Learning from Data
Lecture 10: Principal Component Analysis

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TBSI

December 2, 2022

Today's Lecture

Unsupervised Learning (Part II): PCA

- Motivation
- Linear PCA
- Kernel PCA

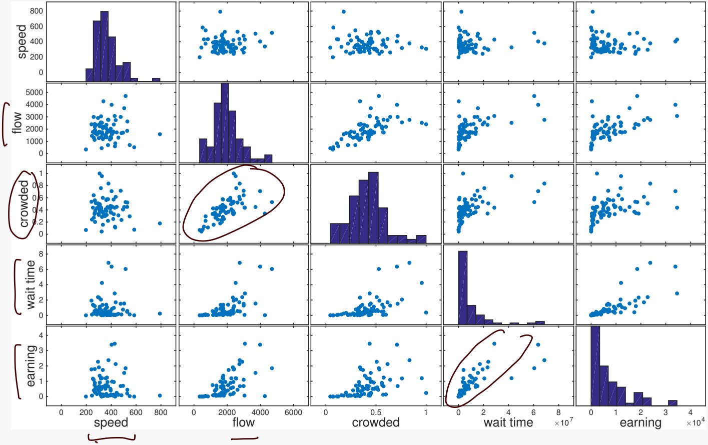
Motivation of PCA

Example: Analyzing San Francisco public transit route efficiency

features	notes
speed	average speed
flow	# boarding passengers per hour
crowded	% passenger capacity reached
wait time	average waiting time at bus stop
earning	net operation revenue
⋮	⋮

Motivation of PCA

Input features contain a lot of redundancy

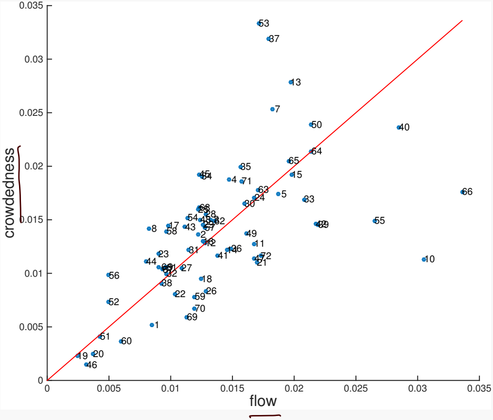


Scatter plot matrix reveals pairwise correlations among 5 major features

Motivation of PCA

Example of linearly dependent features

- Flow: average # boarding passengers per hour
- Crowdedness: $\frac{\text{average \# passengers on train}}{\text{train capacity}}$



Motivation of PCA

Example of linearly dependent features

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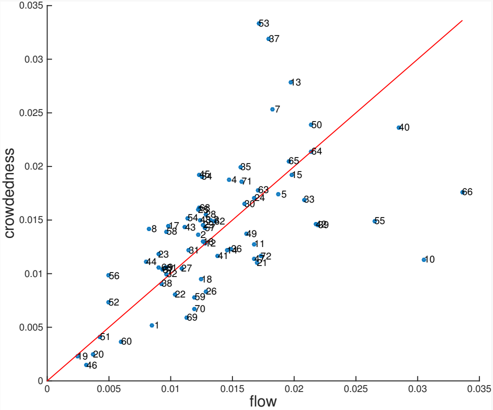


How can we automatically detect and remove this redundancy?

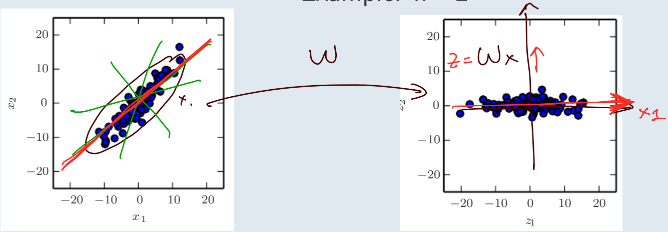
- geometric approach ← *start here!*
- diagonalize covariance matrix approach

How to remove feature redundancy?

Given $\{x^{(1)}, \ldots, x^{(m)}\}$, $x^{(i)} \in \mathbb{R}^n$.

- Find a linear, orthogonal transformation $W : \mathbb{R}^n \to \mathbb{R}^k$ of the input data
- W aligns the direction of maximum variance with the axes of the new space.

Example: $n = 2$



features x_1 and x_2 are strongly correlated

variations in $z = x^T W$ is mostly along the x-axis. *x can be represented in 1D!* z.

