CS 2750 Machine Learning
Lecture 20

Feature selection
Dimensionality reduction

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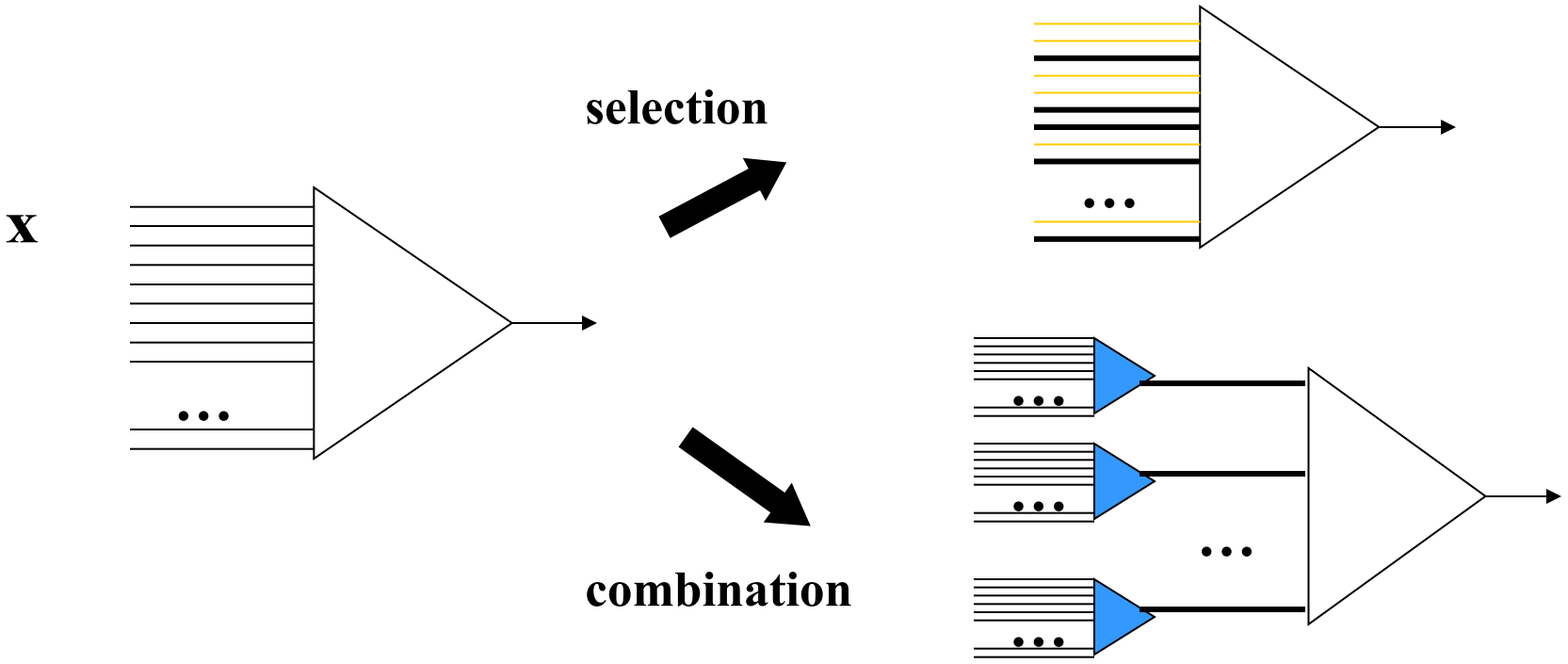
Dimensionality reduction. Motivation.

- **ML methods are sensitive to the dimensionality *d* of data**
- **Question:** Is there a lower dimensional representation of the data that captures well its characteristics?
- **Objective of dimensionality reduction:**
  - **Find a lower dimensional representation of data**
- **Two learning problems:**
  - **Supervised** $D = \{(\mathbf{x_1}, y_1), (\mathbf{x_2}, y_2), ..., (\mathbf{x}_n, , y_n)\}$
    $\mathbf{x}_i = (x_i^1, x_i^2, .., x_i^d)$
  - **Unsupervised** $D = \{\mathbf{x_1}, \mathbf{x_2}, ..., \mathbf{x}_n\}$
    $\mathbf{x}_i = (x_i^1, x_i^2, .., x_i^d)$
- **Goal: replace** $\mathbf{x}_i = (x_i^1, x_i^2, .., x_i^d)$
  with $\mathbf{x}_i'$ **of dimensionality d'<< d**

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



Task-dependent feature selection

Assume: Classification problem:

- **x** – input vector, y - output

Objective: Find a subset of inputs/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
  - Regularization methods, decision tree methods

Feature selection through filtering

Assume: **Classification problem**: **x** – input vector, y - output

How to select the features/inputs?

- **Step 1 .** For each input x_i in data calculate $Score(x_i, y)$ reflecting how well x_i predicts the output y alone
- **Step 2.** Pick a subset of inputs with the best scores $Score(x_i, y)$ (or equivalently eliminate/filter the inputs with the worst scores)

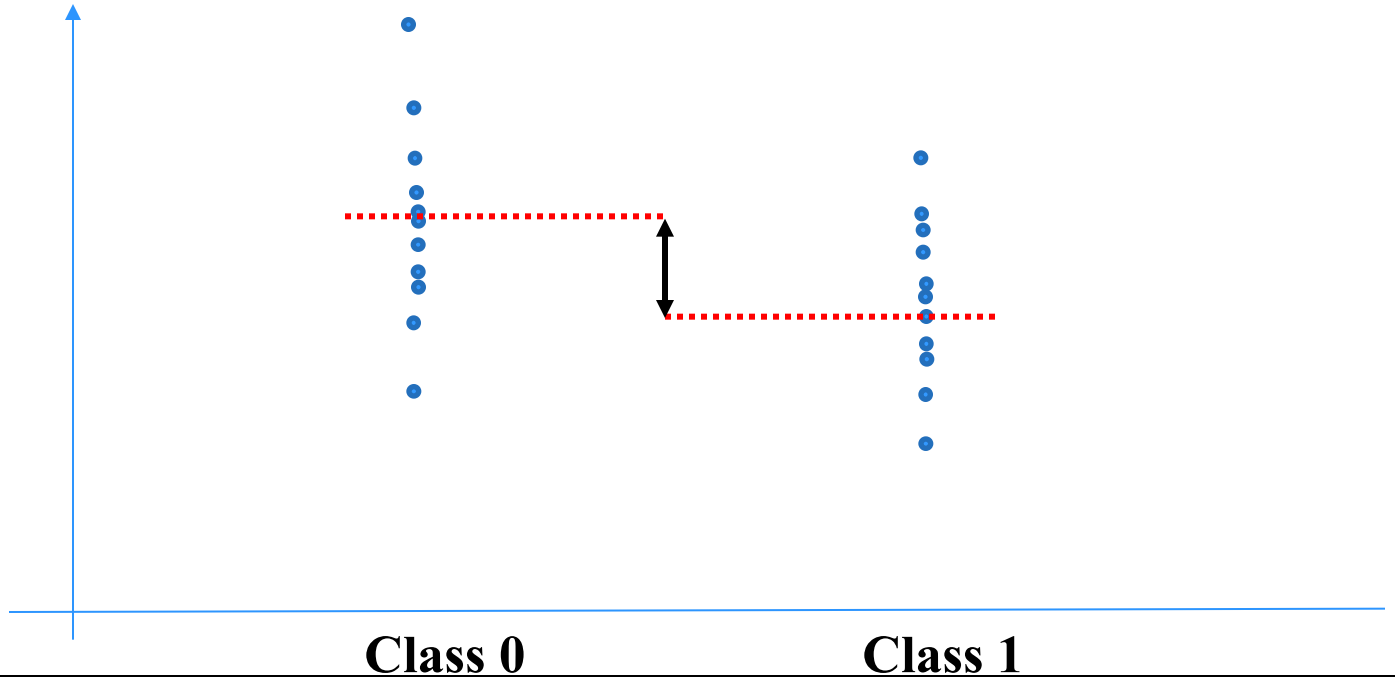
x_1	x_2	x_3		x_{100}	y
1.2	3.3	0.2		9.3	1
7.5	3.7	8.6		2.1	0
1.3	2.6	6.5		7.5	1

