

Machine Learning FS2019

<https://github.com/taneher/HSLU/tree/master/FS19/ML>

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1 Introduction

There are two popular definitions of Machine Learning:

“Field of study that gives computers the ability to learn without being explicitly programmed” (Arthur Samuel, IBM, 1959)

“A computer program is said to learn from experience E with respect to some task T and some performance measure P , if its performance on T , as measured by P , improves with experience E ” (Tom Mitchell, 1998)

So summarizing these two quotes, it can be said, that machine learning is defined as **the process in which machines learn something (mostly) on their own**.

1.1 Disciplines

There are different disciplines in machine learning:

Supervised Learning: The algorithm is given **labeled training data** and learns to **predict the labels** of yet unseen examples.

Unsupervised Learning: The algorithm is given **unlabeled data** and **creates labels by itself** based on the structure of the given data

Semi-Supervised Learning: A **mixture** of supervised and unsupervised learning. This approach is usually chosen if there is only **very little labeled test data**

Reinforcement Learning: No data is available, but the algorithm is **being rewarded**. The algorithm searches the ideal behaviour that maximizes its reward (Not subject of this lecture)

These classifications can be subdivided even more:

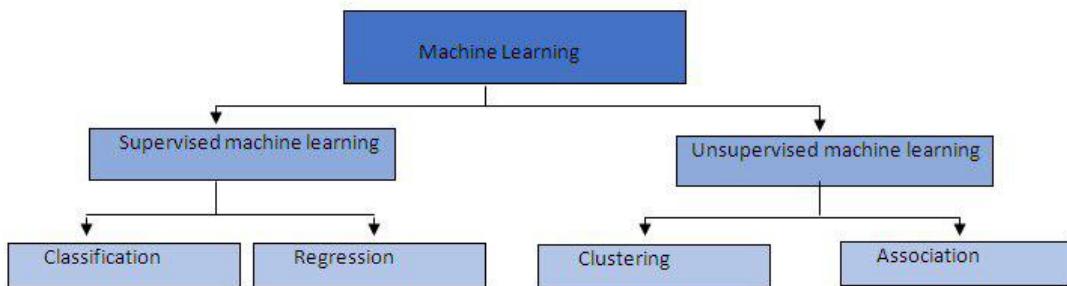


Figure 1.1: Distinction between supervised and unsupervised learning

The main difference between **classification** and **regression** is that when using classification, the result is **categorical**, whereas regression returns **numerical** results.

Clustering is similar to classification. However, while classification algorithms sort the given data into given groups, clustering algorithms determine these groups **by themselves**. This means, you can give a clustering algorithm a seemingly random dataset and the algorithm finds some kind of structure in it.

2 Data Quality

Data is categorized into **numerical** and **categorical** data.

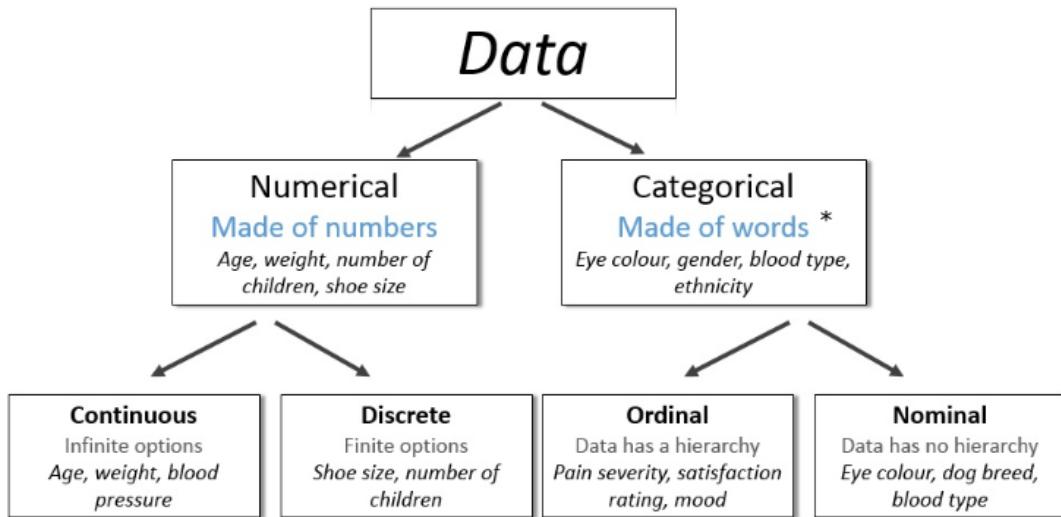


Figure 2.1: Classification of Data

Before any machine learning can take place, the quality of the given data has to be assessed and in some cases improved. Because every prediction made by machine learning algorithms is shit if the data quality is shit.

