

Principal Component Analysis (PCA)

CE-717: Machine Learning
Sharif University of Technology
Spring 2016

Soleymani

Dimensionality Reduction: Feature Selection vs. Feature Extraction

▶ Feature **selection**

- ▶ Select a subset of a given feature set

▶ Feature **extraction**

- ▶ A linear or non-linear transform on the original feature space

$$\begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \rightarrow \begin{bmatrix} x_{i_1} \\ \vdots \\ x_{i_{d'}} \end{bmatrix}$$

Feature
Selection
($d' < d$)

$$\begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \rightarrow \begin{bmatrix} y_1 \\ \vdots \\ y_{d'} \end{bmatrix} = f \left(\begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \right)$$

Feature
Extraction

Feature Extraction

- ▶ Mapping of the original data to another space
 - ▶ Criterion for feature extraction can be different based on problem settings
 - ▶ Unsupervised task: minimize the information loss (reconstruction error)
 - ▶ Supervised task: maximize the class discrimination on the projected space
- ▶ Feature extraction algorithms
 - ▶ Linear Methods
 - ▶ Unsupervised: e.g., Principal Component Analysis (PCA)
 - ▶ Supervised: e.g., Linear Discriminant Analysis (LDA)
 - Also known as Fisher's Discriminant Analysis (FDA)

Feature Extraction

▶ Unsupervised feature extraction:

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & \cdots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \cdots & x_d^{(N)} \end{bmatrix}$$



A mapping $f: \mathbb{R}^d \rightarrow \mathbb{R}^{d'}$

Or

only the transformed data

$$\mathbf{X}' = \begin{bmatrix} x'_1^{(1)} & \cdots & x'_{d'}^{(1)} \\ \vdots & \ddots & \vdots \\ x'_1^{(N)} & \cdots & x'_{d'}^{(N)} \end{bmatrix}$$

▶ Supervised feature extraction:

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & \cdots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \cdots & x_d^{(N)} \end{bmatrix}$$

$$\mathbf{Y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(N)} \end{bmatrix}$$



A mapping $f: \mathbb{R}^d \rightarrow \mathbb{R}^{d'}$

Or

only the transformed data

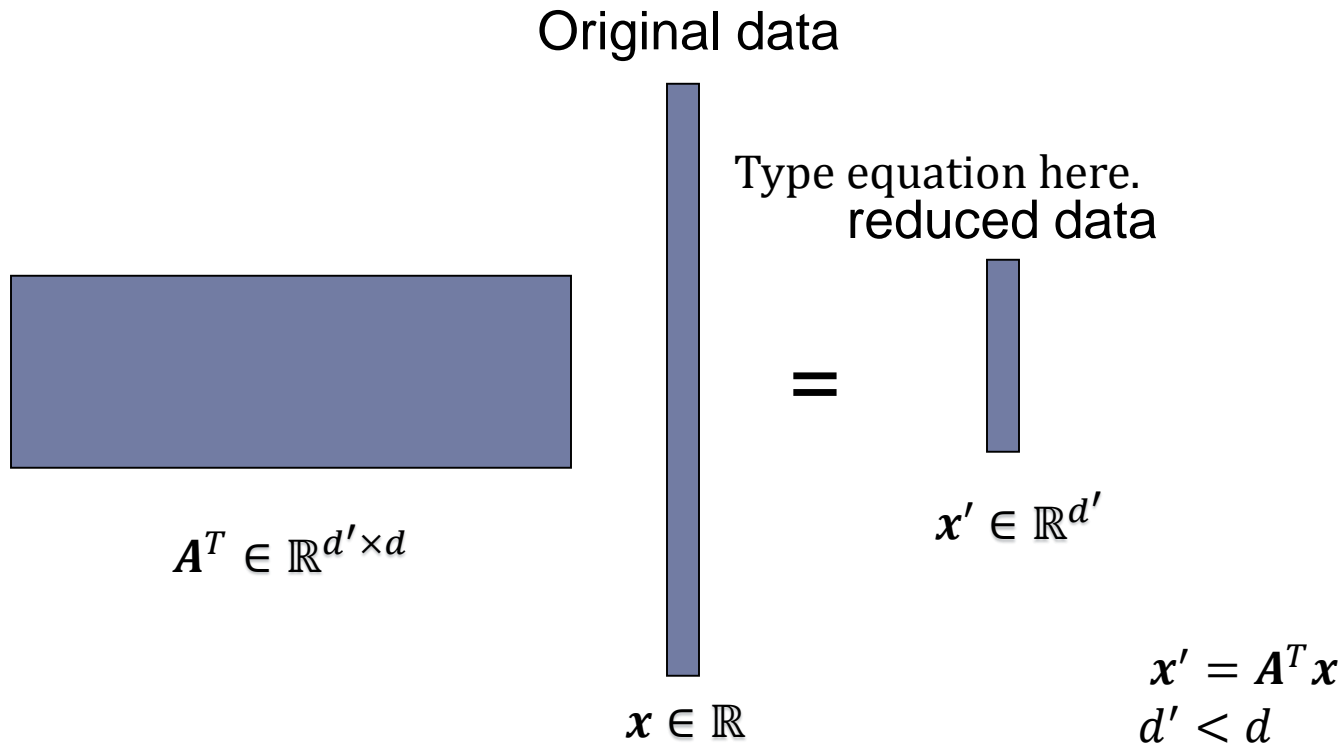
$$\mathbf{X}' = \begin{bmatrix} x'_1^{(1)} & \cdots & x'_{d'}^{(1)} \\ \vdots & \ddots & \vdots \\ x'_1^{(N)} & \cdots & x'_{d'}^{(N)} \end{bmatrix}$$

Unsupervised Feature Reduction

- ▶ Visualization: projection of high-dimensional data onto 2D or 3D.
- ▶ Data compression: efficient storage, communication, or and retrieval.
- ▶ Pre-process: to improve accuracy by reducing features
 - ▶ As a preprocessing step to reduce dimensions for supervised learning tasks
 - ▶ Helps avoiding overfitting
- ▶ Noise removal
 - ▶ E.g, “noise” in the images introduced by minor lighting variations, slightly different imaging conditions, etc.

