CS 2750 Machine Learning
Lecture 19

Dimensionality reduction
Feature selection

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Dimensionality reduction. Motivation.

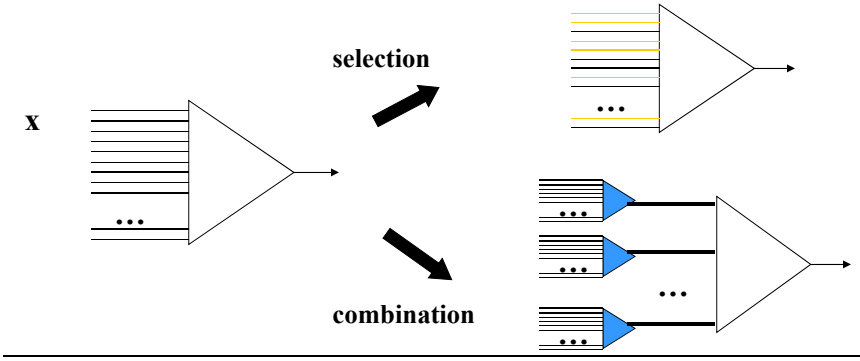
- **Is there a lower dimensional representation of the data that captures well its characteristics?**
- **Assume:**
  - We have an data $\{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}$ such that $\mathbf{x}_i = (x_i^1, x_i^2, ..., x_i^d)$
  - Assume the dimension d of the data point $\boldsymbol{x}$ is very large
  - We want to analyze $\boldsymbol{x}$
- **Methods of analysis are sensitive to the dimensionality d**
- **Our goal: Find a lower dimensional representation of data**
- **Two learning problems:**
  - **supervised**
  - **unsupervised**

Dimensionality reduction for classification

- **Classification problem example:**
  - We have an input data $\{\mathbf{x}_1, \mathbf{x}_2, .., \mathbf{x}_N\}$ such that
    $$\mathbf{x}_i = (x_i^1, x_i^2, .., x_i^d)$$
    and a set of corresponding output labels $\{y_1, y_2, .., y_N\}$
  - Assume the dimension d of the data point $\boldsymbol{x}$ is very large
  - We want to classify $\boldsymbol{x}$
- **Problems with high dimensional input vectors**
  - **A large number of parameters** to learn, if a dataset is small this can result in:
    - Large variance of estimates and overfit
  - **it becomes hard to explain what features are important in the model (**too many choices some can be substitutable**)**

Dimensionality reduction

- **Solutions**:
  - **Selection of a smaller subset** of inputs (features) from a large set of inputs; train classifier on the reduced input set
  - **Combination of high dimensional inputs** to a smaller set of features $\phi_k(\mathbf{x})$; train classifier on new features



Feature selection

How to find a good subset of inputs/features?

- **We need**:
  - A criterion for ranking good inputs/features
  - Search procedure for finding a good set of features
- **Feature selection process can be**:
  - **Dependent on the learning task**
    - e.g. classification
    - Selection of features affected by what we want to predict
  - **Independent of the learning task**
    - Unsupervised methods
    - may lack the accuracy for classification/regression tasks

Task-dependent feature selection

Assume:

- **Classification problem**: $\mathbf{x}$ – input vector, y - output
- Feature mappings $\boldsymbol{\varphi} = \{\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots \phi_k(\mathbf{x}), \ldots\}$

Objective: Find a subset of features that gives/preserves most of the output prediction capabilities

Selection approaches:

- **Filtering approaches**
  - Filter out features with small predictive potential
  - done before classification; typically uses univariate analysis
- **Wrapper approaches**
  - Select features that directly optimize the accuracy of the multivariate classifier
- **Embedded methods**
  - Feature selection and learning closely tied in the method

Feature selection through filtering

- **Assume:**
  - **Classification problem**: **x** – input vector, y - output
  - Inputs in x or feature mappings $\phi_k(\mathbf{x})$
- **How to select the feature:**
  - **Univariate analysis**
    - Pretend that only one variable, x_k, exists
    - See how well it predicts the output y alone
  - **Example:** differentially expressed features (or inputs)
    - Good separation in binary (case/control settings)

Differentially expressed features

- **Scores for measuring the differential expression**
  - T-Test score (Baldi & Long)
    - Based on the test that two groups come from the same population
  - Fisher Score $Fisher\ (i) = \dfrac{\mu_i^{(+)^2} - \mu_i^{(-)^2}}{\sigma_i^{(+)^2} + \sigma_i^{(-)^2}}$
  - Area under Receiver Operating Characteristic (AUC) score

Problems:

- if many random features, the features with a good differentially expressed score must arise
- Techniques to reduce FDR (False discovery rate) and FWER (Family wise error).

