PCA and kernel PCA

Kaiwen Chang
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Outline

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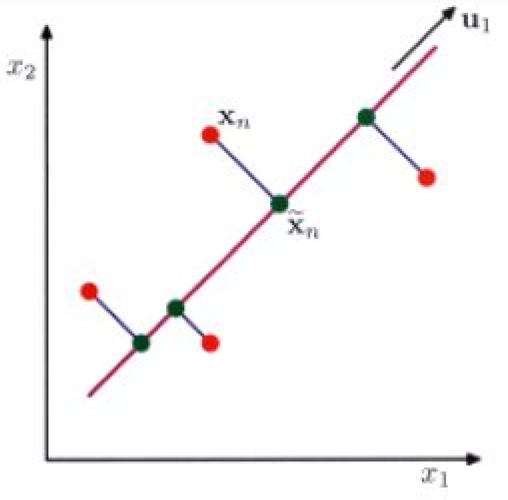
II. Kernel PCA

1. Why kernel
2. Solution
3. Example

I. PCA

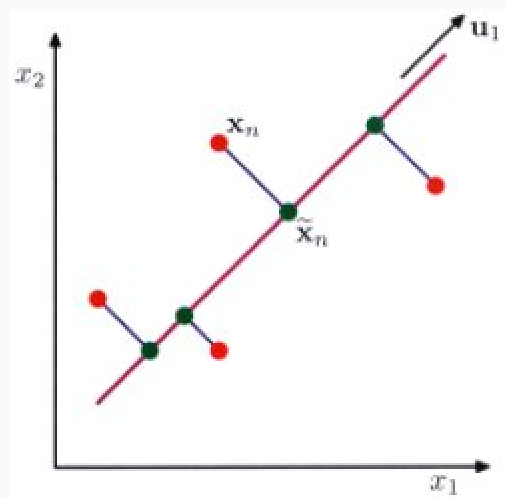
1. Definitions

1. The orthogonal projection of the data onto a lower dimensional linear space (principal subspace), such that the **variance** of the projected data is maximized



Magenta line: principal subspace

2. The linear projection that minimizes the average projection cost (the mean squared distance between the data points and their projections)



Blue line: projection error

2. Solution

Data set $\{\mathbf{x}_n\}$ n = 1,2,...,N

$\mathbf{x}_n$: column vector with dimension D

Aim: project data onto a space with dimension M < D, while maximizing the variance of projected points

Projection of $\mathbf{x}_n$: $\mathbf{u}_1^{\mathrm{T}}\mathbf{x}_n$

($\mathbf{u}_1$: the direction of space, dimension D)

Mean of projected data: $\mathbf{u}_1^{\mathrm{T}}\overline{\mathbf{x}}$ $\overline{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{x}_n$

Variance: $$\frac{1}{N}\sum_{n=1}^{N}\left\{\mathbf{u}_1^{\mathrm{T}}\mathbf{x}_n - \mathbf{u}_1^{\mathrm{T}}\overline{\mathbf{x}}\right\}^2 = \mathbf{u}_1^{\mathrm{T}}\mathbf{S}\mathbf{u}_1$$

Covariance matrix: $$\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N}(\mathbf{x}_n - \overline{\mathbf{x}})(\mathbf{x}_n - \overline{\mathbf{x}})^{\mathrm{T}}$$

Maximize variance $\mathbf{u}_1^{\mathrm{T}}\mathbf{S}\mathbf{u}_1$ with constraint $\mathbf{u}_1^{\mathrm{T}}\mathbf{u}_1 = 1.$

Maximize $$\mathbf{u}_1^{\mathrm{T}}\mathbf{S}\mathbf{u}_1 + \lambda_1\left(1 - \mathbf{u}_1^{\mathrm{T}}\mathbf{u}_1\right)$$

λ_1: lagrange multiplier

Setting the derivative to zero:

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

$\mathbf{u}_1$: an eigenvector of S

$$\mathbf{u}_1^{\mathrm{T}}\mathbf{S}\mathbf{u}_1 = \lambda_1$$

Largest eigenvalue $\longrightarrow$ maximum variance

$\mathbf{u}_1$: first principal component

Additional principal component $\mathbf{u}_n$: choosing a new direction among all possible directions orthogonal to $\mathbf{u}_1$, $\mathbf{u}_2$, ... $\mathbf{u}_{n-1}$, that maximize the projected variance