Linear Transformation

- ▶ For linear transformation, we find an explicit mapping $f(\mathbf{x}) = \mathbf{A}^T \mathbf{x}$ that can transform also new data vectors.



Linear Transformation

- ▶ Linear transformation are simple mappings

$$\mathbf{x}' = \mathbf{A}^T \mathbf{x} \quad \mathbf{A} = \begin{bmatrix} a_{11} & \cdots & a_{1d'} \\ \vdots & \ddots & \vdots \\ a_{d1} & \cdots & a_{dd'} \end{bmatrix}$$

\mathbf{a}_1 $\mathbf{a}_{d'}$

$$\begin{bmatrix} x'_1 \\ \vdots \\ x'_{d'} \end{bmatrix} = \begin{bmatrix} a_{11} & \cdots & a_{d1} \\ \vdots & \ddots & \vdots \\ a_{1d'} & \cdots & a_{d'd} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$

\mathbf{a}_1^T $\mathbf{a}_{d'}^T$

$$x'_j = \mathbf{a}_j^T \mathbf{x} \quad j = 1, \dots, d'$$

Linear Dimensionality Reduction

- ▶ Unsupervised
 - ▶ Principal Component Analysis (PCA) [we will discuss]
 - ▶ Independent Component Analysis (ICA) [we will discuss]
 - ▶ Singular Value Decomposition (SVD)
 - ▶ Multi Dimensional Scaling (MDS)
 - ▶ Canonical Correlation Analysis (CCA)

Principal Component Analysis (PCA)

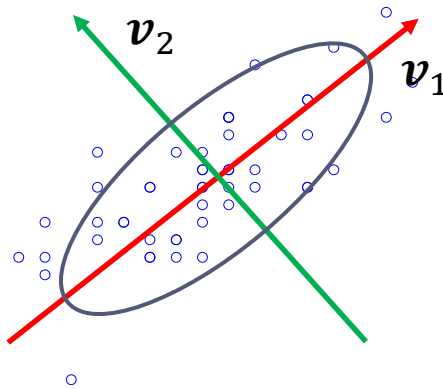
- ▶ Also known as Karhonen-Loeve (KL) transform
- ▶ Principal Components (PCs): orthogonal vectors that are ordered by the fraction of the total information (variation) in the corresponding directions
 - ▶ Find the directions at which data approximately lie
 - ▶ When the data is projected onto first PC, the variance of the projected data is maximized
- ▶ PCA is an orthogonal projection of the data into a subspace so that the variance of the projected data is maximized.

Principal Component Analysis (PCA)

- ▶ The “best” linear subspace (i.e. providing least reconstruction error of data):
 - ▶ Find mean reduced data
 - ▶ The axes have been rotated to new (principal) axes such that:
 - ▶ Principal axis 1 has the highest variance
 -
 - ▶ Principal axis i has the i -th highest variance.
 - ▶ The principal axes are uncorrelated
 - ▶ Covariance among each pair of the principal axes is zero.
- ▶ Goal: reducing the dimensionality of the data while preserving the variation present in the dataset as much as possible.
- ▶ PCs can be found as the “best” eigenvectors of the covariance matrix of the data points.

Principal components

- ▶ If data has a Gaussian distribution $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, the direction of the largest variance can be found by the eigenvector of $\boldsymbol{\Sigma}$ that corresponds to the largest eigenvalue of $\boldsymbol{\Sigma}$



PCA: Steps

- ▶ Input: $N \times d$ data matrix \mathbf{X} (each row contain a d dimensional data point)
 - ▶ $\boldsymbol{\mu} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}^{(i)}$
 - ▶ $\tilde{\mathbf{X}} \leftarrow$ Mean value of data points is subtracted from rows of \mathbf{X}
 - ▶ $\mathbf{C} = \frac{1}{N} \tilde{\mathbf{X}}^T \tilde{\mathbf{X}}$ (Covariance matrix)
 - ▶ Calculate eigenvalue and eigenvectors of \mathbf{C}
 - ▶ Pick d' eigenvectors corresponding to the largest eigenvalues and put them in the columns of $\mathbf{A} = [\mathbf{v}_1, \dots, \mathbf{v}_{d'}]$
 - ▶ $\mathbf{X}' = \tilde{\mathbf{X}}\mathbf{A}$
 - First PC
 - d'-th PC

Covariance Matrix

$$\boldsymbol{\mu}_x = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_d \end{bmatrix} = \begin{bmatrix} E(x_1) \\ \vdots \\ E(x_d) \end{bmatrix}$$

$$\boldsymbol{\Sigma} = E[(\mathbf{x} - \boldsymbol{\mu}_x)(\mathbf{x} - \boldsymbol{\mu}_x)^T]$$

- ▶ ML estimate of covariance matrix from data points $\{\mathbf{x}^{(i)}\}_{i=1}^N$:

