Advanced Data Analysis and Machine Learning: Lecture

Data Preprocessing, Feature and Model Selection

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Outline

Data characteristics

- Different sources of information represent a target object or process. In many cases, the data arises from a direct or indirect measurement action.
- The data from the different sources has (naturally) different characteristics.
- From the viewpoint of further processing and usage of the data, the data can be generally characterised with the following attributes:
    - Encoding of each data element/item/set (integer/real/complex, bits per sample, sampling rate, . . .).
    - Sources of noise and signal-to-noise ratio (SNR).
    - Number of dimensions in the data item/set.
- If the data from multiple sources is to be combined, special care must be taken to characterise and preprocess/transform the data into a form enabling appropriate data fusion and information gain.

Normalisation and redistribution

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- Problem: original raw data/features do not have desired characteristics for the data analysis task.
- Examples:
  - One or more data variables dominate the variation in the data set.
  - One or more data variables have skewed value distribution.
  - Two or more variables correlate significantly.
- If the data/features are preprocessed appropriately, the advantages include the following: unbiased, more representative data/features, faster model parameter estimation/learning and more representative models/better generalization.

Data normalisation

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- Minmax-scaling (of features):

$$x_k^{min} = \min_i x_{ki}, \quad x_k^{max} = \max_i x_{ki}, \quad k = 1, 2, \ldots, l$$

$$\hat{x}_{ik} = \frac{x_{ik} - x_k^{min}}{x_k^{max} - x_k^{min}}$$

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- One-to-one mapping between the original and normalised values which does not cause distortion to the data distribution.
- The result can be sensitive to outliers.
- Future data can have a different value range: samples can be used despite this, can be clipped to the original range, or the samples can be ignored. Alternatives: reserve "space" for the out-of-range values or squashing.

Data normalisation

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- Mean and variance normalization/standardization (of features):

$$\bar{x}_k = \frac{1}{N}\sum_{i=1}^{N} x_{ik}, \quad k = 1, 2, \ldots, l$$

$$\sigma_k^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_{ik} - \bar{x}_k)^2$$

$$\hat{x}_{ik} = \frac{x_{ik} - \bar{x}_k}{\sigma_k}$$

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- One-to-one mapping between the original and normalised values which does not cause distortion to the data distribution.
- Dependent on the number of samples available to estimate the mean and STD $\Rightarrow$ can still have problems related to future data with out-of-range values.

Data normalisation

- Softmax-scaling

$$
\begin{aligned}
y_{ik} &= \frac{x_{ik} - \bar{x}_k}{\sigma_k} \\
\hat{x}_{ik} &= \frac{1}{1 + e^{-y_{ik}}}
\end{aligned}
$$

Data normalisation

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$$

- Possible that very large numbers do not have unique normalised value.
- Can be controlled by λ specifying the linear portion, for example, $y_{ik} = \frac{x_{ik} - \bar{x}_k}{(\lambda/2\pi)\sigma_k}$.

Data redistribution

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- Problems:
  - Methods generally expect the data distributions to be uniform or normal.
  - Significantly varying densities can cause problems.

Data redistribution

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- Problems:
  - Methods generally expect the data distributions to be uniform or normal.
  - Significantly varying densities can cause problems.
- Possibilities for data preprocessing:
  - Requantisation: samples close to each other are merged.
  - Redistribution: sample distribution is transformed to be either equalised (target distribution is uniform), or specified (target distribution any type).

Outliers

- Outlier, *n. Statistics.* An observation whose value lies outside the set of values considered likely according to some hypothesis (usually one based on other observations); an isolated point. (OED)
  $\Rightarrow$ Unexpected, non-typical or out-of-range samples.
- Resulting from noise, human error or malfunctioning measurement/data processing equipment.
- The problem of defining outliers in a generally acceptable manner is nontrivial.

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- The problem of defining outliers in a generally acceptable manner is nontrivial.
- Note: according to information theory [1], the most improbable events carry the most information!