Optimal linear projection: eigenvectors $\mathbf{u}_1$, $\mathbf{u}_2$, ... $\mathbf{u}_M$ of covariance matrix S corresponding to M largest eigenvalues

Summary

1. Evaluating the mean and covariance matrix **S** of data set
2. Finding the M eigenvectors of S corresponding to M largest eigenvalues

Computation cost: $O(MD^2)$

Example: http://sebastianraschka.com/Articles/2014_pca_step_by_step.html

$$\widetilde{\mathbf{x}}_n = \sum_{i=1}^{M} z_{ni}\mathbf{u}_i + \sum_{i=M+1}^{D} b_i\mathbf{u}_i$$

$$J = \frac{1}{N}\sum_{n=1}^{N} \|\mathbf{x}_n - \widetilde{\mathbf{x}}_n\|^2$$

3. Example

Applications:

Dimensionality reduction

Lossy data compression

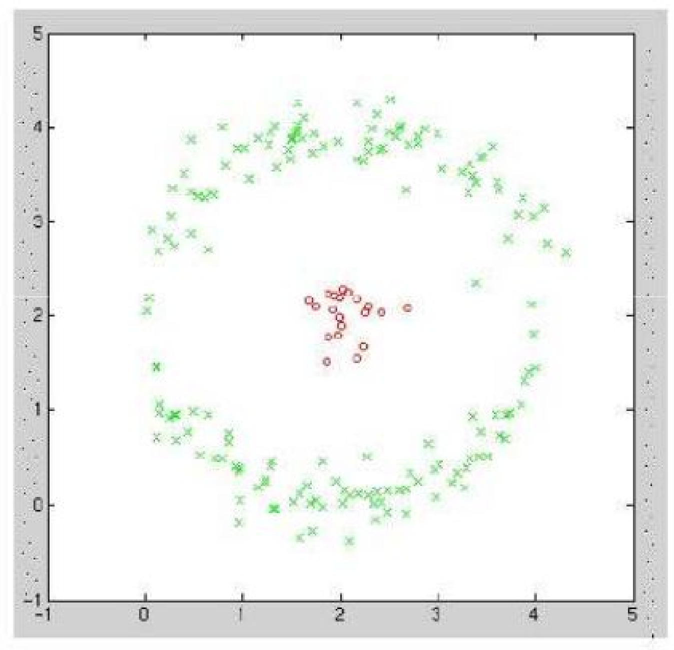
Feature extraction

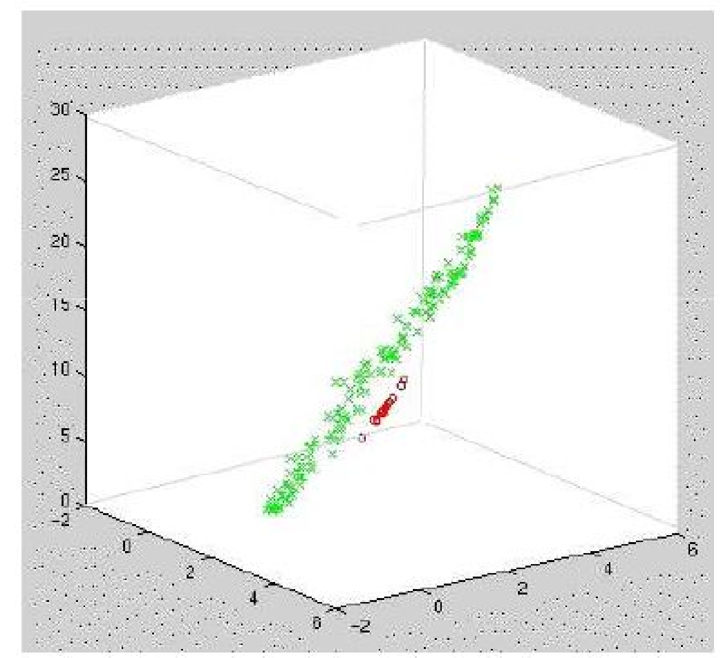
Data visualization

http://scikit-learn.org/stable/auto_examples/decomposition/plot_pca_iris.html#sphx-glr-auto-examples-decomposition-plot-pca-iris-py