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{N} \sum_{i=1}^N (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})(\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}})^T = \frac{1}{N} (\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})$$

$$\tilde{\mathbf{X}} = \begin{bmatrix} \tilde{\mathbf{x}}^{(1)} \\ \vdots \\ \tilde{\mathbf{x}}^{(N)} \end{bmatrix} = \begin{bmatrix} \mathbf{x}^{(1)} - \hat{\boldsymbol{\mu}} \\ \vdots \\ \mathbf{x}^{(N)} - \hat{\boldsymbol{\mu}} \end{bmatrix} \quad \hat{\boldsymbol{\mu}} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}^{(i)}$$

Correlation matrix

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix}$$

$$\begin{aligned} \frac{1}{N} \mathbf{X}^T \mathbf{X} &= \frac{1}{N} \begin{bmatrix} x_1^{(1)} & \dots & x_1^{(N)} \\ \vdots & \ddots & \vdots \\ x_d^{(1)} & \dots & x_d^{(N)} \end{bmatrix} \begin{bmatrix} x_1^{(1)} & \dots & x_d^{(1)} \\ \vdots & \ddots & \vdots \\ x_1^{(N)} & \dots & x_d^{(N)} \end{bmatrix} \\ &= \frac{1}{N} \begin{bmatrix} \sum_{n=1}^N x_1^{(n)} x_1^{(n)} & \dots & \sum_{n=1}^N x_1^{(n)} x_d^{(n)} \\ \vdots & \ddots & \vdots \\ \sum_{n=1}^N x_d^{(n)} x_1^{(n)} & \dots & \sum_{n=1}^N x_d^{(n)} x_d^{(n)} \end{bmatrix} \end{aligned}$$

Two Interpretations

▶ Maximum Variance Subspace

- ▶ PCA finds vectors \mathbf{v} such that projections on to the vectors capture maximum variance in the data

- ▶
$$\frac{1}{N} \sum_{n=1}^N (\mathbf{a}^T \mathbf{x}^{(n)})^2 = \frac{1}{N} \mathbf{a}^T \mathbf{X}^T \mathbf{X} \mathbf{a}$$

▶ Minimum Reconstruction Error

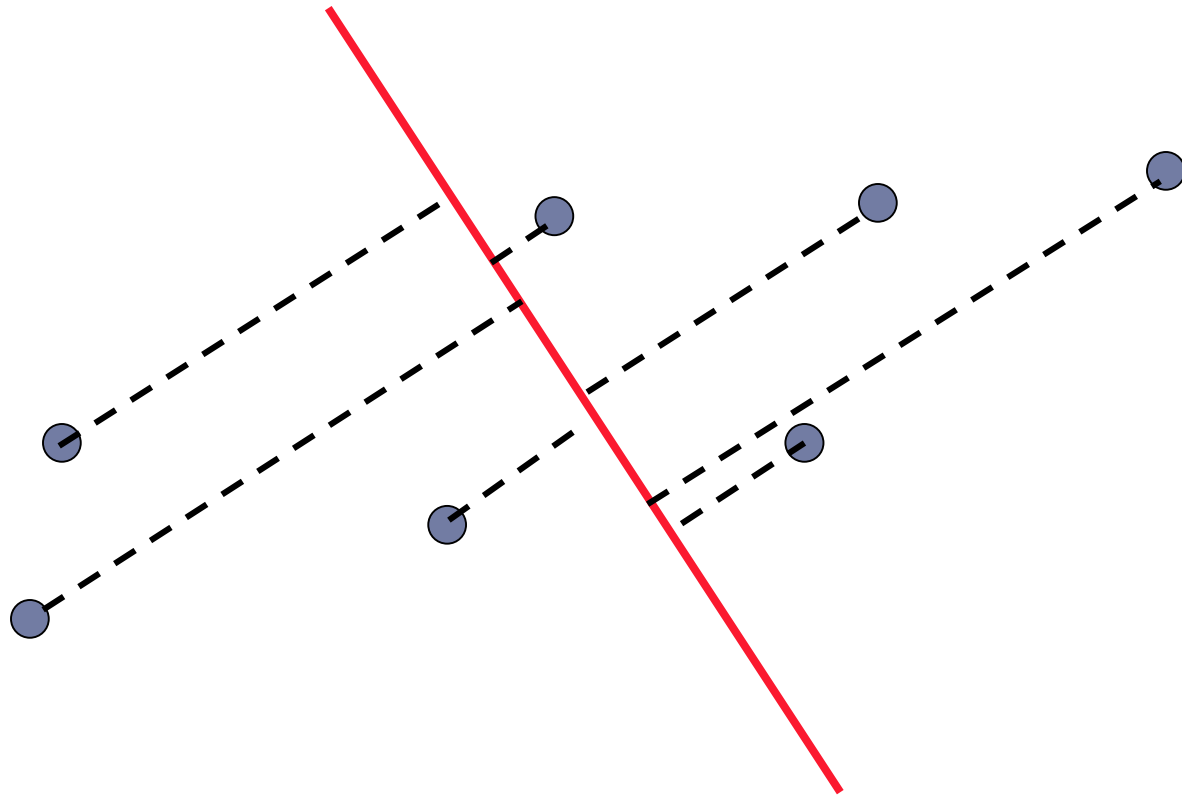
- ▶ PCA finds vectors \mathbf{v} such that projection on to the vectors yields minimum MSE reconstruction

- ▶
$$\frac{1}{N} \sum_{n=1}^N \|\mathbf{x}^{(n)} - (\mathbf{a}^T \mathbf{x}^{(n)}) \mathbf{a}\|^2$$

