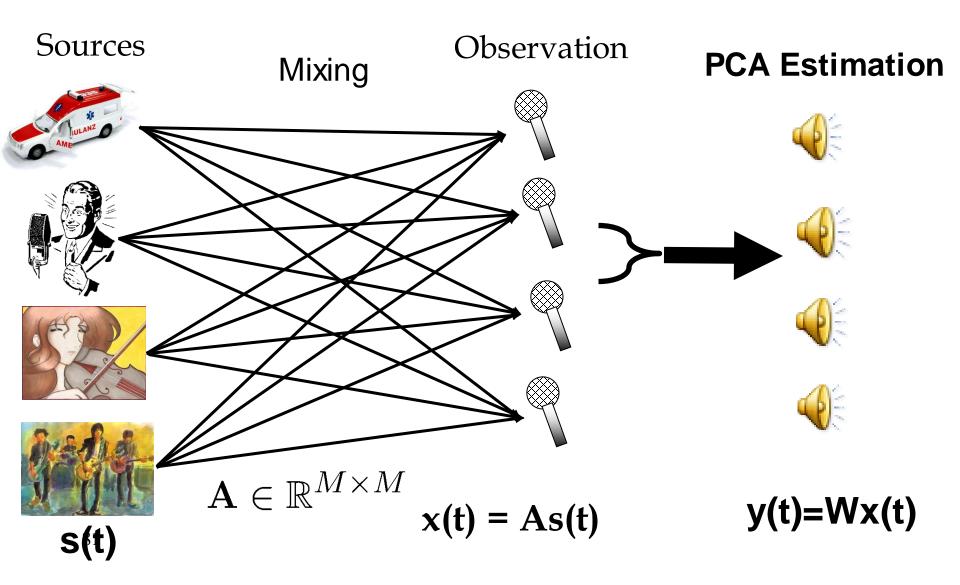
- Let
$$w_{p+1} = w_{p+1} - \sum_{j=1}^{p} w_{p+1}^{T} w_{j} w_{j}$$

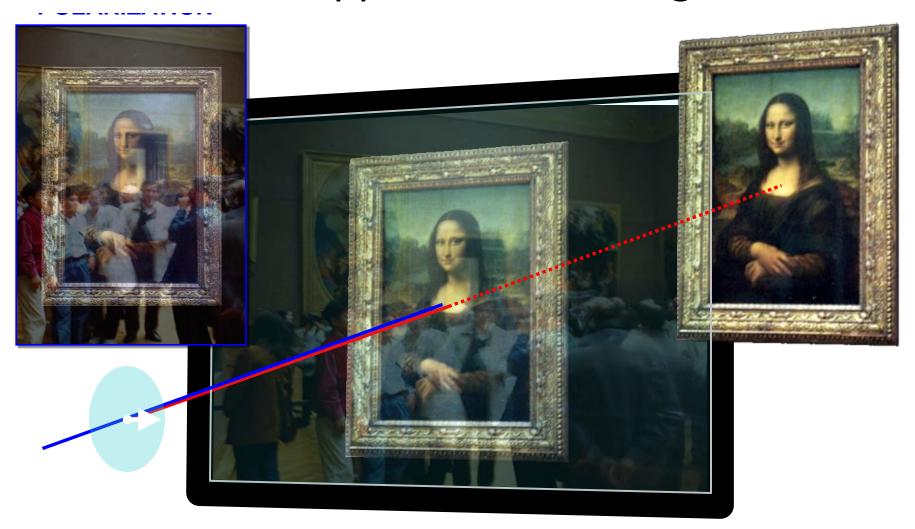
- Let
$$w_{p+1} = w_{p+1} / \sqrt{w_{p+1}^T w_{p+1}}$$

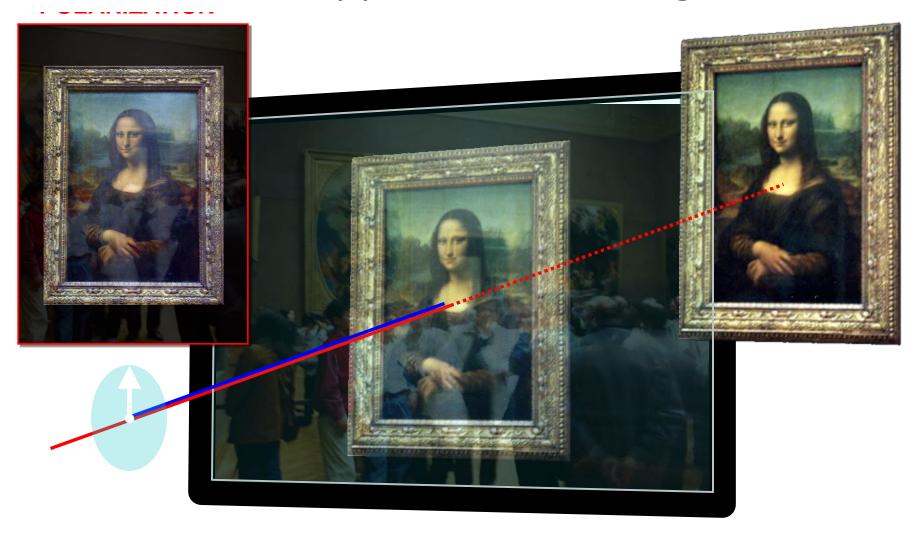
鸡尾酒会问题ICA求解 The Cocktail Party Problem Solving with ICA