There are many reasons why the data quality could be poor:

- Ill-designed, inadequate or inconsistent data formats
- Programming errors or technical issues (e.g. sensor outage)
- Data decay (e.g. outdated e-mail addresses)
- Poorly designed data entry forms (e.g. data fields without verification)
- Human errors in data export or data pre-processing
- Deliberate errors and false information (e.g. due to privacy concerns everybody is called Hans Muster and lives at Musterstrasse 123)

2.1 Data Quality Assessment

Before even starting to assess the data-quality, it is seldomly a bad idea to **clean** the data first.

1. Identify and remove duplicates
2. Replace null-values (do not delete them because that might falsify the mean and median of the data)
3. Make data formats more machine-friendly (so-called *data-wrangling* e.g. store the gender as boolean)

If you change anything from the original data set, you should always

- Document all the changes
- Use a SVN (e.g. git)
- Let the data provider know that his data quality is shit (maybe they'll improve in the future)
- Investigate the origins of the poor data quality

2.2 Approaches to Data Quality Assessment

Identify data sources and their trustworthiness

Interpret statical key figures: See following sections

Visualize selected portions of the data: e.g. with Pair Plots (See Abb. 2.2)

Manually check data ranges Negative Salaries, People more than 200 years old...

Validate plausibility of attribute correlation: e.g. are mileage and number of seats in a core correlated? Can one of the columns be removed for redundancy?

Measure data redundancy: Can certain columns be removed due to not adding any real value to the data

Check for anomalies in syntax and semantics: Outliers can really distort a dataset and render the whole algorithm useless. Can be prevented by e.g. normalization of the data or removal of the outlier

Replace NULL Values and remove duplicate values

There are different ways to cope with NULL variables, but they have to be addressed, as most machine learning algorithms do not play well with them.

- Delete all rows with NULL values
Might be the easiest way if you have loads of data
- Fill in the missing values manually (e.g. from other sources)
Might be the hardest way if you have loads of data
- Fill in a global constant like N/A, UNKNOWN
- Use a measure for central tendency
e.g. take the mean if your data is symmetric or take the median if its skewed
- Use a measure for central tendency per class
e.g. take different values for healthy and sick people
- Use e.g Regression to 'guess' the missing values

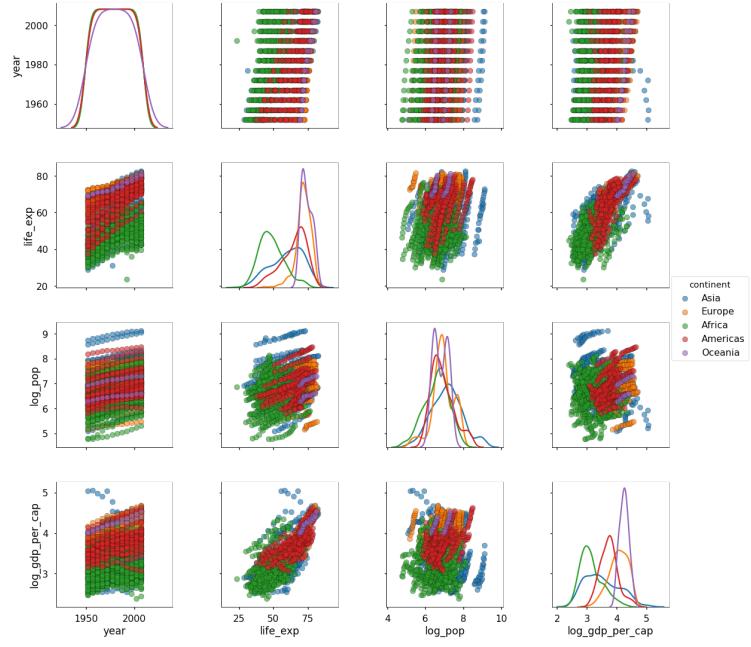


Figure 2.2: Visualisation of Data with Pair Plots

2.3 Statistical Key Figures

These figures can give you a rough overview about the whereabouts of your data-magnitude.