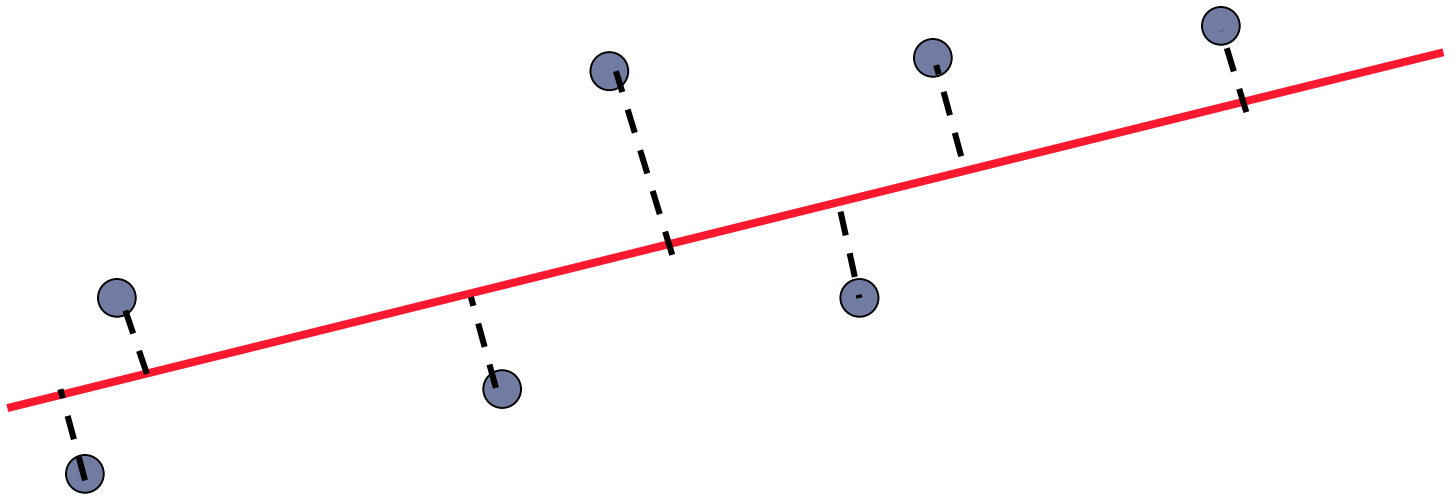
Least Squares Error Interpretation

- ▶ PCs are linear least squares fits to samples, each orthogonal to the previous PCs:
 - ▶ First PC is a minimum distance fit to a vector in the original feature space
 - ▶ Second PC is a minimum distance fit to a vector in the plane perpendicular to the first PC
 - ▶ And so on

