CS 2750 Machine Learning
Lecture 21

Dimensionality reduction
Feature selection

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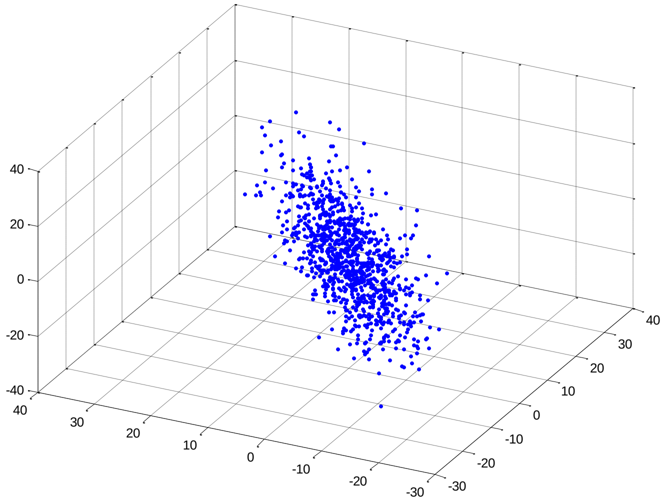
Dimensionality reduction

- **Is there a lower dimensional representation of the data that captures well its characteristics?**
- **Assume:**
  - We have an data $\{\mathbf{x_1}, \mathbf{x_2}, .., \mathbf{x_N}\}$ such that
    $\mathbf{x}_i = (x_i^1, x_i^2, .., x_i^d)$
  - Assume the dimension *d* of the data point ***x*** is very large
  - We want to analyze ***x***
- **Methods of analysis are sensitive to the dimensionality *d***
- **Our goal:**
  - **Find a lower dimensional representation of data of dimension *d'* < *d***

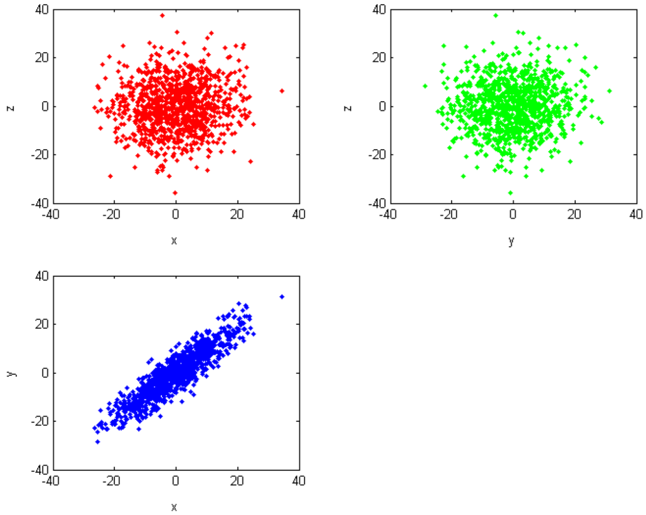
Principal component analysis (PCA)

- **Objective:** We want to replace a high dimensional input with a small set of features (obtained by combining inputs)
  - Different from the feature subset selection !!!
- **PCA:**
  - A linear transformation of *d* dimensional input *x* to M dimensional feature vector *z* such that $M < d$ under which the retained variance is maximal.
  - Equivalently it is the linear projection for which the sum of squares reconstruction cost is minimized.