Direction of Maximum Variance

- Suppose $\mu = mean(x) = 0$, $\sigma_j = var(x_j) = 1$ (variance of jth feature)

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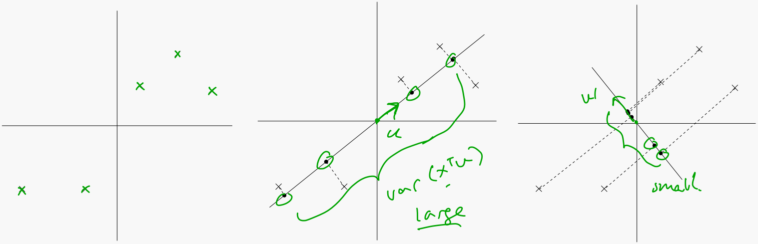
- Find **major axis of variation** unit vector u:



input observations

projections on u have large variance

projections on u have small variance

u maximizes the variance of the projections

Principal Component Analysis (PCA)

Pearson, K. (1901), Hotelling, H. (1933) "Analysis of a complex of statistical variables into principal components". Journal of Educational Psychology.

PCA goals

- Find principal components $u_1, \dots, u_n$ that are mutually orthogonal (uncorrelated)
- Most of the variation in x will be accounted for by k principal components where $k \ll n$.

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- Find principal components $u_1, \ldots, u_n$ that are mutually orthogonal (uncorrelated)
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Main steps of (full) PCA:

1. Standardize x such that $Mean(x) = 0$, $Var(x_j) = 1$ for all j
2. Find projection of x, $u_1^T x$ with maximum variance
3. For $j = 2, \ldots, n$,
   Find another projection of x, $u_j^T x$ with maximum variance, where u_j is orthogonal to $u_1, \ldots, u_{j-1}$

u1 : 1st principal component.

Step 1: Standardize data

Normalize x such that $\underline{Mean(x) = 0}$ and $\underline{Var(x_j) = 1}$

$$x^{(i)} := \underline{x^{(i)} - \mu} \leftarrow \text{recenter}$$

$$\underline{x_j^{(i)} := x_j^{(i)}/\sigma_j} \leftarrow \text{scale by } stdev(x_j)$$

Check:

$$\frac{x_j^{(i)}}{\sigma_j} - \frac{\mu_j}{\sigma_j} \qquad \sigma_j = Var(x_j)$$

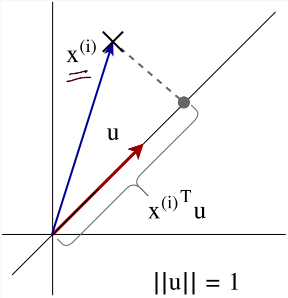
$$\underline{var\left(\frac{x_j}{\sigma_j}\right)} = \underline{\frac{1}{m}\sum_{i=1}^{m}}\left(\frac{x_j^{(i)} - \mu_j}{\sigma_j}\right)^2 = \boxed{\frac{1}{\sigma_j^2}}\underbrace{\frac{1}{m}\sum_{i=1}^{m}\left(x_j^{(i)} - \mu_j\right)^2}_{\sigma_j^2}$$

$$\underline{= \frac{1}{\sigma_j^2}\sigma_j^2 = 1}$$

Step 2: Find Projection with Maximum Variance

$$X = \underbrace{\begin{bmatrix} -x^{(1)}- \\ -x^{(2)}- \\ \vdots \\ x^{(m)} \end{bmatrix}}_{n.} \Big\} m \qquad \underset{(n\times n)}{\mathrm{Cov}(X)} = \begin{bmatrix} \sigma_{11}^2 & \sigma_{12}^2 & & \\ & \sigma_{12}^2 & & \\ & & \ddots & \\ & & & \sigma_{nn}^2 \end{bmatrix}$$

Since $\underline{\|u\| = 1}$, the length of $x^{(i)}$'s projection on u is $\underline{{x^{(i)}}^T u}$.