Feature filtering

Other univariate scores:

- **Correlation coefficients** $\rho(\phi_k, y) = \frac{Cov(\phi_k, y)}{\sqrt{Var(\phi_k)Var(y)}}$
  - Measures **linear dependences**
- **Mutual information**

$$I(\phi_k, y) = \sum_i \sum_j \tilde{P}(\phi_k = j, y = i) \log_2 \frac{\tilde{P}(\phi_k = j, y = i)}{\tilde{P}(\phi_k = j)\tilde{P}(y = i)}$$

- **Univariate assumptions:**
  - Only one feature and its effect on y is incorporated in the mutual information score
  - Effects of two features on y are independent
- What to do if the combination of features gives the best prediction?

Feature selection: dependent features

Filtering with dependent features

- Let $\boldsymbol{\varphi}$ be a current set of features (starting from complete set)
- We can remove feature $\phi_k(\mathbf{x})$ from it when:
  $\tilde{P}(y \mid \boldsymbol{\varphi} \setminus \phi_k) \approx \tilde{P}(y \mid \boldsymbol{\varphi})$ for all values of ϕ_k, y
- Repeat removals until the probabilities differ.

Problem: how to compute/estimate $\tilde{P}(y \mid \boldsymbol{\varphi} \setminus \phi_k), \tilde{P}(y \mid \boldsymbol{\varphi})$?

Solution: make some simplifying assumption about the underlying probabilistic model

- **Example: use a Naïve Bayes**
- **Advantage:** speed, modularity, applied before classification
- **Disadvantage:** may not be as accurate

Feature selection: wrappers

Wrapper approach:

- The feature selection is driven by the prediction accuracy of the classifier (regressor) we actually want to built

How to find the appropriate feature set?

- **If the dimension is d then there 2d**
- **Idea: Greedy search in the space of classifiers**
  - Gradually add features improving most the quality score
  - Gradually remove features that effect the accuracy the least
  - Score should reflect the accuracy of the classifier (error) and also prevent overfit
- **Standard way to measure the quality:**
  - Internal cross-validation (m-fold cross validation)

Internal cross-validation

- **Split train set: to internal train and test sets**
- **Internal train set: train different models** (defined e.g. on different subsets of features)
- **Internal test set/s**: **estimate the generalization error** and select the best model among possible models
- **Internal cross-validation (*m*-fold):**
  - Divide the train data into m equal partitions (of size N/m)
  - Hold out one partition for validation, train the classifiers on the rest of data
  - Repeat such that every partition is held out once
  - The estimate of the generalization error of the learner is the mean of errors of on all partitions

Feature selection: wrappers

- **Greedy (forward) search:**
  - logistic regression model with features

Start with $p(y=1|\mathbf{x},\mathbf{w}) = g(w_o)$

Choose feature x_i with the best error (in the internal step)

$$p(y=1|\mathbf{x},\mathbf{w}) = g(w_o + w_i x_i)$$

Choose feature x_j with the best error (in the internal step)

$$p(y=1|\mathbf{x},\mathbf{w}) = g(w_o + w_i x_i + w_j x_j)$$

Etc.

When to stop ?

Goal: Stop adding features when the error on the data stops descreasing

Embedded methods

- **Feature selection + classification model learning** done together
- **Embedded models:**
  - **Regularized models**
    - Models of higher complexity are explicitly penalized leading to 'virtual' removal of inputs from the model
    - Regularized logistic/linear regression
    - **Support vector machines**
      - Optimization of margins penalizes nonzero weights
  - **CART/Decision trees**

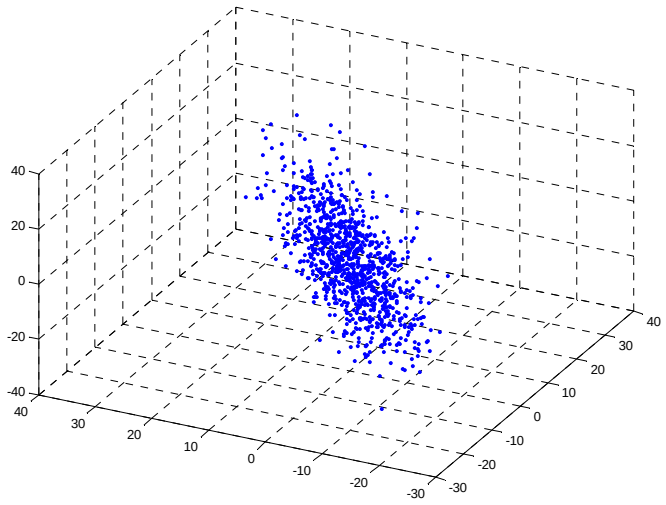
Dimensionality reduction

- **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 $\boldsymbol{x}$ is very large
  - We want to analyze $\boldsymbol{x}$
- **Methods of analysis are sensitive to the dimensionality d**
- **Our goal:**
  - **Find a lower dimensional representation of data of dimension $d' < d$**