Example

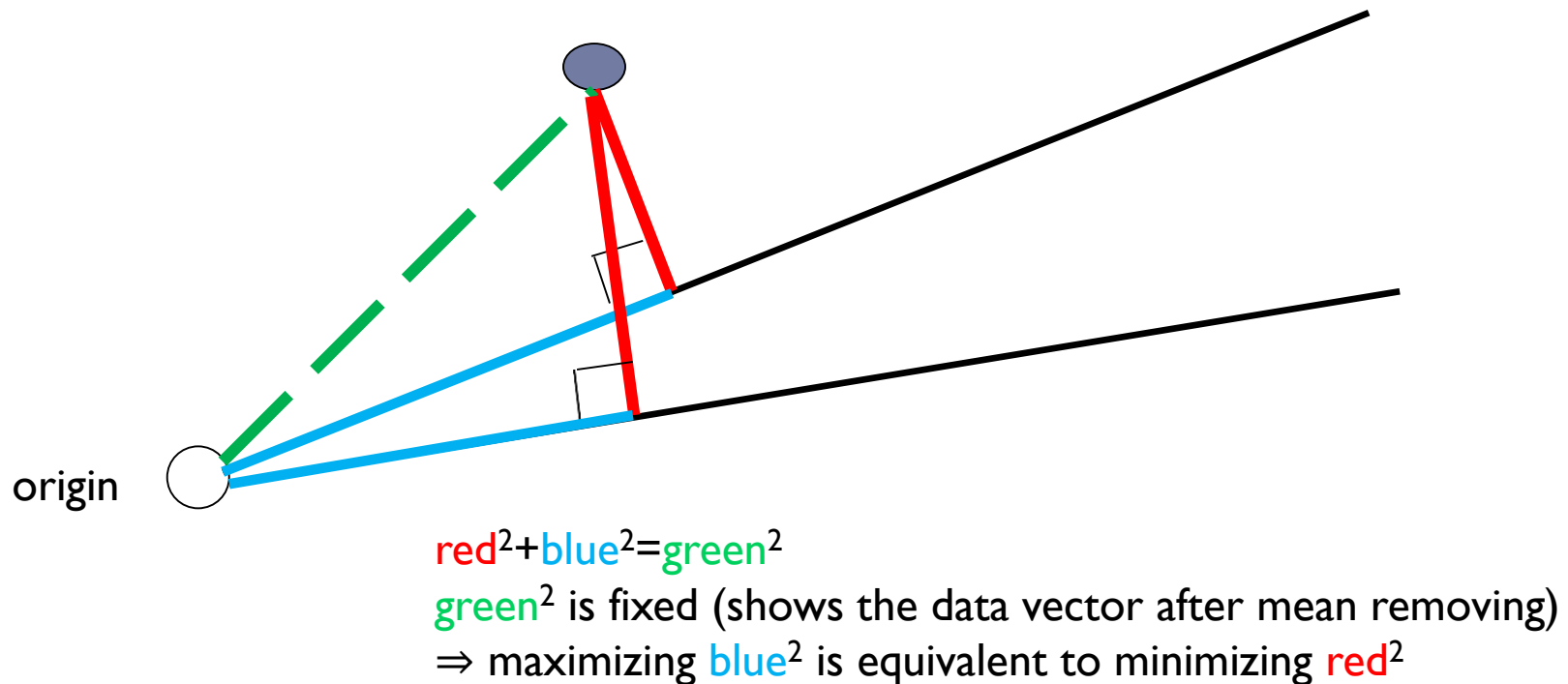


Example



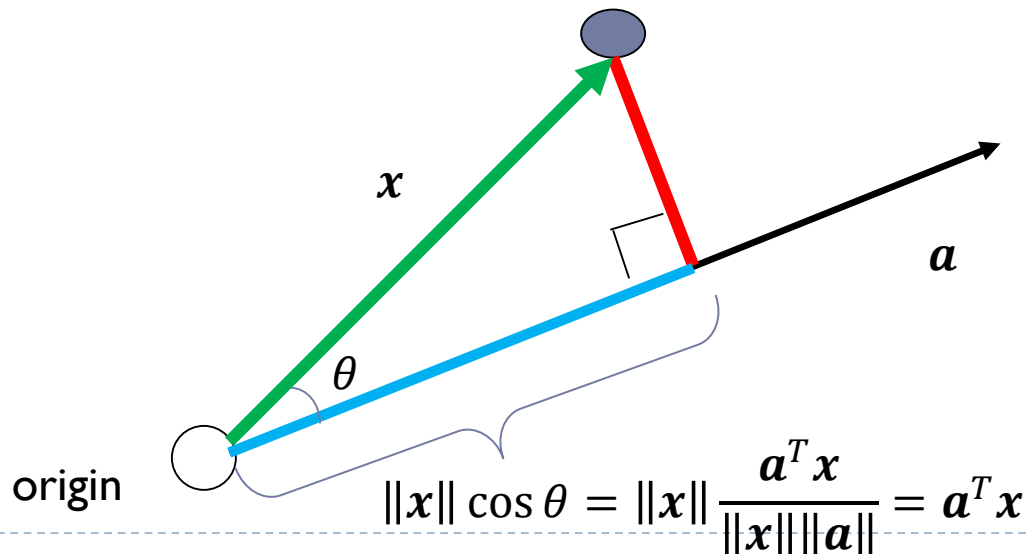
Least Squares Error and Maximum Variance Views Are Equivalent (1-dim Interpretation)

- ▶ Minimizing sum of square distances to the line is equivalent to maximizing the sum of squares of the projections on that line (Pythagoras).



First PC

- ▶ The first PC is direction of greatest variability in data
- ▶ We will show that the first PC is the eigenvector of the covariance matrix corresponding the maximum eigen value of this matrix.
- ▶ If $\|a\| = 1$, the projection of a d-dimensional x on a is $a^T x$



First PC

$$\begin{aligned} \operatorname{argmax}_{\mathbf{a}} \frac{1}{N} \sum_{n=1}^N (\mathbf{a}^T \mathbf{x}^{(n)})^2 &= \frac{1}{N} \mathbf{a}^T \mathbf{X}^T \mathbf{X} \mathbf{a} \\ \text{s.t. } \mathbf{a}^T \mathbf{a} &= 1 \end{aligned}$$

$$\frac{\partial}{\partial \mathbf{a}} \left(\frac{1}{N} \mathbf{a}^T \mathbf{X}^T \mathbf{X} \mathbf{a} + \lambda(1 - \mathbf{a}^T \mathbf{a}) \right) = 0 \Rightarrow \boxed{\frac{1}{N} \mathbf{X}^T \mathbf{X} \mathbf{a} = \lambda \mathbf{a}}$$

- ▶ \mathbf{a} is the eigenvector of sample covariance matrix $\frac{1}{N} \mathbf{X}^T \mathbf{X}$
- ▶ The eigenvalue λ denotes the amount of variance along that dimension.
 - ▶ Variance = $\frac{1}{N} \mathbf{a}^T \mathbf{X}^T \mathbf{X} \mathbf{a} = \mathbf{a}^T \left(\frac{1}{N} \mathbf{X}^T \mathbf{X} \mathbf{a} \right) = \mathbf{a}^T \lambda \mathbf{a} = \lambda$
- ▶ So, if we seek the dimension with the largest variance, it will be the eigenvector corresponding to the largest eigenvalue of the sample covariance matrix

PCA: Uncorrelated Features

$$\mathbf{x}' = \mathbf{A}^T \mathbf{x}$$

$$\mathbf{R}_{\mathbf{x}'} = E[\mathbf{x}' \mathbf{x}'^T] = E[\mathbf{A}^T \mathbf{x} \mathbf{x}^T \mathbf{A}] = \mathbf{A}^T E[\mathbf{x} \mathbf{x}^T] \mathbf{A} = \mathbf{A}^T \mathbf{R}_x \mathbf{A}$$