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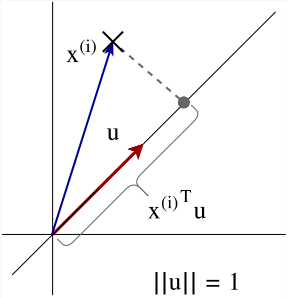

Variance of the projections:

$$\underline{\frac{1}{m}\sum_{i=1}^{m}({x^{(i)}}^T u - \underline{0})^2} = \frac{1}{m}\sum_{i=1}^{m}\underline{u^T x^{(i)} {x^{(i)}}^T} u$$

Step 2: Find Projection with Maximum Variance

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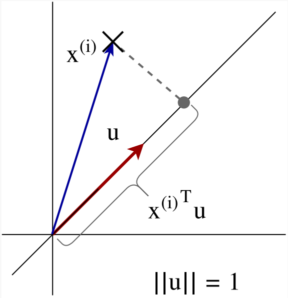

Variance of the projections:

$$\frac{1}{m}\sum_{i=1}^{m}\left({x^{(i)}}^T u - 0\right)^2 = \frac{1}{m}\sum_{i=1}^{m} \underline{u}^T x^{(i)} {x^{(i)}}^T \underline{u}$$

$$= u^T \left(\underbrace{\frac{1}{m}\sum_{i=1}^{m} x^{(i)} {x^{(i)}}^T}_{cov(x) = \Sigma}\right) u$$

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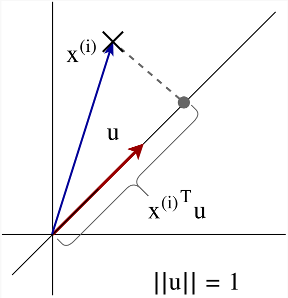

Variance of the projections:

$$\frac{1}{m}\sum_{i=1}^{m}({x^{(i)}}^T u - 0)^2 = \frac{1}{m}\sum_{i=1}^{m} u^T x^{(i)} {x^{(i)}}^T u$$

$$= u^T \left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)} {x^{(i)}}^T\right) u$$

$$= u^T \Sigma u$$

Σ : the sample covariance matrix of $x^{(1)} \dots x^{(m)}$.

1st Principal Component

Find unit vector u_1 that maximizes variance of projections:

$$\underline{u_1} = \underset{u:\underline{\|u\|=1}}{\operatorname{argmax}}\ \underline{u}^T \Sigma u \tag{1}$$

(definition)

$\underline{u_1}$ is the **1st principal component** of X

u_1 can be solved using optimization tools, but it has a more efficient solution:

Proposition 1

$\underline{u_1}$ is the largest eigenvector of covariance matrix Σ

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Proof. $\square$

$\max u^T\Sigma u \Rightarrow. \min -\underline{u^T\Sigma u}$

$\|u\|=1.$

↑

$\underline{u^Tu-1=0}$

Proposition 1

u_1 is the largest eigenvector of covariance matrix $\underline{\Sigma}$

Proof. Generalized Lagrange function of Problem **??**:

$$L(u) = \underline{-u^T\Sigma u + \bigcirc\!\!\!\!\beta\,(u^Tu-1)}$$

Proposition 1

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Proof. Generalized Lagrange function of Problem ??:

$$L(u) = -u^T \Sigma u + \underline{\beta(u^T u} - 1)$$

To minimize $L(u)$,

$$\frac{\delta L}{\delta u} = -2\Sigma u + 2\beta u = 0 \Longrightarrow \underline{\Sigma u = \underline{\beta} u}$$

Therefore u_1 must be an eigenvector of Σ.

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Therefore u_1 must be an eigenvector of Σ.
Let $u_1 = \boxed{v_j,}$ the eigenvector with the jth largest eigenvalue $\underline{\lambda_j}$,

$$\underline{u_1^T \Sigma u_1} = \underline{v_j^T \overset{\lambda v_j}{\Sigma v_j}} = \underline{\lambda_j v_j^T v_j} = \underline{\lambda_j}.$$

Hence $\underline{u_1} = \underline{v_1}$, the eigenvector with the largest eigenvalue $\underline{\lambda_1}$. □

Proposition 2

The j**th principal component** *of* X , u_j *is the* j*th largest eigenvector of* Σ *.*

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Proof. Consider the case $\underline{j = 2,}$

$$u_2 = \underset{\underline{u}:\|u\|=1,\boxed{u_{\mathbf{1}}^T u=0}}{\operatorname{argmax}} u^T \Sigma u \tag{2}$$

Proposition 2

The jth **principal component** *of X, u_j is the jth largest eigenvector of Σ.*

Proof. Consider the case $j = 2$,

$$u_2 = \underset{u:\|u\|=1,\underline{u_1^T u=0}}{\operatorname{argmax}} u^T \Sigma u \qquad (2)$$