Outlier detection

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- For low-dimensional data, outliers are easy to identify visually.
- Possible task formulation: Given a set of n data points and k, the expected number of outliers, find the top k samples that are considerably dissimilar, exceptional or inconsistent with the rest of the data.
- Data models can be used to represent the "valid" data, but the representativeness/validity of the model can significantly affect the outlier detection result.

Outlier detection

- Possible solutions for outlier detection:
  - Statistical distribution-based methods:
    Assumed distribution and its parameters; working/alternative hypothesis; statistical significance.
  - Distance-based methods:
    At least a fraction of data points lie at a distance greater than a threshold.
  - Density-based methods:
    Non-uniform distributions; local outliers and reachability; degree of being an outlier (not binary).
  - Deviation-based methods:
    Subsets of data points; greatest reduction of dissimilarity metric or the statistical method within cubes.
  - Regression methods:
    Robust regression; residual error.

Variable/feature selection

- Dimensionality:
  - Variable/feature space volume is exponential w.r.t. the number of variables/features.
  - Large number of variables/features requires much data to be representative, and processing can be slow.
  - Adding more variables/features does not necessarily add more information (because of noise, correlation between variables).
- Goals:
  - Simpler models easier to interprete
  - Faster model building/analysis/training
  - Representativeness, and improved generalisation without overfitting

Variable/feature selection

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- Selection is dependent on the data analysis task.
- Favorable properties for variables/features: invariance to occurring transformations.
- Two approaches:
    - Individual variable/feature selection
    - Variable/feature subset selection

Variable/feature selection

- General variable/feature selection methods:
  - Wrappers:
    Scoring of variables/features with a predictive model and error rate (of the hold-out subset).
  - Filters:
    Usefulness instead of error rate; proxy measure (mutual information[1], Pearson correlation coefficient, . . .).
  - Embedded methods:
    Selection through penalisation/exclusion of variables/features as part of the model building.
  - Heuristics:
    Combination of different approaches.

[1] joint dist. *vs.* factored marginal dist. product

Variable/feature subset selection

- Number of subsets large: for selecting l features from a total of m

$$\binom{m}{l}.$$

- Difficult problem to exhaustively select the best combination.

Variable/feature subset selection

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- Number of subsets large: for selecting l features from a total of m

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- Difficult problem to exhaustively select the best combination.
- Possible solutions:
  - Greedy search (does not guarantee global optimum)
  - Nondeterministic (random sampling) methods

Method-independent selection

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- Example context: Binary classification.
- Why do we need many different approaches?
- Generalization *vs.* overfitting?
- Improving classification performance by combining classifiers
- Improving classification performance by modifying training data

No classifier is superior – Occam's razor

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- No classifier is superior over all problems.
- Occam's razor: "When you have two competing theories which make exactly the same predictions, the one that is simpler is the better."
  - In other words: "One should not make more assumptions than the minimum needed."
  - For a given set of observations or data, there is always an infinite number of possible models explaining those same data.
  - The simplest model should be selected because it minimizes the number of your incorrect assumptions.

No classifier is superior – no free lunch

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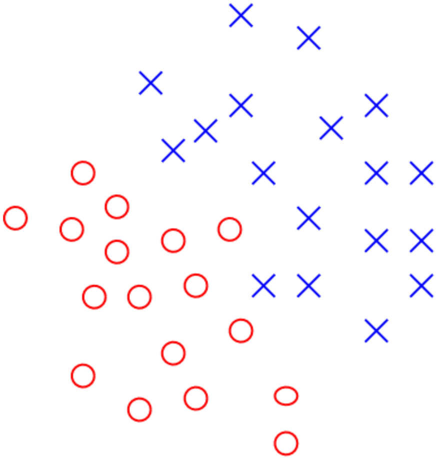
- No Free Lunch theorem: "No algorithm is superior to any other over all classification problems."
    - In the absence of prior information about a problem, there are no reasons to prefer one classifier over another.
    - Comparing generalization performance, there is no problem-independent best pattern recognition method.
    - Opposite viewpoint: The prior information (e.g. homogeneity of decision regions in the feature space) makes classifiers work.

