Learning from Data
Lecture 10: Principal Component Analysis

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TBSI

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Today's Lecture

Unsupervised Learning (Part II): PCA

- Motivation
- Linear PCA
- Kernel PCA

Motivation

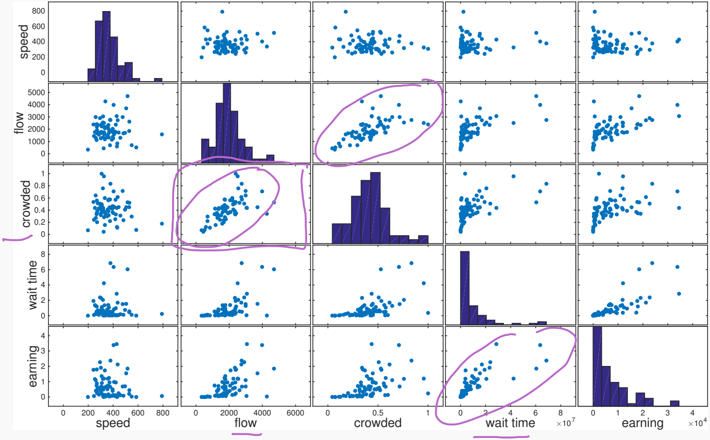
Motivation of PCA

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

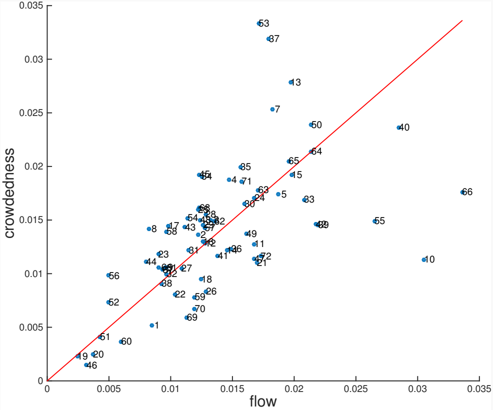


Scatter plot matrix reveals pairwise correlations among 5 major features

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

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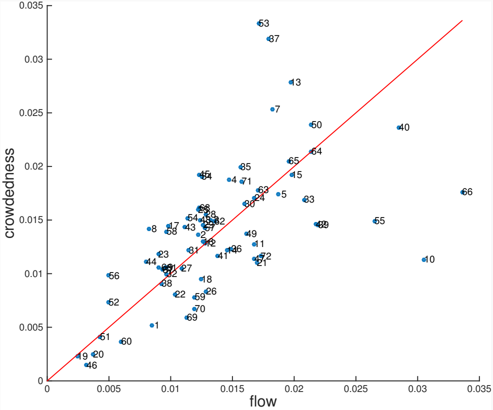


How can we automatically detect and remove this redundancy?

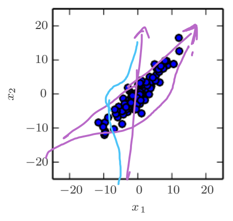
- geometric approach ← *start here!*
- diagonalize covariance matrix approach

How to remove feature redundancy?

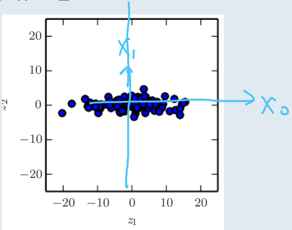
Given $\{x^{(1)}, \ldots, x^{(m)}\}$, $x^{(i)} \in \mathbb{R}^n$.

- 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!*

Direction of Maximum Variance

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

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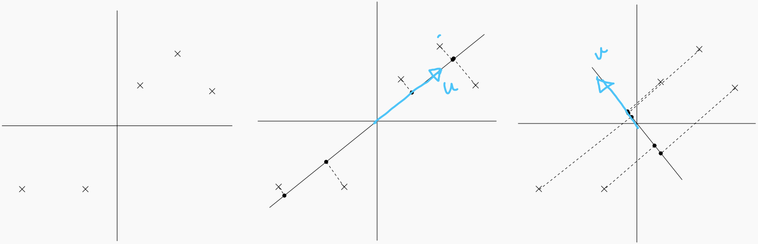
- Find **major axis of variation** unit vector u:



input observations | projections on u have large variance | projections on u have small variance

u maximizes the variance of the projections

Linear PCA

Principal Component Analysis (PCA)

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

axes of maximum variation.