The Lagrangian function:

$$L(u) = -u^T \Sigma u + \beta_1(u^T u - 1) + \underline{\beta_2(u_1^T u)}$$

$$\downarrow$$

Minimizing $L(u)$ yields:

$$\underline{\beta_2 = 0}, \underline{\underline{\Sigma u = \beta_1 u}}$$

$$\frac{\partial L(u)}{\partial u} = -2\Sigma u + 2\beta_1 u = 0.$$

$$\Sigma u = \beta_1 u.$$

$$\frac{\partial L(u)}{\partial u} = -2\Sigma u + 2\beta_1 u + \beta_2 u_1 = 0.$$

Multiply by u_1^T : $-2\,\underline{u_1^T \Sigma u} + 2\beta_1 u_1^T u + \beta_2 u_1^T u_1 = 0.$

$$\Rightarrow \underbrace{\lambda u_1^T u}_{=0} + 2\beta_1 \underbrace{u_1^T u}_{=0} + \beta_2 \underbrace{u_1^T u_1}_{1} = 0.$$

$$\beta_2 = 0.$$

$$\left(\frac{\partial L}{\partial \beta_2} = 0 \Rightarrow u_1^T u = 0\right)$$

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The Lagrangian function:

$$L(u) = -u^T \Sigma u + \beta_1 (u^T u - 1) + \beta_2 (u_1^T u)$$

Minimizing $L(u)$ yields:

$$\beta_2 = 0, \Sigma u = \beta_1 u$$

To maximize $\underline{u^T \Sigma u =} \lambda$, u_2 must be the eigenvector with the second largest eigenvalue $\beta_1 = \lambda_2$. The same argument can be generalized to cases $j > 2$. *(Use induction to prove for* $j = 1 \dots n$ *)* □

Summary

We can solve PCA by solving an eigenvalue problem!
Main steps of (full) PCA:

1. Standardize x such that $Mean(x) = 0, Var(x_j) = 1$ for all j
2. Compute $\Sigma = cov(x)$
3. Find principal components $u_1, \dots, u_n$ by eigenvalue decomposition: $\Sigma = U \Lambda U^T$. $\leftarrow$ *U is an orthogonal basis in $\mathbb{R}^n$*

Next we project data vectors x to this new basis, which spans the **principal component space**.

PCA Projection

- Projection of sample $\underline{x} \in \mathbb{R}^n$ in the principal component space:

projection ↓

$$\underline{z^{(i)}} = \begin{bmatrix} {x^{(i)}}^T \underline{u_1} \\ \vdots \\ {x^{(i)}}^T \underline{u_n} \end{bmatrix} \in \mathbb{R}^n$$

PCA Projection

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- Matrix notation:

$$z^{(i)} = \begin{bmatrix} | & & | \\ u_1 & \dots & u_n \\ | & & | \end{bmatrix}^T x^{(i)} = U^T x^{(i)}, \text{ or } Z = XU$$

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- The truncated transformation $Z_k = XU_k$ keeping only the first k principal components is used for **dimension reduction**.

Properties of PCA

- The variance of principal component projections are

$$\text{Var}(\underline{x^T u_j}) = \underline{{u_j}^T \overset{\swarrow\ \text{cov}(x)}{\Sigma} u_j} = \underline{\lambda_j} \text{ for } j = 1, \ldots, n$$

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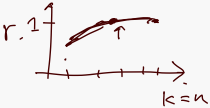
Var

- % of variance explained by the jth principal component: $\frac{\lambda_j}{\boxed{\sum_{i=1}^{n} \lambda_i}}$.

  i.e. projections are uncorrelated

Properties of PCA



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r. - % of variance accounted for by retaining the first k principal components $(\underline{k \leq n})$: $\dfrac{\sum_{j=1}^k \lambda_j \}}{\sum_{j=1}^n \lambda_j \}}$ var. of first k. pc projections.

Another geometric interpretation of PCA is minimizing projection residuals. (see homework!)

Covariance Interpretation of PCA

$x = \mathrm{cov}(x) = \Sigma$

PCA removes the “redundancy” (or noise) in input data X:

Let $\underline{Z} = \underline{\boxed{X}U}$ be the PCA projected data,

$$\underline{\mathrm{cov}(Z)} = \frac{1}{m}\underline{Z^TZ} = \frac{1}{m}\underline{(XU)}^T\underline{(XU)} = \underline{U}^T\underbrace{\left(\frac{1}{m}X^TX\right)}_{\Sigma}\underline{U} = \underline{U^T\overset{\overset{\mathrm{cov}(x)}{\downarrow}}{\Sigma}}U$$