- ▶ If $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_d]$ where $\mathbf{a}_1, \dots, \mathbf{a}_d$ are orthonormal eigenvectors of \mathbf{R}_x :

$$\mathbf{R}_{\mathbf{x}'} = \mathbf{A}^T \mathbf{R}_x \mathbf{A} = \mathbf{A}^T (\mathbf{A} \mathbf{\Lambda} \mathbf{A}^T) \mathbf{A} = \mathbf{\Lambda}$$

$$\Rightarrow \forall i \neq j (i, j = 1, \dots, d) E[\mathbf{x}'_i \mathbf{x}'_j] = 0$$

then mutually uncorrelated features are obtained

- ▶ Completely uncorrelated features avoid information redundancies

PCA Derivation: Mean Square Error Approximation

- ▶ Incorporating all eigenvectors in $A = [\mathbf{a}_1, \dots, \mathbf{a}_d]$:

$$\begin{aligned}\mathbf{x}' &= A^T \mathbf{x} \Rightarrow A \mathbf{x}' = A A^T \mathbf{x} = \mathbf{x} \\ &\Rightarrow \mathbf{x} = A \mathbf{x}'\end{aligned}$$

- ▶ \Rightarrow If $d' = d$ then \mathbf{x} can be reconstructed exactly from \mathbf{x}'

PCA Derivation:

Relation between Eigenvalues and Variances

- ▶ The j -th largest eigenvalue of \mathbf{R}_x is the variance on the j -th PC:

$$\text{var}(x'_j) = \lambda_j$$

$$\begin{aligned}\text{var}(x'_j) &= E[x'_j x'_j] \\ &= E[\mathbf{a}_j^T \mathbf{x} \mathbf{x}^T \mathbf{a}_j] = \mathbf{a}_j^T E[\mathbf{x} \mathbf{x}^T] \mathbf{a}_j \\ &= \mathbf{a}_j^T \mathbf{R}_x \mathbf{a}_j = \mathbf{a}_j^T \lambda_j \mathbf{a}_j = \lambda_j\end{aligned}$$

Eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \dots$

- The 1st PC is the the eigenvector of the sample covariance matrix associated with the largest eigenvalue
 - The 2nd PC v_2 is the the eigenvector of the sample covariance matrix associated with the second largest eigenvalue
 - And so on ...
-

PCA Derivation: Mean Square Error Approximation

- ▶ Incorporating only d' eigenvectors corresponding to the largest eigenvalues $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_{d'}]$ ($d' < d$)
- ▶ It minimizes MSE between \mathbf{x} and $\hat{\mathbf{x}} = \mathbf{A}\mathbf{x}'$:

$$\begin{aligned} J(\mathbf{A}) &= E[\|\mathbf{x} - \hat{\mathbf{x}}\|^2] = E[\|\mathbf{x} - \mathbf{A}\mathbf{x}'\|^2] \\ &= E\left[\left\|\sum_{j=d'+1}^d x'_j \mathbf{a}_j\right\|^2\right] \\ &= E\left[\sum_{j=d'+1}^d \sum_{k=d'+1}^d x'_j \mathbf{a}_j^T \mathbf{a}_k x'_k\right] = E\left[\sum_{j=d'+1}^d x_j'^2\right] \\ &= \sum_{j=d'+1}^d E[x_j'^2] = \sum_{j=d'+1}^d \lambda_j \quad \text{Sum of the } d - d' \text{ smallest eigenvalues} \end{aligned}$$

PCA Derivation:

Mean Square Error Approximation

- ▶ In general, it can also be shown MSE is minimized compared to any other approximation of x by any d' -dimensional orthonormal basis
 - ▶ without first assuming that the axes are eigenvectors of the correlation matrix, this result can also be obtained.
- ▶ If the data is mean-centered in advance, R_x and C_x (covariance matrix) will be the same.
 - ▶ However, in the correlation version when $C_x \neq R_x$ the approximation is not, in general, a good one (although it is a minimum MSE solution)

PCA on Faces: “Eigenfaces”

▶ ORL Database



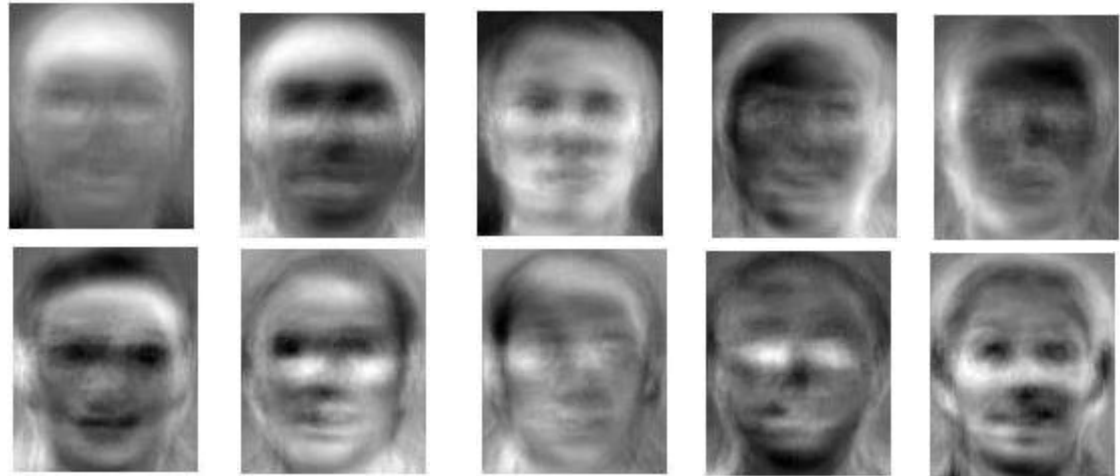
Some Images

PCA on Faces: “Eigenfaces”



