

UNIVERSITY OF STAVANGER, DAT550

## Summary of lecture notes



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Spring 2021

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# 1 Introduction to Data Mining

## 1.1 Data

Data is units of information, and in a technical perspective, data is a set of values of quantitative or qualitative variables about a data object. Data should be understood in the context of information. Information can be thought of as the resolution of uncertainty, though its exact interpretation and meaning differs in different context. Using this vague definition of information it becomes clear how diverse data can be. Everything that removes uncertainty contains information and can potentially be stored and processed as data. Examples of data can be

- Tabular Data like spreadsheets.
- A news article.
- A photograph.
- A TV broadcast.
- And much much more.

Historically, computation has been done on numerical data like tabulated data, but in the later decades data mining and machine learning methods have broadened what data algorithms can use to do inference. One example is Neural Networks and image classification.

## 1.2 Data Mining

Data mining can be described as:

*"Non-trivial extraction of implicit,  
previously unknown and potential useful information from data"*

*"Exploration and analysis, by automatic or semi-automatic means,  
of large quantities of data in order to discover meaningful patterns"*

Data mining is a process of extracting and discovering patterns in large data sets involving methods at the intersection of machine learning, statistics, and database systems. Data mining is an interdisciplinary subfield of computer science and statistics with an overall goal to extract information (with intelligent methods) from a data set and transform the information into a comprehensible structure for further use. [Wikipedia contributors \(2021a\)](#)

## 1.3 Machine Learning

Machine learning can be described as:

*"The field of study that gives computers the ability to learn without being explicitly programmed"*

*"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E"*

Machine learning (ML) is the study of computer algorithms that improve automatically through experience and by the use of data. It is seen as a part of artificial intelligence. Machine learning algorithms build a model based on sample data, known as "training data", in order to make predictions or decisions without being explicitly programmed to do so. Another way to think about it as an abstract mathematical formula.

$$f : \text{input} \rightarrow \text{output}$$

The abstract function  $f$  can be any regression-, classification-, association or calculation problem or anything else that can be thought of as the formula above. In traditional programming, the programmer has collected the input and manually created  $f$  and get the output of interest. I.e. the programmer collects input, the rules  $f$  and calculates the output. In machine learning, the programmer have access to the input and the output and the computer estimates  $f$ . I.e. the programmer collects inputs and outputs and uses the computer to find the rules.

It should be stated that in some cases output is not used in machine learning. There are two different kinds of algorithms, one that learns from outputs called supervised learning but there are also algorithms that do not learn from data tagged by humans but that learn patterns from the data itself. These are called unsupervised learning algorithms. In those cases a metric or criterion is used instead and this is used to learn the rules.

## 1.4 Data Mining or Machine Learning

Data mining is the process of discovering patterns in large data sets involving methods at the intersection of machine learning, statistics, and database systems.

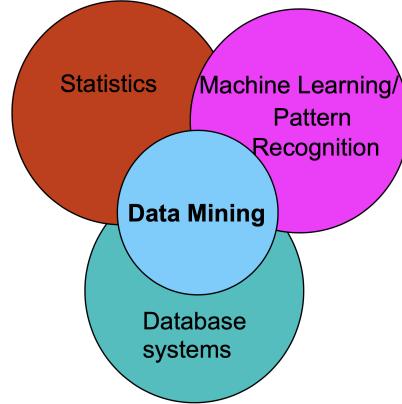


Figure 1.1: Diagram of Data Mining

## 1.5 Data Mining Motivation

### 1.5.1 Commercial viewpoint

Lots of data is being collected and warehoused, such as web data, purchases, and transactions. Computation power has become cheap and powerful, and the competitive pressure is strong. It is therefore necessary to provide better, customized services for an edge.

### 1.5.2 Scientific Viewpoint

Data is collected and stored at enormous speeds, up to multiple terabytes per hour. Such data can be generated from the large hadron collider and from scanning the universe. Such data can not be interpreted by traditional techniques, and requires data mining to classify and segment the data, and form hypothesis formations.

### 1.5.3 KDD Process

Knowledge Discovery in Databases (KDD) refers to the overall process of discovering useful knowledge from data.

KDD is an integration of multiple technologies for data management such as database management and data warehousing, statistic machine learning, decision support, and others such as visualisation and parallel computing.

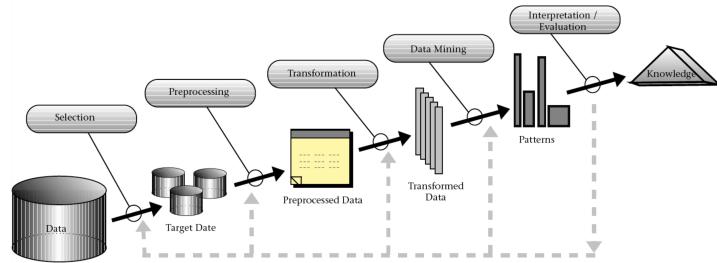


Figure 1.2: The KDD Process

## 1.6 Data Mining tasks

- Prediction methods
  - Use some variables to predict unknown or future values of other variables.
    - \* Supervised (classification or regression)
    - \* Unsupervised (clustering)
    - \* Semi-supervised
- Descriptive methods
  - Find human-interpretable patterns that describe the data.
    - \* Rule mining
    - \* Frequent patterns
    - \* Anomaly detection

## 1.7 Supervised Learning

$$f : \text{input} \rightarrow \text{output}$$

Supervised learning follow the equation above where it uses the input and output of example data to estimate the decision function  $f$ . This is in contrast with traditional programming where the programmer designed the rules or decision function  $f$  and performed calculations to get an output based on inputs. Different algorithms in the class of supervised learning are in essence, just different ways of estimating  $f$ .  $f$  can

have many possible configurations and parameters and selecting appropriate  $f$  estimation methods and tuning the correct parameters of  $f$  are the main workload in supervised machine learning. The terminology used in these cases are **hypothesis space** for  $f$  and its possible estimation methods and parameters. Constraining the hypothesis space must be done to find appropriate algorithms. The parameters that the user manually have to change and give as input to the algorithm is called **hyperparameters**. They are called such because these are parameters the model itself does not have access to. The parameters the model itself tune we call **model parameters**. The hypothesis space is therefore the set of hyperparameters and model parameters.

## 1.8 Unsupervised Learning

- Unsupervised learning includes unlabeled data
- One way of doing this would be to cluster data into groups
  - Group data points which are similar together, while separating dissimilar items as much as possible
  - This is a clustering algorithm

Unsupervised methods does not have the luxury of having the labels of the data, either because there is no natural labelling or because the data has not yet been labeled. These methods must use other metrics than labels to estimate the the decision function  $f$ .

## 1.9 Classification

Given a population  $P$  with subpopulations  $Y$  and a set of attributes for each object in the population  $X$ , a decision function  $f$  must be estimated that is able to capture the true state of nature and correctly identify the correct subpopulation of each object.

$$f : \underset{X \in P}{X} \rightarrow Y$$

## 1.10 Regression

1. Given a set of data points/instances along with “correct” answers or labels (training data)
2. Feed it to an algorithm which can learn a model and predict the correct value for an unseen data point (test data)
3. The learned model is an approximate representation of the training data
4. Predict continuous valued output (price in the previous example)
5. The algorithm should produce more right answers (goal)

Given a variable  $X$  with a continuous variable  $Y$  and a set of observations  $D$ , a decision function  $f$  must be estimated that is able to capture the true state of nature and correctly use  $X$  to predict the corresponding value of  $Y$ .

$$f : X \rightarrow Y \\ X, Y \in D$$

## 1.11 Association Rule Mining

- Given a set of records each of which contain some number of items from a given collection
- Produce dependency rules which will predict occurrence of an item based on occurrences of other items

Such rules can be used for marketing and sales promotion. Rule mining can also be used for inventory management, and much more.

## 1.12 Challenges in Data Mining

- Scalability
- Dimensionality
- Heterogeneous or complex data
- Data ownership and distribution
- Privacy concern
- Data quality
- Evolving/streaming data

# 2 Data

## 2.1 Data Recap

Data is units of information, and in a technical perspective, data is a set of values of quantitative or qualitative variables about a data object. Data should be understood in the context of information. Information can be thought of as the resolution of uncertainty, though its exact interpretation and meaning differs in different context. Using this vague definition of information it becomes clear how diverse data can be. Just see figure 2.1 for examples. Everything that removes uncertainty contains information and can potentially be stored and processed as data.

### 2.1.1 Difference between data and information.

Data and Information is often talked about interchangably but are two different things or rather two different levels of abstraction of the same thing. Data is a structured or unstructured collection of symbols. Information resolves uncertainty and does not take any particular form. Data can represent redundant symbols but can be said to approach information through optimal compression. One of the most common ways to structure data is to have a set of data objects and their attributes.

## 2.2 Attributes

- An attribute is a property or characteristic of an object
  - Attribute are also known as variables, fields, characteristics, or features
- A collection of attributes describe an object
  - Objects are also known as records, points, cases, samples, entries, or instances

### 2.2.1 Values

Attribute values are numbers or symbols assigned to an attribute. The distinction between attributes and attribute values are:

- Same attribute can be mapped to different attribute values
- Different attributes can be mapped to the same set of values

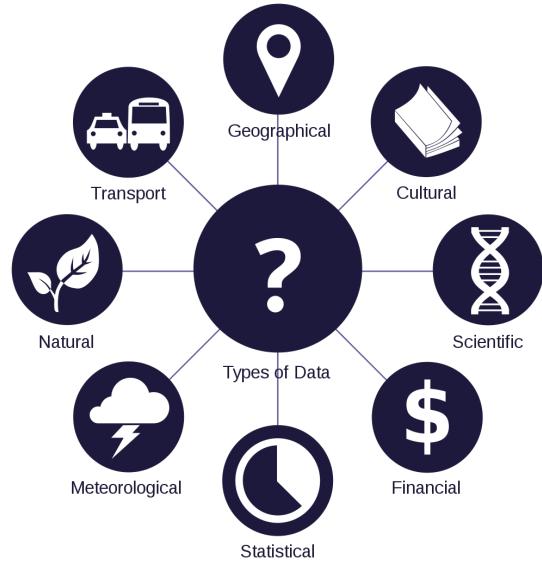


Figure 2.1: Different kinds of data.

### 2.2.2 Types

Attribute Type	Operations	Transformations
Nominal	Mode, Entropy, Contingency, Correlation, $\chi^2$ -test	Any permutation of values
Ordinal	Median, Rank correlation, Percentiles, Run tests, Sign tests	Order-preserving change of values $new\_value = f(old\_value)$ where $f$ is a monotonic function.
Interval	Mean, Standard deviation, $t$ -tests Pearson's correlation, $F$ -tests	$new\_value = a * old\_value + b$ where $a$ and $b$ are constants
Ratio	Geometric mean, Harmonic mean, Percent variation	$new\_value = a * old\_value$

### 2.2.3 Discrete and Continuous Attributes

Discrete attributes:

- Finite or countably infinite set of values

- Often integer or binary variables

Continuous attributes:

- Real numbers as attribute values
- Typically floating-point variables

## 2.3 Datasets

Some important characteristics of structured data are:

- Dimensionality
  - Curse of dimensionality
    - \* As the number of features or dimensions grow, the amount of data needed to generalize accurately grows exponentially.
    - \* When data moves from one dimensions to i.e. three dimensions, the given data fills less and less of the data space. In order to maintain an accurate representation of the space, the data for analysis grows exponentially.
    - \* When sorting or classifying data, low dimensional spaces tend to show the data as very similar, but in higher dimensions, the data might be further away from each other.
- Sparsity
  - Only presence counts
- Resolution
  - Patterns depend on the scale

### 2.3.1 Record Data

Data that consists of a collection of records, each of which consists of a fixed set of attributes.

#### Data Matrix

If data objects have the same fixed set of numeric attributes, then the data objects can be thought of as points in a multi-dimensional space, where each dimension represents a distinct attribute. Such data set can be represented by an  $m$  by  $n$  matrix, where there are  $m$  rows, one for each object, and  $n$  columns, one for each attribute.

#### Document Data

Each document becomes a *term* vector. Each term is a component (attribute) of the vector. The value of each component is the number of times the corresponding term occurs in the document.

### **Transaction Data**

A special type of record data, where each record (transaction) involves a set of items. For example, consider a grocery store. The set of products purchased by a customer during one shopping trip constitute a transaction, while the individual products that were purchased are the items.

### **2.3.2 Graph Data**

Data which can be represented as a collection of edges and vertices. I.e. chemical structures. Graph data can be directional or undirectional.

### **2.3.3 Sequential Data**

Data in which sequence matters. One cannot permute the data in a meaningful way. I.e. time series data or gene sequences.

### **2.3.4 Spatio-temporal Data**

This is data that represents information about both space and time. I.e average temperatures in the world.

## **2.4 Data Quality**

Data Quality is important to measure, detect and improve. Data is elevated to information when optimal data compression is achieved. Problems that reduce the quality of data threatens to damage or skew the information the data is supposed to represent. There are many examples of data quality problems and some of them are addressed in this section.

### **2.4.1 Noise**

Ultimately, Noise can be thought as  $\epsilon$  in the following equation

$$D = S + \epsilon \quad (2.1)$$

Where  $D$  is the collected Data and  $S$  is the true signal. Noise is therefore a modification of original / correct values.

### **2.4.2 Outliers**

Outliers are data objects with characteristics that are considerably different than most of the other data objects in the data set. Though outliers are theoretically possible in many distributions (i.e Normal Distribution) outliers indicate some experimental error or heavy tails. In the former case one either discard the outliers completely or use robust statistics or in the latter case be careful in using statistical tests that assume normal distributions.

### 2.4.3 Missing Values

Reasons for missing values may be that some information is not collected or applicable to all cases.

Handling missing values can be done by:

- Eliminating data objects
- Estimating the missing values
- Ignoring the missing values during analysis
- Replacing the missing values with all possible values weighted by their probabilities

### 2.4.4 Duplicate Data

Data set may include data objects that are duplicates, or almost duplicates of one another. This is a major issue when merging data from heterogenous sources.