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Since Σ is symmetric, it has real eigenvalues. Its eigen decomposition is

$$\Sigma \underline{= U \Lambda U^T}$$

where

$$\underline{U} = \begin{bmatrix} | & & | \\ \underline{u_1} & \dots & \underline{u_n} \\ | & & | \end{bmatrix}, \Lambda = \begin{bmatrix} \underline{\lambda_1} & & \\ & \ddots & \\ & & \underline{\lambda_n} \end{bmatrix}$$

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Then

$$\underline{\text{cov}(Z)} = \underline{\underbrace{U^T(U}_{I}\Lambda\underbrace{U^T)U}_{I}} = \underline{\Lambda}$$

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Then

$$\mathrm{cov}(Z) = U^T(U\Lambda U^T)U = \Lambda$$

The principal component transformation XU diagonalizes the sample covariance matrix of X

Linear PCA Review

PCA Dimension reduction

- Find principal components $\underline{u_1}, \dots, \underline{u_n}$ that are mutually orthogonal (uncorrelated)
- Most of the variations in x will be accounted for by k principal components where $k \ll n$.

Main steps

1. Standardize x such that $Mean(x) = 0, Var(x_j) = 1$ for all j
2. Compute $\underline{\Sigma = cov}(x)$
3. Find principal components $u_1, \dots, u_n$ by eigenvalue decomposition: $\underline{\Sigma = U\Lambda U}^T$. ← *$U$ is an orthogonal basis in $\mathbb{R}^n$*
4. Project data on first the k principal components: $\underline{z = [x^T u_1, \dots, x^T u_k]^T}$

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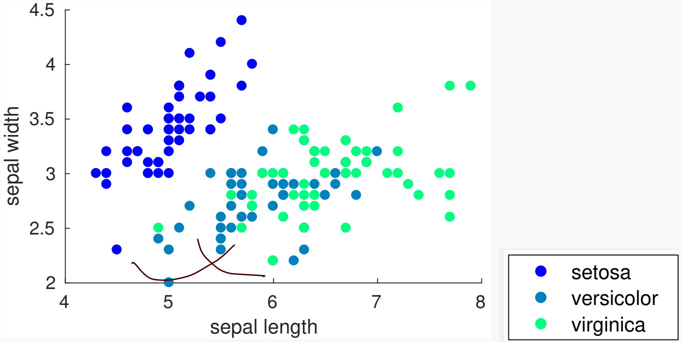
PCA Example: Iris Dataset

- 150 samples
- input feature dimension: 4

First two input attributes



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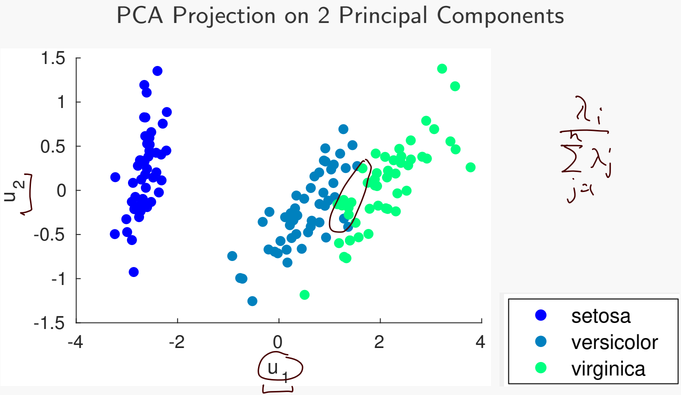

PCA Projection on 2 Principal Components

$$\frac{\lambda_i}{\sum_{j=1}^{n} \lambda_j}$$

% of variance explained by PC1: 73%, by PC2: 22% 95%

PCA Example: Eigenfaces

Learning image representations for face recognition using PCA [Turk and Pentland CVPR 1991]

$$x^{(i)} = \left[\quad\right] \Big\} \underline{900}$$

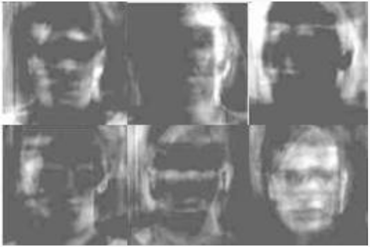
Training data

↓

30×30

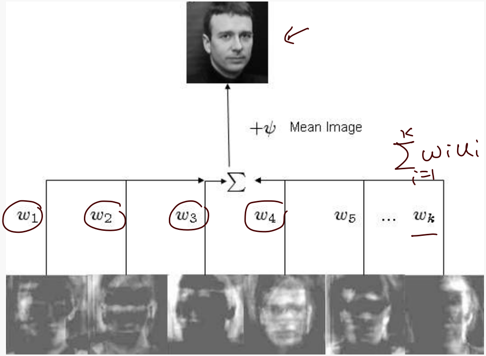
Eigenfaces: k principal components

$\underline{u_1}$ u_2 u_3.