Average
face

→
1st
to 10th
PCs



For eigen faces

“gray” = 0,

“white” > 0,

“black” < 0

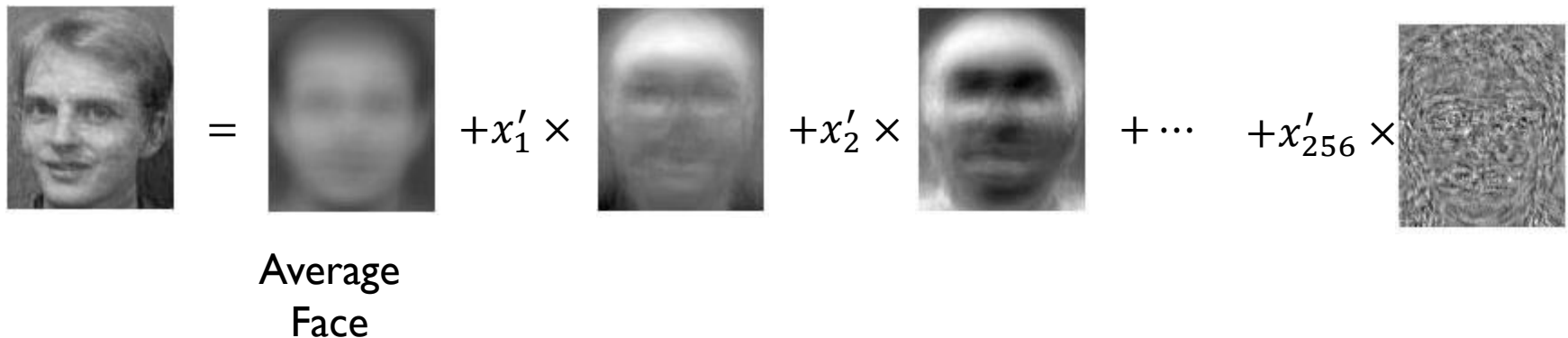
PCA on Faces:



x is a $112 \times 92 = 10304$ dimensional vector containing intensity of the pixels of this image

Feature vector = $[x'_1, x'_2, \dots, x'_{d'}]$

$x'_i = PC_i^T x \longrightarrow$ The projection of x on the i -th PC



PCA on Faces: Reconstructed Face

$d'=1$



$d'=2$



$d'=4$



$d'=8$



$d'=16$



$d'=32$



$d'=64$



$d'=128$



$d'=256$



**Original
Image**

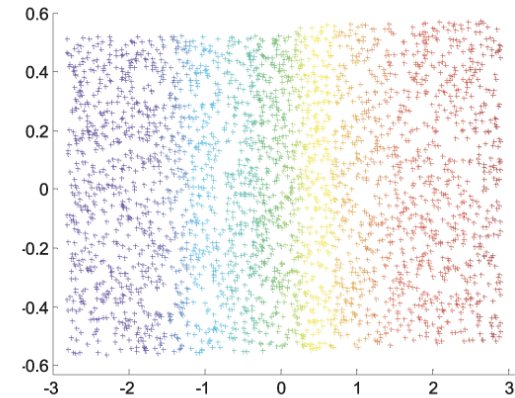
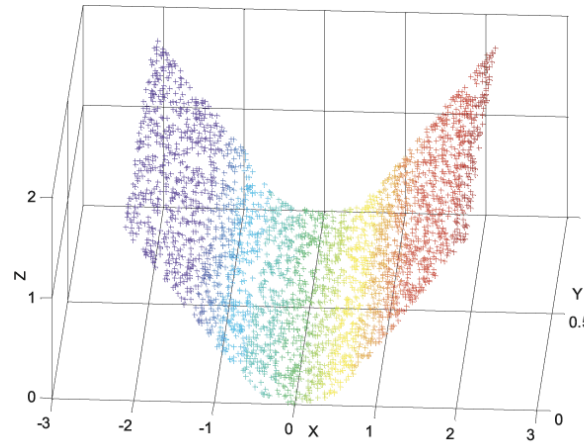
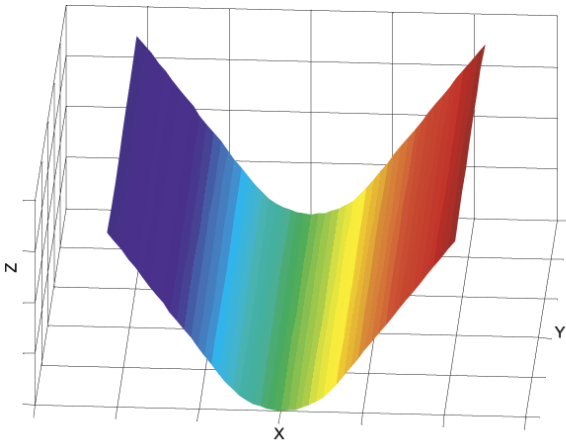


Dimensionality Reduction by PCA

- ▶ In high-dimensional problems, data sometimes lies near a linear subspace (small variability around this subspace can be considered as noise)
- ▶ Only keep data projections onto principal components with large eigenvalue
- ▶ Might lose some info, but if eigenvalues are small, do not lose much