PCA goals

- Find principal components $u_1, \ldots, u_n$ 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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PCA goals

- 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 $u_1, \ldots, u_{j-1}$

Step 1: Standardize data

Normalize x such that $Mean(x) = 0$ and $Var(x_j) = 1$

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

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

Check:

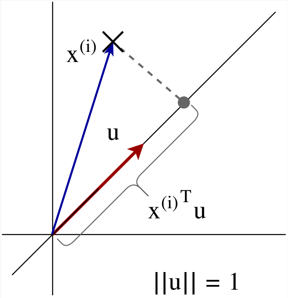
$$var\left(\frac{x_j}{\sigma_j}\right) = \frac{1}{m}\sum_{i=1}^{m}\left(\frac{x_j^{(i)} - \mu_j}{\sigma_j}\right)^2 = \frac{1}{\sigma_j^2}\frac{1}{m}\sum_{i=1}^{m}\left(x_j^{(i)} - \mu_j\right)^2$$

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

Step 2: Find Projection with Maximum Variance

$$X = \begin{bmatrix} - & x^{(1)} & - \\ & \vdots & \\ - & x^{(n)} & - \end{bmatrix} \quad cov(X) = \begin{bmatrix} \sigma_1^2 & \sigma_{12}^2 & \cdots \\ & \ddots & \sigma_n^2 \end{bmatrix}$$

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



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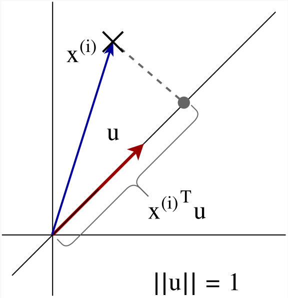

Variance of the projections:

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

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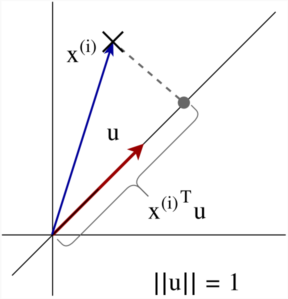

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$\Sigma = cov(X)$

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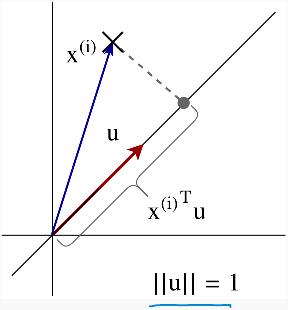

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$$= u^T \Sigma u$$

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

1st Principal Component (Rayleigh-Ritz theorem).

Rayleigh-quotient $R(x) = \frac{x^T A x}{x^T x}$ $(x \neq 0)$

The critical points of $R(x)$ are the eigenvectors of A

Find unit vector u_1 that maximizes variance of projections:

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

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

u_1 is the largest eigenvector of covariance matrix Σ

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Proof.

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Proof. Generalized Lagrange function of Problem 1: $\|u\|_2^2 = 1 = u^T u$

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

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To minimize $L(u)$,

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

Therefore u_1 must be an eigenvector of Σ.

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Therefore u_1 must be an eigenvector of Σ.
Let $u_1 = v_j$, the eigenvector with the jth largest eigenvalue λ_j,

$$u_1^T \Sigma u_1 = v_j^T \Sigma v_j = \lambda_j v_j^T v_j = \lambda_j. = \beta.$$

Hence $u_1 = v_1$, the eigenvector with the largest eigenvalue λ_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 $j = 2$,

$$u_2 = \underset{u:\|u\|=1,\, u_1^T u=0}{\operatorname{argmax}} \; u^T \Sigma u \tag{2}$$

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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:

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

proof

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

Multiply both side by u_1^T.

$$-2 u_1^T \Sigma u + 2\beta_1 u_1^T u + \beta_2 u_1^T u_1 = 0.$$

$u_1^T u = 0$, $u_1^T u_1 = 1$, $u_1^T \Sigma u = \lambda u_1^T u = 0$, then $\beta_2 = 0$

Then $\frac{\partial L}{\partial u} = -2\Sigma u + 2\beta_1 u = 0$

We have: $\Sigma u = \beta_1 u$

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Minimizing $L(u)$ yields:

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

To maximize $u^T \Sigma u = \lambda$, 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 $j = 1 \ldots n$)* □