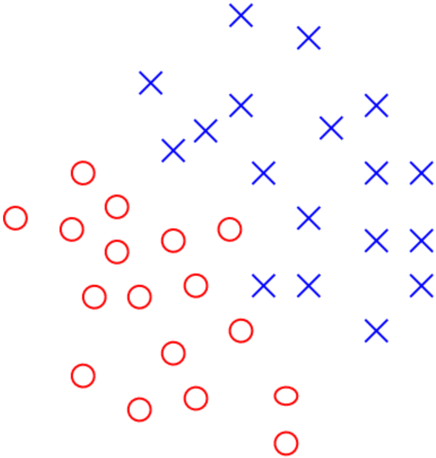
Bias and variance

- A training set is finite and it represents almost always a subset of all possible cases.
- Having few samples, it would be beneficial to use a classifier which is predictable with few samples (typically simple boundaries).
  - Predictability can differ even for classifiers with the same form of boundary.
- Having many samples, we can more confidently use classifiers with more complex boundaries.
- The total error rate of a classifier can be decomposed into two parts:
  - Error rate due to the average performance of the classifier
  - Error rate due to the variation of training set

Example data



Example data



Next look into best possible classifier.

Minimum error classifier

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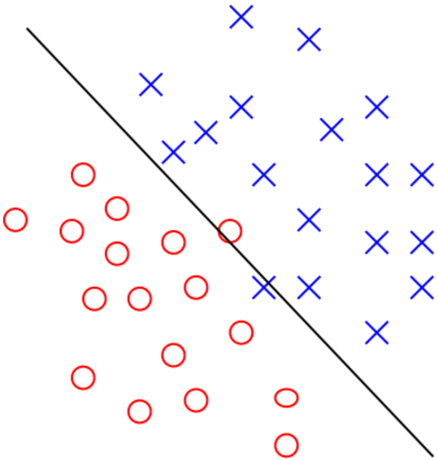
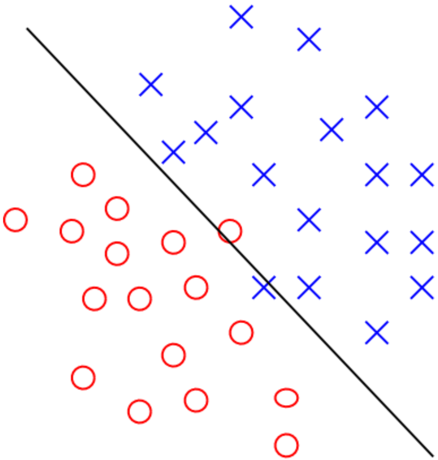


Minimum error classifier



This is the optimal classifier (minimum error).

Worse classification performance

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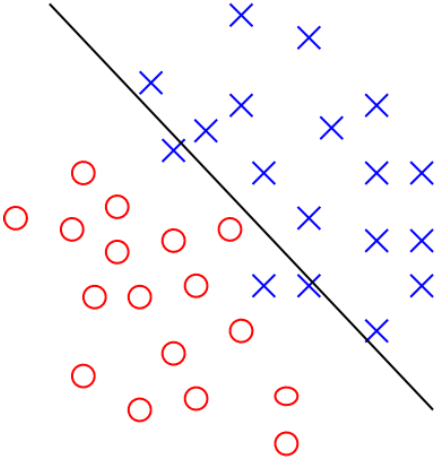