## 2.5 Distance/Similarity Functions

According to [Wikipedia contributors \(2021c\)](#):

In statistics and related fields, a similarity measure or similarity function is a real-valued function that quantifies the similarity between two objects. Although no single definition of a similarity measure exists, usually such measures are in some sense the inverse of distance metrics: they take on large values for similar objects and either zero or a negative value for very dissimilar objects.

- Similarity
  - Numerical measure of how alike two data objects are
  - Higher value means more alike
  - Often falls in the range [0, 1]
- Dissimilarity
  - Numerical measure of how different two data objects are
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- Proximity refers to a similarity or dissimilarity

### 2.5.1 Similarity/Dissimilarity for Simple Attributes

Given that  $p$  and  $q$  are the attribute values for two data objects:

Attribute Type	Dissimilarity	Similarity
Nominal	$d = \begin{cases} 0 & \text{if } p = q \\ 1 & \text{if } p \neq q \end{cases}$	$s = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{if } p \neq q \end{cases}$
Ordinal	$d = \frac{ p-q }{n-1}$	$s = 1 - \frac{ p-q }{n-1}$
Interval/Ratio	$d =  p - q $	$s = -d, s = \frac{1}{1+d}, s = 1 - \frac{d - \min(d)}{\max(d) - \min(d)}$

### 2.5.2 Euclidean distance

Euclidean distance is defined in the following theorem, where  $n$  is the number of dimensions (attributes) and  $p_k$  and  $q_k$  are, respectively, the  $k$ th attributes (components) or data objects  $p$  and  $q$ .

#### Theorem 2.1: Euclidean Distance

The distance between two points in Euclidean space is the length of a line segment between the two points. It can be calculated from the Cartesian coordinates of the points using the Pythagorean theorem. In  $n$  dimensions:

$$\text{distance} = \sqrt{\sum_{k=1}^n (p_k - q_k)^2}$$

Standardization is necessary if scales differ.

### 2.5.3 Minkowski Distance

Minkowski Distance is a generalization of Euclidean Distance where  $r$  is a parameter,  $n$  is the number of dimensions (attributes) and  $p_k$  and  $q_k$  are, respectively, the  $k$ th attributes (components) or data objects  $p$  and  $q$ .

#### Theorem 2.2: Minkowski Distance

$$\text{distance} = \sqrt[r]{\sum_{k=1}^n |p_k - q_k|^r}$$

- $r = 1$ : Manhattan distance

- $r = 2$ : Manhattan distance
- $r \rightarrow \infty$ : "Supremum" distance
  - This is the maximum difference between any component of the vectors

#### 2.5.4 Properties of Distance Functions

Distances, such as the Euclidean distance, have some well known properties.

- Positive definiteness
  - $d(p, q) \geq 0$  for all  $p$  and  $q$
  - $d(p, q) = 0$  only if  $p = q$
- Symmetry
  - $d(p, q) = d(q, p)$  for all  $p$  and  $q$
- Triangle Inequality
  - $d(p, r) \leq d(p, q) + d(q, r)$  for all  $p$ ,  $q$  and  $r$

#### Important 2.3: Metric

A distance that satisfies the properties mentioned above is a metric.

#### 2.5.5 Properties of Similarity Functions

Well known properties of similarities.

- Maximum Similarity
  - $s(p, q) = 1$  (or maximum similarity) only if  $p = q$
- Symmetry
  - $s(p, q) = s(q, p)$  for all  $p$  and  $q$

### 2.6 Similarity/Coefficient

A common situation is that objects,  $p$  and  $q$ , have only binary attributes.

Let's define:

- $M_{01}$  - Number of attributes where  $p$  is 0 and  $q$  is 1
- $M_{10}$  - Number of attributes where  $p$  is 1 and  $q$  is 0
- $M_{00}$  - Number of attributes where  $p$  is 0 and  $q$  is 0
- $M_{11}$  - Number of attributes where  $p$  is 1 and  $q$  is 1

### 2.6.1 Simple Matching Coefficient

$$SMC = \frac{\text{Number of matches}}{\text{Number of attributes}} \quad (2.2)$$

$$SMC = \frac{M_{00} + M_{11}}{M_{01} + M_{10} + M_{00} + M_{11}} \quad (2.3)$$

### 2.6.2 Jaccard Similarity/Coefficient

The Jaccard Similarity/Coefficient is used for categorical attributes and sets.

$$J = \frac{\text{Number of } M_{11}}{\text{Number of non-both-zero attributes}} \quad (2.4)$$

$$J = \frac{M_{11}}{M_{01} + M_{10} + M_{11}} \quad (2.5)$$

$$J(A, B) = \frac{|A \cap B|}{|A \cup B|} = \frac{|A \cap B|}{|A| + |B| - |A \cup B|} \quad (2.6)$$

### 2.6.3 Cosine Similarity

If  $\mathbf{A}$  and  $\mathbf{B}$  are two documented vectors, then

$$\text{similarity} = \cos(\theta) = \frac{\mathbf{A} \cdot \mathbf{B}}{\|\mathbf{A}\| \|\mathbf{B}\|} = \frac{\sum_{i=1}^n A_i B_i}{\sqrt{\sum_{i=1}^n A_i^2} \sqrt{\sum_{i=1}^n B_i^2}} \quad (2.7)$$

## 2.7 Dot Product

Given two vectors  $a$  and  $b$ :

$$\vec{a} \cdot \vec{b} = \sum_{i=1}^n a_i b_i = a_1 b_1 + a_2 b_2 + \dots + a_n b_n \quad (2.8)$$

## 2.8 Data Preprocessing

### 2.8.1 Aggregation

Aggregation is to combine two or more attributes (or objects) into a single attribute (or object).

Purpose:

- Data reduction
- Reduce the number of attributes or objects
- Change of scale

- More "stable" data
- Often reduce variability

### 2.8.2 Data Sampling

Data sampling is the main technique employed for data selection. It is often used for both the preliminary investigation of the data and the final data analysis. Statisticians sample because obtaining the entire set of data of interest is too expensive or time consuming. Sampling is used in data mining because processing the entire set of data of interest is too expensive or time consuming. A good strategy for choosing the sample size is to aim for a sample size that is 10% of the population, as long as the sample size is smaller than 1000. It is also important to have a large enough sample size so that all attributes/groups are represented.

Sampling is effective when:

- The sample is representative
- The sample has approximately the same properties (of interest) as the original set of data

Types of sampling:

- Simple random sampling
  - Equal probability of selecting any item.
- Sampling without replacement
  - As each item is selected, it is removed from the population.
- Sampling with replacement
  - Objects are not removed from the population as they are selected for the sample.
- Stratified sampling
  - Split the data into several partitions, then draw random samples from each partition.

### Reservoir Sampling

**The problem:** We want to perform a simple random sample (uniform random sample) on a continuous stream of data of unknown size. Reservoir sampling achieves this.

#### Theorem 2.4: Reservoir Sampling

Keep a reservoir of  $r$  samples

1. Keep the first  $r$  items in memory

2. When the  $i^{th}$  item arrives ( $i > r$ )
  - a) Keep the new item with probability  $\frac{r}{i}$ ,  
or discard the new item with probability  $1 - \frac{r}{i}$
  - b) Discard one of the items in the reservoir at random  
if the new item was kept.

This means that as  $i$  increases, the probability of a new item being kept in the reservoir reduces.

## 2.9 Dimensionality Reduction

- Purpose
  - Avoid curse of dimensionality
  - Reduce amount of time and memory required by data mining
  - Allow data to be more easily visualized
  - May help eliminate irrelevant features or reduce noise
- Techniques
  - Principle Component analysis
  - Singular Value Decomposition

# 3 Exploring Data

## 3.1 Summary Statistics

summary statistics are used to summarize a set of observations, in order to communicate the largest amount of information as simply as possible. The most common types are measurements of location and spread. Below are a collection of examples of summary statistics.

- Frequency
- Mode
- Percentiles
- Mean
- Median
- Range
- Variance

### 3.1.1 Frequency and Mode

The frequency of an attribute value is the percentage of time the value occurs in the data set. The mode of an attribute is the most frequent attribute value. These metrics are often used on categorical data.

#### Theorem 3.1: Frequency

$$\text{Frequency}(x) = N_x = \text{No of occurrences of value } x$$

#### Theorem 3.2: Mode

$$\text{Mode}(X) = \operatorname{argmax}_{x} \text{Frequency}(x)$$

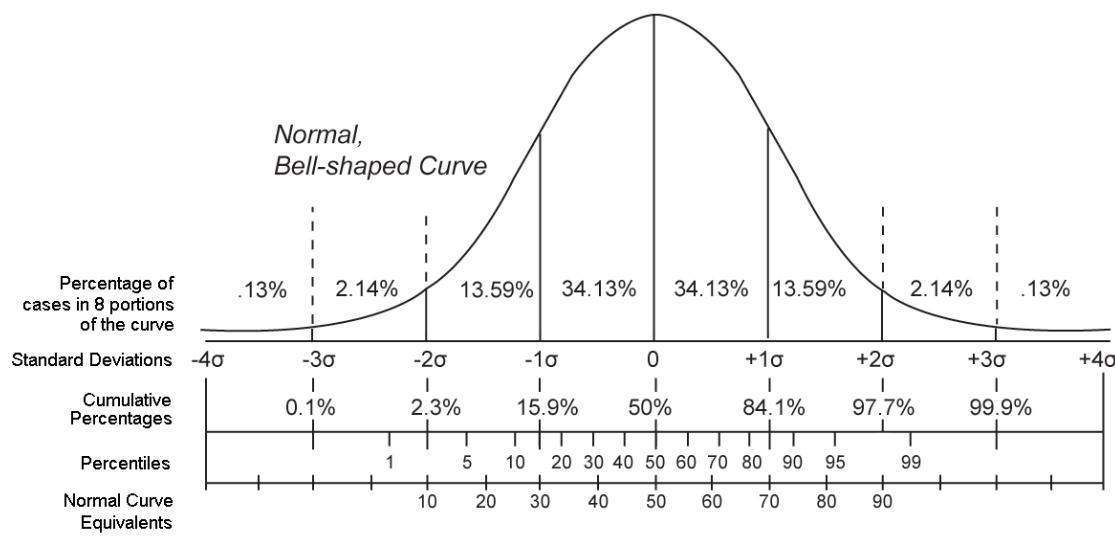


Figure 3.1: Example of gaussian and it's percentiles

### 3.1.2 Percentile

In statistics, a percentile is a score below which a given percentage of scores in its frequency distribution falls or a score at or below which a given percentage falls. See figure 3.1.

### 3.1.3 Measurements of location

The most common measurement of location is the mean.

#### Theorem 3.3: Mean

$$\text{mean}(x) = \bar{x} = \frac{1}{m} \sum_{i=1}^m x_i$$

though the mean is very sensitive to outliers. There are many ways to combat this sensitivity. One is to use the median.

#### Theorem 3.4: Median

$$\text{median}(x) = \begin{cases} x_{(r+1)} & \text{if } m = 2r + 1 \\ \frac{1}{2} (x_{(r)} + x_{(r+1)}) & \text{if } m = 2r \end{cases}$$

Median is not affected by outliers in the same way since it only cares about the index of the sorted observations and not the value of the observations itself.

### 3.1.4 Measurements of Spread

After we have calculated the location of our distribution, using mean, median or any other location metric. But this metric only tells us of where the center of the data lies. The most used metric to describe the spread of data is variance:

#### Theorem 3.5: Variance

$$\text{variance}(x) = s_x^2 = \frac{1}{m-1} \sum_{i=1}^m (x_i - \bar{x})^2$$

Variance as a statistic, like mean, is sensitive to outliers. Therefore there exists other statistics of spread that are robust.

#### Theorem 3.6: Average Absolute Deviation

$$AAD(x) = \frac{1}{m} \sum_{i=1}^m |x_i - \bar{x}|$$

#### Theorem 3.7: Mean Absolute Deviation

$$MAD(x) = \text{median} (\{|x_1 - \bar{x}|, \dots, |x_m - \bar{x}|\})$$

## 3.2 Visualisation

Visualisation is the conversion of data into a visual or tabular format so that the characteristics of the data and the relationships among data items or attributes can be analyzed or reported. Visualisation allows humans to detect general patterns and trends, as well as detect outliers and unusual patterns. Visualisation therefore is one step of transforming Data into information.

### 3.2.1 Representation

The representation is the mapping of information to a visual format. Data objects, their attributes, and the relationships among data objects are translated into graphical elements such as points, lines, shapes, and colors.

### 3.2.2 Arrangement

Arrangement is the placement of visual elements within a display. This can make a large difference in how easy it is to understand the data.

### 3.2.3 Selection

Selection is the elimination or the de-emphasis of certain objects and attributes. Such selections may involve choosing a subset of attributes, or choosing a subset of objects. Only selecting some attributes can be done through dimensionality reduction, while selecting some objects can be done through stratified sampling. Some things to keep in mind when using data selection is to contain the diversity of the objects.

### 3.2.4 Visualisation Techniques

- Histogram plot
- Box plot
- Scatter plot
- Matrix plot
- Parallel coordinates plot
- Star plot

# 4 Decision Trees

## 4.1 Classification Definition

Given a collection of records (a training set) where each record contains a set of attributes, the classification has to find a model for one particular attribute (the class) as a function of the values of other attributes. The goal is for previously unseen records to have the class attribute assigned as accurately as possible. A test set is used to determine the accuracy of the model. Usually, the given data set is divided into training and test sets, with the training set, used to build the model, and the test set used to validate it.