PCA Example: Eigenfaces

Each face image is a linear combination of the **eigenfaces** (principal components)



$\sum_{i=1}^{k} w_i u_i + \psi.$

Each image is represented by k weights

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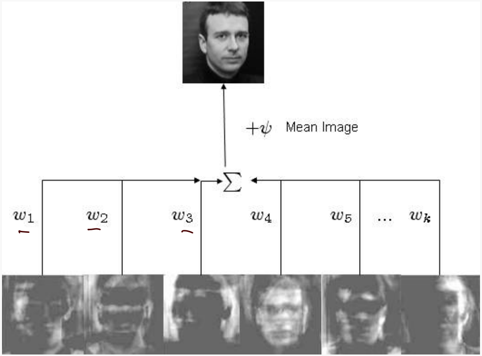
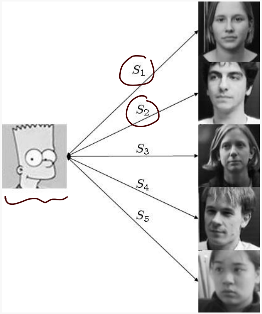


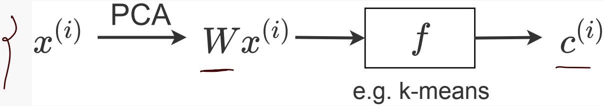
Each image is represented by k weights

Recognize faces by classifying the weight vectors. e.g. k-Nearest Neighbor



Kernel PCA

Feature extraction using PCA



Linear PCA assumes data are separable in $\mathbb{R}^n$

Kernel PCA

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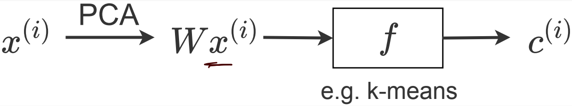

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A non-linear generalization

- Project data into higher dimension using feature mapping $\phi : \underline{\mathbb{R}^n} \to \underline{\mathbb{R}^d}$ $(\underline{d \geq n})$

Kernel PCA

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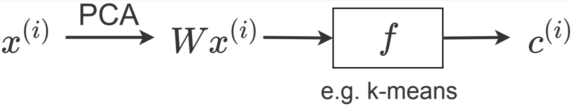

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A non-linear generalization

- Project data into higher dimension using feature mapping $\phi : \mathbb{R}^n \to \mathbb{R}^d \ (d \geq n)$
- Feature mapping is defined by a kernel function $\underline{K\left(x^{(i)}, x^{(j)}\right) = \phi(x^{(i)})^T \phi(}x^{(j)})$ or kernel matrix $K \in \mathbb{R}^{m \times m}$

Kernel PCA

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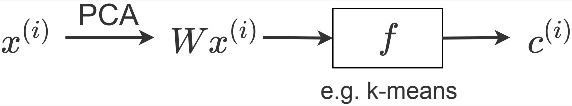

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A non-linear generalization

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- Feature mapping is defined by a kernel function $K\left(x^{(i)}, x^{(j)}\right) = \phi(x^{(i)})^T \phi(x^{(j)})$ or kernel matrix $K \in \mathbb{R}^{m \times m}$
- We can now perform standard PCA in the feature space

Kernel PCA

(Bernhard Schoelkopf, Alexander J. Smola, and Klaus-Robert Mueller. 1999. *Kernel principal component analysis*. In Advances in kernel methods) Sample covariance matrix of feature mapped data (assuming $\phi(x)$ is centered)

$$\underline{\Sigma} = \frac{1}{m}\sum_{i=1}^{m}\underline{\phi(x^{(i)})}\,\underline{\phi(x^{(i)})}^T \in \underline{\mathbb{R}^{d\times d}}$$

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How to avoid evaluating $\phi(x)$ explicitly?