Kernel PCA

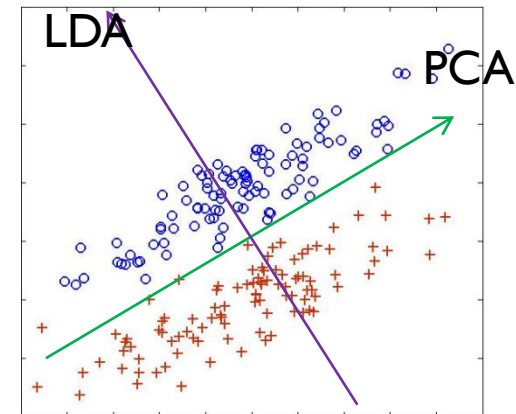
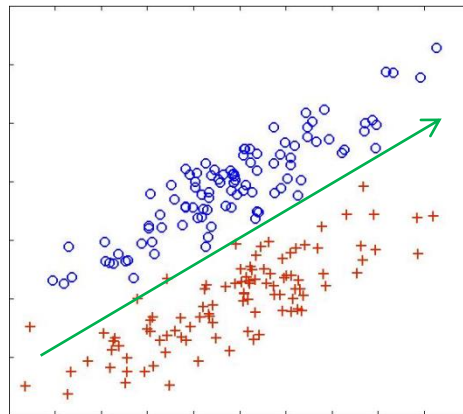
▶ Kernel extension of PCA



data (approximately) lies on
a lower dimensional non-linear space

PCA and LDA: Drawbacks

- ▶ PCA drawback: An excellent information packing transform does not necessarily lead to a good class separability.
 - ▶ The directions of the maximum variance may be useless for classification purpose



- ▶ LDA drawback
 - ▶ Singularity or under-sampled problem (when $N < d$)
 - ▶ Example: gene expression data, images, text documents
 - ▶ Can reduce dimension only to $d' \leq C - 1$ (unlike PCA)

PCA vs. LDA

- ▶ Although LDA often provide more suitable features for classification tasks, PCA might outperform LDA in some situations:
 - ▶ when the number of samples per class is small (overfitting problem of LDA)
 - ▶ when the number of the desired features is more than $C - 1$
- ▶ Advances in the last decade:
 - ▶ Semi-supervised feature extraction
 - ▶ E.g., PCA+LDA, Regularized LDA, Locally FDA (LFDA)

Singular Value Decomposition (SVD)

- ▶ Given a matrix $X \in \mathbb{R}^{N \times d}$, the SVD is a decomposition:

$$X = USV^T$$

$$\begin{array}{c} \boxed{\begin{array}{c} X \\ (N \times d) \end{array}} = \boxed{\begin{array}{c} U \\ (N \times d) \end{array}} \boxed{\begin{array}{c} \sigma_1 \quad 0 \\ 0 \quad \sigma_2 \quad \dots \end{array}} \boxed{\begin{array}{c} V^T \\ (d \times d) \end{array}} = \sum_i \sigma_i u_i v_i^T \\ \mathbf{S} \\ (d \times d) \end{array}$$

- ▶ S is a diagonal matrix with the singular values $\sigma_1, \dots, \sigma_d$ of X .
- ▶ Columns of U, V are orthonormal matrices

Singular Value Decomposition (SVD)

- ▶ Given a matrix $X \in \mathbb{R}^{N \times d}$, the SVD is a decomposition:

$$X = USV^T$$

- ▶ SVD of X is related to eigen-decomposition of $X^T X$ and XX^T .
 - ▶ $X^T X = VSU^T USV^T = VS^2V^T$
 - ▶ so V contains eigenvectors of $X^T X$ and S^2 includes its eigenvalues ($\lambda_i = \sigma_i^2$)
 - ▶ $XX^T = USV^T VSU^T = US^2U^T$
 - so U contains eigenvectors of XX^T and S^2 includes its eigenvalues ($\lambda_i = \sigma_i^2$)
- ▶ In fact, we can view each row of US as the coordinates of an example along the axes given by the eigenvectors.

Independent Component Analysis (ICA)

▶ PCA:

- ▶ The transformed dimensions will be uncorrelated from each other
- ▶ Orthogonal linear transform
- ▶ Only uses second order statistics (i.e., covariance matrix)

▶ ICA:

- ▶ The transformed dimensions will be as independent as possible.
- ▶ Non-orthogonal linear transform
- ▶ High-order statistics can also used

Uncorrelated and Independent

Uncorrelated: $cov(X_1, X_2) = 0$

Independent: $P(X_1, X_2) = P(X_1)P(X_2)$

- ▶ Gaussian
 - ▶ Independent \Leftrightarrow Uncorrelated
- ▶ Non-Gaussian
 - ▶ Independent \Rightarrow Uncorrelated
 - ▶ Uncorrelated \nRightarrow Independent

ICA: Cocktail party problem

▶ Cocktail party problem

- ▶ d speakers are speaking simultaneously and any microphone records only an overlapping combination of these voices.
 - Each microphone records a different combination of the speakers' voices.
- ▶ Using these d microphone recordings, can we separate out the original d speakers' speech signals?

▶ Mixing matrix A :

$$\mathbf{x} = A\mathbf{s}$$

▶ Unmixing matrix A^{-1} :

$$\mathbf{s} = A^{-1}\mathbf{x}$$

$s_j^{(i)}$: sound that speaker j was uttering at time i .

$x_j^{(i)}$: acoustic reading recorded by microphone j at time i .

ICA

- ▶ Find a linear transformation $\mathbf{x} = \mathbf{A}\mathbf{s}$
- ▶ for which dimensions of $\mathbf{s} = [s_1, s_2, \dots, s_d]^T$ are statistically independent

$$p(s_1, \dots, s_d) = p_1(s_1)p_2(s_2) \dots p_d(s_d)$$

- ▶ Algorithmically, we need to identify matrix \mathbf{A} and sources \mathbf{s} where $\mathbf{x} = \mathbf{A}\mathbf{s}$ such that the mutual information between s_1, s_2, \dots, s_d is minimized:

$$I(s_1, s_2, \dots, s_d) = \sum_{i=1}^d H(s_i) - H(s_1, s_2, \dots, s_d)$$