Aalto University
School of Electrical Engineering

CS-C3240 – Machine Learning D

Feature Engineering

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Learning goals

Understand the concepts of

- feature engineering
- feature selection
- challenges with high dimensional feature spaces
- Principle Component Analysis
- Kernel methods

Outline

Feature Engineering

Strategies to cope with common challenges

Principle Component Analysis

Kernel methods

Feature engineering

Feature pre-processing

→ Normalisation

→ Detection of outliers

→ Are features independent?

Feature engineering

Simple normalization: Scaling

For each sample x_i from a set $\mathcal{X}$, compute the scaled value as

$$x_i' = \frac{x_i - \min(\mathcal{X})}{\max(\mathcal{X}) - \min(\mathcal{X})}$$

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after scaling, it is common to center the values around e.g. 0 or their arithmetic mean, median, centre of mass etc.

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Standardization to zero mean/unit variance

Given a set of values $x_i; i \in \{1..n\}$ from a set $\mathcal{X}$ with mean μ and standard deviation σ, we derive the standardized values x_i' as

$$x_i' = \frac{x_i - \mu}{\sigma}$$

Feature pre-processing

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Using the variance σ^2 instead of σ is called variance scaling

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Important:

When normalizing on the training set input, this need to be applied identically ot the test set input. Do not normalize the test set input on the test set data.

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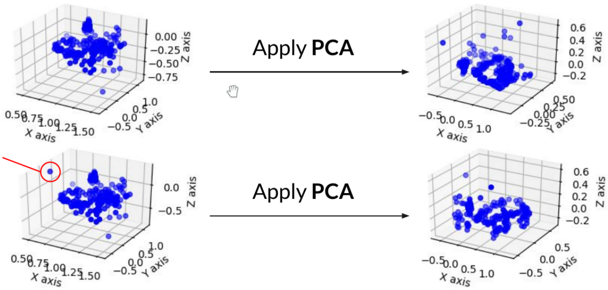

Feature pre-processing

→ Normalisation

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Feature engineering

Common pitfalls in outlier handling:

It is not unusual to find values that clearly depart from the rest.

Example: In insurance, most claims are small but a few are large. Removing the large claims will completely invalidate an insurance model.

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Common pitfalls in outlier handling:

It is not unusual to find values that clearly depart from the rest.

Example: In insurance, most claims are small but a few are large. Removing the large claims will completely invalidate an insurance model.

Caution: Do <u>not</u> throw away outliers, unless you have evidence that they are errors

Darell Huff, How to lie with Statistics, 1954

Feature pre-processing

→ Normalisation

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Feature engineering

Common pitfalls in outlier handling:

It is not unusual to find values that clearly depart from the rest.

Approach: If outliers are present, use algorithms that are robust to outliers. For instance, covarianceor mean are sensitive to outliers. $\rightarrow$ replace mean with median.

Feature pre-processing

$\rightarrow$ Normalisation

$\rightarrow$ Detection of outliers

$\rightarrow$ Are features independent?

Feature engineering

Common pitfalls in outlier handling:

It is not unusual to find values that clearly depart from the rest.

$\rightarrow$ Outliers behave sometimes different than the rest $\rightarrow$ train separate model on outliers

Detection clustering, density estimation,

Feature pre-processing

$\rightarrow$ Normalisation

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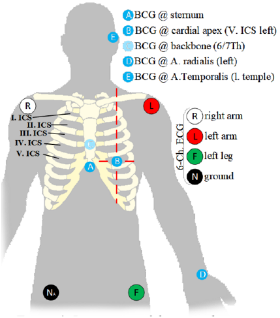
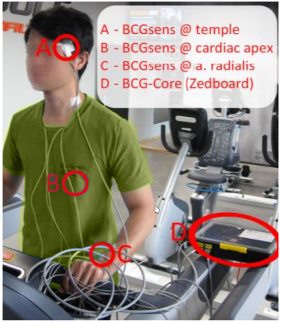
Feature engineering

Example: walking speed vs. heart rate



(a) Positioning of the sensors



(b) Subject performing the study

Feature pre-processing

→ Normalisation

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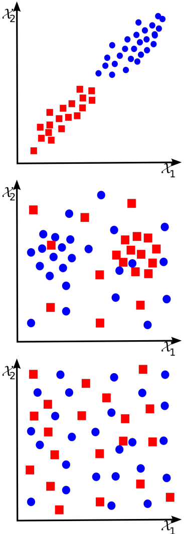
Feature Selection

A large portion of the performance of Machine Learning algorithms is due to the right choice and processing of features.