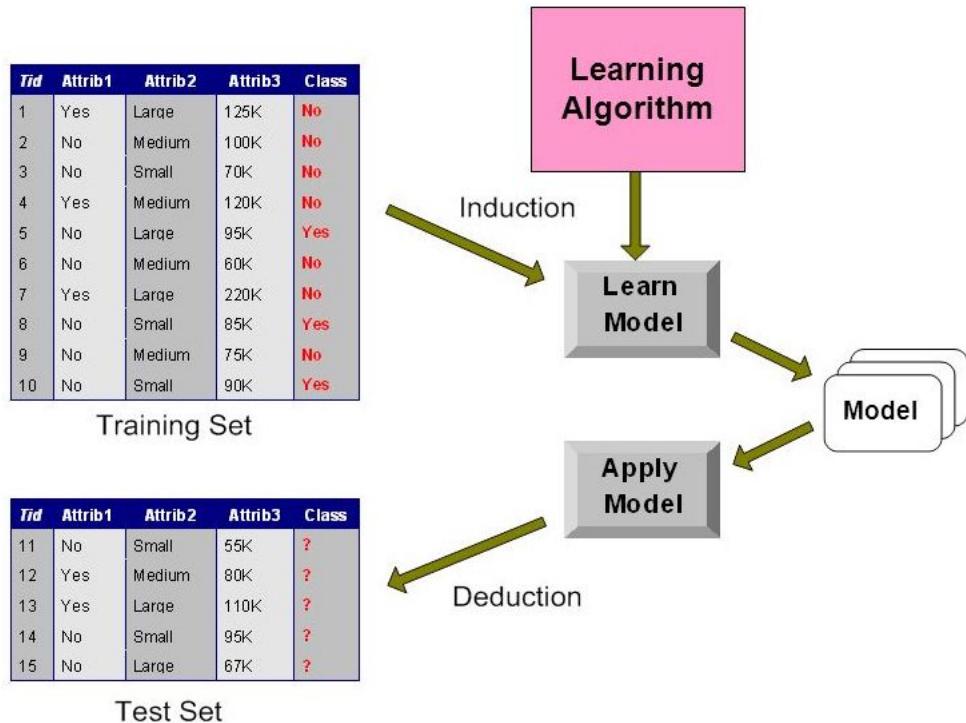


Figure 4.1: Typical Classification Task

### 4.1.1 Decision Tree

A tree is built by splitting the source set, constituting the root node of the tree, into subsets, which constitute the successor children. The splitting is based on a set of splitting

rules based on classification features. This process is repeated on each derived subset in a recursive manner called recursive partitioning. The recursion is completed when the subset at a node has all the same values of the target variable, or when splitting no longer adds value to the predictions. This process of top-down induction of decision trees is an example of a greedy algorithm, and it is by far the most common strategy for learning decision trees from data.

Decision trees used in data mining are of two main types:

- Classification tree analysis - When the predicted outcome is the class (discrete) to which the data belongs.
- Regression tree analysis - When the predicted outcome can be considered a real number.

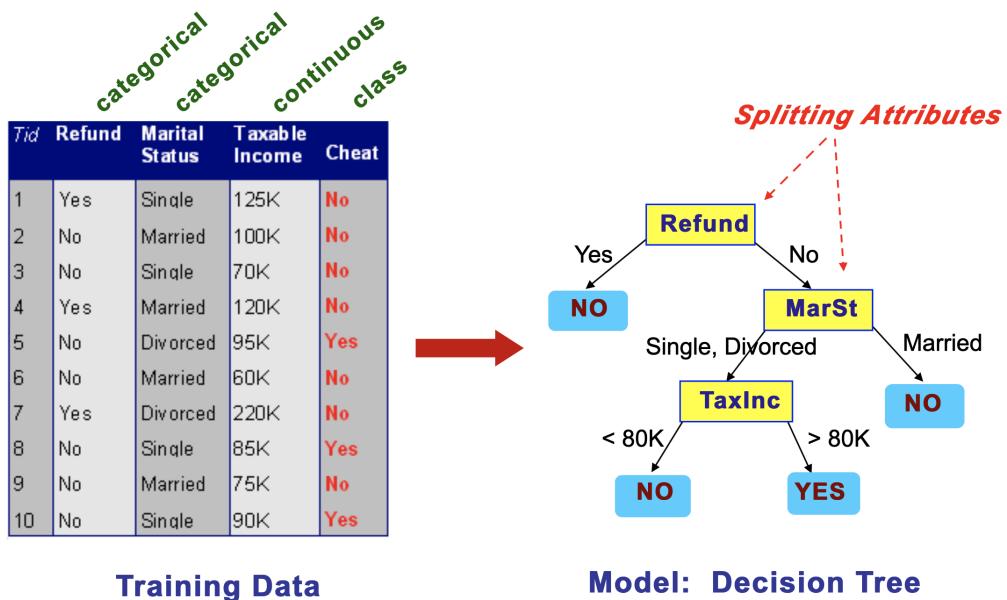


Figure 4.2: Typical Decision Tree

## 4.2 Hunt's Algorithm

- Let  $D_t$  be the set of training records that reach a node  $t$ .
- General procedure:
  - If  $D_t$  contains records that belong to the same class as  $y_t$ , then  $t$  is a leaf node labeled as  $y_t$ .
    - \* This is a pure node.
  - If  $D_t$  is an empty set, then  $t$  is a leaf node labeled by the default class  $y_d$ .
  - If  $D_t$  contains records that belong to more than one class, use an attribute test to split the data into smaller subsets. Recursively apply the procedure to each subset.
    - \* This is an impure node.

## 4.3 Building Trees

### 4.3.1 Tree Induction

The greedy strategy splits the records based on an attribute test that optimizes a certain criterion.

Issues with this approach include:

- How to split the records. How should the attribute test condition be specified, and how is the best split determined?
- Determining when to stop.

#### Specifying the Attribute Test Condition

A proper test condition depends on the attribute type, which can be nominal, ordinal, or continuous.

The condition also depends on the number of ways to split. This can be either a two-way split (binary) or a multi-way split. The binary split is often preferred as of the bushiness of the multi-way split. This means that very few records will match the leaf-nodes, and will therefore be overfitted.

Ordinal attributes can be split the same way as nominal attributes, with some limitations if the order is to be preserved.

For continuous attributes, there are two ways of handling splitting:

- Discretization to form an ordinal categorical attribute.
  - Static - discretize once at the beginning.
  - Dynamic - ranges can be found by equal interval bucketing, equal frequency bucketing, or clustering.

- Binary decision.
  - Consider all possible splits and find the best cut.
  - Can be more compute intensive.

### Determine Best Split

When it comes to greedy approaches, nodes with a homogeneous class distribution are preferred.



Figure 4.3: Class distributions

## 4.4 Measures of Node Impurity

Finding the best split follows closely to this process:

1. Define the set of records as  $M_0$ , where some records belong to class  $C_0$ , while the rest belongs to  $C_1$ .
2. Define some splitting criterias  $A$  and  $B$ .
3. Use each criteria to generate new sets of records. The new sets of records now has a different (or equal) distribution of  $C_0$ - and  $C_1$ -records.
  - $M_1$  and  $M_2$  from  $A$ , collected into  $M_{12}$
  - $M_3$  and  $M_4$  from  $B$ , collected into  $M_{34}$
4. The gain in purity can be measured as such:  $Gain = M_0 - M_{12}$  vs.  $M_0 - M_{34}$
5. The greedy algorithm can then choose the attribute that gives the greatest gain in purity.

### 4.4.1 Gini

The Gini Index measures the degree of probability of a particular variable being wrongly classified when it is randomly chosen.

#### Theorem 4.1: Gini Index

$$GINI(t) = 1 - \sum_j^{n_c} [p(j|t)]^2$$

$$\text{Maximum: } (1 - \frac{1}{n_c}) \quad \text{Minimum: } 0.0 \text{ (pure)}$$

Note:  $p(j|t)$  is the relative frequency of class  $j$  at node  $t$ .

Gini can be used when splitting nodes. When a node  $p$  is split into  $k$  partitions (children), the quality of split follows the theorem:

#### Theorem 4.2: Gini Split

$$GINI_{split} = \sum_{i=1}^k \frac{n_i}{n} GINI(i)$$

$n_i$  = Number of records at child  $i$ .

$n$  = Number of records at node  $p$ .

Compute the Gini Index for continuous attributes can often be quite expensive as all values have to be evaluated for splitting. One process (to be done for each attribute) for finding a good split is as such:

1. Sort the attribute on values.
2. Linearly scans the values, each time choosing the mean of the current value and the next value as the splitting point position and compute the Gini Index.
3. Choose the split position that has the least Gini Index.

Cheat	No	No	No	Yes	Yes	Yes	No	No	No	No	
Annual Income											
Sorted Values	60	70	75	85	90	95	100	120	125	220	
Split Positions	55	65	72	80	87	92	97	110	122	172	230
<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >	<= >
Yes	0 3	0 3	0 3	0 3	1 2	2 1	3 0	3 0	3 0	3 0	3 0
No	0 7	1 6	2 5	3 4	3 4	3 4	3 4	4 3	5 2	6 1	7 0
Gini	0.420	0.400	0.375	0.343	0.417	0.400	0.300	0.343	0.375	0.400	0.420

Figure 4.4: Gini Index of Continuous Attributes

### 4.4.2 Entropy

Entropy is a measure of the uncertainty associated with a random variable. Entropy is a splitting criterion based on information gain and measures the homogeneity of a node.

#### Theorem 4.3: Entropy

$$\text{Entropy}(t) = - \sum_j^{n_c} p(j|t) \log_2 p(j|t)$$

Maximum:  $(\log_2 n_c)$       Minimum: 0.0

Note:  $p(j|t)$  is the relative frequency of class  $j$  at node  $t$ .

In the same way Gini can be used to split nodes, so can Entropy:

#### Theorem 4.4: Entropy Split

$$GAIN_{split} = \text{Entropy}(p) - \left( \sum_{i=1}^k \frac{n_i}{n} \text{Entropy}(i) \right)$$

Parent node  $p$  is split into  $k$  partitions.

$n_i$  is the number of records in partition  $i$

The gain measures reduction in entropy achieved from the split. Choose the split that achieves the most reduction, that is, maximizes gain. The disadvantage is that Entropy tends to prefer splits that result in a large number of partitions, each being small but pure (overfitting). This is fixed by including the number of partitions in the equation.

#### Theorem 4.5: Entropy Split Ratio

$$GainRatio_{split} = \frac{Gain_{split}}{SplitInfo}$$

$$SplitInfo = - \sum_{i=1}^k \frac{n_i}{n} \log \frac{n_i}{n}$$

Parent node  $p$  is split into  $k$  partitions.

$n_i$  is the number of records in partition  $i$

### 4.4.3 Misclassification error

The Classification error measures the misclassification error made by a node.

Classification error at node  $t$ :

**Theorem 4.6: Classification Error**

$$\text{Error}(t) = 1 - \max P(i|t)$$

$$\text{Maximum: } (1 - \frac{1}{n_c}) \quad \text{Minimum: } 0.0$$

### 4.4.4 Comparison among Splitting Criterias

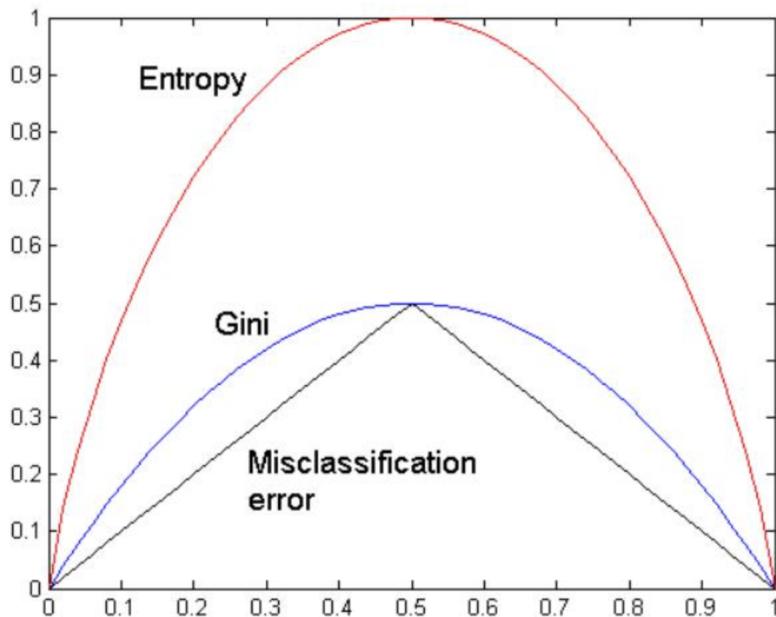


Figure 4.5: Splitting Criterias for a two-class problem

## 4.5 Stopping Criteria for Tree Induction

- Stop expanding a node when all the records belong to the same class.
- Stop expanding a node when all the records have similar attribute values.
- Early termination (probably for limiting tree depth).

## 4.6 Advantages of Decision Tree based Classification

- Inexpensive to construct.
- Extremely fast at classifying unknown records.
- Easy to interpret for small-sized trees.
- Accuracy is comparable to other classification techniques for many simple data sets.

## 4.7 Classification Issues

### 4.7.1 Underfitting and Overfitting

- Underfitting: When a model cannot capture the underlying trend of the data. Intuitively, underfitting occurs when the model or the algorithm does not fit the data well enough. Specifically, underfitting occurs if the model or algorithm shows low variance but high bias. Underfitting is often a result of an excessively simple model. Overfitting can also arise from insufficient data points.
- Overfitting: When a model captures the noise of the data. Intuitively, overfitting occurs when the model or the algorithm fits the data too well. Specifically, overfitting occurs if the model or algorithm shows low bias but high variance. Overfitting is often a result of an excessively complicated model, and it can be prevented by fitting multiple models and using validation or cross-validation to compare their predictive accuracies on test data.