$Score(x_1, y)$ $Score(x_2, y)$ $Score(x_3, y)$ $Score(x_{100}, y)$

Feature scoring for classification

Scores for measuring the differential expression

- **T-Test score** (Baldi & Long): Based on the test that two groups come from the same population
  - Null hypothesis: **is mean of class 0 = mean of class 1**
  - Larger **t score** → the groups are more different
  - Smaller t score → the groups are more similar

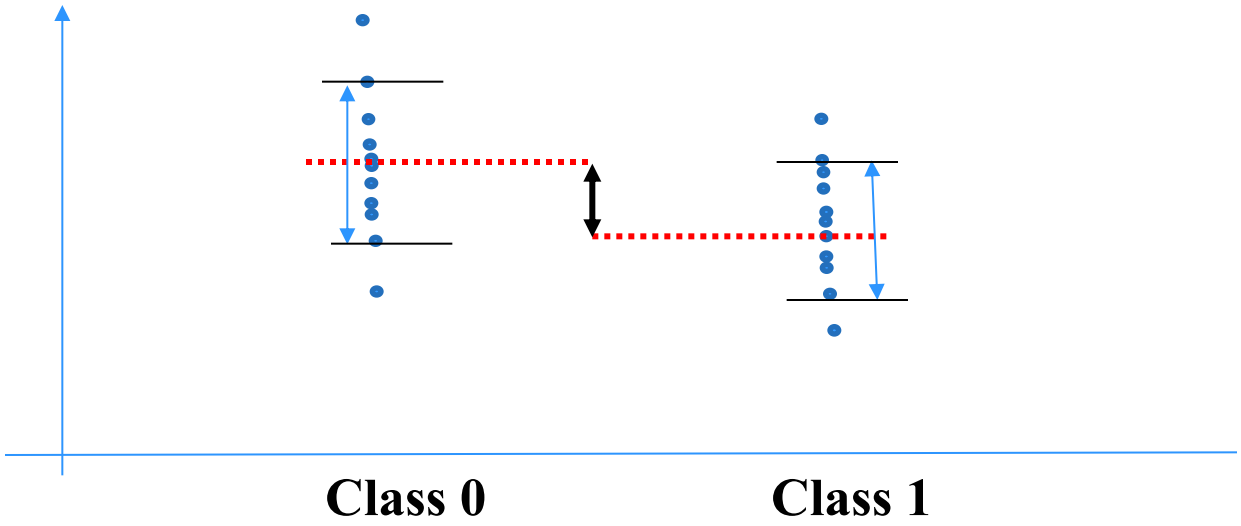


Feature scoring for classification

Scores for measuring the differential expression

- **Fisher Score**

$$Fisher(i) = \frac{(\mu_i^{(+)} - \mu_i^{(-)})^2}{\sigma_i^{(+)2} + \sigma_i^{(-)2}}$$

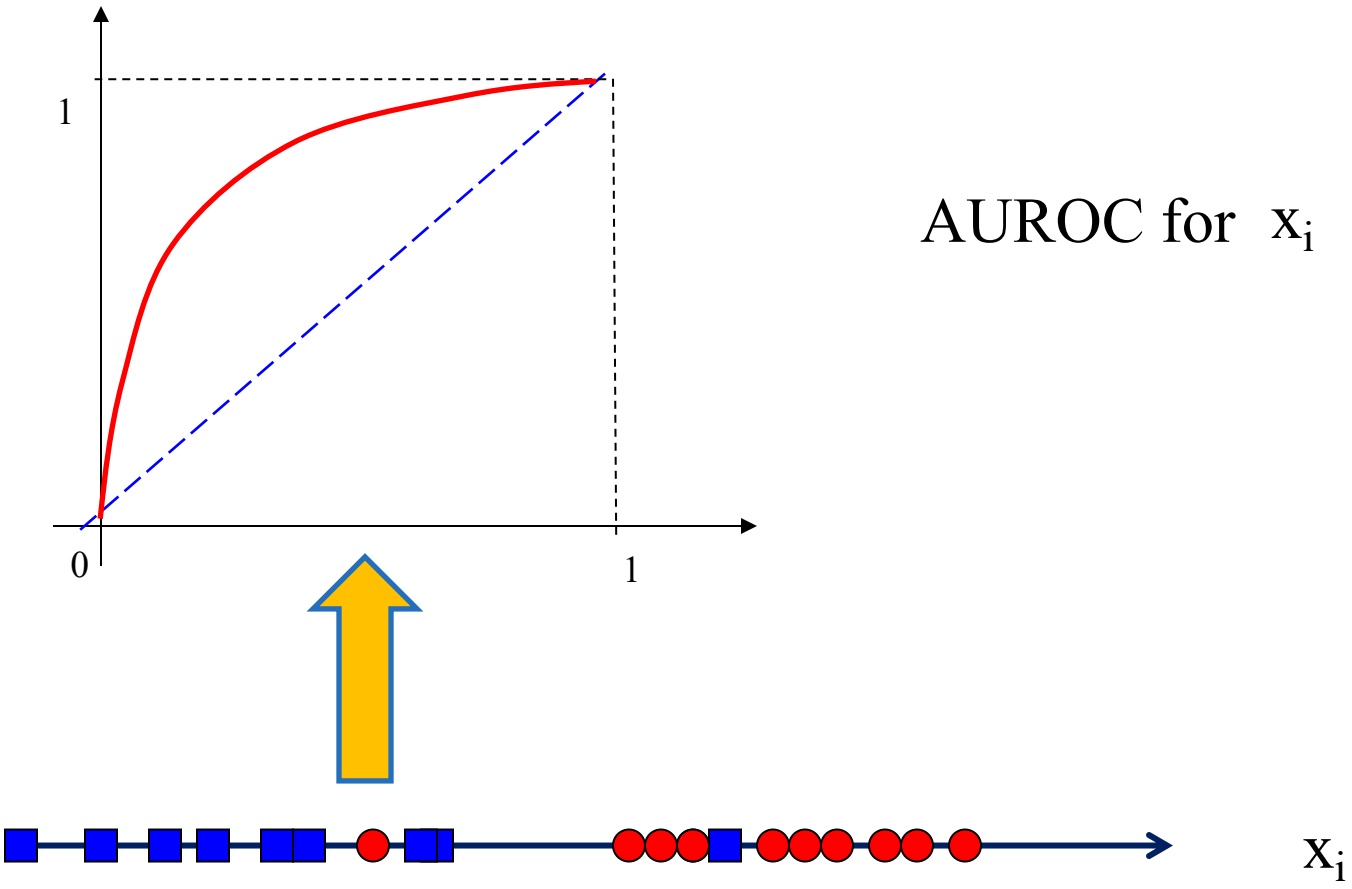


- **AUROC score:** Area under Receiver Operating Characteristic curve

Feature scoring for classification

Scores for measuring the differential expression

- **AUROC score:** Area under Receiver Operating Characteristic curve



Feature scoring for classification

- **Correlation coefficients**
  - **Measures linear dependences**

$$\rho(x_k, y) = \frac{Cov(x_k, y)}{\sqrt{Var(x_k)Var(y)}}$$

- **Mutual information**
  - **Measures dependences**
  - **Needs discretized input values**