Summary

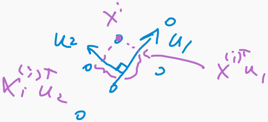
$$\Sigma = \begin{bmatrix} | & & | \\ u_1 & \dots & u_n \\ | & & | \end{bmatrix} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \begin{bmatrix} - u_1 - \\ \\ - u_n - \end{bmatrix}^T.$$

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: $\Sigma = U \Lambda U^T$. ← *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 $x \in \mathbb{R}^n$ in the principal component space:

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

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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

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

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- % of variance explained by the jth principal component: $\frac{\lambda_j}{\sum_{i=1}^{n} \lambda_i}$.
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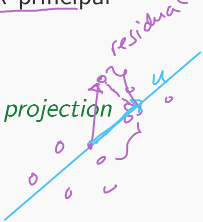
- % of variance accounted for by retaining the first k principal components ($k \leq n$): $\frac{\sum_{j=1}^{k} \lambda_j}{\sum_{j=1}^{n} \lambda_j}$

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



Covariance Interpretation of PCA

previous PCA alg.: $\frac{1}{m}X^TX = \Sigma = U\Lambda U^T$

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

Let $Z = XU$ be the PCA projected data,

$$\text{cov}(Z) = \frac{1}{m}Z^TZ = \frac{1}{m}(XU)^T(XU) = U^T\left(\frac{1}{m}X^TX\right)U = U^T\Sigma U$$

($\frac{1}{m}X^TX$ is Σ)

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

$$\Sigma = U \Lambda U^T$$

where

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

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Then

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

← diagonal matrix !

$(U^TU)\Lambda(U^TU)$, $U^TU = I$

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Then

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

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

Linear PCA Review

PCA Dimension reduction

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

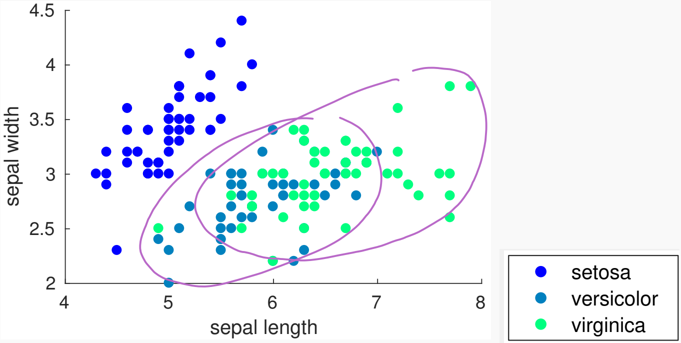
Main steps

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

PCA Example: Iris Dataset

- 150 samples
- input feature dimension: 4

First two input attributes



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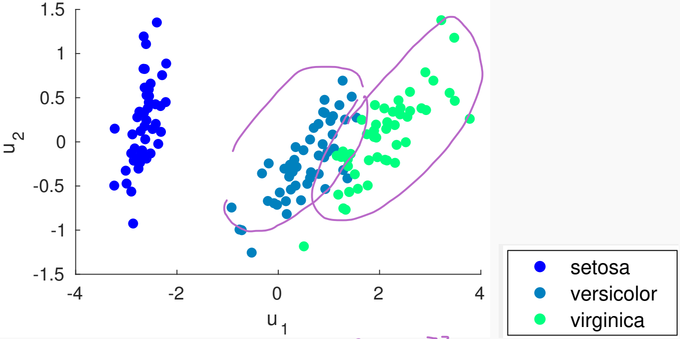
PCA Projection on 2 Principal Components