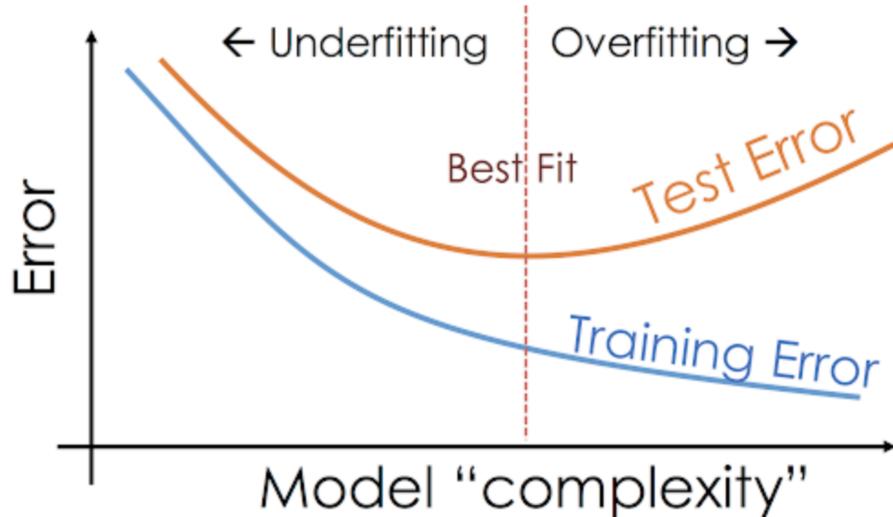


Figure 4.6: Overfitting and underfitting

### 4.7.2 Address Overfitting

#### Decision Tree Pruning

Pre-Pruning (Early Stopping Rule):

- Stop the algorithm before it becomes a fully-grown tree.
  - Stop if all instances belong to the same class.
  - Stop if all the attribute values are the same.
  - Stop if the number of records in a node are lower than the user-specified threshold.
  - Stop if splitting a node does not improve the impurity measure.

Post-Pruning:

1. Grow decision tree to its entirety.
2. Trim the nodes of the decision tree in a bottom-up fashion.
3. If generalization error improves after trimming, replace sub-tree by a leaf node.
4. The class label of a leaf node is determined from the majority class of instances in the sub-tree.

#### Occam's Razor

- Given two models of similar generalization errors, one should prefer the simpler model over the more complex model.
- For complex models, there is a greater chance that it was fitted accidentally by the error in data.
- Therefore, one should include model complexity when evaluating a model.

### 4.7.3 Generalization Errors

Generalization error is a measure of how accurately a model can predict outcome values for previously unseen data. The measure is calculated from the ratio of misclassifications that can occur when choosing the majority class for all records in the node.

- Training errors: Error on training ( $\sum_{t=1}^n e(t)$ )
- Generalization errors: Error on validation ( $\sum_{t=1}^n e'(t)$ )

Methods for estimating generalization errors:

- Optimistic approach:  $e'(t) = e(t)$

- Pessimistic approach:
  - For leaf each leaf node,  $e'(t_i) = e(t_i) + \frac{1}{2}$
  - Total error:  $e'(T) = e(T) + N\frac{1}{2}$  ( $N$  = number of leaf nodes)
- Reduced error pruning (REP)
  - Uses validation data set to estimate generalization error.

#### 4.7.4 Handling Missing Attribute Values

Missing attribute values affect the decision tree in three major ways:

- How impurity measures are computed.
- How to distribute instance with missing value to child nodes.
- How a test instance with missing value is classified.

##### Computing Impurity Measure (Impurity Gain)

One way of computing the information gain is as normal, without including the instances with the missing attribute. This means that the entropy-computation for the parent is as normal, but for the children, instances with the missing attributes should be omitted, but included in the denominator. Finally, the gain is computed as normal but is multiplied by the fraction of "valid" records.

##### Distributing Instances

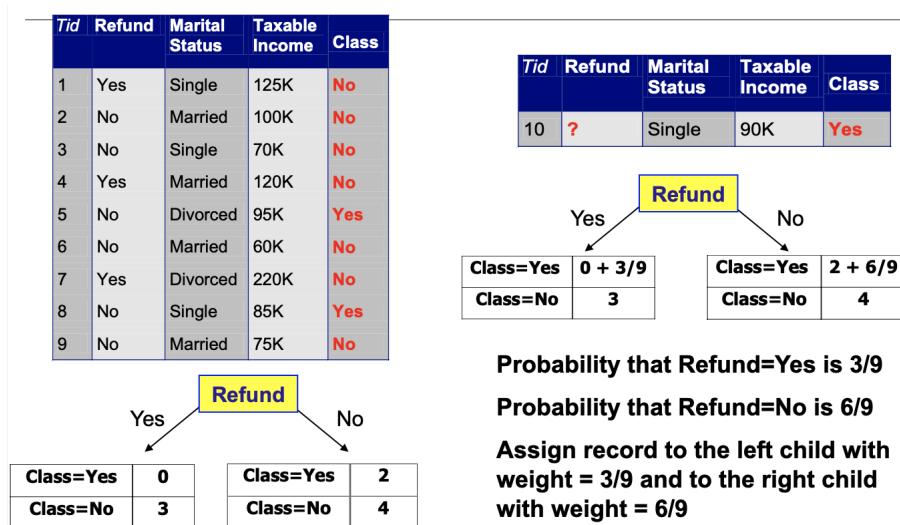


Figure 4.7: Distributing Instances

The figure explains that since the instance with the unknown attribute corresponds to the class yes, it is distributed on both nodes, affecting the yes-class in each node. The distribution ratio is based on the number of instances of the same class, divided by the total number of instances.

### **Classify Instances**

To classify an instance with an unknown class, as well as having the current attribute unknown, can be done by understanding what option is more likely. If most of the instances are of attribute 1 the instance with the unknown attribute is assumed to also have attribute 1 and follows the tree accordingly.

### **4.7.5 Other Issues**

#### **Data Fragmentation**

- The number of instances gets smaller as you traverse down the tree.
- Number of instances at the leaf node could be too small to make any statistically significant decision.

#### **Search Strategy**

- Finding an optimal decision tree is NP-hard (exponentially).
- The algorithm presented so far uses a greedy, top-down, recursive partitioning strategy to induce a reasonable solution.
- Could use bottom-up or bi-directional algorithms.

#### **Expressiveness**

Decision trees provide expressive representation for learning discrete-valued functions, but they do not generalize well to certain types of boolean functions like parity functions. Also, decision trees are not expressive enough for modeling continuous variables.

#### **Decision Boundary**

The borderline between two neighboring regions of different classes is known as a decision boundary.

A decision boundary is parallel to the axes because the test conditions only involve a single attribute at a time.

This could be fixed with oblique decision trees, but includes more expressive representation and can be computationally expensive.

#### **Tree Replication**

The same subtree appears in multiple branches.

# 5 Model Evaluation

## 5.1 Metrics for Performance Evaluation

Metrics for performance evaluation focuses on the predictive capability of a model, that is, how well a model can predict the class of the test data, and evaluate the performance of the training-data. Speed and scalability is not discussed in this section.

### 5.1.1 Confusion Matrix

One of the most common ways of doing this is through the confusion matrix:

		Predicted		Precision
		FALSE	TRUE	
Actual	FALSE	True Negative (TN)	False Positive (FP)	
	TRUE	False Negative (FN)	True Positive (TP)	
				Recall

Figure 5.1: Confusion Matrix

The confusion matrix in this example has one axis for the true classes and one axis for the predicted classes. A correct classification is therefore on the diagonal. From this confusion almost all other metrics used in classification can be derived. A confusion matrix can also contain more than two classes.  $TP$ ,  $TN$ ,  $FP$  and  $FN$  is in those cases calculated with respect to each class. One of the most common and widely-used metric for evaluating the performance is accuracy:

#### Theorem 5.1

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}$$

The accuracy metric has some limitations, among those are the ability to evaluate two-class problems where almost all instances are of class 0, while only a few are of

class 1. The accuracy metric will result in 99.9% accuracy, which is misleading if the model predicts all instances to belong to class 0. Accuracy can also be calculated for each individual class where one calculates  $TP$ ,  $TN$ ,  $FP$  and  $FN$  for the respected class as positive against all other classes considered negative. This may help combat some of the limitations from using overall accuracy.

### 5.1.2 Cost Matrix

One way of solving the issue is to use a cost matrix instead:

		PREDICTED CLASS		
		C(i j)	Class=Yes	Class>No
ACTUAL CLASS	Class=Yes	C(Yes Yes)	C(No Yes)	
	Class>No	C(Yes No)	C(No No)	

Figure 5.2: Cost Matrix

Here,  $C(i|j)$  is the cost of misclassifying class  $j$  as class  $i$ . The cost equals the weighted sum of all predictions.

If true positives and true negatives are equally weighted, as well as the false positives and the false negatives, the accuracy is proportional to the cost. This results in the following equation:

$$Cost = N[q - (q - p) * Accuracy] \quad (5.1)$$

Where  $N = TP + TN + FP + FN$ ,  $q = FP$ , and  $p = TP$ .

### 5.1.3 Cost-Sensitive Measures

Some cost-sensitive measures that are preferred over accuracy:

$$\text{Precision}(p) = \frac{TP}{TP + FP} \quad (5.2)$$

$$\text{Recall}(r) = \frac{TP}{TP + FN} \quad (5.3)$$

$$\text{F-measure}(F) = \frac{2TP}{2TP + FP + FN} \quad (5.4)$$

- Precision is biased towards  $TP$  and  $FP$
- Recall is biased towards  $TP$  and  $FN$
- F-measure is biased towards all except  $TN$

$$\text{Weighted Accuracy} = \frac{\omega_1 TP + \omega_4 TN}{\omega_1 TP + \omega_2 FN + \omega_3 FP + \omega_2 TN} \quad (5.5)$$

## 5.2 Methods for Performance Evaluation

Methods on how to obtain a reliable estimate of performance.

The performance of a model may depend on other factors besides the learning algorithm:

- Class distribution.
- Cost of misclassification.
- Size of training and test sets.

### 5.2.1 Learning Curve

Learning curves show how accuracy changes with varying sample sizes.

Learning curves require a sampling schedule:

- Arithmetic sampling. (Linear)
- Geometric sampling. (Exponential)

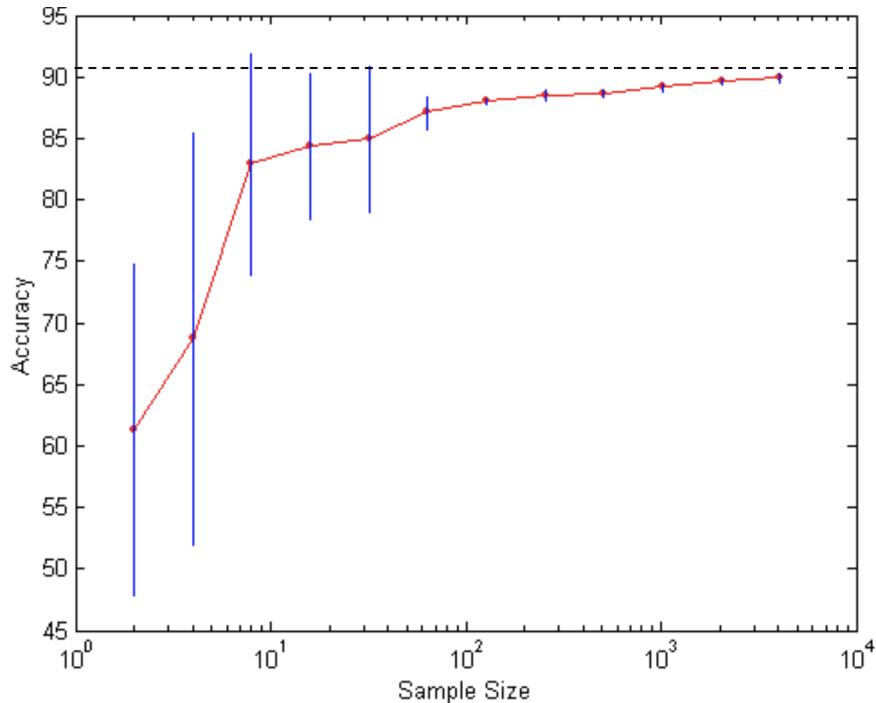


Figure 5.3: A Learning Curve

The effects of small sample sizes includes:

- Bias in the estimate (Underfitting)
- Variance of estimate (Overfitting)

### 5.2.2 Other Methods of Estimation

- Holdout
  - Reserve 80% for training and 20% for testing.
- Random subsampling
  - Repeated holdouts
- Cross validation (popular)
  - Partition data into  $k$  disjoint subsets.
  - $k$ -fold: Train on  $k - 1$  partitions, test on the remaining one.
  - Leave-one-out:  $k = n$
- Stratified sampling
  - Oversampling

- Undersampling
- Bootstrap
  - Sampling with replacement

## 5.3 Methods for Model Comparison

Methods for model comparison explains how to compare the relative performance among competing models.

### 5.3.1 Receiver Operating Characteristic (ROC)

ROC was developed in the 1950s to characterize the trade-off between true positives and false positives.

A ROC curve plots  $TP$  on the  $y$ -axis against  $FP$  on the  $x$ -axis, where the performance of each classifier is represented as a point on the ROC curve. The point changes based on the threshold of the algorithm, the sample distribution, and/or the cost matrix.

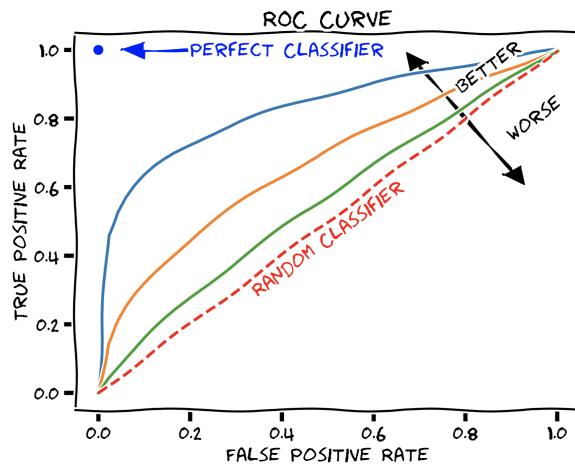


Figure 5.4: ROC Curve

In some cases when comparing the ROC curve for different models, no models consistently outperform the others. Evaluating such models can be based on the area under the ROC curve (AUC), or which model fits better to the desired outcome.