The Kernel Trick

Represent projection $\phi(x^{(l)})^T u_k$ using kernel function K:

- Write $\underline{u_k}$ as a linear combination of $\underline{\phi(x^{(1)})}, \ldots, \underline{\phi(x^{(m)})}$:

$$\underline{u_k} = \sum_{i=1}^{m} \alpha_k^i \underline{\phi(x^{(i)})}$$

$$\Sigma u_k = \lambda_k u_k$$

$$\left(\frac{1}{m} \sum_{i=1}^{m} \phi(x^{(i)}) \phi(x^{(i)})^T \right) u_k = \lambda_k u_k.$$

$$\frac{1}{m \lambda_k} \sum_{i=1}^{m} \underbrace{\phi(x^{(i)}) \phi(x^{(i)})^T u_k} = u_k.$$

$$\sum_{i=1}^{m} \underbrace{\frac{1}{m\lambda_k} \phi(x^{(i)})^T u_k}_{\alpha_k^i} \underline{\phi(x^{(i)})} = \underline{u_k}.$$

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$$\underline{\phi(x^{(l)})}^T \underline{u_k} = \underline{\phi(x^{(l)})}^T \underbrace{\sum_{i=1}^{m} \alpha_k^i \underline{\phi(x^{(i)})}} = \sum_{i=1}^{m} \alpha_k^i \underline{K(x^{(l)}, x^{(i)})}$$

How to find $\underline{\alpha_k^i\text{'s directly}}$?

The Kernel Trick

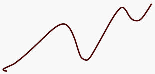
Kth eigenvector equation:

$$\Sigma u_k = \left(\frac{1}{m} \sum_{i=1}^{m} \phi(x^{(i)}) \phi(x^{(i)})^T \right) u_k = \lambda_k u_k$$

- Substitute $u_k = \sum_{i=1}^{m} \alpha_k^{(i)} \phi(x^{(i)})$, we obtain

  $$K \alpha_k = \lambda_k m \alpha_k$$

  where $\alpha_k = \begin{bmatrix} \alpha_k^1 \\ \vdots \\ \alpha_k^m \end{bmatrix}$ can be solved by eigen decomposition of K



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- Normalize α_k such that $u_k^T u_k = 1$:

$$u_k^T u_k = \sum_{i=1}^{m} \sum_{j=1}^{m} \alpha_k^i \alpha_k^j \phi(x^{(i)})^T \phi(x^{(j)}) = \alpha_k^T K \alpha_k = \lambda_k m (\alpha_k^T \alpha_k)$$

$$\|\alpha_k\|^2 = \frac{1}{\lambda_k m}$$

Kernel PCA

When $\mathbb{E}[\phi(x)] \neq 0$, we need to center $\phi(x)$:

$$\widetilde{\phi}(x^{(i)}) = \phi(x^{(i)}) - \frac{1}{m}\sum_{l=1}^{m}\widetilde{\phi}(x^{(l)})$$

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$$\widetilde{\phi}(x^{(i)}) = \phi(x^{(i)}) - \frac{1}{m}\sum_{l=1}^{m}\widetilde{\phi}(x^{(l)})$$

The "centralized" kernel matrix is

$$\tilde{K}_{i,j} = \widetilde{\phi}(x^{(i)})^T\widetilde{\phi}(x^{(j)})$$

In matrix notation:

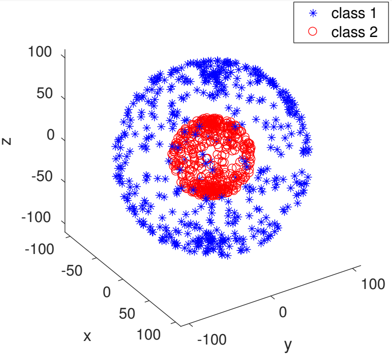
$$\widetilde{K} = K - 1_m K - K 1_m + 1_m K 1_m$$

where $1_m = \begin{bmatrix} 1/m & \dots & 1/m \\ \vdots & \ddots & \vdots \\ 1/m & \dots & 1/m \end{bmatrix} \in \mathbb{R}^{mxm}$