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

Feature scoring for classification: dependences

Univariate score assumptions:

- Only one input and its effect on *y* is incorporated in the score
- Effects of two features on *y* are considered to be independent

Correlation based feature selection

- A partial solution to the above problem
- **Idea:** good feature subsets contain features that are highly correlated with the class but independent of each other
- **Assume a set of features S of size *d*.** Then

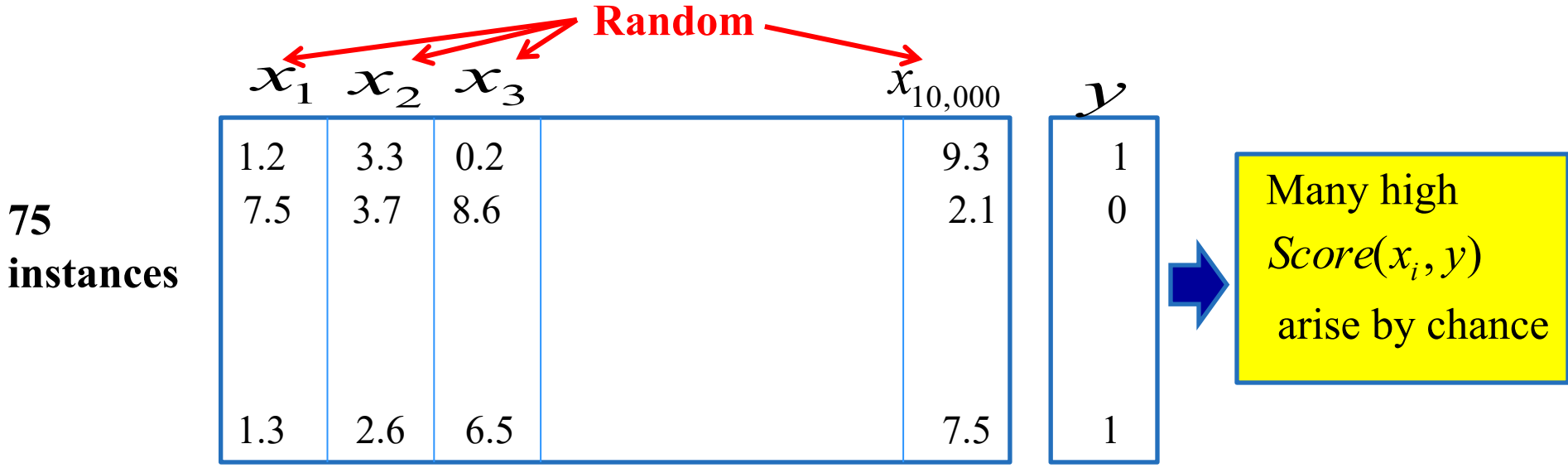
$$M(S) = \frac{d\bar{r}_{yx}}{\sqrt{d + d(d+1)\bar{r}_{xx}}}$$

- Average correlation between x and class y $\bar{r}_{yx}$
- Average correlation between pairs of xs $\bar{r}_{xx}$

Feature selection: low sample size

Problems: Many inputs and low sample size

- if we have many random features, and not many instances to learn from, the features with a good predictive score **may arise simply by chance.** The probability of this can be quite large.



- Techniques to address the problem:
  - reduce **FDR** (False discovery rate) and
  - **FWER** (Family wise error)

Feature selection: wrappers

Wrapper approach:

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

Two problems:

How to judge the quality of a subset of inputs on the model?

How to find the best subset of inputs out of d inputs efficiently?

Feature selection: wrappers

Wrapper approach:

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Two problems:

How to judge the quality of a subset of inputs on the model?

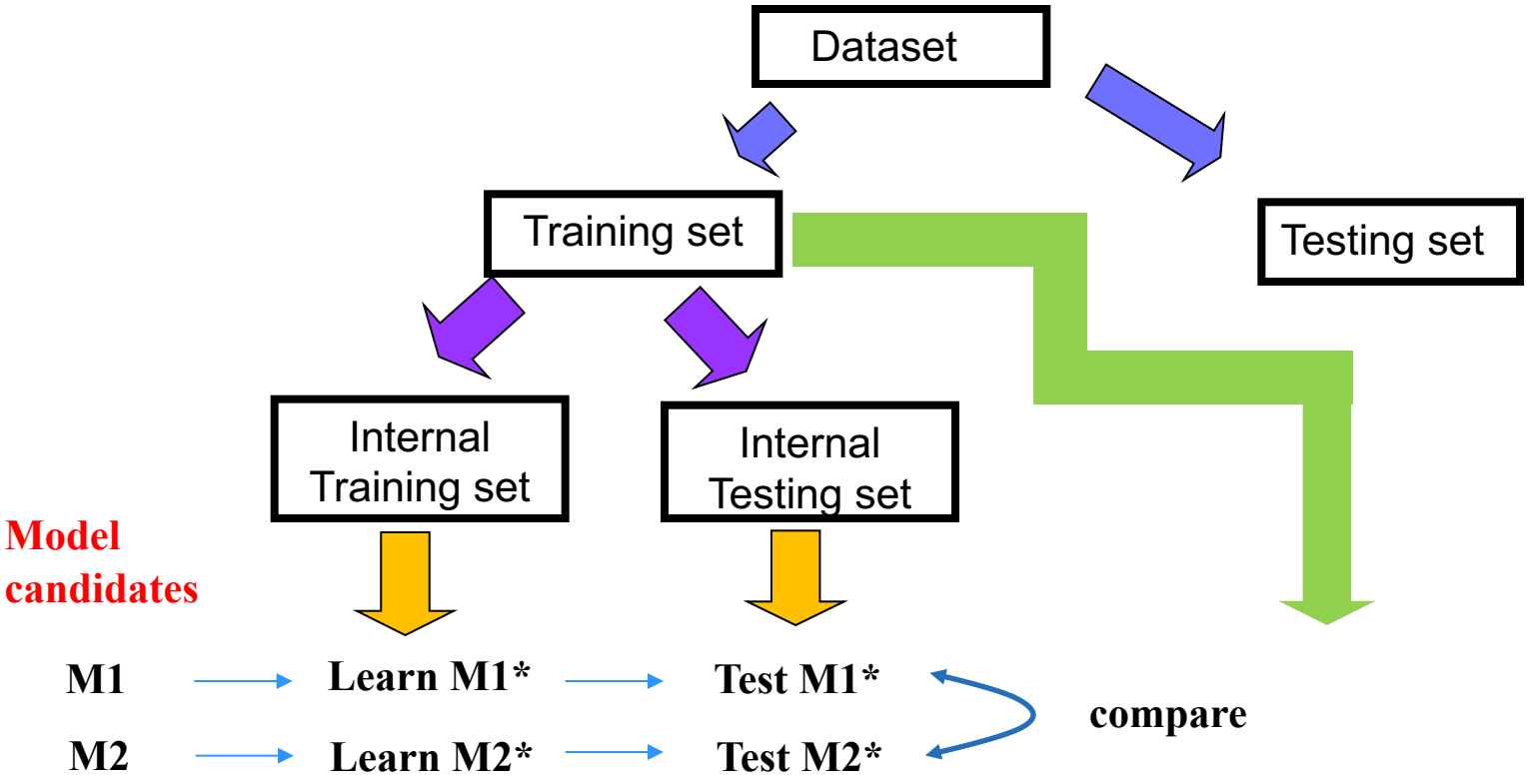
- Internal cross-validation (k-fold cross validation)