#### Constructing a ROC curve

1. Use a classifier that produces posterior probability for each test instance  $P(+|A)$ .
2. Sort the instances according to  $P(+|A)$  in descending order.
3. Apply threshold at each unique value of  $P(+|A)$ .
4. Count the number of  $TP$ ,  $FP$ ,  $TN$  and  $FN$  at each threshold.

- $TPR = \frac{TP}{TP+FN}$

- $FPR = \frac{FP}{FP+TN}$

# 6 Regression Trees and Ensemble methods

## 6.1 Regression Trees

In a decision tree, there is typically a data set with  $N$  features  $(X_1, X_2, \dots, X_N)$ . Each of the features has a domain, with the domain type being dependent on the type of data the feature contains (categorical or numerical). The output variable  $Y$  will have a domain  $D_y$ .

- Categorical - Classification
- Numerical - Regression

### 6.1.1 Constructing a Regression Tree

We have already explored the classification algorithm of decision trees and how entropy, gini and information gain is used to calculate node impurity which is used to determine the splits. But what do we use when the dependent variable  $Y$  is a continuous / numerical value? Most literature use two metrics for regression trees are *Least Squares* and the other *Least Absolute deviations*. Loh (2011) In both cases the spread in the nodes is used as a metric for *information*, in the same way as entropy. The split that has the least variance in its child nodes compared to the parent is the split that contains the most information.

1. Find a split  $(X_i, v)$  that creates two child nodes  $D_L$  and  $D_R$  from the parent node  $D$ . The split should maximize the weighted sum of the variances.
  - For ordered domains, sort  $X_i$  and consider a split between each pair of adjacent values.
  - For categorical  $X_i$  find the best split based on subsets (Breiman's algorithm).

$$\text{Weighted Variance} = |D| * \text{Var}(D) - (|D_L| * \text{Var}(D_L) + |D_R| * \text{Var}(D_R)) \quad (6.1)$$

$$\text{Var}(D) = \frac{1}{n} \sum_{i=1}^{|D|} (y_i - \bar{y})^2 \quad (6.2)$$

### Stopping a Tree

- When the leaf is pure, i.e.  $Var(D) < \epsilon$
- When the number of instances in the leaf ( $|D|$ ) is too small.

### Predictor

- Regression - Average value of  $y_i$  of the instances in the leaf.
- Classification - Choose the most common  $y_i$  in the leaf.

## 6.2 Ensemble Methods

In addition to using pruning to construct more generalised trees. Two other methods exist to generalise models. These are ensemble and resample methods. Ensemble methods construct a set of classifiers from a given training data. The classification is done by predicting class values from previously unseen records by aggregating predictions made by multiple classifiers.

The general idea of ensemble methods is to have the original training data and then:

1. Create multiple data sets from the training data (resampling).
2. Build multiple classifiers corresponding to the data sets.
3. Combine the predictions of the classifiers.

Ensemble methods work the sum of the error rate of multiple independent classifiers are lower than the error rate itself. The following equation calculates the probability that the ensemble classifier makes a wrong prediction, having  $\epsilon$  as the error rate.

$$\sum_{i=N/2(+1)}^N \binom{N}{i} \epsilon^i (1-\epsilon)^{N-i} \quad (6.3)$$

## 6.3 Manipulating the Training set

### Bagging

Bagging is sampling with replacement (bootstrapping).

1. Let  $k$  be the number of bootstrap samples.
2. `for i in range(k):`
  - a) Create a bootstrap sample of size  $N$ ,  $D_i$ .
  - b) Train a base classifier  $C_i$  on the bootstrap sample  $D_i$ .

$$C^*(x) = \operatorname{argmax} (\sum_i \delta(C_i(x) = y))$$

$\delta = 1$  if the argument is true and 0 otherwise (the majority class is chosen).  
Bagging can also increase the complexity of simple classifiers such as decision stumps.

## Boosting

Boosting is an iterative procedure to adaptively change the distribution of training data by focusing more on previously misclassified records. Initially, all  $N$  records are assigned equal weights.

Unlike bagging, the weights of the records may change at the end of each boosting round.

- Records that are wrongly classified will have their weights increased.
- Records that are classified correctly will have their weights decreased.

One way of boosting is to use the AdaBoost algorithm:

---

**Algorithm 5.7** AdaBoost algorithm.

---

```

1:  $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \dots, N\}$ . {Initialize the weights for all  $N$  examples.}
2: Let  $k$  be the number of boosting rounds.
3: for  $i = 1$  to  $k$  do
4:   Create training set  $D_i$  by sampling (with replacement) from  $D$  according to  $\mathbf{w}$ .
5:   Train a base classifier  $C_i$  on  $D_i$ .
6:   Apply  $C_i$  to all examples in the original training set,  $D$ .
7:    $\epsilon_i = \frac{1}{N} [\sum_j w_j \delta(C_i(x_j) \neq y_j)]$  {Calculate the weighted error.}
8:   if  $\epsilon_i > 0.5$  then
9:      $\mathbf{w} = \{w_j = 1/N \mid j = 1, 2, \dots, N\}$ . {Reset the weights for all  $N$  examples.}
10:    Go back to Step 4.
11:   end if
12:    $\alpha_i = \frac{1}{2} \ln \frac{1-\epsilon_i}{\epsilon_i}$ .
13:   Update the weight of each example according to Equation 5.69.
14: end for
15:  $C^*(\mathbf{x}) = \underset{y}{\operatorname{argmax}} \sum_{j=1}^T \alpha_j \delta(C_j(\mathbf{x}) = y))$ .
```

---

Figure 6.1: AdaBoost Algorithm

## 6.4 Manipulating the Features

### Random Forest

A random forest is a class of ensemble methods specifically designed for decision tree classifiers. It combines the predictions made by multiple decision trees where each tree is generated based on the values of an independent sample set. The samples are generated from a fixed probability distribution.

As in bagging, we build decision trees on bootstrapped training samples. Each time a split in a tree is considered, a random sample of  $F$  features is chosen as split candidates from the full set of  $m$  features.

(If  $F = m$ , we have bagging)

A random forest algorithm can look like this:

- `for i in range(B):`
1. Draw a bootstrap sample  $D^*$  of size  $N$  from the training data.
    - a) Grow a random forest tree to the bootstrapped data.
      - i. Select  $F$  features at random from the  $m$  variables.
      - ii. Pick the best variable/split point among the  $F$ s.
      - iii. Split the node into two child nodes.
  - Output the ensemble of trees.

Prediction at a new point  $x$  can be done:

- For regression - Average of the results.
- For classification - Majority vote.

### Random Forest Recommendations

- For classification, the default value for  $F$  is  $\sqrt{m}$  and the minimum node size is one.
- For regression, the default value for  $F$  is  $\frac{m}{3}$  and the minimum node size is five.

# 7 Locality-Sensitive Hashing

## 7.1 Definition

Locality-sensitive hashing (LSH) is an algorithmic technique that hashes similar input items into the same "buckets" with high probability. Since similar items end up in the same buckets, this technique can be used for data clustering and nearest neighbor search. It differs from conventional hashing techniques in that hash collisions are maximized, not minimized. Alternatively, the technique can be seen as a way to reduce the dimensionality of high-dimensional data; high-dimensional input items can be reduced to low-dimensional versions while preserving relative distances between items.

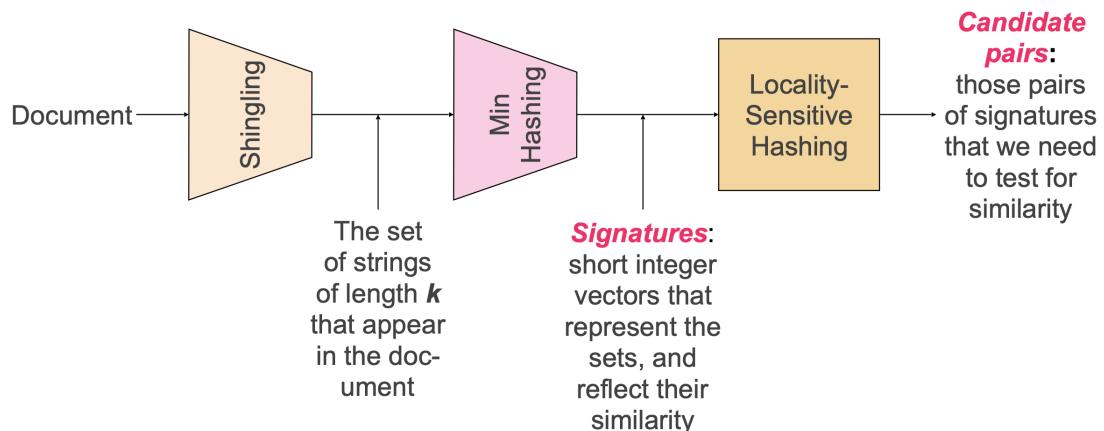


Figure 7.1: Locality-Sensitive Hashing

## 7.2 LSH Steps

1. Shingling: Convert documents into sets of shingles.
2. Min-Hashing: Convert large sets of short signatures, while preserving similarity (i.e. Jaccard similarity).
3. Locality-Sensitive Hashing: Focus on pairs of signatures likely to be from similar documents.
  - This results in candidate pairs, which are likely candidates with a high probability of being similar to the input document.

## 7.3 Shingling

Shingling is the process of converting documents to sets. Some simple approaches are to transform the document into sets of unique words, or "important" words. The main problem is that the ordering of words has to be taken into account:

### 7.3.1 Shingles

A  $k$ -shingle (or  $k$ -gram) for a document is a sequence of  $k$  tokens that appears in the document.

- Tokens can be characters, words, or something else, depending on the application.

A modification of the  $k$ -shingle is to use shingles as a bag (multiset), and therefore counting equal sequences multiple times instead of only one.

#### Similarity Metric for Shingles

- Document  $D_i$  is a set of its  $k$ -shingles  $C_i = S(D_i)$
- In this setting, each unique shingle is a dimension.
- The vectors will be very sparse as most documents does not contain most of the shingles.

A natural similarity measure is the **Jaccard Similarity**:

$$\text{sim}(D_1, D_2) = \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|} \quad (7.1)$$

#### Working Assumptions

- Documents that have lots of shingles in common have similar text, even if the text appears in different orders.
- $k = 5$  is ok for short documents.
- $k = 10$  is better for long documents.

## 7.4 Min-Hashing

Using pairwise Jaccard similarity directly to find near-duplicate documents would result in operations too complex and time consuming to handle. This is why min-hashing is used.

Min-hashing provides signatures (short integer vectors) that represent the sets and their similarity.

### Encoding Sets as Bit Vectors

Many similarity problems can be formalized as:

Finding subsets that have a significant intersection.

This can be done efficiently by encoding sets using boolean vectors.

Documents (N)				
Shingles (D)	1	1	1	0
	1	1	0	1
	0	1	0	1
	0	0	0	1
	1	0	0	1
	1	1	1	0
	1	0	1	0

$$\text{Note: } d(C_1, C_2) = 1 - \frac{|C_1 \cap C_2|}{|C_1 \cup C_2|} = 1 - \frac{3}{6}$$

Figure 7.2: Boolean Matrix

#### 7.4.1 Hashing Columns

The key idea of hashing is to hash each column  $C$  to a small signature  $h(C)$  so that:

- $h(C)$  is small enough to fit in the RAM.
- The Jaccard similarity is preserved.

The goal is to find a hash function so that if  $\text{sim}(C_1, C_2)$  is high, there is a high probability that  $h(C_1) = h(C_2)$ , and vice versa. The hash function places columns into a bucket, with the expected outcome being that most pairs of near-duplicate documents hash into the same bucket.

A suitable hash function for the Jaccard similarity is called **Min-Hashing**.

#### 7.4.2 Definition

- Imagine the rows of the boolean matrix permuted under random permutation  $\pi$ .
- Define a hash function  $h_\pi(C) =$  the index of the first row in which column  $C$  is *True*.

- Use several independent hash functions (that is, permutations) to create a signature of a column.

$$h_\pi(C) = \min_\pi \pi(C) \quad (7.2)$$

Each unique combination of 1s and 0s can be classified as different types.

I.e.  $A = 1, 1$ ,  $B = 1, 0$ ,  $C = 0, 1$ ,  $D = 0, 0$ . If lower case letters denote the number of rows corresponding to the corresponding type, we get the following Jaccard similarity:

$$\text{sim}(C_1, C_2) = \frac{a}{a + b + c} \quad (7.3)$$

And the probability:

$$\Pr[h_\pi(C_1) = h_\pi(C_2)] = \text{sim}(C_1, C_2) \quad (7.4)$$

And the thought-process is:

1. Look down the columns  $C_1$  and  $C_2$  until the first 1 appears.
2. If the row is of type  $A$ , then  $h(C_1) = h(C_2)$ .
3. If the row is of type  $B$  or  $C$ , then  $h(C_1) \neq h(C_2)$ .

### Similarity for Signatures

- The similarity of two signatures is the fraction of the hash functions in which they agree.
- Because of the Min-Hash property, the similarity of columns is the same as the expected similarity of their signatures.