Avoid non-important features

- Noisy data
- Non-correlation between features and classes
- Correlated features
- Sometimes, less is better



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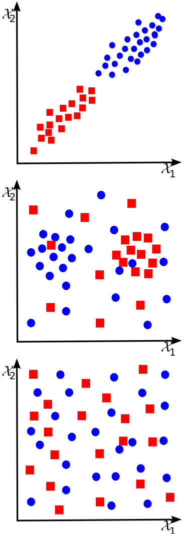

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Choosing the most important features

- Reduces training and evaluation time
- Reduces complexity of a model (easier to interpret)
- Improves prediction/recall of a model
- Reduces overfitting

Feature selection algorithms

How to identify good/meaningful features?

Feature selection

For a set of features $\{\mathcal{X}\}$, how to find a good subset $\{\mathcal{X}\}_s \subseteq \mathcal{X}\}$ which is best suited to distinguish between the considered classes $\mathcal{Y}_i \in \{\mathcal{Y}\}$?

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Las Vegas Filter

Repeatedly generate random feature subsets $\{\mathcal{X}\}_s \subseteq \mathcal{X}\}$, train a classifier $\hat{h}_s(\overrightarrow{\hat{w}_s}, \cdot) = \min_{i\in\{\mathcal{X}_s\}} \mathcal{L}\left(h(\overrightarrow{w}, \overrightarrow{x}^{(i)}), y^{(i)}\right)$ and validate $\hat{h}_s(\overrightarrow{\hat{w}_s}, \cdot)$ for its classification performance

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Focus algorithm

1. Train and evaluate a classifier for singleton feature $\mathcal{X}_o$
2. Evaluate each set of two features $\mathcal{X}_o, \mathcal{X}_p$

$\vdots$

Until consistent solution is found

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Complexity:

$$\binom{|\mathcal{X}|}{k} = \frac{|\mathcal{X}|!}{(|\mathcal{X}|-k)!(k!)} \rightarrow \mathcal{O}(2^{|\mathcal{X}|})$$

$$\binom{|\mathcal{X}|}{1} \cdot \binom{|\mathcal{X}|}{2} \cdots \binom{|\mathcal{X}|}{|\mathcal{X}|}$$

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Relief algorithm

Given a collection of values $x_i; i \in \{1..n\}$ of a feature $\mathcal{X}$, compute

$$\frac{\text{Closest distance to all other samples of the same class}}{\text{Closest distance to all samples not in that class}}$$

Rationale: Feature more relevant the more it separates a sample from samples in other classes and the less it separates from samples in same class

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Pearson Correlation Coefficient

$$r(\mathcal{X}_1, \mathcal{X}_2) = \frac{\mathrm{Cov}(\mathcal{X}_1, \mathcal{X}_2)}{\sqrt{\mathrm{Var}(\mathcal{X}_1)\mathrm{Var}(\mathcal{X}_2)}}$$

- Identifies linear relation between features $\mathcal{X}_i$

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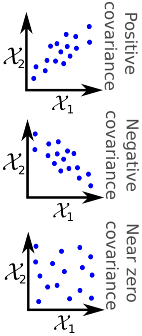

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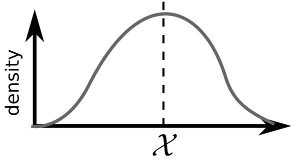
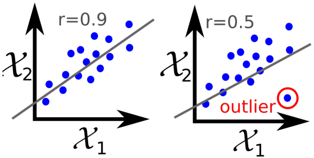
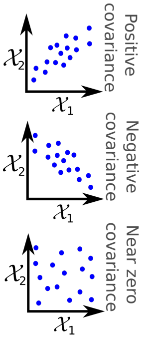