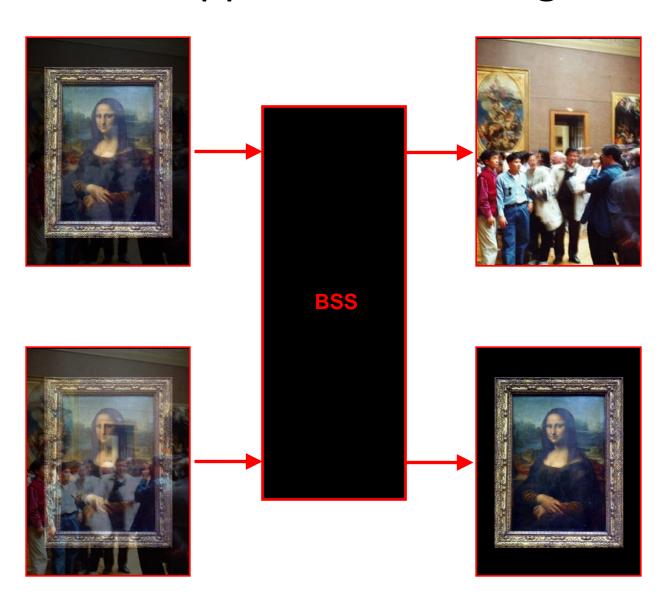


鸡尾酒会问题ICA求解 The Cocktail Party Problem Solving with PCA

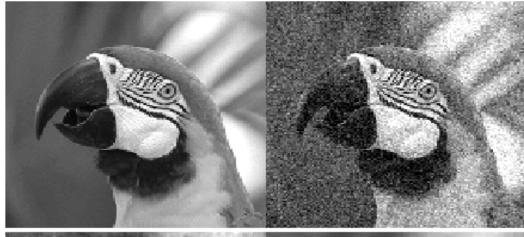






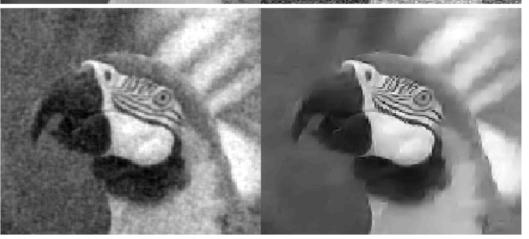


Original image



Noisy image

Wiener filtering

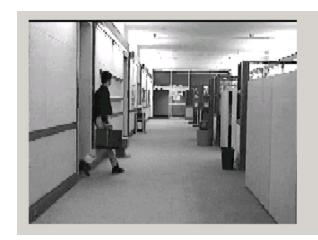


ICA filtering

视频问题ICA求解 ICA Application on Video



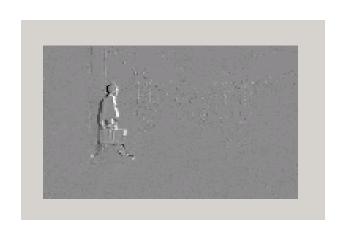






Source images

视频问题ICA求解 ICA Application on Video

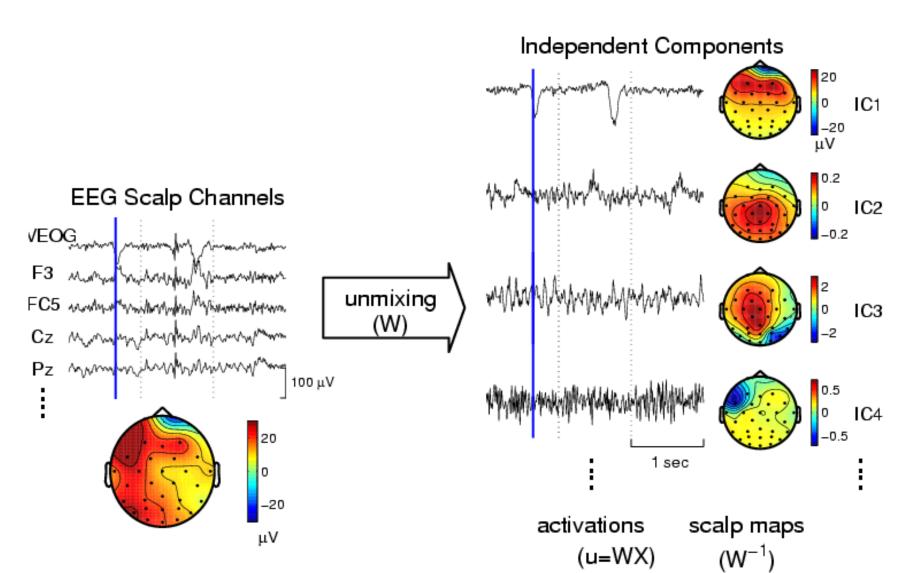




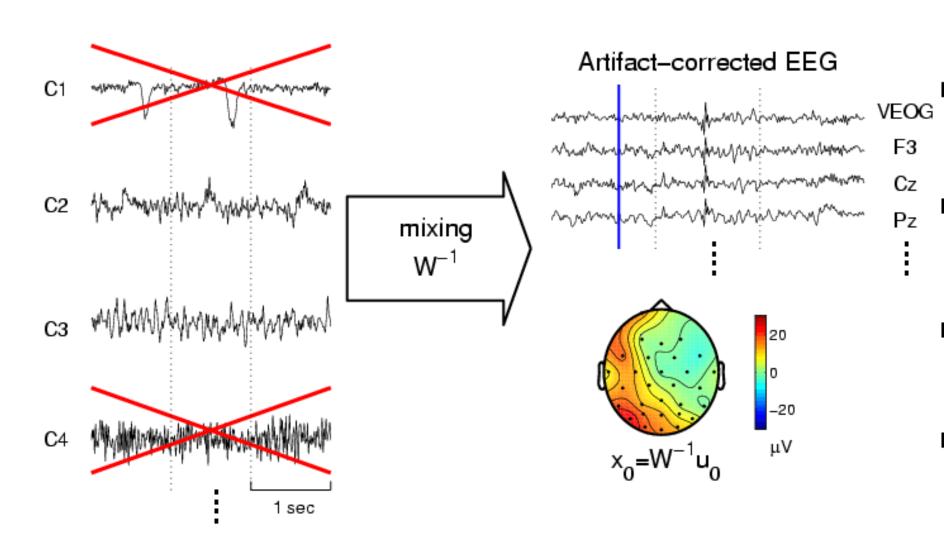
- EEG ~ Neural cocktail party
- Severe contamination of EEG activity by