PCA



PCA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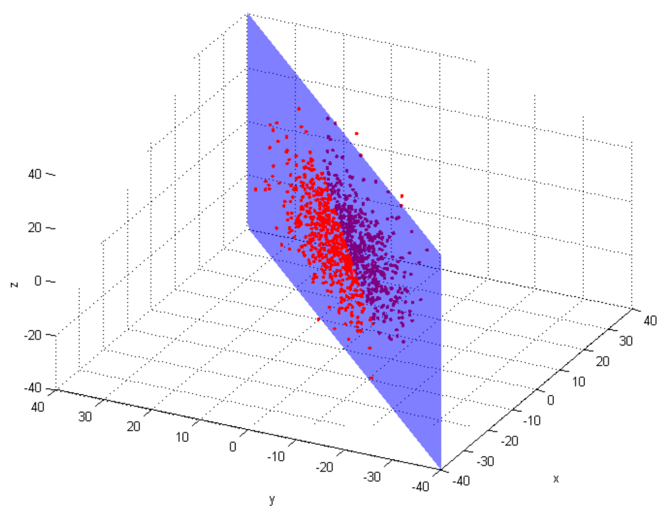
PCA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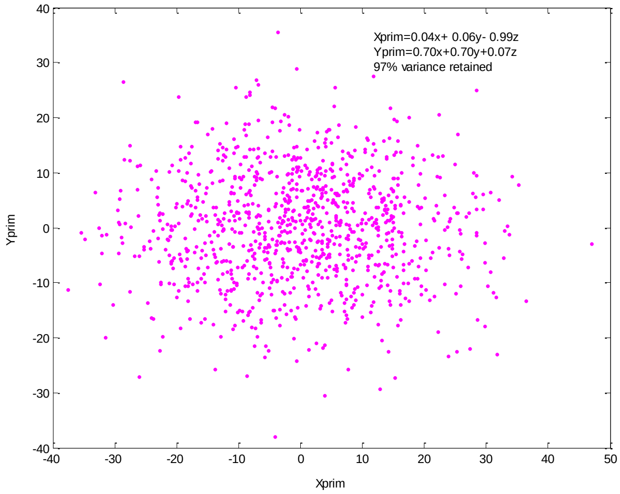
PCA



Principal component analysis (PCA)

- **PCA:**
  - linear transformation of a *d* dimensional input **x** to M dimensional vector **z** such that $M < d$ under which the retained variance is maximal.
  - Task independent
- **Fact:**
  - A vector **x** can be represented using a set of orthonormal vectors **u**

$$\mathbf{x} = \sum_{i=1}^{d} z_i \mathbf{u}_i$$

  - Leads to transformation of coordinates (from **x** to **z** using **u**'s)

$$z_i = \mathbf{u}_i^T \mathbf{x}$$

PCA

- **Idea:** replace *d* coordinates with *M* of z_i coordinates to represent *x*. We want to find the subset *M* of basis vectors.

$$\tilde{\mathbf{x}} = \sum_{i=1}^{M} z_i \mathbf{u}_i + \sum_{i=M+1}^{d} b_i \mathbf{u}_i$$

b_i - constant and fixed

- **How to choose the best set of basis vectors?**
  - We want the subset that gives the best approximation of data *x* in the dataset on average (we use least squares fit)

Error for data entry $\mathbf{x}^n$ $\quad \mathbf{x}^n - \tilde{\mathbf{x}}^n = \sum_{i=M+1}^{d} (z_i^n - b_i)\mathbf{u}_i$

Reconstruction error

$$E_M = \frac{1}{2}\sum_{n=1}^{N} \left\| \mathbf{x}^n - \tilde{\mathbf{x}}^n \right\| = \frac{1}{2}\sum_{n=1}^{N} \sum_{i=M+1}^{d} (z_i^n - b_i)^2$$

PCA

- **Differentiate the error function** with regard to all b_i and set equal to 0 we get:

$$b_i = \frac{1}{N}\sum_{n=1}^{N} z_i^n = \mathbf{u}_i^T \bar{\mathbf{x}} \qquad \bar{\mathbf{x}} = \frac{1}{N}\sum_{n=1}^{N} \mathbf{x}^n$$

- Then we can rewrite:

$$E_M = \frac{1}{2}\sum_{i=M+1}^{d} \mathbf{u}_i^T \mathbf{\Sigma} \mathbf{u}_i \qquad \mathbf{\Sigma} = \sum_{n=1}^{N} (\mathbf{x}^n - \bar{\mathbf{x}})(\mathbf{x}^n - \bar{\mathbf{x}})^T$$

- The error function is optimized when basis vectors satisfy:

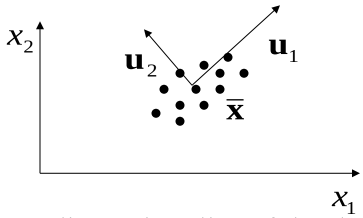
$$\mathbf{\Sigma}\mathbf{u}_i = \lambda_i \mathbf{u}_i \qquad E_M = \frac{1}{2}\sum_{i=M+1}^{d} \lambda_i$$

The best *M* basis vectors: discard vectors with *d-M* smallest eigenvalues (or keep vectors with M largest eigenvalues)