All features should follow a normal distribution



Data should have no significant outliers



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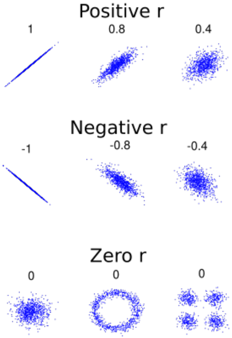

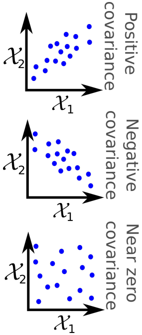

Outline

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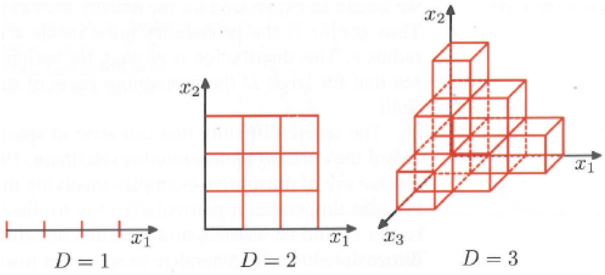
Strategies to cope with common challenges

Principle Component Analysis

Kernel methods

Issues related to high dimensional input data

Exponential growth Volume of the space grows exponentially with dimension



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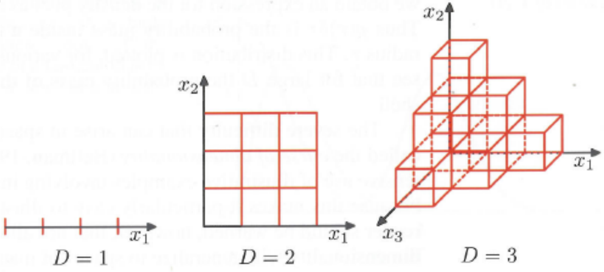
Too sparse samples across regions to estimate a distribution in that space
(Problematic for methods that require statistical significance)



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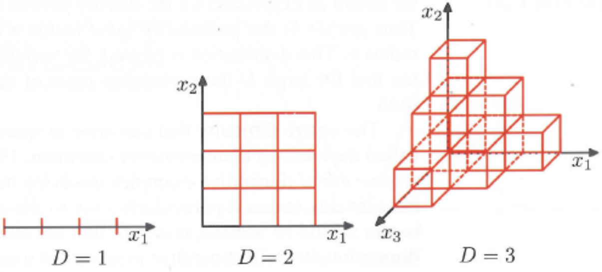
Hughes (peaking) phenomenon

Predictive power of classifier first increases with dimension, then decreases



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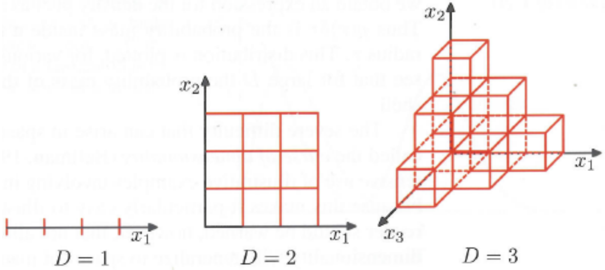
Counter-intuitive properties in higher dimensional spaces



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Example – Volume of a sphere

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$V_D(r) = \delta_D r^D$ for appropriate δ_D

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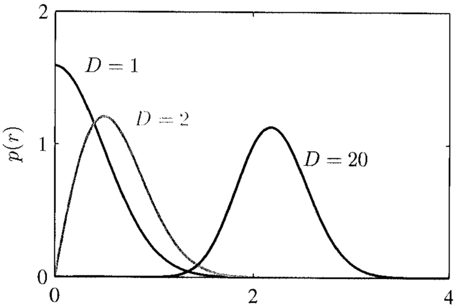
For large D, this fraction tends to 1