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 (*k*-fold):**
  - Divide the train data into *m* equal partitions (of size *N/k*)
  - 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

Internal train and test

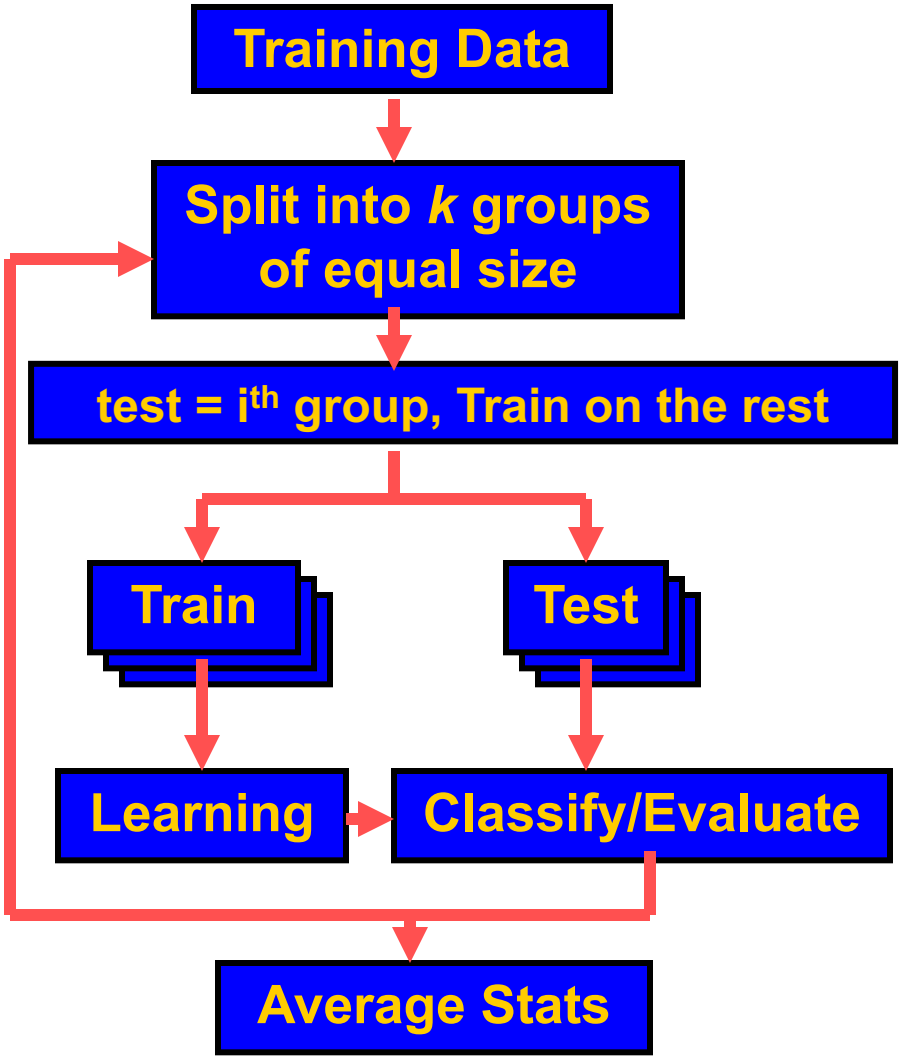
Internal train and test splitting. Hold some data out of the training set (called validation set) to decide on the model first, than train the picked model



Internal k-fold cross-validation

Cross-validation (k-fold)

- Divide data into k disjoint groups, validate on k-th group/train on the rest
- Typically 5-fold cross-validation

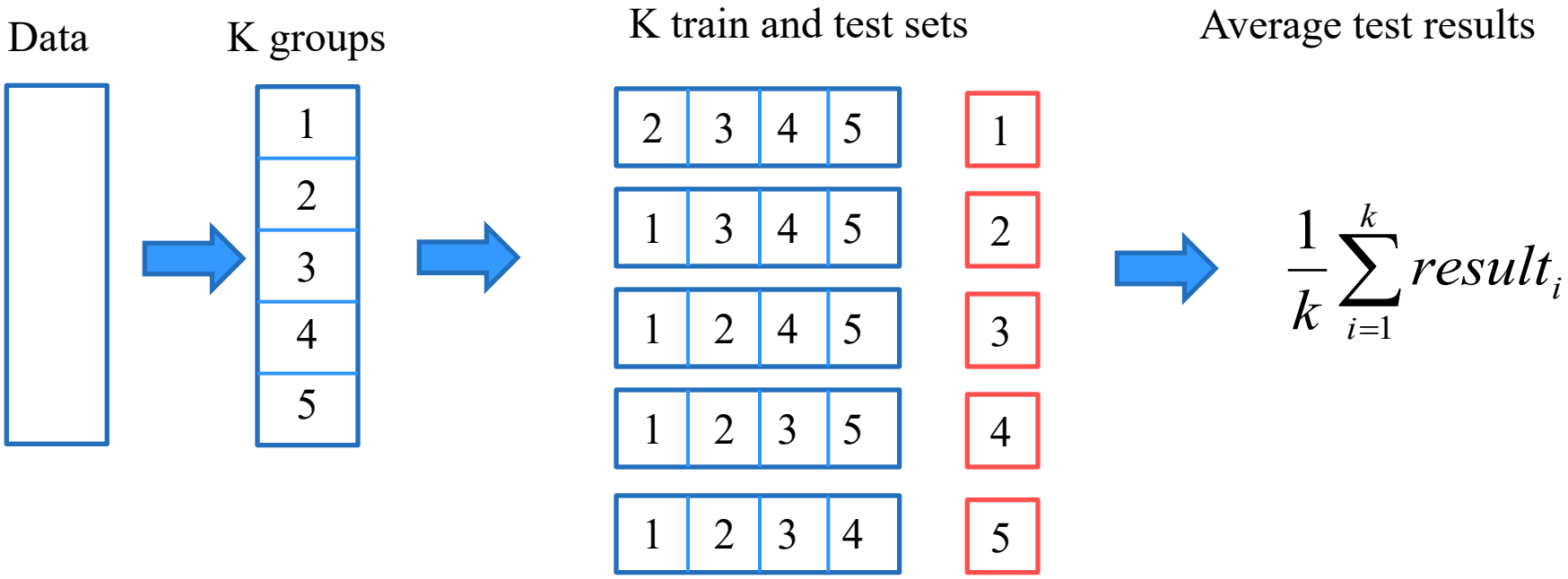


Evaluation of models using k-fold cross-validation

Cross-validation (k-fold)

- Divide data into k disjoint groups,
- For every group i, test on i-th group and train on the rest
- Gives k models and k test results

Example: k=5 (5-fold crossvalidation)



Feature selection: wrappers

Wrapper approach:

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

Two problems:

How to judge the quality of a subset of inputs on the model?