II. Kernel PCA

1. Why kernel





Not linear

Kernel trick $K(x_i, x_j) = \phi(x_i)^T \phi(x_j)$

2. Solution

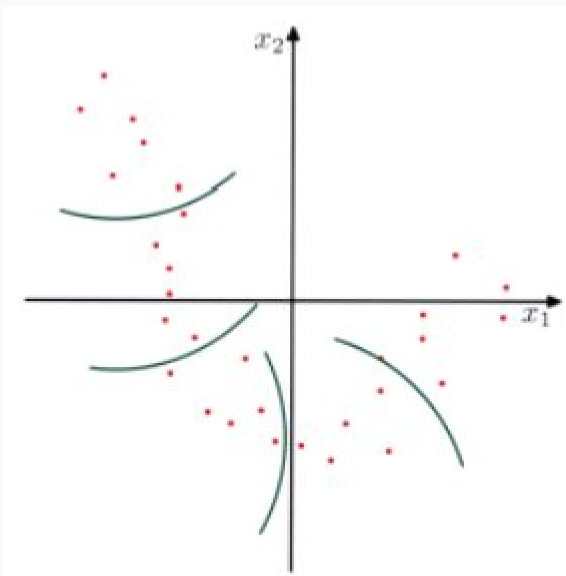
$\sum_n \mathbf{x}_n = \mathbf{0}.$

Covariance matrix $$\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^{\mathrm{T}}$$

$\phi(\mathbf{x})$: a nonlinear transformation into an M-dimensional feature space (M > D)

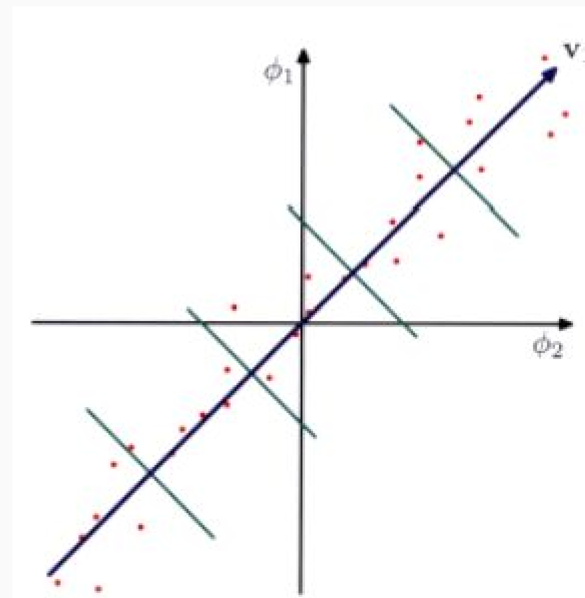
$\mathbf{x}_n \longrightarrow \phi(\mathbf{x}_n)$

Perform standard PCA in feature space



Original data space

Nonlinear projection



Feature space

Principal components

Assume $\sum_n \phi(\mathbf{x}_n) = \mathbf{0}$.

Covariance matrix in feature space:

$$\mathbf{C} = \frac{1}{N} \sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^{\mathrm{T}}$$

$$\mathbf{C}\mathbf{v}_i = \lambda_i \mathbf{v}_i$$

$$\frac{1}{N} \sum_{n=1}^{N} \phi(\mathbf{x}_n) \left\{\phi(\mathbf{x}_n)^{\mathrm{T}}\mathbf{v}_i\right\} = \lambda_i \mathbf{v}_i$$

$$\mathbf{v}_i = \sum_{n=1}^{N} a_{in}\phi(\mathbf{x}_n)$$

Goal: solve the problem without having to work explicitly in the feature space

$$\frac{1}{N}\sum_{n=1}^{N}\boldsymbol{\phi}(\mathbf{x}_n)\boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}}\sum_{m=1}^{N}a_{im}\boldsymbol{\phi}(\mathbf{x}_m) = \lambda_i\sum_{n=1}^{N}a_{in}\boldsymbol{\phi}(\mathbf{x}_n)$$

Kernel function: $k(\mathbf{x}_n, \mathbf{x}_m) = \boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_m)$

Multiply by $\boldsymbol{\phi}(\mathbf{x}_l)^{\mathrm{T}}$

$$\frac{1}{N}\sum_{n=1}^{N}k(\mathbf{x}_l, \mathbf{x}_n)\sum_{m=1}^{m}a_{im}k(\mathbf{x}_n, \mathbf{x}_m) = \lambda_i\sum_{n=1}^{N}a_{in}k(\mathbf{x}_l, \mathbf{x}_n)$$