 - eye movements
 - blinks
 - muscle
 - heart, ECG artifact
 - vessel pulse
 - electrode noise
 - line noise, alternating current (60 Hz)
- ICA can improve signal
 - effectively detect, separate and remove activity in EEG records from a wide variety of artifactual sources.
 - (Jung, Makeig, Bell, and Sejnowski)
- ICA weights help find location of sources

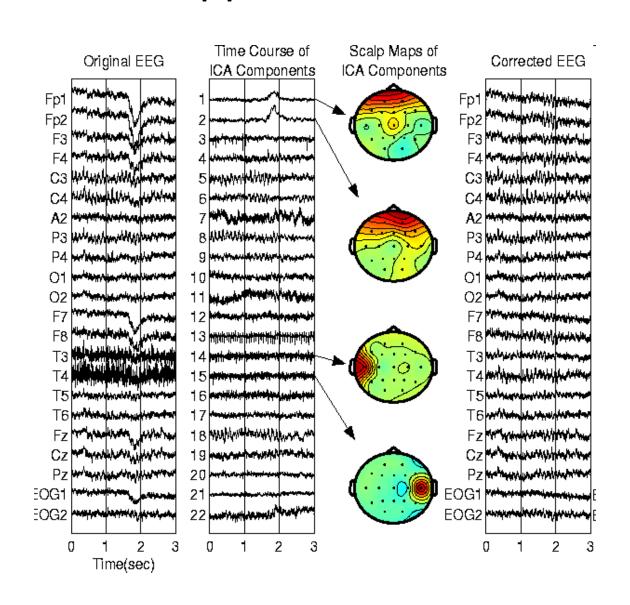


ICA decomposition



Summed Projection of Selected Components

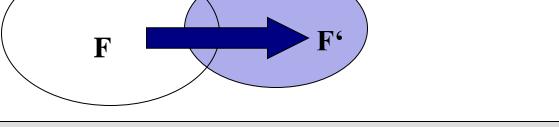




降维与特征选择

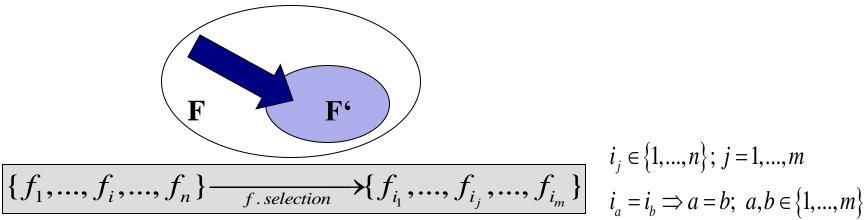
Dimensionality reduction & Feature selection