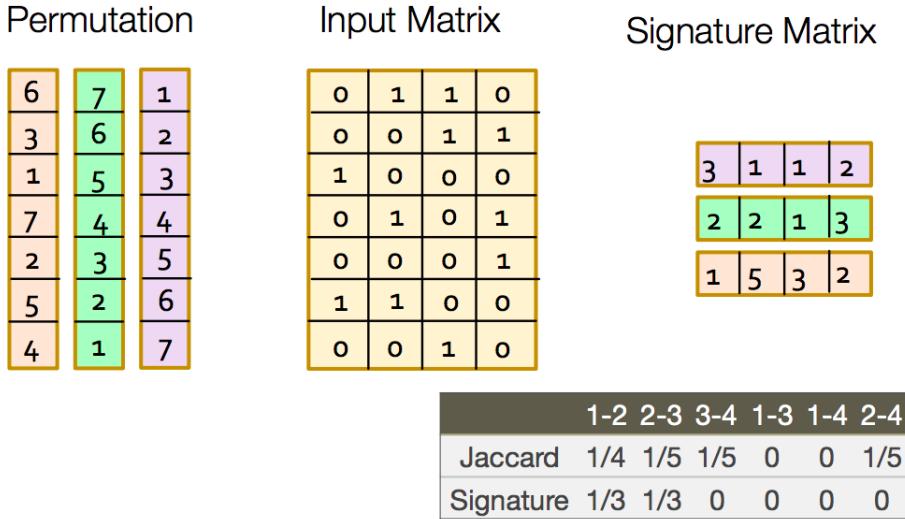


Figure 7.3: Min-Hashing

### 7.4.3 Process

1. Pick  $k = 100$  random permutations of the rows.
2. Think of  $\text{sig}(C)$  as a column vector.
3.  $\text{sig}(C)[i] =$  The index of the first row that has the value of 1 in column  $C$ , given the  $i_{th}$  permutation.
4.  $\text{sig}(C)[i] = \min(\pi_i(C))$

## 7.5 LSH

The goal of the locality-sensitive hashing process is to find documents with Jaccard similarity over some similarity threshold  $s$ .

The general idea is to use a function  $f(x, y)$  that tells whether  $x$  and  $y$  is a candidate pair; a pair of elements whose similarity must be evaluated.

For Min-Hash matrices:

- Hash columns of the signature matrix  $M$  into many buckets,
- Each pair of documents that hashes into the same bucket is a candidate pair.

Columns  $x$  and  $y$  of  $M$  are a candidate pair if their signatures agree on at least the fraction  $s$  of their rows.  $M(i, x) = M(i, y)$  for at least the fraction  $s$  of  $i$ . It is expected that the documents  $x$  and  $y$  have the same Jaccard similarity as their signatures.

The main idea of LSH for Min-hashing is to hash columns of the signature matrix  $M$  several times. Then, arrange the columns so that only similar columns are likely to hash to the same bucket, with a high probability. Finally, the candidate pairs are those columns that hash to the same bucket.

### 7.5.1 Process of LSH

1. Divide matrix  $M$  into  $b$  bands of  $r$  rows.
2. For each band, hash its portion of each column to a hash table with  $k$  buckets, while making  $k$  as large as possible.
3. The candidate column pairs are those bands that hash to the same bucket for more than one band.
4. Tune  $b$  and  $r$  to catch most similar pairs, and minimize the number of non-similar pairs.

### Simplified Assumptions

- There are enough buckets that columns are unlikely to hash to the same bucket unless they are identical in a particular band.
- It is assumed that all bands in the bucket are identical.
- These assumptions are only needed to simplify the analysis, not for the correctness of the algorithm.

### Some Probabilities

Given the columns  $C_1$  and  $C_2$  with the similarity  $s$ , and that  $b$  bands with  $r$  rows is selected:

- The probability that all rows in the band are equal =  $s^r$
- The probability that some rows in the band are unequal =  $1 - s^r$
- The probability that no bands are identical after  $b$  bands =  $(1 - s^r)^b$
- The probability that at least one band is identical after  $b$  bands =  $1 - (1 - s^r)^b$

### 7.5.2 LSH Decisions

Some parameters have to be adjusted to balance the false positives and negatives and get the most desired result when using LSH. This includes:

- The number of Min-Hashes (rows of  $M$ ).
- The number of bands  $b$ .
- The number of rows  $r$  per band.

### 7.5.3 Summary

- Tune  $M$ ,  $b$ , and  $r$  to get almost all pairs with similar signatures, but eliminate most pairs that do not have similar signatures.
- Check in the main memory that candidate pairs do have similar signatures.
- Optional: In another pass through the data, check that the remaining candidate pairs represent similar documents.

# 8 Dimensionality reduction

## 8.1 Dimensionality Reduction

The purpose of dimensionality reduction is to:

- Avoid curse of dimensionality.
- Reduce the amount of time and memory required by data mining algorithms.
- Allow data to be more easily visualized.
- May help to eliminate irrelevant features or reduce noise.
- Recommender systems

Some of the techniques used for dimensionality reduction are:

- Principle Component Analysis
- Singular Value Decomposition

This is done by searching for a plane with a lower count of dimensions, which approximately fits the data values.

### Data compression

By compressing the data, data mining algorithms can be trained faster. Besides, redundant data such as equal measures, but in different units, could be compressed/merged.

### Visualization

Dimensionality reduction can improve how we display information in a tractable manner for human consumption. This is important because visually understandable information often helps to develop algorithms.

## 8.2 Singular Value Decomposition (SVD)

**Theorem 8.1: SVD**

$$A_{[m \cdot n]} = U_{[m \cdot r]} \Sigma_{[r \cdot r]} V_{[n \cdot r]}^T$$

Where:

$A$  = Input data matrix

I.E m documents, n terms

$U$  = Left Singular vectors

I.E m documents, r concepts

$\Sigma$  = Singular values

r - rank of matrix  $A$

$V$  = Right Singular vectors

I.E n terms, r concepts

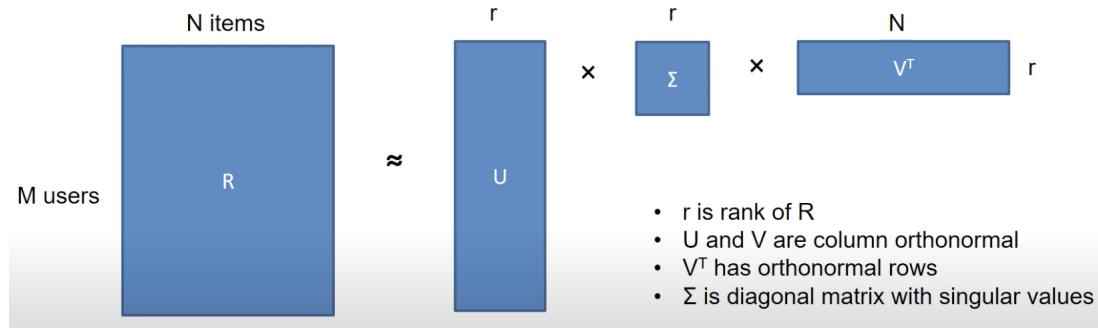


Figure 8.1: Single Value Decomposition

For information on how to compute the singular value decomposition (with examples), visit: [Singular Value Decomposition \(SVD\) tutorial](#).

## 8.3 Principal Component Analysis (PCA)

PCA is the most commonly used dimensionality reduction method.

### 8.3.1 Goal

The goal of the PCA is to find a single line (or plane in higher dimensions) onto which to project the input data.

The line/plane can be found by finding a lower-dimensional surface so the sum of squares onto that surface is minimized.

### 8.3.2 General Case

- Given an  $m * n$  matrix, the goal is to find an  $m * k$  matrix.
- Find a set of vectors which we project the data onto the linear subspace spanned by that set of vectors.
- We can define a point in a plane with  $k$  dimensional vectors.

### 8.3.3 Algorithm

The PCA Algorithm requires some preprocessing to work properly.

- Step 1: Preprocessing
  - Mean normalization - Replace each  $x_{ji}$  with  $x_{ji} - \mu_j$ , subtract the mean from the value, so the mean is re-scaled to be 0.
  - Feature scaling (dependent on data) - If the features have very different scales, normalize them by changing  $x_{ji}$  to  $\frac{x_{ij} - \mu_j}{s_j}$ , where  $s_j$  is some measure of the range, i.e. *max*, *min*, or *standard deviation*.
- Step 2: Compute the covariance matrix
  - $COV(x, y) = \frac{1}{n-1} \sum_{i=1}^n (x_i - \hat{x})(y_i - \hat{y})$
  - This results in an  $[n * n]$  matrix.
  - $x_i$  and  $y_i$  are  $[m * 1]$  vectors.
- Step 3: SVD
  - Compute the SVD on the covariance matrix C.
  - $[U, \Sigma, V^T] = SVD(C)$
  - The U matrix is an  $[n * r]$  matrix.
  - To reduce the system from  $n$ -dimensions to  $k$ -dimensions, take the first  $k$  vectors from  $U$  (The first  $k$  columns).

### 8.3.4 Transformation

To change  $X$  (which is  $n$  dimensional) to  $z$  (which is  $k$  dimensional):

1. Take the first  $k$  columns of the  $U$  matrix and stack in columns. This gives the  $n * k$  matrix  $U_{Reduced}$ .
2. Calculate  $z$ :  $z = U_{Reduced}^T * X$
3.  $[[k * n]] * [[n * 1]]$
4. This generates a matrix which is  $k * 1$  per data row.

### 8.3.5 Measure Quality of PCA

To measure how good the implemented PCA is, we can measure the reconstruction error:

- Given the reduced data  $U_{Reduced}$  in  $K$  dimensions .
- $X_{Approx} = U_{Reduce} * Z$

$$\frac{\frac{1}{m} \sum_{i=1}^m \|x_i - x_i^{approx}\|^2}{\frac{1}{m} \sum_{i=1}^m \|x_i\|^2} \leq 0.01 \quad (8.1)$$

### 8.3.6 Choosing the Parameter k

We want to choose the  $k$  value which results in the smallest ratio between the averaged squared projection error with the total variation in the data. This makes sense, as we want  $x_i \approx x_i^{Approx}$  to retain as much information as possible.

# 9 Advanced Classifiers (Naive Bayes)

## 9.1 Probability theory recap

Probability theory is a branch of mathematics concerning numerical descriptions of how likely an event is to occur. Formalised by Andrey Kolmogorov in 1933. [Kolmogorov \(1960\)](#) He formalised the modern interpretation of probability theory. The axioms from this publication is:

**The First Axiom:** The Probability of an event  $E$  is a non-negative real number.

$$P(E) \in \mathbb{R}, P(E) \geq 0, \quad \forall E \in F \quad (9.1)$$

where  $F$  is the event space.

**The Second Axiom:** The Probability of at least one element occurring in the sample space is 1

$$P(\Omega) = 1 \quad (9.2)$$

**The Third Axiom:** The probability of the union of disjoint sets is equal to the sum of the probabilities of the disjoint sets.

$$P\left(\bigcup_{i=1}^{\infty} E_i\right) = \sum_{i=1}^{\infty} P(E_i) \quad (9.3)$$

## 9.2 Conditional Probability Recap

$$P(A | B) = \frac{P(A \cap B)}{P(B)}$$

This is read as: Probability of event A given B.

## 9.3 Bayes Theorem

Bayes theorem is derived from the definition of conditional probability. Given that

$$P(A \cap B) = P(B \cap A)$$

Since the intersection operator does not care about order. We can rearrange equation and get

$$P(A \cap B) = P(A | B)P(B) = P(B | A)P(A)$$

and we can substitute  $P(A \cap B)$  with the equation above and get:

**Theorem 9.1**

$$P(A | B) = \frac{P(B | A)P(A)}{P(B)}$$

## 9.4 Bayes Theorem for Continuous Values

We need to assume that the values we are interested in have a Gaussian distribution.

- Find the mean  $\mu$
- Find the variance  $\sigma^2$
- Use the Gaussian distribution to calculate the probability  $P(A)$

For conditional probabilities:

- Find the mean  $\mu_B$  for only the condition  $B$
- Find the variance  $\sigma_B^2$  for only the condition  $B$
- Use the Gaussian distribution to calculate the conditional probability  $P(A|B)$

For inequalities, we need to integrate the Gaussian density (preferably by computing the standard Gaussian density first).

## 9.5 Bayesian Classifiers

### 9.5.1 Goal

Given a record with attributes  $(A_1, A_2, \dots, A_n)$ , the goal of the bayesian classifier is to predict the class  $C$ . Specifically, we want the classifier to find the value of  $C$  that maximizes  $P(C|A_1, A_2, \dots, A_n)$ .

### 9.5.2 Approach

1. Compute the posterior probability for all values of  $C$  based on Bayes theorem.
2. Choose the value of  $C$  that maximizes the posterior probability.

- This is equivalent to choosing the value of  $C$  that maximizes  $P(A_1, A_2, \dots, A_n|C)P(C)$ , because the denominators are equal

Computing  $P(A_1, A_2, \dots, A_n|C)P(C)$  is done as such:

1. Assume independence among attributes  $A_i$  when the class is given:
  - $P(A_1, A_2, \dots, A_n|C) = P(A_1|C_j)P(A_2|C_j) \cdots P(A_n|C_j)$
2. Estimate  $P(A_i|C_j)$  for all  $A_i$  and  $C_j$
3. The new point is classified to  $C_j$  if  $P(C_j) \prod P(A_i|C_j)$  is maximal

### 9.5.3 Estimating Probabilities from Data

For continuous attributes:

1. Discretize the range into bins:
  - One ordinal attribute per bin
  - Violates independence assumption
2. Two-way split
  - Choose only one of the two splits as a new attribute
3. Probability density estimation
  - Assume that the attribute follows a normal distribution
  - Estimate the mean and the variance
  - Estimate the conditional probability  $P(A_i|C)$  from the known distribution

**Given a Test Record:**

$$X = (\text{Refund} = \text{No}, \text{Married}, \text{Income} = 120\text{K})$$

naive Bayes Classifier:

```

P(Refund=Yes|No) = 3/7
P(Refund=No|No) = 4/7
P(Refund=Yes|Yes) = 0
P(Refund=No|Yes) = 1
P(Marital Status=Single|No) = 2/7
P(Marital Status=Divorced|No)=1/7
P(Marital Status=Married|No) = 4/7
P(Marital Status=Single|Yes) = 2/7
P(Marital Status=Divorced|Yes)=1/7
P(Marital Status=Married|Yes) = 0

For taxable income:
If class=No:    sample mean=110
                sample variance=2975
If class=Yes:   sample mean=90
                sample variance=25
  
```

- $P(X|\text{Class}=\text{No}) = P(\text{Refund}=\text{No}|\text{Class}=\text{No}) \times P(\text{Married}|\text{Class}=\text{No}) \times P(\text{Income}=120\text{K}|\text{Class}=\text{No}) = 4/7 \times 4/7 \times 0.0072 = 0.0024$
- $P(X|\text{Class}=\text{Yes}) = P(\text{Refund}=\text{No}|\text{Class}=\text{Yes}) \times P(\text{Married}|\text{Class}=\text{Yes}) \times P(\text{Income}=120\text{K}|\text{Class}=\text{Yes}) = 1 \times 0 \times 1.2 \times 10^{-9} = 0$

Since  $P(X|\text{No})P(\text{No}) > P(X|\text{Yes})P(\text{Yes})$   
Therefore  $P(\text{No}|X) > P(\text{Yes}|X)$   
 $\Rightarrow \text{Class} = \text{No}$

Figure 9.1: Example of deciding class

#### 9.5.4 Naive Bayes Classifier problems

In the previous figure, one of the conditional probabilities is zero, meaning that the entire expression becomes zero. This is often an effect of having an incomplete training set. This means that the class, given the conditional probability, will never be chosen.