Worse classification performance

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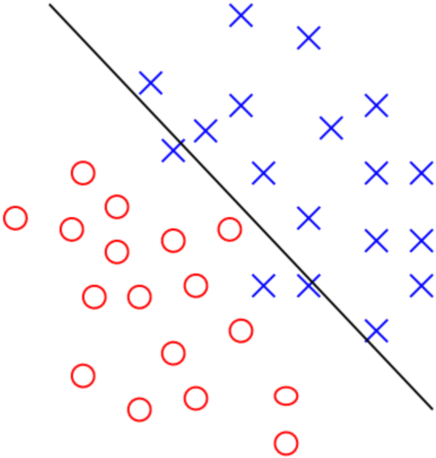
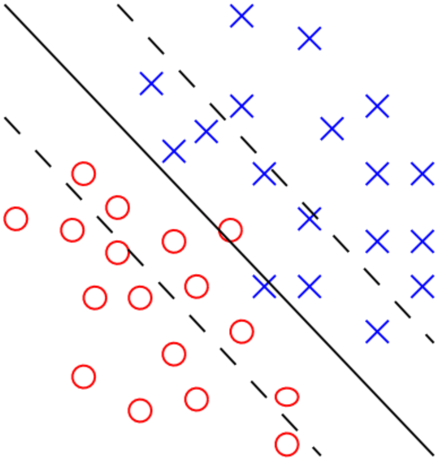


But what if these are the average performances?

Optimal on average, varies a lot



Optimal on average, varies a lot

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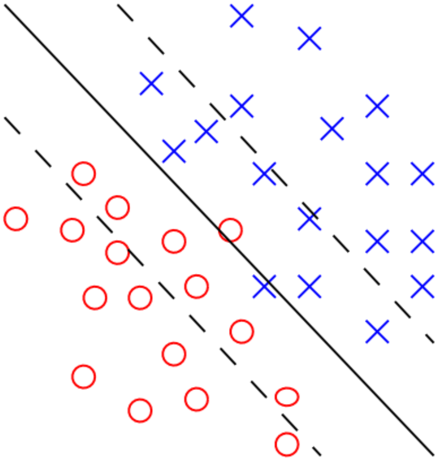

Optimal on average, but varies much for different training sets.

Worse average, but varies little

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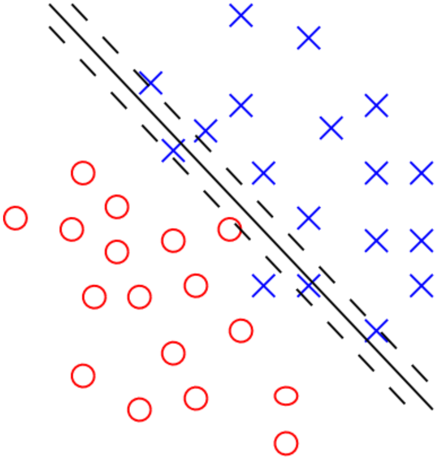

Worse average, but varies little

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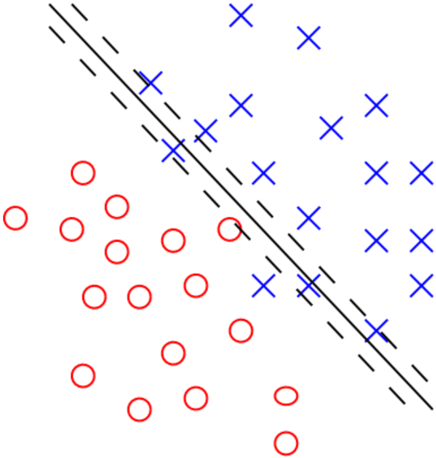

Worse on average, but smaller variance.

Bias and variance for classification

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- Bias:
  - How far is the average performance from the optimal one?
- Variance:
  - How much does the performance vary over different training sets?
  - How much does the boundary vary over different training sets?
- Small variance often more important than small bias if the bias is relatively small.

Resampling

- Could we decrease the variance somehow?
- How to take an "average" classifier over different data sets?
- Resampling of the data produces several different data sets.

Summary

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- Original raw data/features can have less than optimal characteristics for the data analysis task $\Rightarrow$ data preprocessing is needed.
- Data normalisation methods have different properties and consequences of using them should be understood.
- Outliers are non-typical samples in the data set, and a few approaches exist for their detection.
- Simpler models with fewer variables/features have benefits.

Claude E. Shannon.
A mathematical theory of communication.
Bell System Technical Journal, 27(3):379–423, 1948.