Dimensionality reduction: creating a subset of new features by combinations of the existing features



$$\{f_1,...,f_i,...,f_n\} \xrightarrow{f.extraction} \{g_1(f_1,...,f_n),...,g_j(f_1,...,f_n),...,g_m(f_1,...,f_n)\}$$

Feature Selection: choosing a subset of all the features

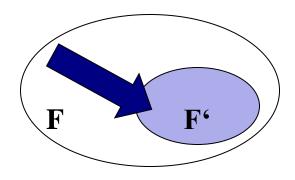


$$i_j \in \{1,...,n\}; j = 1,...,m$$

 $i_a = i_b \Rightarrow a = b; a,b \in \{1,...,m\}$

特征选择 Feature selection

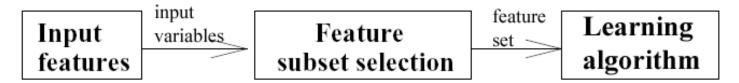
Find the optimal feature subset.



- Filter Methods
- Wrapper Methods
- Embedded Methods

过滤法 Filter Methods

Select subsets of variables as a pre-processing step, independently of the used classifier!!



Features could be evaluated by

- Distance
- Information
- dependency(correlation)
- ...

过滤法 Filter Methods

Relief (Relevant Features)

$$\delta^j = \sum_i -\operatorname{diff}(x_i^j, x_{i, \text{nh}}^j)^2 + \operatorname{diff}(x_i^j, x_{i, \text{nm}}^j)^2$$

• Fischer's ratio.
$$\frac{|S_b|}{|S_w|} = \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2}$$

information gain

$$Gain(A) = Ent(D) - \sum_{v=1}^{V} \frac{|D^v|}{|D|} Ent(D^v)$$

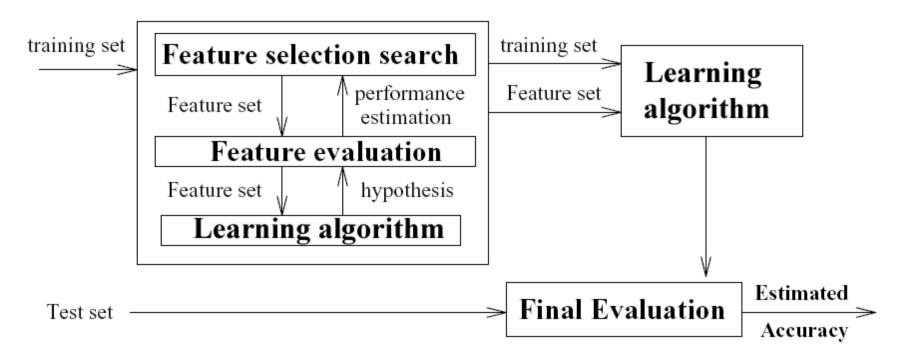
coefficient scores

$$\Re(i) = \frac{\operatorname{cov}(X_i, Y)}{\sigma(X_i) \times \sigma(Y)}$$

过滤法 Filter Methods

- usually fast
- provide generic selection of features
- feature set not optimized for used classifier
- sometimes used as a preprocessing step for other methods

包裹法 Wrapper Methods



Features could be evaluated by classifier error rate (the classifier themselves).

包裹法 Wrapper Methods

- The problem of finding the optimal subset is NP-hard!
- A wide range of heuristic search strategies can be used. Two different classes:
 - Forward selection (start with empty feature set and add features at each step)
 - Backward elimination (start with full feature set and discard features at each step)
- predictive power is usually measured on a validation set or by cross-validation
- By using the learner as a black box wrappers are universal and simple!
- Criticism: a large amount of computation is required.

嵌入法 Embedded Methods

Specific to a given learning machine!

- Performs feature selection (implicitly) in the process of training
- E.g. LASSO [Tibshirani, 1996]

$$\min_{oldsymbol{w}} \sum_{i=1}^m (y_i - oldsymbol{w}^ op oldsymbol{x}_i)^2 + \lambda \|oldsymbol{w}\|_1$$

Random Forest and Gradient Boosting

问题: 简述你所了解到的特征降 维的几种方法及其特点