This can be "fixed" by using some type of smoothing:

- Original:  $P(A_i|C) = \frac{N_{ic}}{N_c}$
- Laplace:  $P(A_i|C) = \frac{N_{ic}+1}{N_c+c}$
- m-estimate:  $P(A_i|C) = \frac{N_{ic}+mp}{N_c+m}$

Where  $c$  = number of classes,  $p$  = prior probability, and  $m$  = own parameter.

### 9.6 Bayesian Belief Network (BBN)

- Conditional independence assumption is not always practical.
- A Bayesian belief network provides a graphical representation of dependencies.
  - A directed acyclic graph (dag) encoding the dependence relationships among a set of variables.
  - A probability table associating each node to its immediate parent node.
- Calculating the probability of a variable, which is dependent on some other variables, can often be simplified to only depend on the direct parent(s).

## 9.7 Summary of Naive Bayes

- Robust to isolated noise points.
- Handle missing values by ignoring the instance during probability estimate calculations.
- Robust to irrelevant attributes.
- Independence assumption may not hold for some attributes.
  - Use other techniques such as Bayesian Belief Networks (BBN).

# 10 Advanced Classifiers (Linear Regression)

## 10.1 Regression Analysis

In statistical modeling, regression analysis is a set of statistical processes for estimating the relationships between a dependent variable (often called the 'outcome variable') and one or more independent variables (often called 'predictors', 'covariates', or 'features'). [Wikipedia contributors \(2021b\)](#) Recall from chapter 1 that given a variable  $X$  with a continuous variable  $Y$  and a set of observations  $D$ , a decision function  $f$  must be estimated that is able to capture the true state of nature and correctly use  $X$  to predict the corresponding value of  $Y$ .

$$f : X \rightarrow Y \\ X, Y \in D$$

The equation above is a general equation for how regression models relate the independent variables  $X$  and the outcome variable  $Y$ . Though the exact implementation of the model of this relationship varies throughout different methods. One of which we will discuss in this chapter, linear regression.

## 10.2 Solving Linear Regression

For Ordinary Least Squares (OLS) there exists a closed-form solution to calculate the solution parameters. Given a feature matrix  $X$  and outcome vector  $Y$  and minimisation of squared errors, the solution parameter matrix  $\theta$  is calculated as

$$\theta = (X^T X)^{-1} X^T$$

This calculation is done only once and is the optimal solution. But there are constraints which will lead us to use a gradient descent approach instead. According to [Pedregosa et al. \(2011\)](#), the complexity of the analytical solution is

$$O(n_{\text{samples}} n_{\text{features}}^2)$$

And compare this with the complexity of the Stochastic Gradient Descent approach is

$$O(knp\bar{p})$$

where  $k$  is the number of epochs in the gradient descent,  $n$  the number of samples and  $\bar{p}$  the average number of non-zero attributes in the samples. Plotting the complexity of the two methods against increasing sample and features size we get

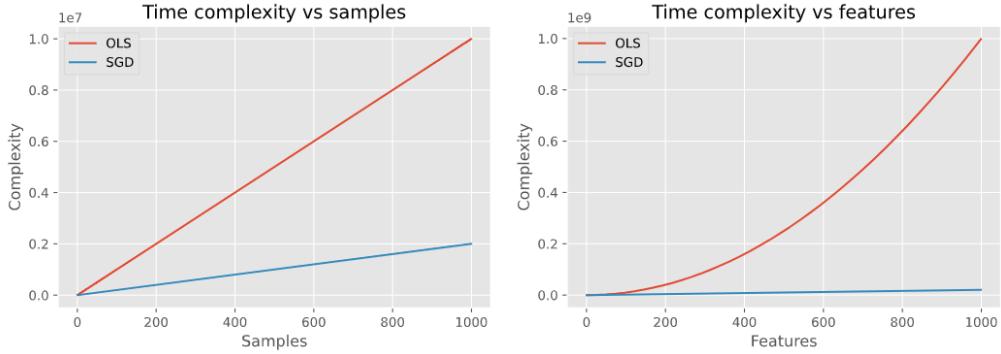


Figure 10.1: Complexities of the two methods.

We see that the analytical solution does not handle increasing samples and especially not increasing features due to the exponential growth in complexity as features increase. While SGD is much cheaper and robust. For big data tasks, using gradient descent is almost always the least demanding way of getting a solution to the problem.

### 10.3 Notation

- $m$  = The number of training examples
- $x$  = The input variables / features
- $y$  = The output variable/"target" variables
- $(x_i, y_i)$  = A specific example ( $i_{th}$  training example)

Passing the features into a learning algorithm that outputs a function (denoted  $h$  = hypothesis), resulting in the function:

$$h_\theta(x) = \theta_0 + \theta_1 x$$

where  $\theta_i$  are parameters,  $\theta_0$  is the zero condition, and  $\theta_1$  is the gradient.

### 10.4 Cost Function

Recall from the decision tree section on decision trees and regression trees. There we somehow need to mathematically describe information and how much information the model is able to explain. In regression trees we used variance. Since a model that contains a lot of information about the true state of nature will have a low variance in its predictions. A cost function that lets us figure out how to fit the best linear prediction line is needed. We want to solve a minimization problem where we minimize  $(h_\theta(x) - y)^2$ .

The most common cost function is the mean squared error (MSE):

$$J(\theta_0, \theta_1) = \frac{1}{m} \sum_{i=1}^m (h_\theta(x_i) - y_i)^2$$

Note that multiplying the cost function by  $\frac{1}{2}$  does not change the location of the minima, which is why we use it to form the following cost function:

One half mean squared error:

$$J(\theta_0, \theta_1) = \frac{1}{2m} \sum_{i=1}^m (h_\theta(x_i) - y_i)^2$$

The cost function determines the parameters, and the values associated with the parameters determine how the hypothesis behaves. Different values generate different hypotheses.

The MSE cost function is convex.

Finding the global minima in linear regression can be done with a gradient descent algorithm.

#### 10.4.1 Cost Function for Multiple Variables

$$J(\theta_0, \theta_1, \dots, \theta_n) = \frac{1}{2m} \sum_{i=1}^m (h_\theta(x_i) - y_i)^2$$

### 10.5 Batch Gradient Descent Algorithm (BGD)

- In each step you look at all the training data

#### Progress

1. Start with initial guesses, i.e.  $(0, 0)$
2. Keep changing  $\theta_0$  and  $\theta_1$  a little bit to reduce  $J(\theta_0, \theta_1)$
3. Each time the parameters change, select the gradient which reduces  $J(\theta_0, \theta_1)$  the most
4. Repeat until we converge to a local/global minima

Different starting points will often result in different minimas.

## Formal progress

- Do the following until convergence:
  - $\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$
  - For  $j = 0$  and  $j = 1$  in this example.
- $\alpha$  is the learning rate
- $\alpha$  controls how aggressive the gradient descent is

"For  $j = 0$  and  $j = 1$ " means that we update both parameters simultaneously. This is done by first solving the derivative for  $\theta_0$  and storing it in a temporary variable. Do the same for  $\theta_1$ , and then update the original  $\theta_j$ -values.

## Partial Derivatives

$$\begin{aligned}\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1) &= \frac{\partial}{\partial \theta_j} \frac{1}{2m} \sum_{i=1}^m (\theta_0 + \theta_1 x_i - y_i)^2 \\ \frac{\partial}{\partial \theta_0} J(\theta_0, \theta_1) &= \frac{1}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x_i - y_i) * 1 \\ \frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) &= \frac{1}{m} \sum_{i=1}^m (\theta_0 + \theta_1 x_i - y_i) x_i^{(1)} \\ \frac{\partial}{\partial \theta_j} J(\theta_0, \dots, \theta_n) &= \frac{1}{m} \sum_{i=1}^m (\theta_0 + \dots + \theta_n x_i - y_i) x_i^{(j)}\end{aligned}$$

### 10.5.1 Gradient Descent in Practice

- Feature Scaling (normalize)
  - Problems with multiple features should be scaled to a more even scale across the features.
  - One common way is to use the mean to scale all data into the range  $[-1, 1]$ .
  - Try to create a range between  $[-3, 3]$  and  $[-\frac{1}{3}, \frac{1}{3}]$ .
  - This is done by  $x_i = \frac{x_i - \hat{x}}{\max(x) - \min(x)}$
- Running gradient descent on this kind of cost function can take a long time to find the global minima.

## 10.6 Practical Tips

- Plot  $\min(J(\theta))$  with the number of iterations to clearly illustrate the convergence.
- Start with a low learning rate, and gradually increase it. It is normal to go for roughly treefold increments (multiply by 3).
- We could also use a polynomial regression on the form  $(\theta_0 + \theta_1x + \theta_2x^2)$ .

# 11 Advanced Classifiers (Logistic Regression)

## 11.1 The Logistic Classifier

The logistic regression model is a binary classification problem. Linear regression for binary classification is not a viable option as the decision boundary will not separate the two categories correctly because of the nature of the mean square error. The classifier should output either 1 or 0, depending on the data. Where the classifier outputs the probability of the class given the observations. The problem is that a regression model has a domain of  $(-\infty, \infty)$  and we want to somehow map this to the probability of observing a class which has the domain  $(0, 1)$ . To do this we introduce odds:

$$\text{odds} = \frac{p}{1-p}$$

The odds is the ratio of successes to failures. Colloquially we talk about odds all the time. Statements like *For every 4 people 1 are....* This is in an odds of 4 : 1 or just 4. The probability on the other hand for the same statement is *1 out of 5 are...* or *There is a one in fifth chance of....* Odds have the domain of  $(0, \infty)$ , which is closer to that of a regression model but still not quite there. Taking the log of the odds

$$\ell = \log_b \frac{p}{1-p}$$

we map the odds to the domain  $(-\infty, \infty)$ . Now, we assume a linear relationship between the feature and the log-odds

$$\ell = \log_b \frac{p}{1-p} = \theta^T x$$

And we can now recover the odds by exponentiation the log odds

$$\frac{p}{1-p} = b^{\theta^T x}$$

And by algebraic manipulation we get

$$p = \frac{1}{1 + b^{-\theta^T x}}$$

In most litterature, the classification hypothesis representation used for logistic regression uses  $b = e$ :

$$h_{\theta}(x) = g(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$$

This is the sigmoid function (the logistic function).

The function is used as such:

$$\begin{cases} 1 & \text{if } h_{\theta}(x) > 0.5 \\ 0 & \text{otherwise} \end{cases} \quad (11.1)$$

### 11.1.1 Logistic Classifier for Higher-Order Terms

As in polynomial regression, the logistic classifier can be used for higher order terms by adding higher order terms. I.e.  $g(\theta_0 + \theta_1 x_1 + \theta_3 x_1^2 + \theta_4 x_2^2)$

## 11.2 Problems with the Linear Regression Cost Function

The mean square error function results in a convex PDF when given it is given linear values. This is not the case for logistic regression. This means that the MSE would most likely only find a local minimum, not a global one.

## 11.3 Logistic Regression Cost Function

$$Cost(h_{\theta}(x), y) = \begin{cases} -\ln(h_{\theta}(x)) & \text{if } y = 1 \\ -\ln(1 - h_{\theta}(x)) & \text{if } y = 0 \end{cases} \quad (11.2)$$

This can be rewritten into a single function:

$$Cost(h_{\theta}(x), y) = -y \ln(h_{\theta}(x)) - (1 - y) \ln(1 - h_{\theta}(x)) \quad (11.3)$$

## 11.4 Process

The process forwards is the same as in the linear regression chapter.

## 11.5 Multiclass Classifier for Logistic Regression

Extending the logistic regression from a binary classifier to a multiclass classifier can be done in a "one vs. all" classification.

This means that the algorithm is conducted multiple times, each time changing which class is the positive class (where all the other classes are negative).

# 12 Classification (Regularization)

## 12.1 Addressing Overfitting

Multiple strategies can be used to check if overfitting occurs:

- Plot the hypothesis to check for overfitting. Might not always work.
- Reduce the number of features
- Regularization

## 12.2 Regularization

Regularization is the process of adding information in order to solve an ill-posed problem or to prevent overfitting. Normally in machine learning regularization is done by introducing a regularization term  $R(f)$  to the loss function

$$\min_f \sum_{i=1}^n V(f(x_i), y_i) + \lambda R(f)$$

Where  $V$  is the underlying loss function and  $R(f)$  is typically chosen to impose a penalty on the complexity of  $f$ . Regularization in one way imposes occam's razor on the solution, the principle that the simpler explanation (model) is usually the best. Another perspective is the Bayesian one where prior knowledge is applied to the model parameters.

- Small values for parameters correspond to a simpler hypothesis (you effectively get rid of some of the terms).
- A simpler hypothesis is less prone to overfitting.

### 12.2.1 Cost function optimization

We can penalize some of the higher-order  $\theta$  parameters and make them very small:

$$\min \frac{1}{2m} \sum_{i=1}^m (h_\theta(x_i) - y_i)^2 + 1000\theta_3^2 + 1000\theta_4^2$$

### 12.2.2 Regularization on features

Unlike in a polynomial, we don't know which parameters are the high-order terms. The solution for this is to penalize all the parameters.

