CS 2750 Machine Learning
Lecture 22

Dimensionality reduction
Feature selection

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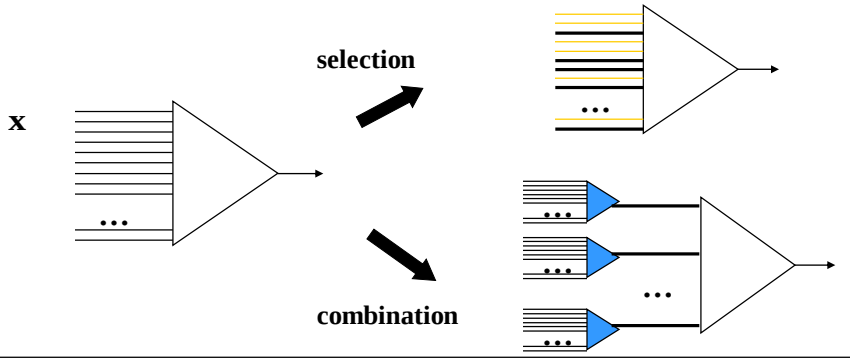
Dimensionality reduction. Motivation.

- **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:

- $\mathbf{x}$ – 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?

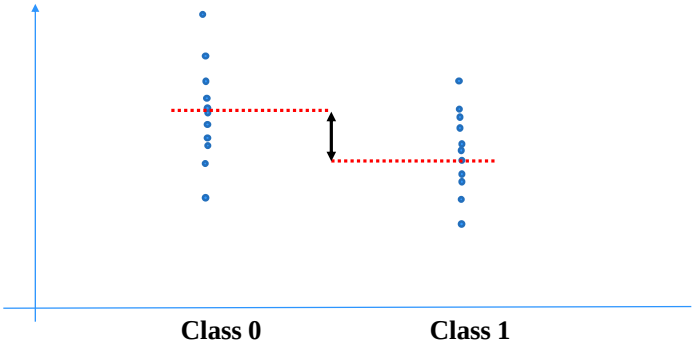
- **Step 1 .** For each input x_i in data calculate $Score(x_i, y)$ reflecting how well x_i predicts the output y alone
- **Step 2.** Pick a subset of inputs with the best scores $Score(x_i, y)$ (or equivalently eliminate/filter the inputs with the worst scores)

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**

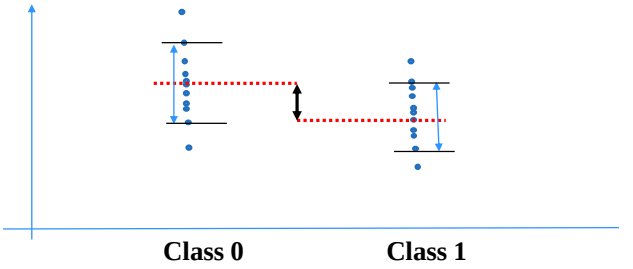


Feature scoring for classification

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

- **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/input 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

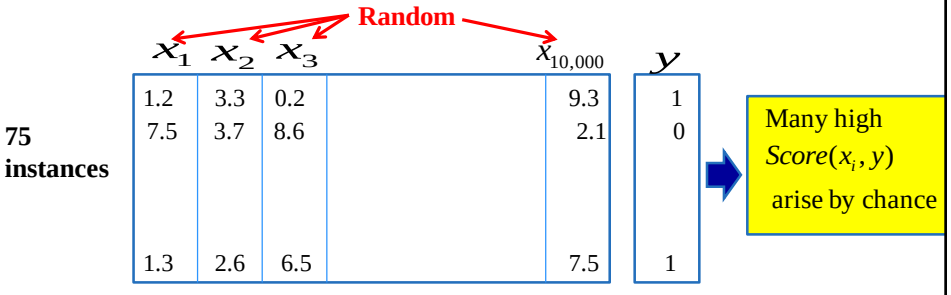
$$M(S) = \frac{d\bar{r}_{yx}}{\sqrt{d + d(d+1)\bar{r}_{xx}}}$$

- 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 many random features, and not many instances we can 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

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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

Feature selection: wrappers

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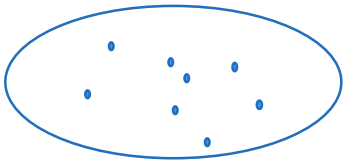

d inputs

Feature selection: wrappers

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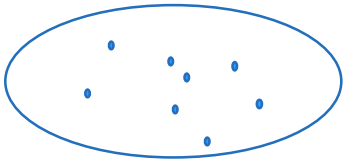

d inputs

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

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Feature selection: wrappers

How to find the appropriate feature subset S efficiently?