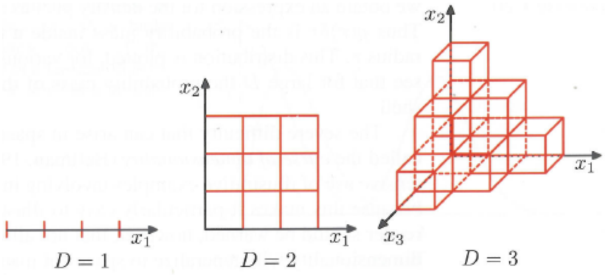
In high dimensions, most of the volume of a sphere concentrates near the surface

Issues related to high dimensional input data

Example – Gaussian distribution

Probability mass concentrated in a thin shell
(here plotted as distance from the origin in a polar coordinate system)





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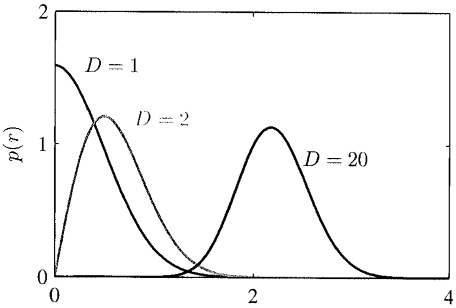

Curse of Dimensionality

Mechanisms to efficiently reduce dimensions or classifiers that respect properties of high-dimensional spaces required.

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Principle Component Analysis

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Find lower dimensional surface onto which to project the data

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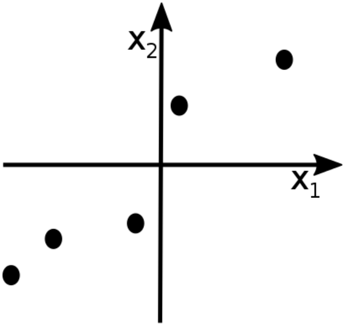

Principle Component Analysis

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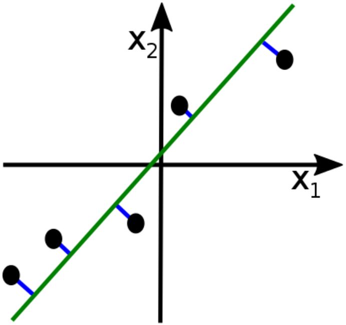

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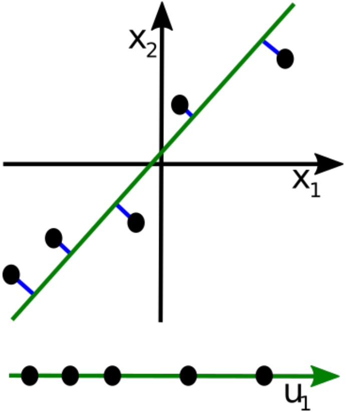

Principle Component Analysis

PCA finds k vectors $\overrightarrow{u_1}, \ldots, \overrightarrow{u_k}$ onto which to project the data such that the projection error is minimized.

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$\rightarrow$ In particular, find $\overrightarrow{z_i} = z_i^{(1)} \ldots z_i^{(n)}$ to represent the $\overrightarrow{x_i} = x_i^{(1)} \ldots x_i^{(n)}$ in this k-dimensional vector space spanned by the $\overrightarrow{u_i}$

Principle Component Analysis

1. Compute the covariance matrix from the $x^{(i)}$:

$$C = \frac{1}{n} \underbrace{\underbrace{\boldsymbol{X}}_{\boldsymbol{n} \times \boldsymbol{m}\text{-dim.}} \underbrace{\boldsymbol{X}^{\boldsymbol{T}}}_{\boldsymbol{m} \times \boldsymbol{n}\text{-dim.}}}_{m \times m\text{-dim.}}$$

(We assume that all features are mean-normalized and scaled into $[0, 1]$)

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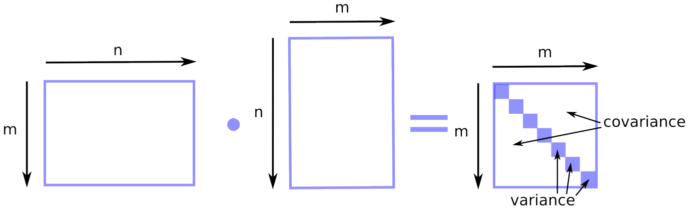

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Covariance

A measure of spread of a set of points around their center of mass

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2. The pricipal components are found by computing the eigenvectors and eigenvalues of C (solving $(C - \lambda I_m)u = 0$)

Principle Component Analysis

When a matrix C is multiplied with a vector u', this usually results in a new vector Cu' of different direction than u'.