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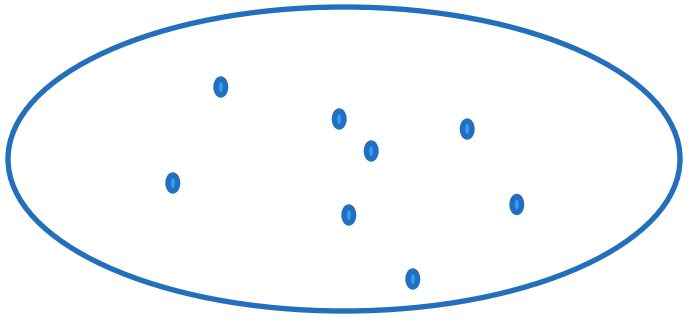
How to find the best subset of inputs out of d inputs efficiently?



d inputs

Feature selection: wrappers

Wrapper approach:

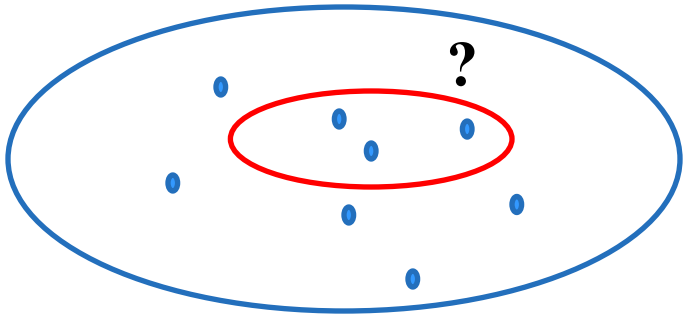
- The input/feature selection is driven by the prediction accuracy of the classifier (regressor) we actually want to built

Two problems:

How to judge the quality of a subset of inputs on the model?

- Internal cross-validation (k-fold cross validation)

How to find the best subset of inputs out of d inputs efficiently?



d inputs

For *d* inputs/features there are 2^d different input subsets to evaluate and compare

Feature selection: wrappers

How to find the appropriate feature subset S efficiently?

- For *d* inputs/features there are 2^d different feature subsets

- **Solution : Greedy search in the space of classifiers**
  - **Option 1: Build the set incrementally**
    - Add features one by one. Add features that improve the quality of the model the most
  - **Option 2: Gradually remove features**
    - Remove features that effect the accuracy the least

- **Model quality:**
  - Internal cross-validation (k-fold cross validation)

Feature selection: wrappers

Greedy selection

Level 1

$\{x_1\}$ $\{x_2\}$ $\{x_3\}$ $\cdots$ $\{x_{100}\}$

$M_{\{x_1\}}$ $M_{\{x_2\}}$ $M_{\{x_3\}}$ $\cdots$ $M_{\{x_{100}\}}$

$e(M_{\{x_1\}})$ $e(M_{\{x_2\}})$ $e(M_{\{x_3\}})$ $\cdots$ $e(M_{\{x_{100}\}})$

Best score

selected $\{x_2\}$

Level 2

$\{x_2, x_1\}$ $\{x_2, x_3\}$ $\cdots$ $\{x_2, x_{100}\}$

$M_{\{x_2,x_1\}}$ $M_{\{x_2,x_3\}}$ $\cdots$ $M_{\{x_2,x_{100}\}}$

$e(M_{\{x_2,x_1\}})$ $e(M_{\{x_2,x_3\}})$ $\cdots$ $e(M_{\{x_2,x_{100}\}})$

Best score

selected $\{x_2, x_3\}$

Level 3

$\{x_2, x_3, x_1\}$ $\cdots$ $\{x_2, x_3, x_{100}\}$

Feature selection: wrappers

Stopping criterion:

- **Compare:**
  - The best score at the previous level k-1
  - The best score at the current level k
- Stop when there is a decrease in performance on the set of features at level k

Embedded methods

Feature selection + model learning done jointly

- **Examples of embedded methods:**
  - **Regularized models**
    - Models of higher complexity are explicitly penalized leading to 'virtual' removal of inputs from the model
    - **Covers:**
      - Regularized logistic/linear regression
      - Support vector machines
        - » Optimization of margins penalizes nonzero weights

$$\underbrace{J_n(\mathbf{w}, D)}_{\text{Function to optimize}} = \underbrace{L(\mathbf{w}, D)}_{\text{Loss function (fit of the data)}} + \underbrace{R(\mathbf{w})}_{\text{Regularization penalty}}$$

  - **CART/Decision trees**

Unsupervised dimensionality reduction

- **Is there a lower dimensional representation of the data that captures well its characteristics?**
- **Assume:**
  - We have data $D = \{\mathbf{x_1}, \mathbf{x_2}, .., \mathbf{x_N}\}$ 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***, there is no class label *y*
- **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 vector with a lower dimension vector (obtained by combining inputs)

- Different from the feature subset selection !!!

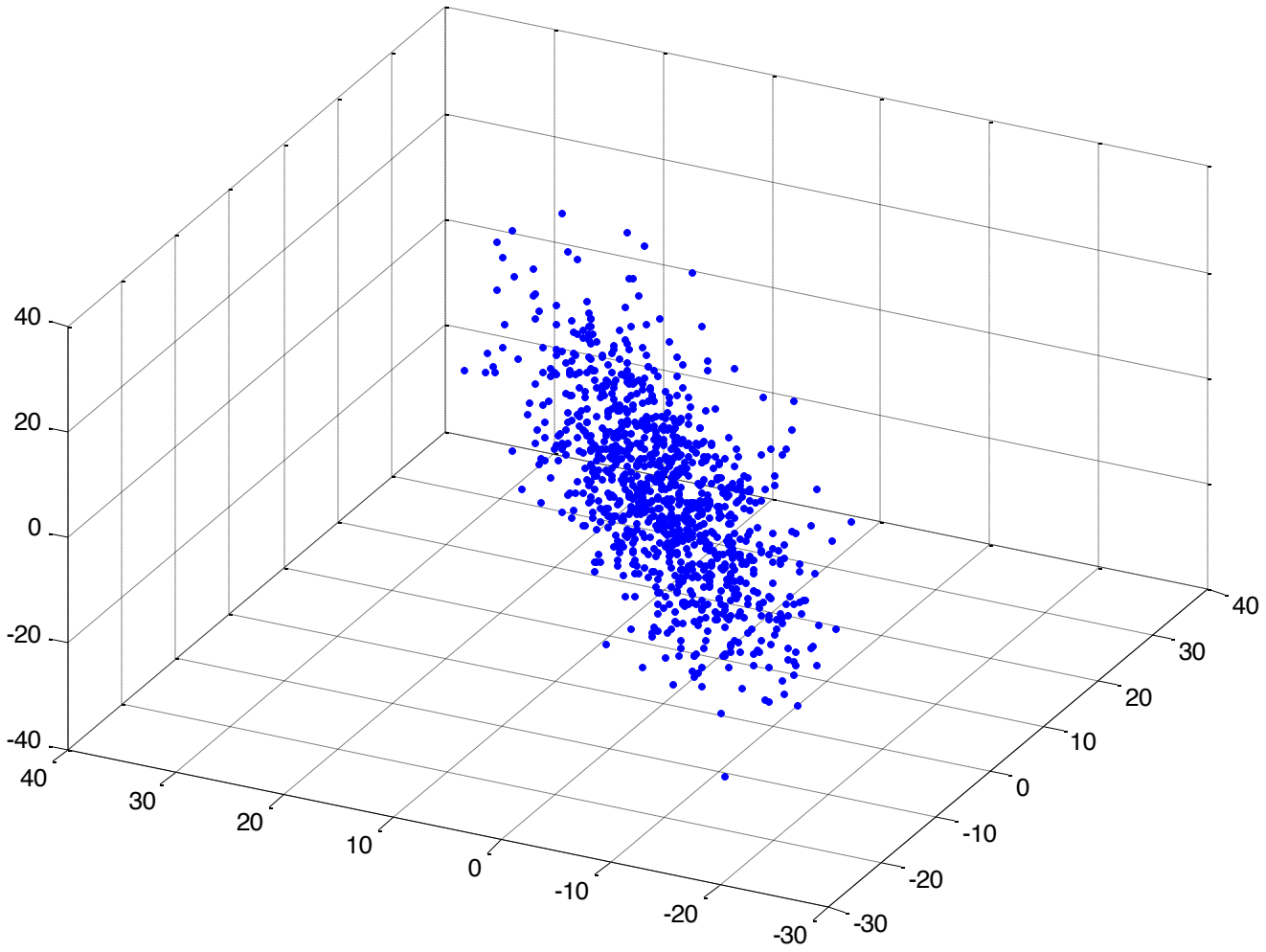
PCA:

- A linear transformation of the d dimensional input x to the M dimensional feature vector z such that $M < d$

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

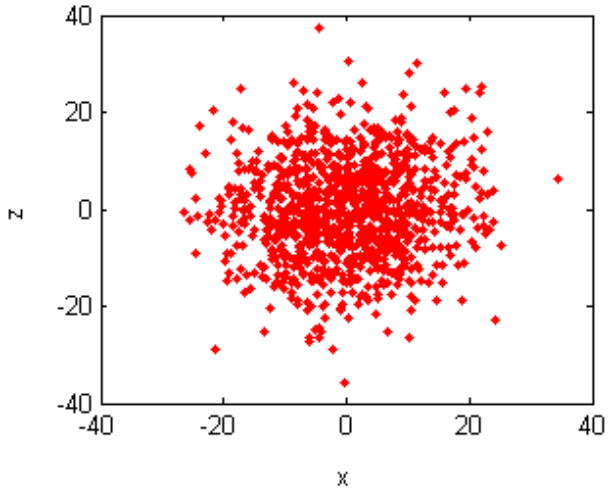
- Many different transformations exists, which one to pick?
- PCA –selects the linear transformation for which **the retained variance is maximal**
- Or, equivalently it is the linear transformation for which the sum of squares reconstruction cost is minimized