$\lambda_1 = 0.73$ 0.22 → 0.95

% of variance explained by PC1: 73%, $\sum_{i=1}^{4} \lambda_i$ by PC2: 22%

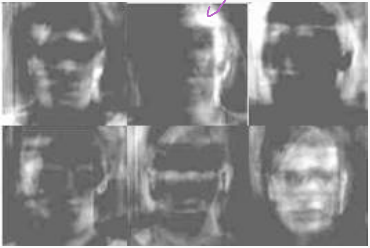
PCA Example: Eigenfaces

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

reshape

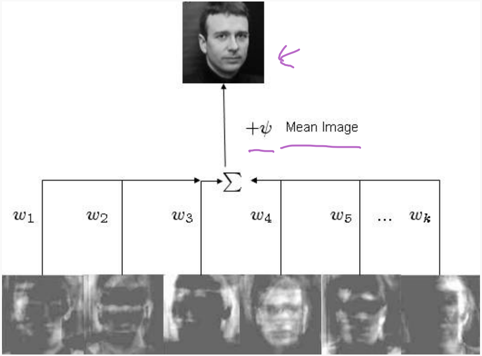
Training data

Eigenfaces: k principal components



PCA Example: Eigenfaces

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



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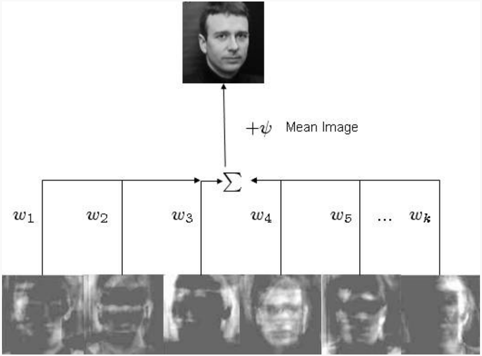

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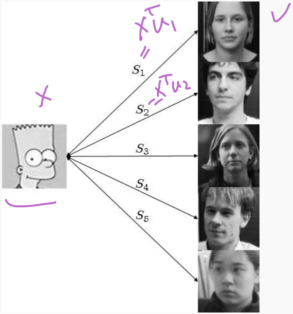
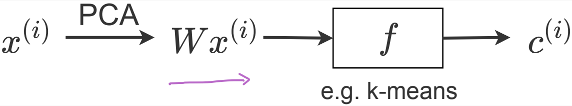
Recognize faces by classifying the weight vectors. e.g. k-Nearest Neighbor



Kernel PCA

Kernel PCA

Feature extraction using PCA



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

Kernel PCA

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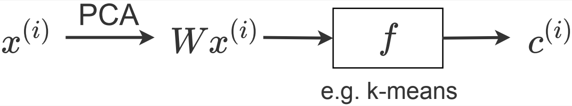

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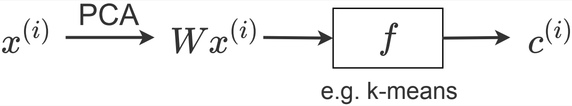
A non-linear generalization

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

Kernel PCA

Feature extraction using PCA



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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 $K \in \mathbb{R}^{m \times m}$

Kernel PCA

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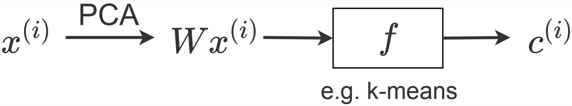

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- Feature mapping is defined by a kernel function $K\left(x^{(i)}, x^{(j)}\right) = \phi(x^{(i)})^T \phi(x^{(j)})$ or kernel matrix $K \in \mathbb{R}^{m \times m}$
- We can now perform standard PCA in the feature space

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)

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

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Let $(\lambda_k, u_k), k = 1, \ldots, d$ be the eigen decomposition of Σ:

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

k th principal component

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

$$\Sigma u_k = \lambda_k u_k$$

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

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

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

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

- PCA projection of $x^{(l)}$ using kernel function K:

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

How to find α_k^i's directly ?

$\alpha_k^i \phi(x^l)^T \phi(x^i)$

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

algebra

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

eigenvalue of 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 $\phi(x)$:

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

Kernel PCA

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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

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

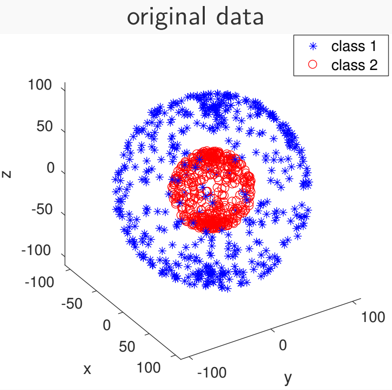
In matrix notation:

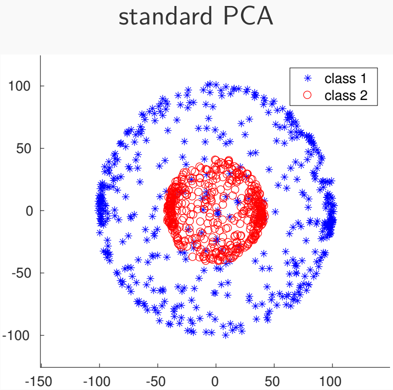
$$\widetilde{K} = K - \mathbf{1}_m K - K\mathbf{1}_m + \mathbf{1}_m K \mathbf{1}_m$$

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

Use $\widetilde{K}$ to compute PCA

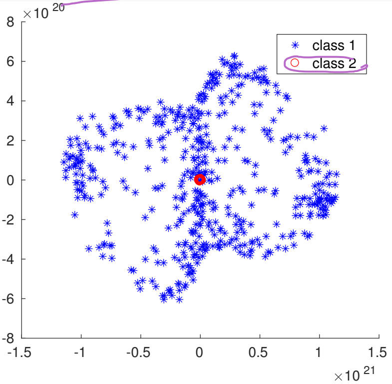
Kernel PCA Example





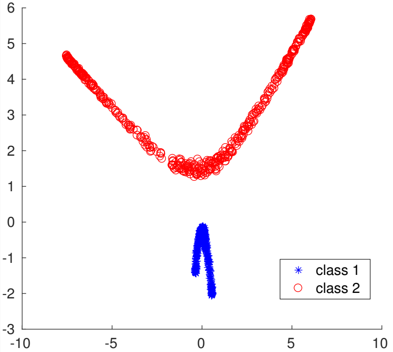
Kernel PCA Example

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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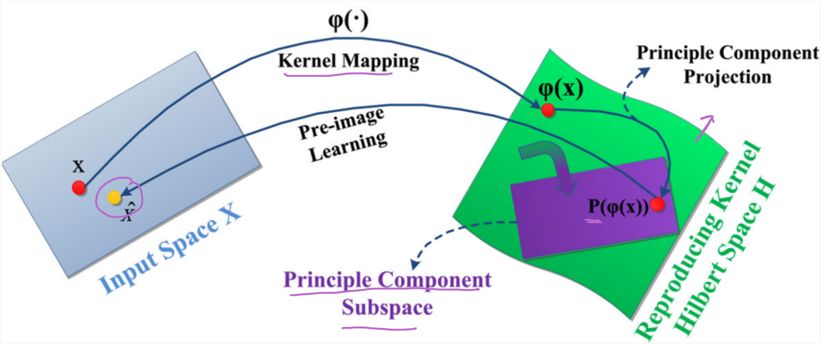
K

Discussions of kernel PCA

- Often used in clustering, abnormality detection, etc
- 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

x_j

- 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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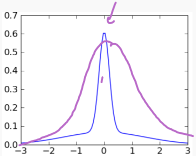
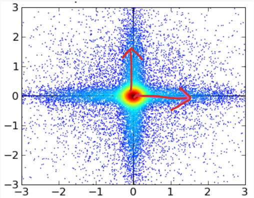
Example of strongly non-normal distributed input:

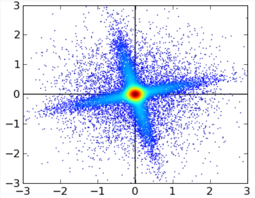
PDF



Original Input



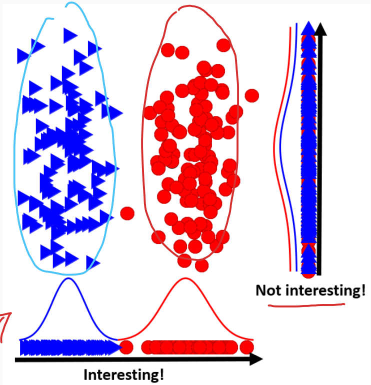
PCA Projection

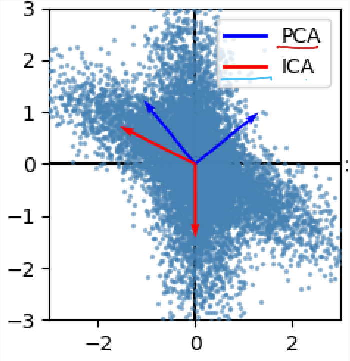


PCA Limitations

PCA results may not be useful when

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





Summary

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 (clustering)	✓	✓	
Laplacian eigenmap spectral embedding	✓		✓
PCA	✓		✓