$$\mathbf{K}^2\mathbf{a}_i = \lambda_i N\mathbf{K}\mathbf{a}_i$$

a_i : N dimensional column vector with a_{in}

Kernel matrix

$$\mathbf{K} = \phi(\mathbf{X})\phi(\mathbf{X})^{\mathrm{T}} = \begin{bmatrix} \kappa(\mathbf{x}_1, \mathbf{x}_1) & \kappa(\mathbf{x}_1, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_1, \mathbf{x}_N) \\ \kappa(\mathbf{x}_2, \mathbf{x}_1) & \kappa(\mathbf{x}_2, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_2, \mathbf{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(\mathbf{x}_N, \mathbf{x}_1) & \kappa(\mathbf{x}_N, \mathbf{x}_2) & \cdots & \kappa(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

$$\mathbf{K}\mathbf{a}_i = \lambda_i N \mathbf{a}_i$$

Normalization

$$1 = \mathbf{v}_i^{\mathrm{T}}\mathbf{v}_i = \sum_{n=1}^{N}\sum_{m=1}^{N} a_{in}a_{im}\boldsymbol{\phi}(\mathbf{x}_n)^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_m) = \mathbf{a}_i^{\mathrm{T}}\mathbf{K}\mathbf{a}_i = \lambda_i N \mathbf{a}_i^{\mathrm{T}}\mathbf{a}_i$$

Projection

$$y_i(\mathbf{x}) = \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\mathbf{v}_i = \sum_{n=1}^{N} a_{in}\boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n) = \sum_{n=1}^{N} a_{in}k(\mathbf{x}, \mathbf{x}_n)$$

Centralizing projected data:

$$\widetilde{\phi}(\mathbf{x}_n) = \phi(\mathbf{x}_n) - \frac{1}{N}\sum_{l=1}^{N}\phi(\mathbf{x}_l)$$

Element of the Gram matrix

$$\begin{aligned}
\widetilde{K}_{nm} &= \widetilde{\phi}(\mathbf{x}_n)^{\mathrm{T}}\widetilde{\phi}(\mathbf{x}_m) \\
&= \phi(\mathbf{x}_n)^{\mathrm{T}}\phi(\mathbf{x}_m) - \frac{1}{N}\sum_{l=1}^{N}\phi(\mathbf{x}_n)^{\mathrm{T}}\phi(\mathbf{x}_l) - \frac{1}{N}\sum_{l=1}^{N}\phi(\mathbf{x}_l)^{\mathrm{T}}\phi(\mathbf{x}_m) + \frac{1}{N^2}\sum_{j=1}^{N}\sum_{l=1}^{N}\phi(\mathbf{x}_j)^{\mathrm{T}}\phi(\mathbf{x}_l) \\
&= k(\mathbf{x}_n, \mathbf{x}_m) - \frac{1}{N}\sum_{l=1}^{N}k(\mathbf{x}_l, \mathbf{x}_m) - \frac{1}{N}\sum_{l=1}^{N}k(\mathbf{x}_n, \mathbf{x}_l) + \frac{1}{N^2}\sum_{j=1}^{N}\sum_{l=1}^{N}k(\mathbf{x}_j, \mathbf{x}_l)
\end{aligned}$$

In matrix notation $\widetilde{\mathbf{K}} = \mathbf{K} - \mathbf{1}_N\mathbf{K} - \mathbf{K}\mathbf{1}_N + \mathbf{1}_N\mathbf{K}\mathbf{1}_N$

1_N: NxN matrix with each element 1/N

1. Pick a kernel

Gaussian $\boxed{K(\vec{x},\vec{x}') = \exp\left(-\beta \|\vec{x} - \vec{x}'\|^2\right)}$

Polynomial $\boxed{K(\vec{x},\vec{x}') = (1 + \vec{x} \cdot \vec{x}')^p}$

2. Construct the normalized kernel matrix of data (NxN)

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

3. Solve an eigenvalue problem: $\widetilde{\mathbf{K}}\mathbf{a}_i = \lambda_i N \mathbf{a}_i$

4. Represent the data point i as

$$y_i(\mathbf{x}) = \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\mathbf{v}_i = \sum_{n=1}^{N} a_{in}\boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n) = \sum_{n=1}^{N} a_{in}k(\mathbf{x},\mathbf{x}_n)$$

3. Example

Example: http://sebastianraschka.com/Articles/2014_kernel_pca.html

RBF: radial basis function

http://scikit-learn.org/stable/auto_examples/plot_digits_pipe.html#sphx-glr-auto-examples-plot-digits-pipe-py

Reference

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   http://sebastianraschka.com/Articles/2014_kernel_pca.html