By convention, we don't penalize  $\theta_0$ , but all other parameters, with the regularization parameter  $\lambda$ .

$$J(\theta) = \frac{1}{2m} \left[ \sum_{i=1}^m (h_\theta(x_i) - y_i)^2 + \lambda \sum_{j=1}^n \theta_j^2 \right]$$

### 12.2.3 Regularized Gradient Descent

$$\theta_j := \theta_j - \alpha \left[ \frac{1}{m} \sum_{i=1}^m (h_\theta(x_i) - y_i) x_i^{(j)} + \frac{\lambda}{m} \theta_j \right]$$

$$\theta_j := \theta_j \left( 1 - \alpha \frac{\lambda}{m} \right) - \alpha \frac{1}{m} \sum_{i=1}^m (h_\theta(x_i) - y_i) x_i^{(j)}$$

Given a typical small learning rate  $\lambda$  and a large number of terms  $m$ , we see that  $\theta_j$  is multiplied by a value close to 1 (around 0.95 – 0.99).

# 13 Deep Learning (Neural Network)

## 13.1 Achievements of Deep Learning

Deep Learning has had an explosion in applications and research and development for the last decade. These applications include:

- Automatic speech recognition
- Image recognition
- Visual art processing
- Natural language processing
- Drug discovery and toxicology
- Customer relationship management
- Recommendation systems
- Bioinformatics

The theoretical foundations of the field is old (mid 19th century), but the playground for these algorithms has just now arrived. These include large datasets, computational hardware and software.

## 13.2 Comparison with traditional machine learning

In traditional machine learning development. One needs domain knowledge for developing good models. Domain knowledge let's you select good features and good features give good models. One example could be a certain visual feature in a certain kind of biomedical image. This field is called **feature engineering**.

## 13.3 Feature Learning

Feature Learning, also known as **Representation Learning** is a set of techniques that allow systems to automatically discover the representation needed for feature detection or classification. Feature learning methods let us replace the manual feature engineering that is done in traditional machine learning development. A lot of deep learning architectures for representation learning have been researched and published in the last decade.

## 13.4 Motivations for deep learning

Deep Learning let's us model nonlinear decision boundaries by introducing nonlinearities in the activation functions and deep architectures. This means that deep learning is especially fit for problems that are too complex for linear methods. One could question whether models like logistic regression could be used with polynomial decision boundaries to achieve the same thing. The problem with using regression is that it achieves this by introducing polynomial features. The number of features the model must take into account is then

$$\sum_{i=1}^k \binom{k+i-1}{i} = \binom{k+n}{n} - 1$$

where  $n$  is the polynomial degree that you want the model to incorporate and  $k$  is the number of features/variables. [Wolfgang \(Wolfgang\)](#) For 100 features, introducing  $k = 2$  gives over 5000 features. This is not feasible.

## 13.5 Artificial Neuron

- Feed input via input nodes
- Logistic unit does some computation
- Sends output

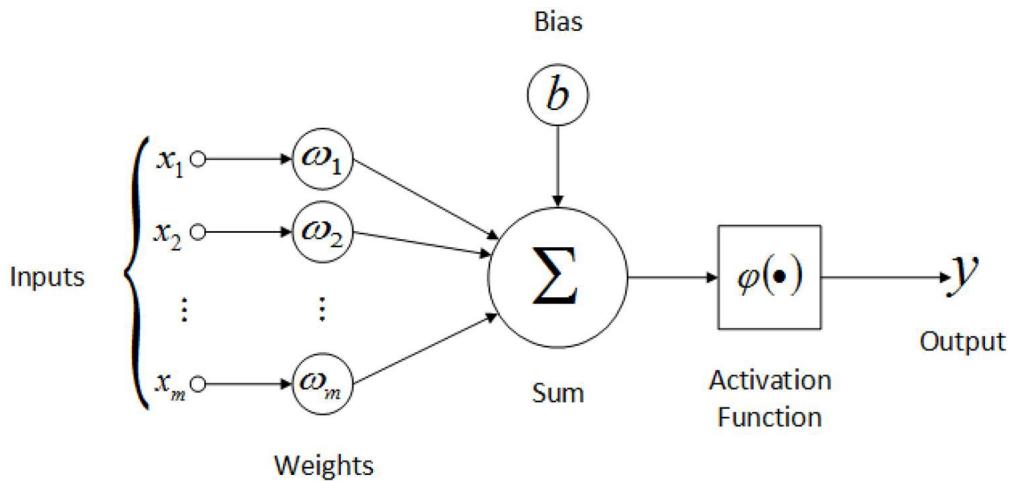


Figure 13.1: Artificial Neuron

The activation function is typically the sigmoid function, a hyperbolic tangent, or a rectified linear unit (ReLU). They must be a non-linear function because several layers of

linear activation functions still yield a linear decision boundary. Deep layers of non-linear activations yield complex decision boundaries.

## 13.6 Notations

- $a_i^{(j)}$  - Activation of unit  $i$  in layer  $j$  (the output of the node)
- $\theta^{(j)}$  - Matrix of parameters (controlling the activation from one layer to the next)
- $g(\theta^T x)$  - The activation function

## 13.7 Multiclass Classification

- Given  $N$  classes:
  - Build a neural network with  $N$  output units
  - Use one-hot encoding to encode the output as an array of  $N - 1$  zeros and one 1.

## 13.8 Cost function for Neural Networks

The cost function can generate  $k$  outputs, meaning that the sigmoid function (or any other cost functions) returns a  $k$  dimensional vector.

The cost function is combined by two parts.

The first part finds the mean of the sum of each training sample  $m$ , over the sum of each class  $k$ . All classes has a "one-vs-all" comparison. This gives the following expression:

$$-\frac{1}{m} \left[ \sum_{i=1}^m \sum_{k=1}^K y_k^{(i)} \log \left( h_\Theta(x^{(i)}) \right)_k + (1 - y_k^{(i)}) \log \left( 1 - (h_\Theta(x^{(i)}))_k \right) \right]$$

The second part is the regularization term. In this part, we sum all layers  $L - 1$ , over all units in each layer  $s_t$ , over all the input layers  $j$ :

$$\frac{\lambda}{2m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_t} \sum_{j=1}^{s_l+1} (\Theta_{ji}^{(l)})^2$$

## 13.9 How to minimise the cost function

To minimise the cost function, we need to change the weights and biases of the neural network such that this cost function is decreased. This is achieved using calculus and gradient descent. Recall from calculus that the gradient can be interpreted as the direction and rate of fastest increase. In gradient descent one therefore wish to iteratively go opposite to the gradient to reach a minima. When performing gradient, convergence

to a local minima is guaranteed. When the cost function is convex, all local minima is also global minima. The nature of the cost function is therefore important to consider. Global optimisation is a field of mathematics concerning this and there exists many deterministic and stochastic methods to achieve this.

## 13.10 Gradient Descent

Here, we will focus on gradient descent as a way to achieve minima. Consider the following algorithm:

---

**Algorithm 1:** Gradient Descent

---

**Result:** Local og global minima

Initialise  $\theta \sim N(0, \sigma^2)$ ,  $\epsilon$ ,  $\alpha$ .

**while**  $\Delta J > \epsilon$  **do**

Compute gradient  $\frac{\partial J(\theta)}{\partial \theta}$ ;

Update weights  $\theta = \theta - \alpha \frac{\partial J(\theta)}{\partial \theta}$ ;

**end**

Return  $\theta$

---

This is a general algorithm for the intuition behind gradient descent. But how do we achieve this for the multivariate case with several layers of activation? Let us introduce **backpropagation**

## 13.11 Backpropagation

When calculating partial derivatives for a neural network. One starts at the output layer and calculate the derivatives backwards. One begins by calculating the error between the activations of the output and the true state of nature.

$$\delta^{(L)} = a^{(L)} - y$$

then compute

$$\delta^{(L-1)} = (\theta^{L-1})^T \delta^{(L)} \cdot g'(z^{(L-1)})$$

and do this until we reach layer 1.

## 13.12 Hyperparameters and model enginnering

After understanding gradient descent, backpropagation, activation function etc, one is ready to start to engineer neural networks for ones needs. But there is one problem, the hyperparameters. In this section some of these hyperparameters and challenges will be discussed.

### 13.12.1 Loss Functions in reality

These are very seldom convex. One may be able to change the loss function to make it more convex, but this may not work. Evolutionary and stochastic algorithms that explore the loss function space may help. Selecting losses and ensuring that these are well behaved is a challenge when creating neural networks.

### 13.12.2 Initialisation of weights

Weights must be initialised and these must be initialised using a gaussian distribution with mean at 0.

### 13.12.3 Learning Rate

Learning rate is a model hyperparameter that must be considered. If learning rate is too low, the model does not explore the cost function space and converges in local minima. If it is too large, it may diverge and cause the exploding gradient problem. Learning rates may be changed over time and so on.

### 13.12.4 Mini-batches

Instead of computing gradients for individual samples, batches may be used instead. This gives a smoother convergence and allows for larger learning rates. This also allows for parallelising computation!

### 13.12.5 Overfitting and regularisation

Neural networks have a quite large hypothesis space and capacity. This allows them to quickly overfit. Large amounts of data is needed to make the model generalisable. Regularisation may also help by introducing a penalty for complexity. Dropout is a much used way to regularise neural networks. It simply removes nodes from the neural network during a training step and forces the model to learn using a smaller capacity.

Early stopping is also an alternative, by using learning curves one should stop the training as soon as one observes that the accuracy of the testing set is getting worse compared to the training accuracy.

# 14 Convolutional Neural Network (CNN)

## 14.1 History of CNN's

CNNs are a special kind of architecture that was popularised in the 2010s. It is vaguely based on biological processes and visual cortices from biology. These kinds of networks are most commonly applied to visual imagery. They are also applicable to other kinds of data. A simple rule of thumb is that data where if swapping columns of the data matrix removes the information contained in the data, convolutional neural networks may be used.

## 14.2 Convolution Layer

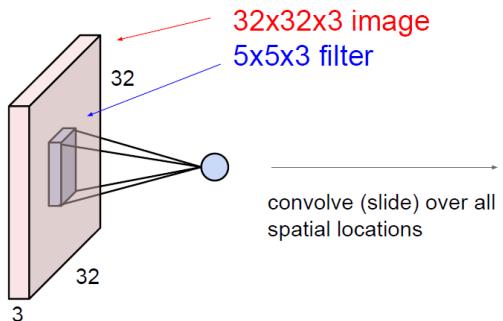


Figure 14.1: Convolution layer

The central concept of CNNs (it is even in its name) is the convolution. A convolution can be thought of as passing a filter or kernel through the image to average it out. The selection of kernel determines what visual features are extracted from the image. Using multiple filters to get different features is not uncommon.

In many convolutional neural networks found in publications, these typically are very deep, have many different convolutions and pooling layers and end in a fully connected layer. The layers before the fully connected layer are there for simply extracting features and preprocessing the data. The fully connected layer is there for inference.

It is not uncommon to use existing CNN architectures from publications and remove the fully connected layer at the end to suit it for your own needs. In those cases one

assume that the existing CNN architecture is able to collect high quality features for ones problem. This saves time on training the CNN part of the network and one can focus on training the inference layer at the end.

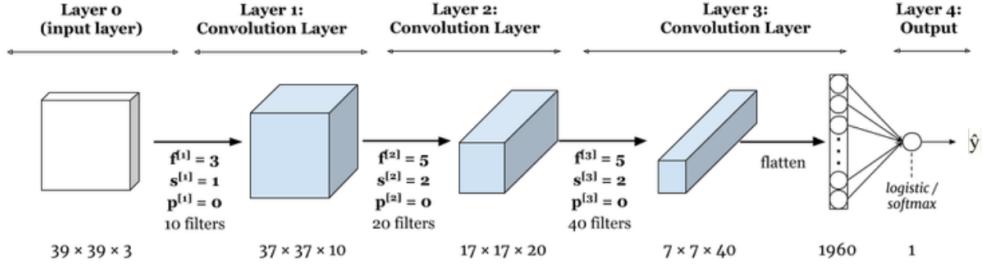


Figure 14.2: CNN architecture

### 14.3 Number of weights after convolution layers

When working with CNNs and Neural Networks in general it is regular to talk about parameters. Parameters are weights in the neural network and is learned through backpropagation. Below is a list of the different layers and their parameters. The numbers and calculations are examples.

#### 14.3.1 Size of output tensor for a conv layer

Let us define

$$O = \text{Size (width) of output image}$$

$$I = \text{Size (width) of input image}$$

$$K = \text{Size (width) of the kernels used in conv layer}$$

$$N = \text{Number of kernels}$$

$$S = \text{Stride of the conv layer}$$

$$P = \text{Padding}$$

The size  $O$  is given Bayes

$$O = \frac{I - K + 2P}{S} + 1 \quad (14.1)$$

**Example:** Let's say we have a image of size  $32 \times 32 \times 3$ , 5 kernels  $5 \times 5 \times 3$ , stride 1 and padding 0 we get

$$O = \frac{32 - 5 - 0}{1} + 1 = 28$$

the image is then  $28 \times 28 \times 5$

### 14.3.2 Size of output of maxpool layer

$O$  = Size (width) of output image

$I$  = Size (width) of input image

$S$  = Stride of the convolution operation

$P$  = Pool size

The output size  $O$  is then given by

$$O = \frac{I - P}{S} + 1$$

### 14.3.3 Number of parameters in a Conv layer

$B$  = Number of biases in conv layer

$P$  = Number of parameters of conv layer

$K$  = Size of kernels used in conv layer

$N$  = Number of kernels

$C$  = Number of channels of the input image

The parameters is then calculated as

$$P = (K^2 \times C \times N) + B$$

Note:  $B = N$

**Example:** Assume that we have the same kernels as above then we get  $P = 28^2 \times 3 \times 5 + 5 = 380$

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