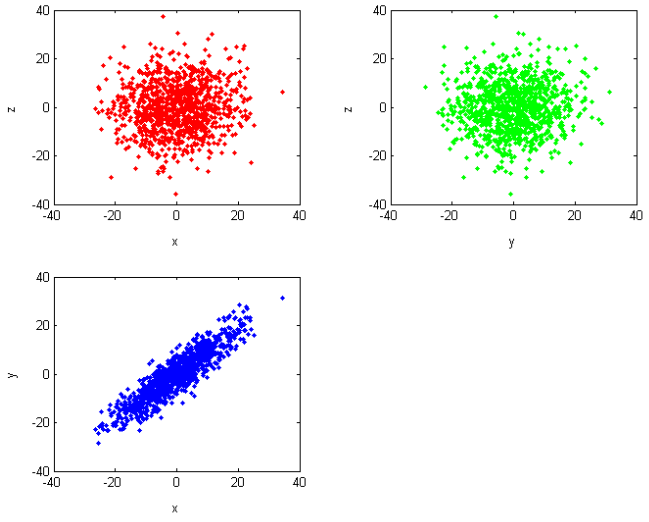
Principal component analysis (PCA)

- **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.

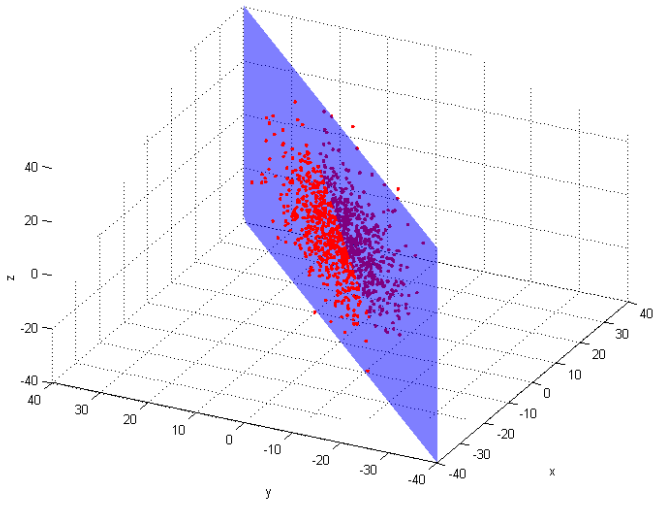
PCA



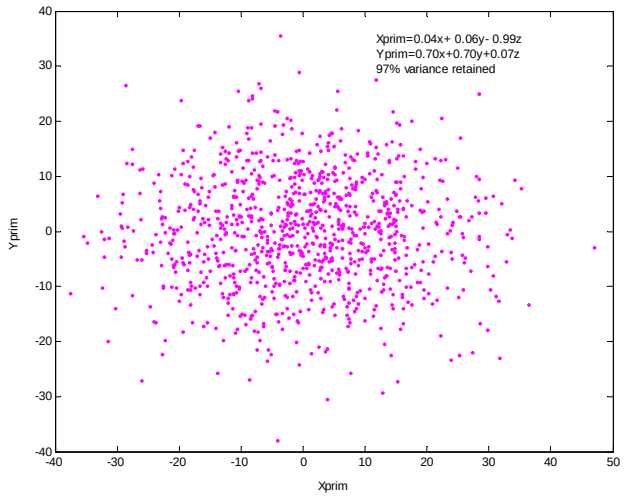
PCA



PCA


z
y
x

PCA


Xprim=0.04x+ 0.06y- 0.99z
Yprim=0.70x+0.70y+0.07z
97% variance retained
Yprim
Xprim

Principal component analysis (PCA)