2.3.1 Central Tendency

Mean

This is the average in a set of numeric data. You add all data and divide it by the number of data points

$$\mu_x = \frac{1}{n} \sum_{i=1}^n x_i \quad (1)$$

Mode

This is the value that occurs the most in a given set of data

Median

This is the middlemost value of a sorted set of data. In contrast to the Mean, the Median can give information concerning the distribution of the data.

Given a dataset of 1, 2, 3, 4, 5, the median and mean are both 3. However, if we have 1, 2, 3, 1000, 10000, the mean is 2201.2 whereas the mean is still 3

2.3.2 Skewness

All of these values can give information concerning the data's **skewness**

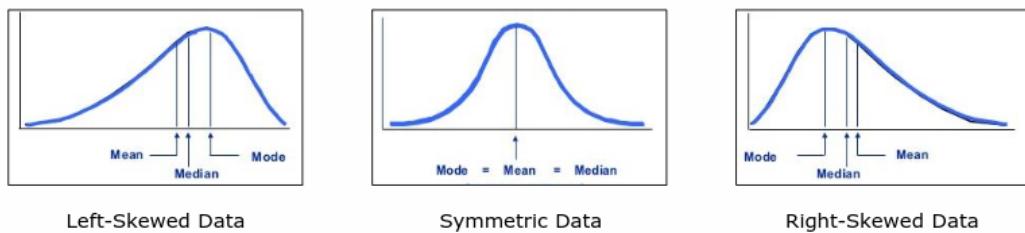


Figure 2.3: Skewness of data

$\text{Mean} - \text{Mode} > 0 \rightarrow$ Negative skewness / Left-skewed data

$\text{Mean} - \text{Mode} = 0 \rightarrow$ Symmetric Data

$\text{Mean} - \text{Mode} < 0 \rightarrow$ Positive skewness / Right-skewed data

2.3.3 Quartile & Interquartile Range (IQR)

The three quartiles divide your data into four equal-sized, consecutive subsets.

To calculate Q_1 , take the median of your data and then again the median of the left half of the data.

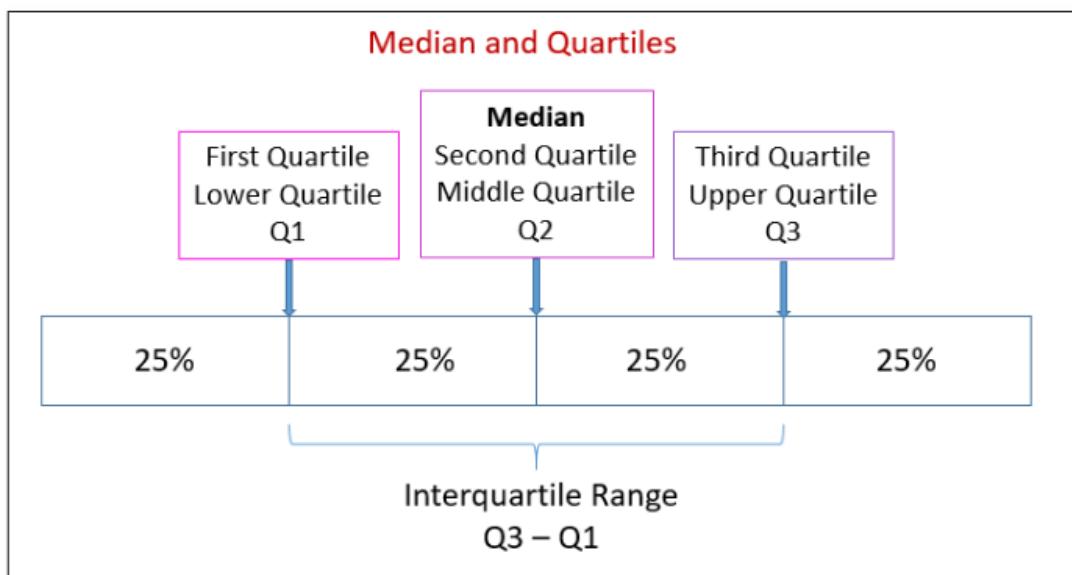


Figure 2.4: Quartiles of a dataset

2.3.4 Five Number Summary

With this method, you can get a pretty good overview of your data. The **Five Number Summary** of a dataset consists of:

- Median Q2
- Quartiles Q1 and Q2
- Smallest individual Value
- Largest individual Value

```

1 import numpy as np
2 import panas as pd
3
4 s = pd.Series(np.random.rand(100))
5 s.describe()

```

Listing 2.1: Five Number Summary in Python

1	mean	0.524559
2	std	0.285565
3	min	0.003933
4	25%	0.298367
5	50%	0.530632
6	75%	0.765907
7	max	0.993293
8		dtype: float64

Listing 2.2: Output

2.3.5 Boxplot

This plot is a **visual representation of the five number summary** and can also give information on potential outliers.

Values $1.5 \cdot IQR$ above the 3rd or below the 1st Quartile can be considered outliers and are displayed with small circles.

2.3.6 Variance

The variance shows **how much the values are spread on average**. This is measured by squaring the sum of all deviations from the mean

$$\frac{1}{1-n} \sum_{i=1}^n (x_i - \mu_x)^2 \quad (2)$$

The standard deviation σ is calculated as $\sqrt{\text{variance}}$

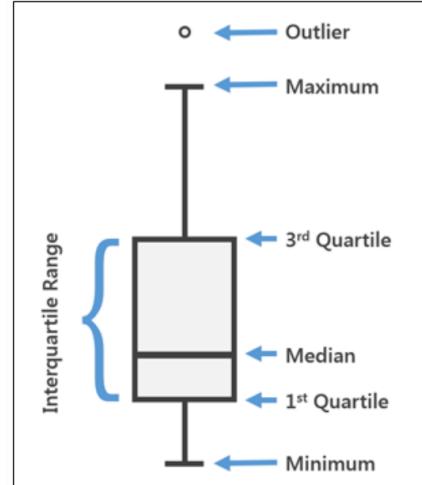


Figure 2.5: Boxplot

2.3.7 Covariance

The covariance is used to determine whether two variables are **connected** to each other.

If both variables are on the same side of the mean, the variance is **positive**, the variables are probably connected. Meaning if the value of one variable is rising, the other one will most likely rise as well.

If one is above and one is below the mean, the variance is **negative**, the variables are most likely **inversely connected** to each other. Meaning if the value of one variable is rising, the other is most likely falling.

If the variables are **independent** from each other, the covariance is zero, as they both cancel each other out.

$$Cov(x, y) = \frac{1}{1-n} \sum_{i=1}^n (x_i - \mu_x)(y_i - \mu_y) \quad (3)$$

The **covariance matrix** shows the covariance from all X with all Y . As $Cov(x, x) = Var(x)$, the covariance matrix has the variance of X in its diagonal

2.3.8 Pearson Correlation

Both the covariance and the variance are connected to the scale of the dataset, so the covariance of $X = [1, 2, 3, 4, 5]/Y = [6, 7, 8, 9, 10]$ is 2.5, whereas the covariance of $X = [1000, 2000, 3000, 4000, 5000]/Y = [6000, 7000, 8000, 9000, 10000]$ is 2'500'000'000. However, the Pearson Correlation is 1 in both examples.

$$\rho(X, Y) = \frac{Cov(X, Y)}{\sigma_x \sigma_y} = \frac{\frac{1}{1-n} \sum_{i=1}^n (x_i - \mu_x)(y_i - \mu_y)}{\sqrt{\frac{1}{1-n} \sum_{i=1}^n (x_i - \mu_x)^2} \cdot \sqrt{\frac{1}{1-n} \sum_{i=1}^n (y_i - \mu_y)^2}} \quad (4)$$

The Pearson Correlation is always between 1 and -1.