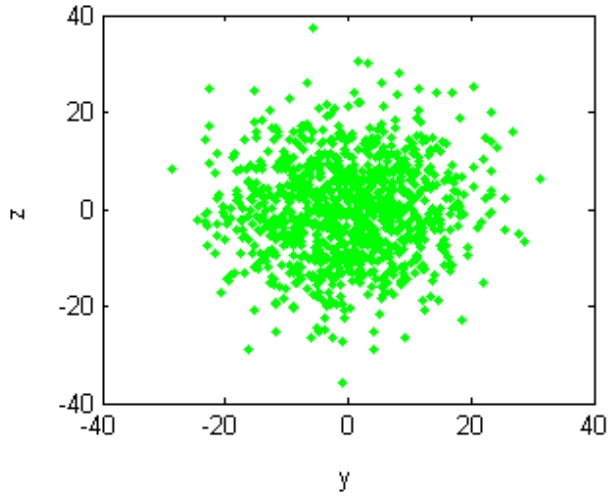
PCA: example

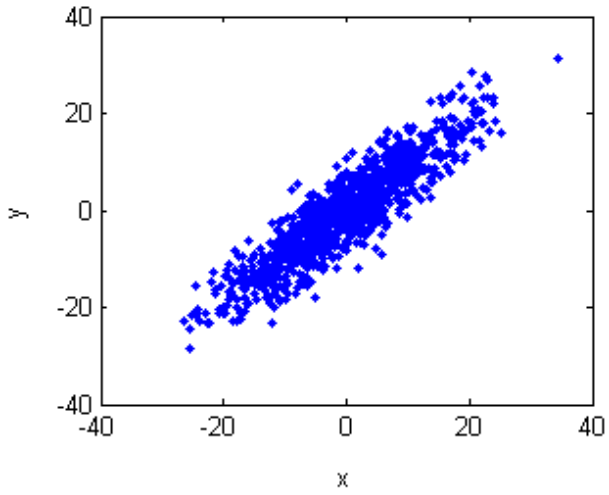


PCA

Projections to different axis

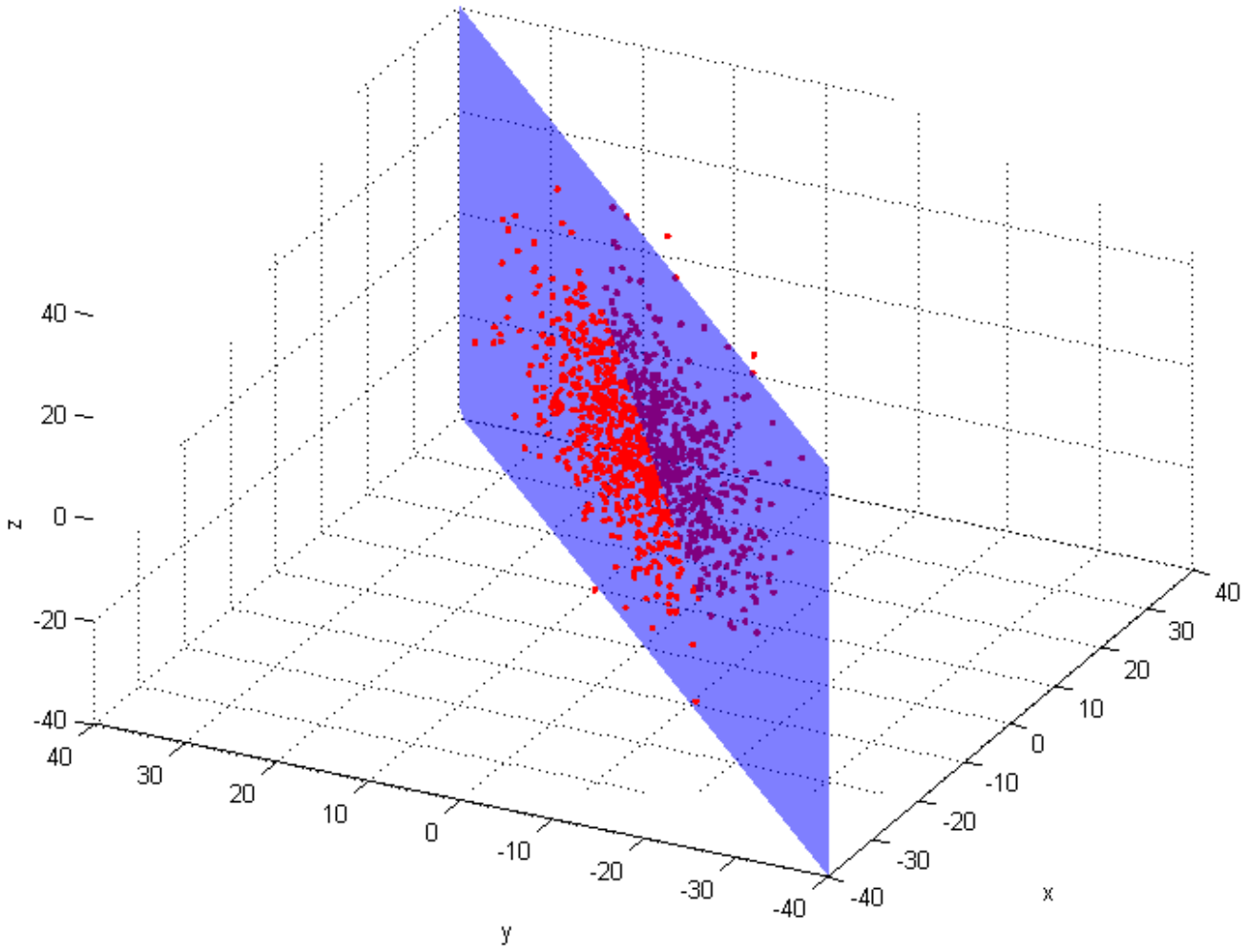






PCA

- PCA projection to the 2 dimensional space



PCA

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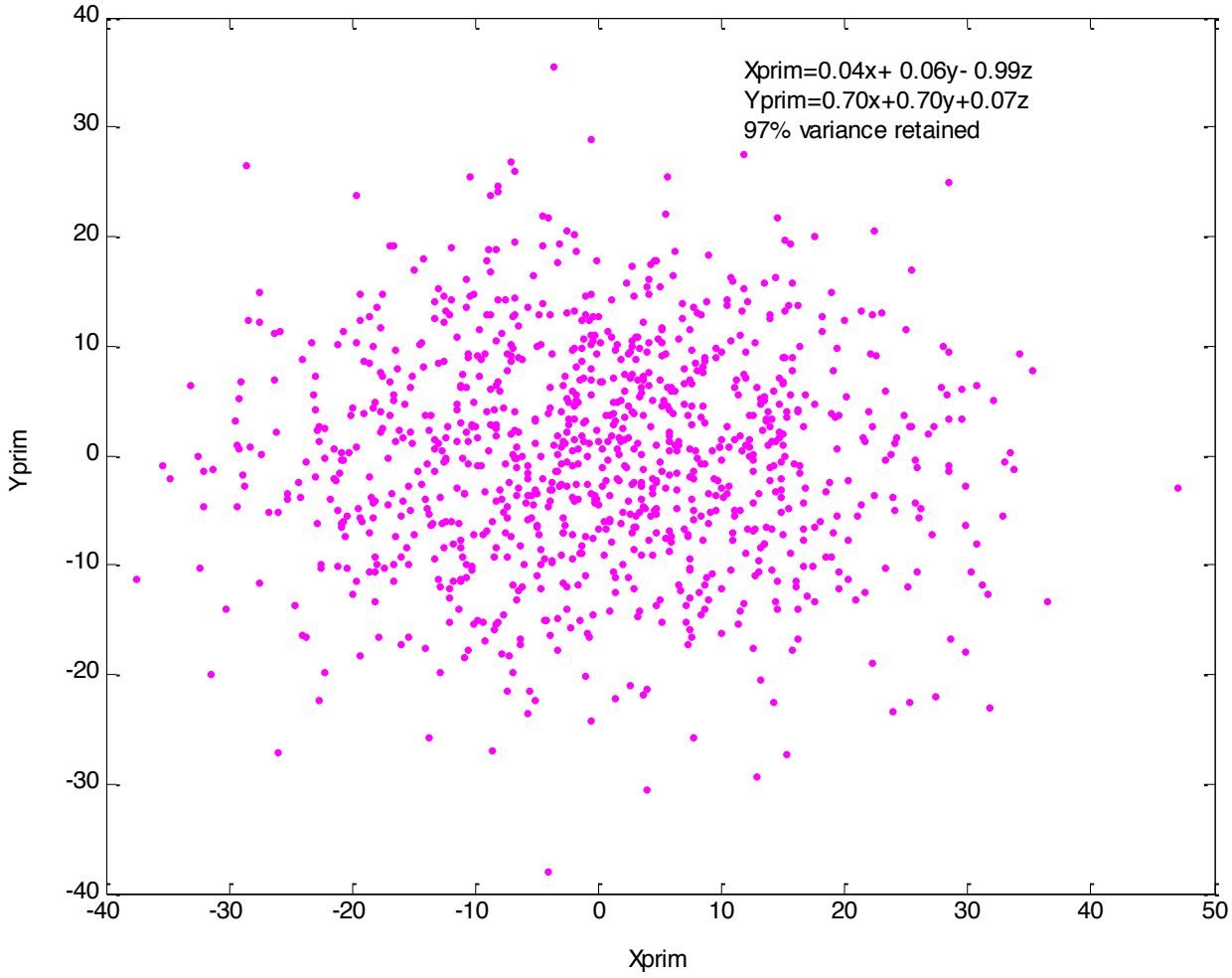

Principal component analysis (PCA)

- **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. **Remember:** no y is needed
- **Fact:**
  - A vector **x** can be represented using a set of orthonormal vectors **u** (basis vectors)

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

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

$$z_i = \mathbf{u}_i^T \mathbf{x} \qquad \mathbf{z} = \mathbf{U}\mathbf{x} \qquad \mathbf{U} = \begin{bmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ .. \\ \mathbf{u}_d^T \end{bmatrix}$$

Principal component analysis (PCA)

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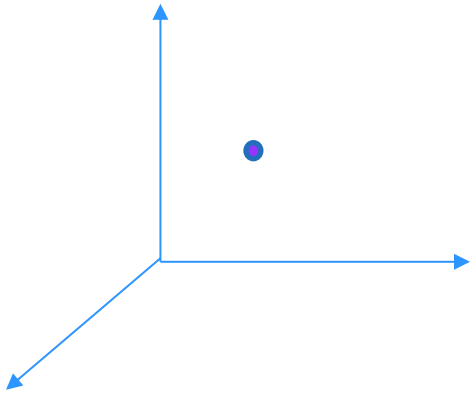
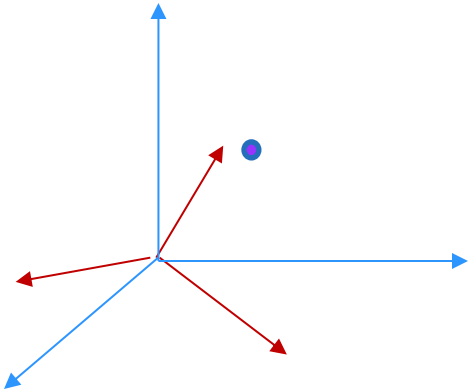


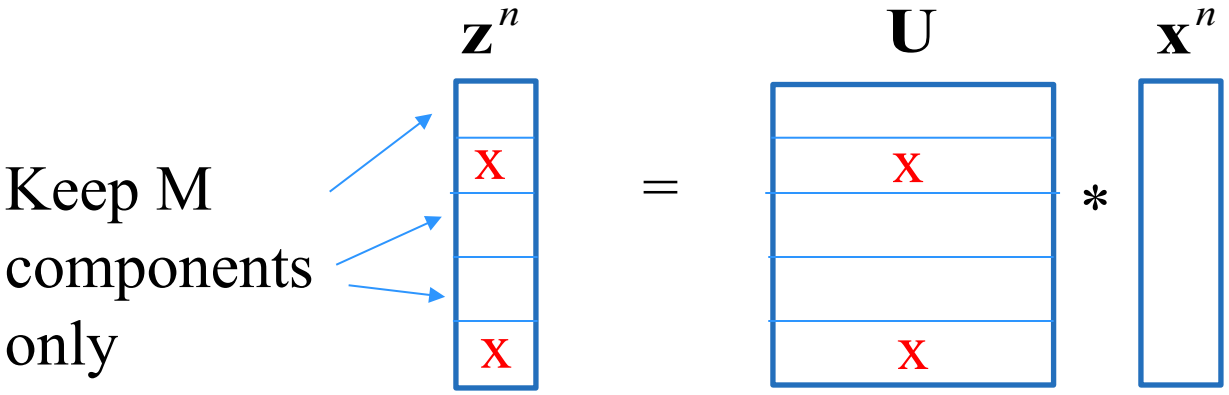
Standard bases:
(1,0,0); (0,1,0); (0,0,1)



New bases: $\mathbf{u}_1$, $\mathbf{u}_2$, $\mathbf{u}_3$

PCA

- **Idea:** represent d-dimensional $\mathbf{x}^n$ with an M-dimensional $\mathbf{z}^n$ formed by subset of z_i coordinates for the bases defined by $\mathbf{U}$.