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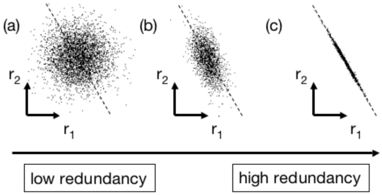
When a matrix C is multiplied with a vector u', this usually results in a new vector Cu' of different direction than u'.

→ There are few vectors u, however, which have the same direction ($Cu = \lambda u$).

These are the eigenvectors of C and λ are the eigenvalues

Principle Component Analysis



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Eigenvectors and Eigenvalues

The (orthogonal) eigenvectors are sorted by their eigenvalues with respect to the direction of greatest variance in the data.

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3. Choose the k eigenvectors with largest eigenvalues to represent the projection space U
4. These k eigenvectors in U are used to transform the inputs x_i to z_i:

$$z^{(i)} = U^T x^{(i)}$$

Principle Component Analysis

How to choose the number k of dimensions?

We can calculate

$$\frac{\text{Average squared projection error}}{\text{Total variation in the data}} \rightarrow \frac{\sum_{i=1}^{k} ||x^{(i)} - x_{\text{approx}}^{(i)}||^2}{\frac{1}{m}\sum_{i=1}^{m} ||x^{(i)}||^2}$$

as the accuracy of the projection using k principle components as a function of the eigenvalues

$$\frac{\sum_{i=1}^{k} \sqrt{\lambda_i}}{\sum_{j=1}^{m} \sqrt{\lambda_j}} = d$$

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as the accuracy of the projection using *k* principle components as a function of the eigenvalues

$$\frac{\sum_{i=1}^{k} \sqrt{\lambda_i}}{\sum_{j=1}^{m} \sqrt{\lambda_j}} = d$$

We say that $100 \cdot (1 - d)\%$ of variance is retained.

(Typically, $d \in [0.01, 0.05]$)