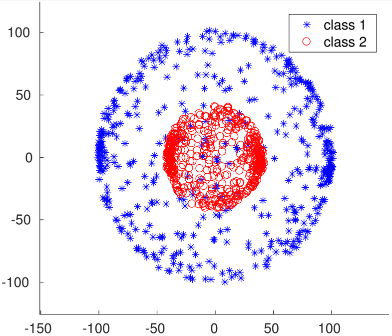
Use $\widetilde{K}$ to compute PCA

Kernel PCA Example

original data

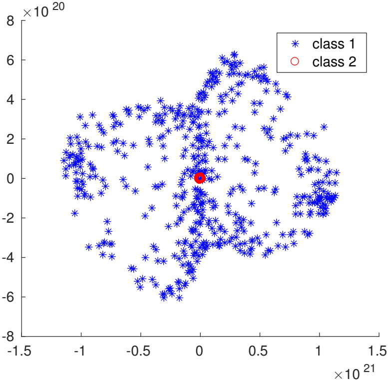


standard PCA



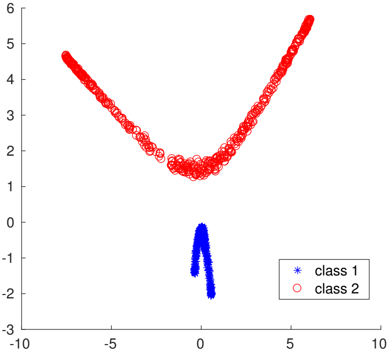
Kernel PCA Example

Polynomial kernel PCA



$$k(x, x') = (x \cdot x' + 1)^5$$

Gaussian kernel PCA



$$k(x, x') = \exp\left(-\frac{\|x-x'\|^2}{2\sigma^2}\right)$$

Discussions of kernel PCA

- Often used in clustering, abnormality detection, etc

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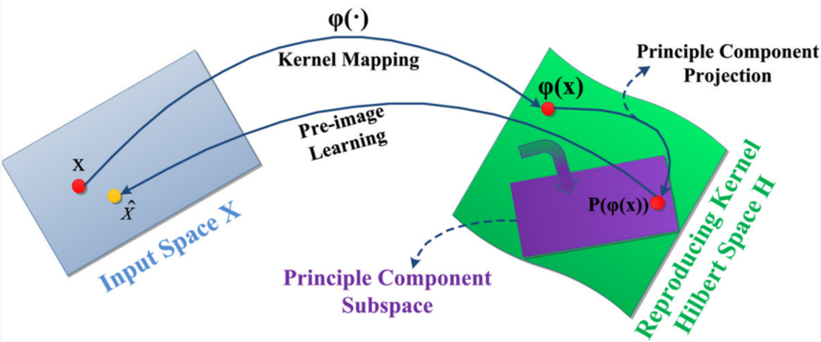
- Requires finding eigenvectors of $m \times m$ matrix instead of $n \times n$
- Dimension reduction by projecting to k-dimensional principal subspace is generally not possible



The Pre-Image problem: reconstruct data in input space x from feature space vectors $\phi(x)$

PCA Limitations

- Assumes input data is real and continuous
- Assumes **approximate normality** of input space (but may still work well on non-normally distributed data in practice) ← *sample mean & covariance must be sufficient statistics*

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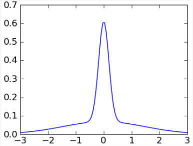
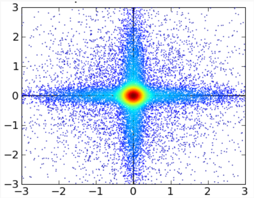
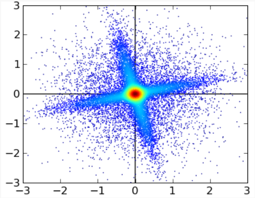
Example of strongly non-normal distributed input:



PDF



Original Input

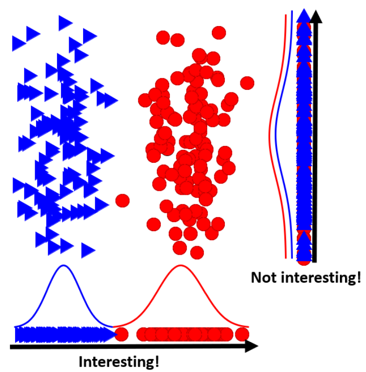


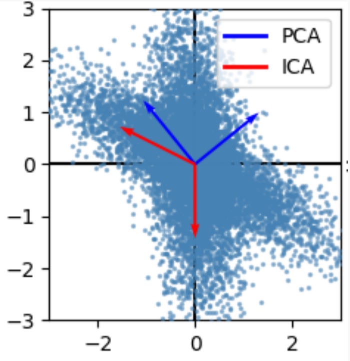
PCA Projection

PCA Limitations

PCA results may not be useful when

- Axes of larger variance is less ‘interesting‘ than smaller ones.
- Axes of variations are not orthogonal;





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Representation learning

- Transform input features into “simpler” or “interpretable” representations.
- Used in feature extraction, dimension reduction, clustering etc

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Unsupervised learning algorithms:

	low dimension	sparse	disentangle variations
k-means	✓	✓	
spectral embedding	✓		✓
PCA	✓		✓