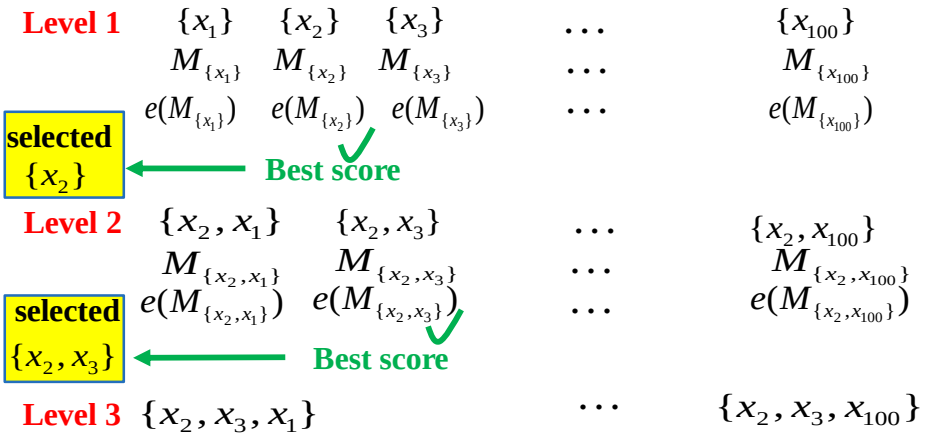
- For *d* inputs/features there are 2^d different feature subsets

- **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



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 $\boldsymbol{x}$ is very large
  - We want to analyze $\boldsymbol{x}$, 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 !!!

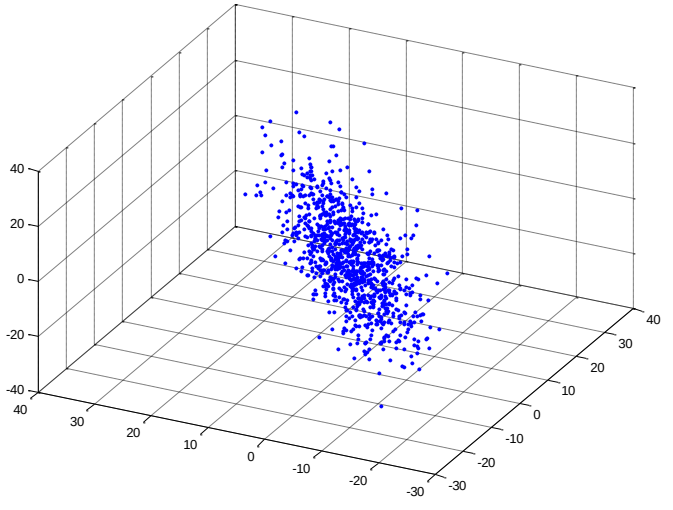
PCA:

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

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

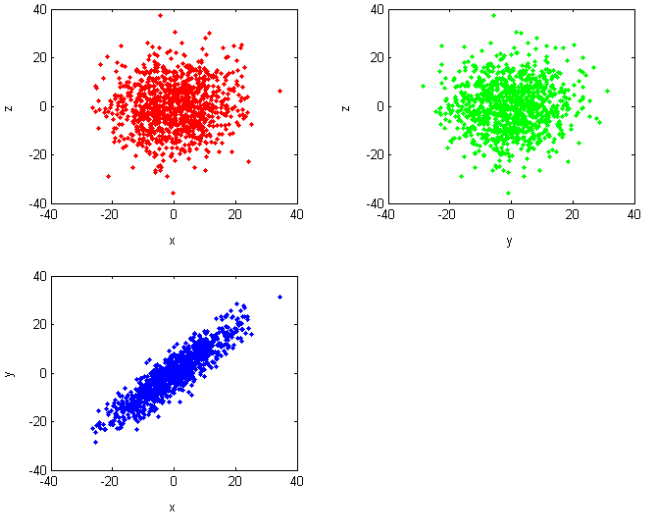
- Many different transformations exists, which one to pick?
- PCA –selects the linear transformation for which **the retained variance is maximal**
- Or, equivalently it is the linear transformation for which the sum of squares reconstruction cost is minimized