Outline

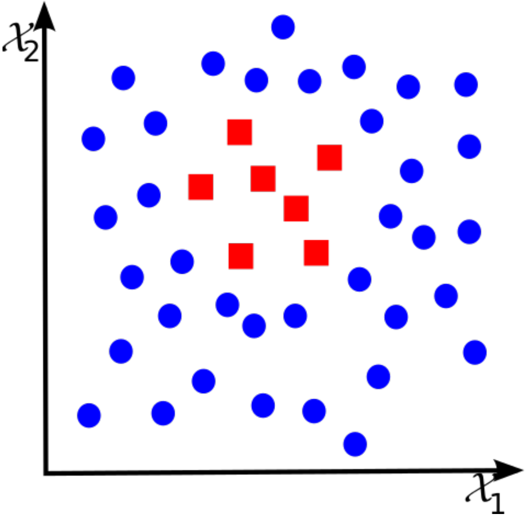
Feature Engineering

Strategies to cope with common challenges

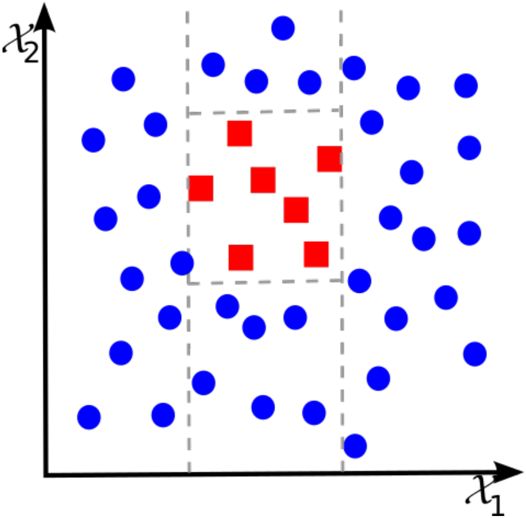
Principle Component Analysis

Kernel methods

Strategies to cope with non-linear problems

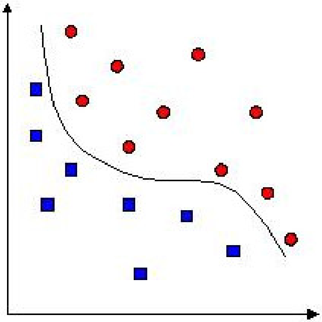


Strategies to cope with non-linear problems



Strategies to cope with non-linear problems

Classifier may search an objective function of sufficient dimension

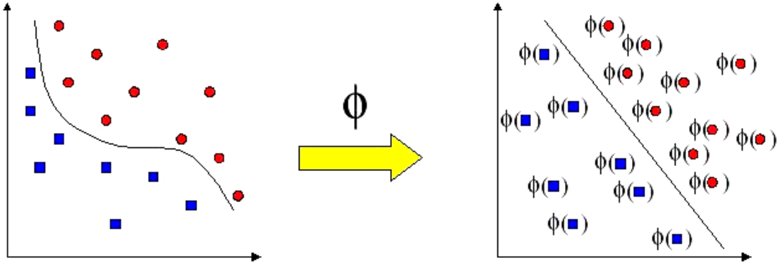


Strategies to cope with non-linear problems

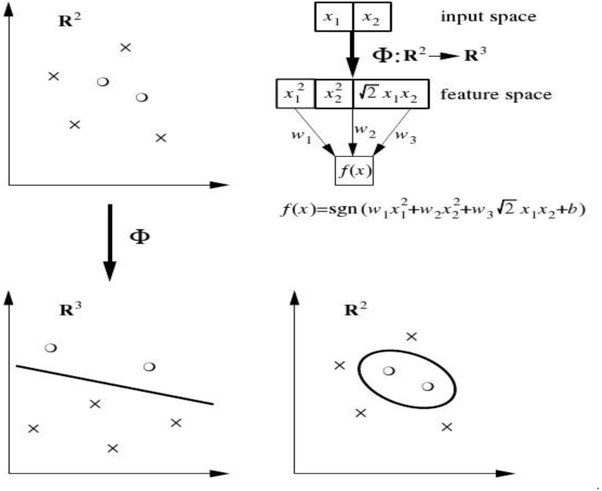
Alternative

Classifier may search an objective function of sufficient dimension for complex non-linear decision boundaries:

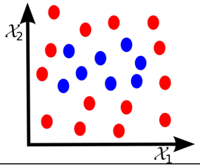
Change dimension of input space so that linear separation is possible



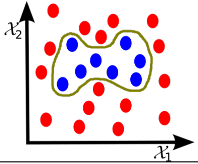
Example: Mapping into linear separable space



Using a kernel function

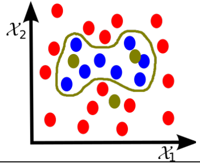


Using a kernel function



Hypothesis $= 1$ if

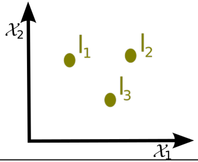
Using a kernel function



Hypothesis $= 1$ if

$$\Rightarrow w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \cdots \geq 0$$

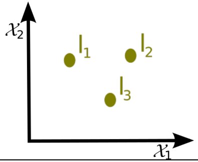
Using a kernel function



$$\Rightarrow \quad w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \ldots$$

Kernel Define kernel via landmarks

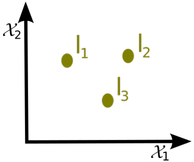
Using a kernel function



$$\Rightarrow w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \dots$$

Gaussian: $k(x, l_i) = e^{-\frac{||x - l_i||^2}{2\sigma^2}}$

Using a kernel function

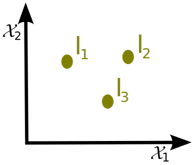


$$\Rightarrow \quad w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \ldots$$