- **Goal:** We want to find:

  (1) **Basis vectors U** and (2) **their subset *of size M***

- **This effectively replaces** $\mathbf{x}^n$ **with its approximation** $\tilde{\mathbf{x}}^n$

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

b_i - constant and fixed for all data-points

PCA

- **Goal:** We want to find:

  Basis vectors ***U*** and a their subset *of size M* to keep

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

  b_i - constant and fixed for all data-points

- **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:

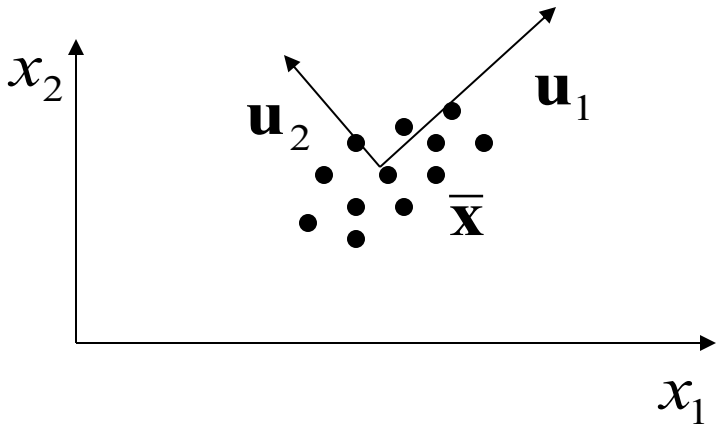
$$\boldsymbol{\Sigma}\mathbf{u}_i = \lambda_i \mathbf{u}_i \qquad E_M = \frac{1}{2}\sum_{i=M+1}^{d} \lambda_i$$

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

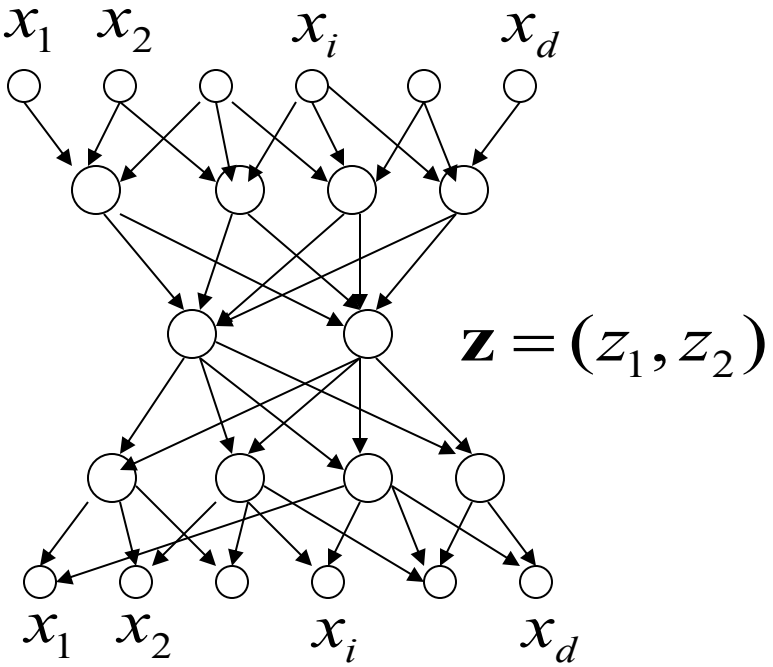
- Once eigenvectors $\mathbf{u}_i$ with largest eigenvalues are identified, they are used to transform the original *d*-dimensional data to *M* dimensions



- 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.
- **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 ($\boldsymbol{x}$)



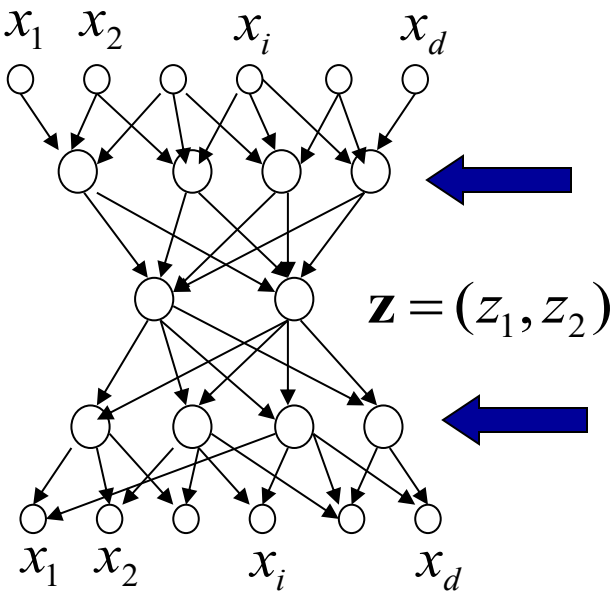
- The middle layer corresponds to the reduced dimensions

Dimensionality reduction with neural nets

- **Error criterion:**

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

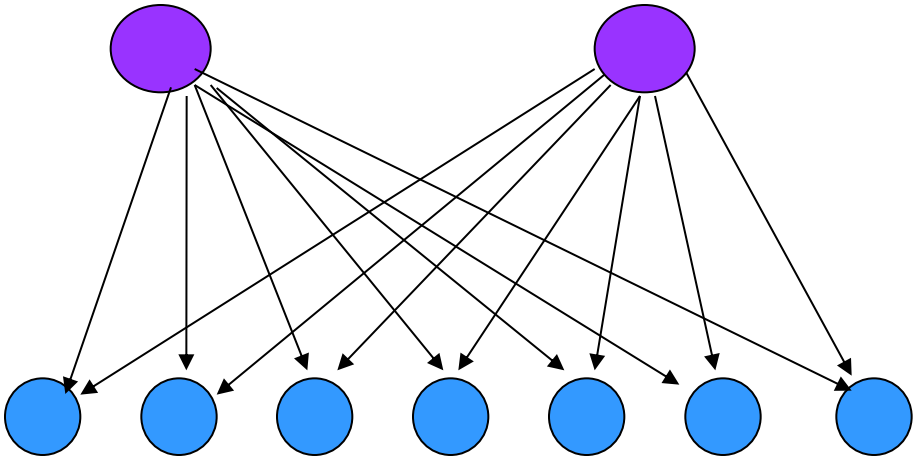
- Error measure tries to recover the original data through limited number of dimensions in the middle layer
- **Non-linearities** modeled through intermediate layers between the middle layer and input/output
- If no intermediate layers are used the model replicates PCA optimization through learning

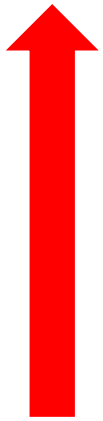


Latent variable models

- **Learning using unsupervised learning**
- **Dimensionality reduction via inference**

Latent variables (s): Dimensionality k





Dimensionality reduction via inference

Observed variables x: real valued vars
Dimensionality d

Cooperative vector quantizer

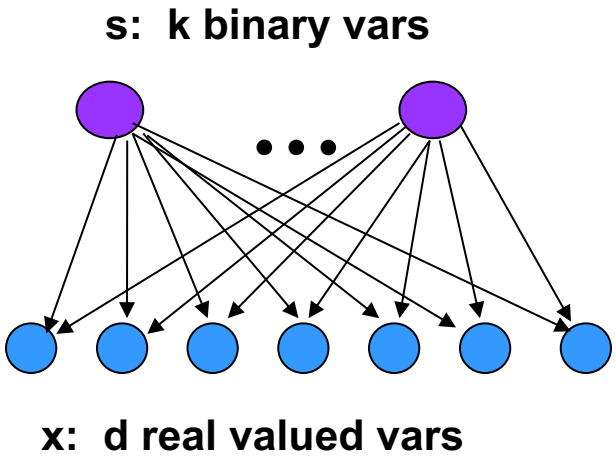
Model:

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: **W, Σ**

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

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:

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