Eigenvector $\mathbf{u}_i$ – is called a **principal component**

PCA

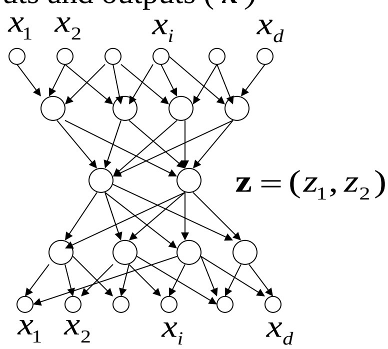
- Once eigenvectors $\mathbf{u}_i$ with largest eigenvalues are identified, they are used to transform the original *d*-dimensional data to *M* dimensions



- To find the "true" dimensionality of the data *d'* we can just look at eigenvalues that contribute the most (small eigenvalues are disregarded)
- **Problem:** PCA is a linear method. The "true" dimensionality can be overestimated. There can be non-linear correlations.
- **Modifications for nonlinearities:** kernel PCA

Dimensionality reduction with neural nets

- **PCA** is limited to linear dimensionality reduction
- To do non-linear reductions we can use neural nets
- **Auto-associative (or auto-encoder) network:** a neural network with the same inputs and outputs ($\boldsymbol{x}$)



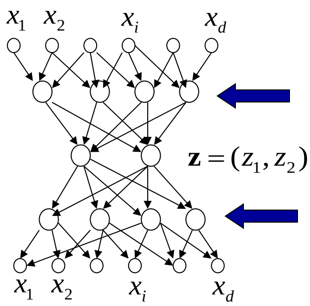
- The middle layer corresponds to the reduced dimensions

Dimensionality reduction with neural nets

- **Error criterion:**

$$E = \frac{1}{2}\sum_{n=1}^{N}\sum_{i=1}^{d}\left(y_i(x^n) - x^n\right)^2$$

- Error measure tries to recover the original data through limited number of dimensions in the middle layer
- **Non-linearities** modeled through intermediate layers between the middle layer and input/output
- If no intermediate layers are used the model replicates PCA optimization through learning



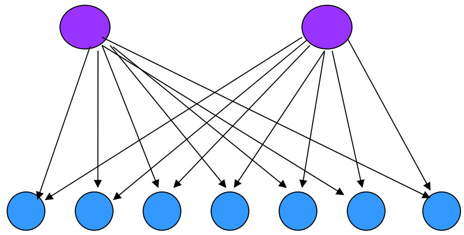
Multidimensional scaling

- Find a lower dimensional space projection such that the distances among data points are preserved
- Used in visualization – d-diminensional data transformed to 3D or 2D
- **Dissimilarities before projection** $\delta_{i,j} = \|x_i - x_j\|$
- **Objective:** Optimize points and their coordinates by fitting the dissimilarities afterwards

$$\min_{\{x_1, x_2, \cdots x_n\}} \sum_{i<j} (\|x_i' - x_j'\| - \delta_{ij})^2$$

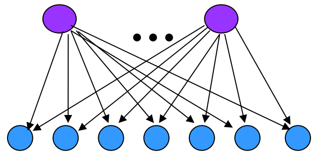
Latent variable models

Latent variables (s): Dimensionality k



Observed variables x: real valued vars
Dimensionality d

Cooperative vector quantizer



Model:

Latent var s_i:

~ Bernoulli distribution

parameter: π_i

$$P(s_i \mid \pi_i) = \pi_i^{s_i}(1-\pi_i)^{1-s_i}$$

Observable variables x:

~ Normal distribution

parameters: $\mathbf{W}, \Sigma$

$$P(\mathbf{x} \mid \mathbf{s}) = N(\mathbf{Ws}, \Sigma)$$

We assume $\Sigma = \sigma I$

$$\mathbf{W} = \begin{pmatrix} w_{11} & w_{12} & .. & w_{1k} \\ w_{21} & & & \\ & .. & & \\ w_{d1} & .. & .. & w_{dk} \end{pmatrix}$$

Joint for one instance of x and s:

$$P(\mathbf{x},\mathbf{s} \mid \Theta) = (2\pi)^{-d/2} \sigma^{-d/2} \exp\left\{ -\frac{1}{2\sigma^2} (\mathbf{x} - \mathbf{Ws})^T (\mathbf{x} - \mathbf{Ws}) \right\} \prod_{i=1}^{k} \pi_i^{s_i} (1-\pi_i)^{(1-s_i)}$$

Other unsupervised methods

- **Factor analysis (a latent variable model)**
- Decompose signal into multiple Gaussian sources

$$\mathbf{x} = \mathbf{A}\mathbf{s}$$ X is a linear combination of values for sources

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

- **Independent component analysis:**
  - Identify independent components/signals/sources in the original data
  - Non-Gaussian signals

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