Gaussian: $k(x, l_i) = e^{-\frac{||x-l_i||^2}{2\sigma^2}}$

$x \approx l_i \Rightarrow k(x, l_i) \approx 1$ (towards 0 else)

Using a kernel function



$$\Rightarrow \quad w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \dots$$

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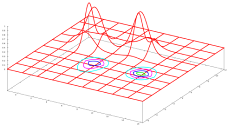
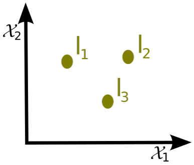


$\sigma = 1$

Using a kernel function



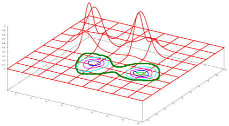
$$\Rightarrow \quad w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \dots$$

Gaussian: $k(x, l_i) = e^{-\frac{||x - l_i||^2}{2\sigma^2}}$

$x \approx l_i \Rightarrow k(x, l_i) \approx 1$ (towards 0 else)

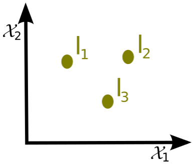
Example: $w_0 = -0.5, w_1 = 1, w_2 = 1, w_3 = 0$

$$h(x) = w_0 + w_1 k(x, l_1) + w_2 k(x, l_2) + w_3 k(x, l_3)$$



$\sigma = 1$

Using a kernel function



$$\Rightarrow \; w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \dots$$

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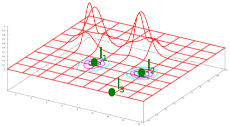
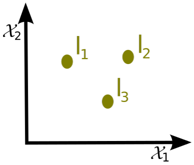


$\sigma = 1$

Using a kernel function



$\Rightarrow \quad w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \dots$

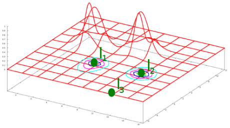
Gaussian: $k(x, l_i) = e^{-\frac{||x - l_i||^2}{2\sigma^2}}$

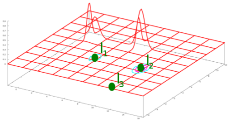
$x \approx l_i \Rightarrow k(x, l_i) \approx 1$ (towards 0 else)

σ controls the width of the Gaussian

Example: $w_0 = -0.5, w_1 = 1, w_2 = 1, w_3 = 0$

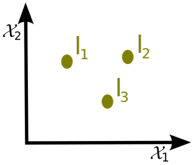
$$h(x) = w_0 + w_1 k(x, l_1) + w_2 k(x, l_2) + w_3 k(x, l_3)$$





$\sigma = 1$ $\qquad$ $\sigma = 0.5$

Using a kernel function



$$\Rightarrow \quad w_0 + w_1 k_1 + w_2 k_2 + w_3 k_3 + \dots$$

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Example: $w_0 = -0.5, w_1 = 1, w_2 = 1, w_3 = 0$

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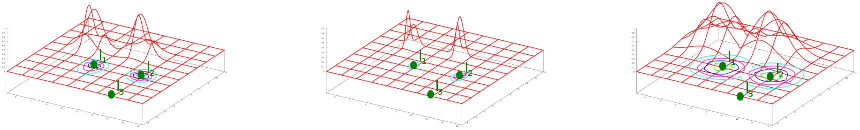

$\sigma = 1$ $\quad$ $\sigma = 0.5$ $\quad$ $\sigma = 2$

Using a kernel function

Kernels – placement of landmarks

Possible choice of initial landmarks: All training-set samples

Training of w_i

$$f_i = \begin{bmatrix} k(x_i, l_1) \\ \vdots \\ k(x_i, l_m) \end{bmatrix}$$

$$\min_W C \sum_{i=1}^{m} y_i \text{cost}_{y_i=1}(W^T f_i) + (1 - y_i) \cdot \text{cost}_{y_i=0}(W^T f_i) + \frac{1}{2} \sum_{j=1}^{m} w_j^2$$

Questions?

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Literature

- C.M. Bishop: Pattern recognition and machine learning, Springer, 2007.
- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001.