- **PCA:**
  - linear transformation of d dimensional input $\mathbf{x}$ to M dimensional feature vector $\mathbf{z}$ such that $M < d$ under which the retained variance is maximal.
  - Task independent
- **Fact:**
  - A vector $\mathbf{x}$ can be represented using a set of orthonormal vectors $\mathbf{u}$
$$\mathbf{x} = \sum_{i=1}^{d} z_i \mathbf{u}_i$$
  - Leads to transformation of coordinates (from $\mathbf{x}$ to $\mathbf{z}$ using $\mathbf{u}$'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:

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

- The error function is optimized when basis vectors satisfy:

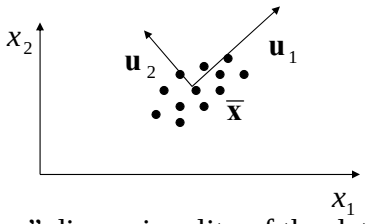
$$\boldsymbol{\Sigma}\mathbf{u}_i = \lambda_i \mathbf{u}_i \qquad E_M = \frac{1}{2}\sum_{i=M+1}^{d} \lambda_i$$

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

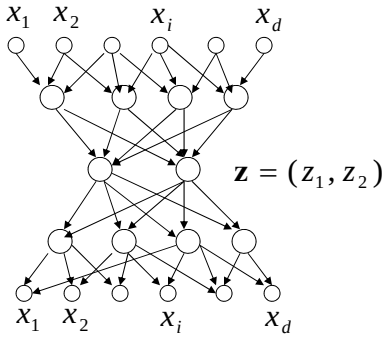
- Once eigenvectors $\mathbf{u}_i$ with largest eigenvalues are identified, they are used to transform the original *d*-dimensional data to *M* dimensions



- 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.

Dimensionality reduction with neural nets

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



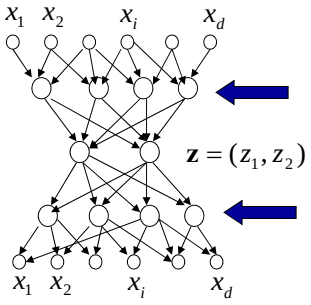
- The middle layer corresponds to the reduced dimensions

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** $\delta_{i,j} = \left\| x_i - x_j \right\|$
- **Objective:** Optimize points and their coordinates by fitting the dissimilarities afterwards

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

Other (unsupervised) methods

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

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

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

Dimensionality reduction through clustering

- **Clustering algorithms**
  - group together "similar" instances in the data sample
- **Dimensionality reduction based on clustering**:
  - Replace a high dimensional data entry with a cluster label
- **Problem:**
  - Determistic clustering gives only one label per input
  - May not be enough to represent the data for prediction
- **Solutions:**
  - Clustering over subsets of input data
  - Soft clustering (probability of a cluster is used directly)

Dimensionality reduction through clustering

- **Soft clustering** (e.g. mixture of Gaussians) attempts to cover all instances in the data sample with a small number of groups
  - Each group is more or less responsible for a data entry (responsibility – a posterior of a group given the data entry)

Mixture of G. responsibility

$$h_{il} = \frac{\pi_i \, p(x_l \mid y_l = i)}{\sum_{u=1}^{k} \pi_u \, p(x_l \mid y_l = u)}$$

- **Dimensionality reduction based on soft clustering**
  - Replace a high dimensional data with the set of group posteriors
  - Feed all posteriors to the learner e.g. linear regressor, classifier

Dimensionality reduction through clustering

- We can use the idea of soft clustering before applying regression/classification learning
- **Two stage algorithms**
  - Learn the clustering
  - Learn the classification
- Input clustering: $\mathbf{x}$ (high dimensional)
- Output clustering (Input classifier): $p(c = i \mid \mathbf{x})$
- Output classifier: y
- **Example: Networks with Radial Basis Functions (RBFs)**
- **Problem:**
  - Clustering learns based on $p(\mathbf{x})$ (disregards the target)
  - Prediction based on $p(y \mid x)$

Networks with radial basis functions

- An alternative to **multilayer NN for non-linearities**
- Radial basis functions: $f(x) = w_0 + \sum_{j=1}^{k} w_j \phi_j(\mathbf{x})$
  - Based on interpolations of prototype points (**mean**s)
  - Affected by the distance between the **x** and the **mean**
  - Fit the outputs of basis functions through the linear model
- Choice of basis functions:

Gaussian $\phi_j(x) = \exp\left\{\frac{\|x - \mu_j\|^2}{2\sigma_j^2}\right\}$

- **Learning:**
  - In practice seem to work OK for up to 10 dimensions
  - For higher dimensions (ridge functions – logistic) combining multiple learners seem to do better job