PCA: example



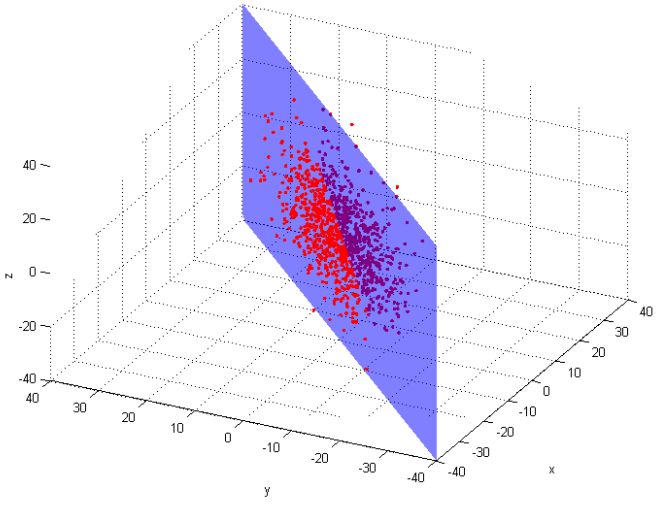
PCA

Projections to different axis



PCA

- PCA projection to the 2 dimensional space



PCA

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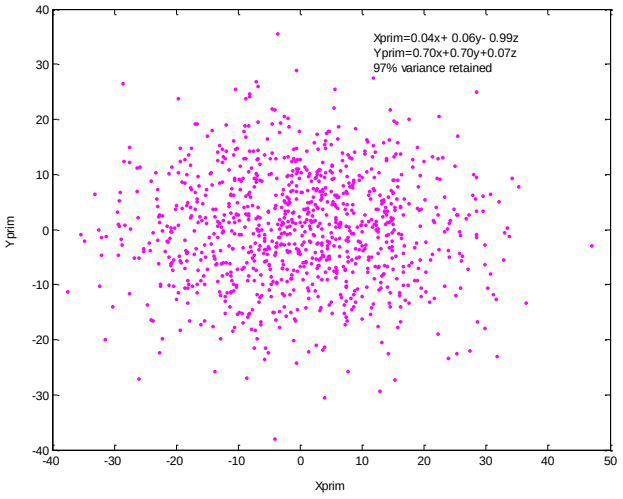

Principal component analysis (PCA)

- **PCA:**
  - linear transformation of a d dimensional input $\mathbf{x}$ to M dimensional vector $\mathbf{z}$ such that $M < d$ under which the retained variance is maximal. **Remember:** no y is needed
- **Fact:**
  - A vector $\mathbf{x}$ can be represented using a set of orthonormal vectors $\mathbf{u}$ (basis vectors)

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

  - Leads to transformation of coordinates (from $\mathbf{x}$ to $\mathbf{z}$ using $\mathbf{u}$'s)

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

Principal component analysis (PCA)

- **Fact:** A vector **x** can be represented using a set of orthonormal vectors **u** (basis vectors)

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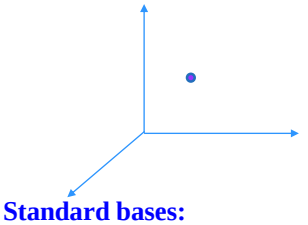
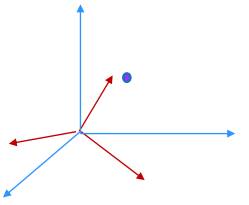


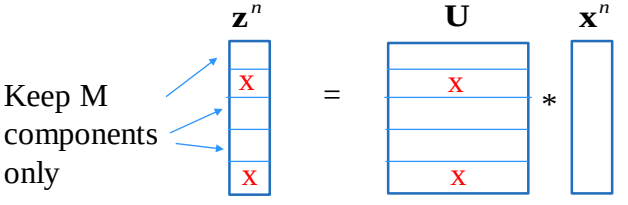
Standard bases: (1,0,0); (0,1,0); (0,0,1)



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 **U** .



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

  (1) Basis vectors U and (2) a subset *of basis of size M* to keep

- **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: z_i

  Basis vectors U and a subset *of basis 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:

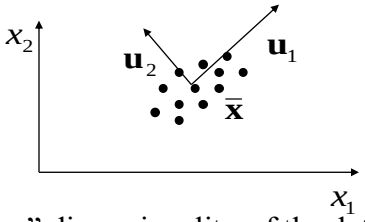
$$\boldsymbol{\Sigma}\mathbf{u}_i = \lambda_i \mathbf{u}_i \qquad E_M = \frac{1}{2}\sum_{i=M+1}^{d} \lambda_i$$

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

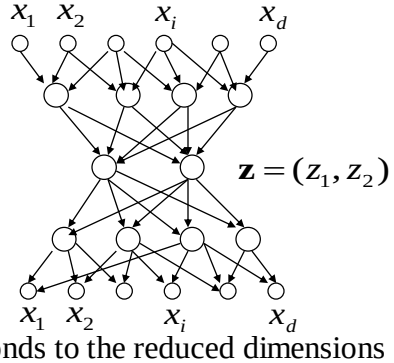
- Once eigenvectors $\mathbf{u}_i$ with largest eigenvalues are identified, they are used to transform the original *d*-dimensional data to *M* dimensions



- 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 (***x***)



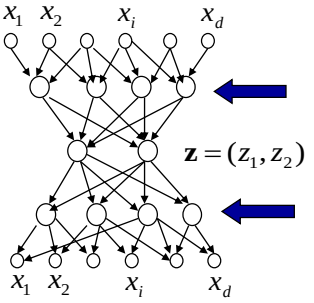
- The middle layer corresponds to the reduced dimensions

Dimensionality reduction with neural nets

- **Error criterion:**

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

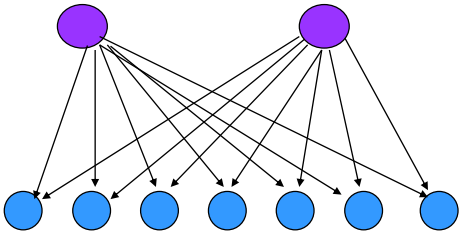
- Error measure tries to recover the original data through limited number of dimensions in the middle layer
- **Non-linearities** modeled through intermediate layers between the middle layer and input/output
- If no intermediate layers are used the model replicates PCA optimization through learning



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