1 means the data is perfectly correlated, whereas -1 means that the data is perfectly incorrelated

2.4 Normalization

It is immensely important that all data is normalized before we run a machine learning algorithm over it. Considering the data in figure 3.2, 'Mileage' and 'Price' are in a completely different scale. If the mileage of the first shown car goes up 500 miles, it's not really a big deal. However, a price increase by 500 would double the car's price.

Such differently scaled data can (and will) falsify the result of every machine learning algorithm you could find. Therefore, **normalization is really important**.

There are two popular normalization approaches: The Min-Max and the Z-Score normalization.

Min-Max normalization

All data is condensed to a value between 0 and 1. The smallest value becomes 0 and the largest one becomes 1.

$$x \rightarrow \frac{x - \min_x}{\max_x - \min_x} \quad (5)$$

Z-Score Normalization

The dataset is transformed in such a way, that the mean becomes 0 (so-called *mean-centering*) and the standard deviation is 1

$$x \rightarrow \frac{x - \mu_x}{\sigma_x} \quad (6)$$

3 Geometry of Data

3.1 Feature Engineering

Sometimes, data has to be modified to be better accessible/processable for machine learning algorithms. These algorithmus can work the best with simple numbers, so that's the data we should be striving for:

Free	Date	Time	Free	Hour	Minute	Year	Month	Day
283	2015-09-27 00:00:00	06:26:46	283	6	26	2015	9	27
282	2015-09-11 00:00:00	05:18:55	282	5	18	2015	9	11
280	2015-09-20 00:00:00	21:14:49	280	21	14	2015	9	20
283	2015-09-25 00:00:00	01:22:47	283	1	22	2015	9	25
0	2015-10-15 00:00:00	08:12:35	0	8	12	2015	10	15
0	2015-10-27 00:00:00	10:02:28	0	10	2	2015	10	27
281	2015-09-13 00:00:00	12:20:54	281	12	20	2015	9	13
168	2015-10-14 00:00:00	08:07:35	168	8	7	2015	10	14
283	2015-09-25 00:00:00	05:42:47	283	5	42	2015	9	25
283	2015-09-18 00:00:00	22:57:50	283	22	57	2015	9	18
279	2015-09-10 00:00:00	20:26:55	279	20	26	2015	9	10
279	2015-10-04 00:00:00	18:37:40	279	18	37	2015	10	4
84	2015-09-17 00:00:00	17:17:51	84	17	17	2015	9	17
86	2015-09-11 00:00:00	08:28:55	86	8	28	2015	9	11
3	2015-10-26 00:00:00	13:51:28	3	13	51	2015	10	26
281	2015-09-30 00:00:00	00:44:44	281	0	44	2015	9	30
252	2015-10-15 00:00:00	07:19:35	252	7	19	2015	10	15
280	2015-09-15 00:00:00	00:41:52	280	0	41	2015	9	15
282	2015-09-09 00:00:00	06:05:56	282	6	5	2015	9	9
0	2015-10-29 00:00:00	12:16:27	0	12	16	2015	10	29

Figure 3.1: Turn 'complicated' data into easier data for better results

3.2 Vector Space Model

As described before, machine learning algorithms work best with **numeric** data. However, the real world isn't that easy and mostly throws categorical data at you. Therefore, you have to convert categorical data to numerical data.

This transformed data can also be visualized in a coordinate system and we can do math with it.

Name	Price	Mileage	Color	Name	Price	Mileage	braun	gelb	grau	grün	rot	schwarz	silber	weiss
ALFA ROMEO 145 1.4 TS 16V L	500	187000	schwarz	ALFA ROMEO 145 1.4 TS 16V L	500	187000	0	0	0	0	0	1	0	0
ALFA ROMEO 145 1.8 TS 16V L	2600	182510	rot	ALFA ROMEO 145 1.8 TS 16V L	2600	182510	0	0	0	1	0	0	0	0
ALFA ROMEO 145 1.9 JTD	3500	116000	grau	ALFA ROMEO 145 1.9 JTD	3500	116000	0	0	1	0	0	0	0	0
ALFA ROMEO 145 2.0 TS 16V Quadrifog.	4900	181000	rot	ALFA ROMEO 145 2.0 TS 16V Quadrifog.	4900	181000	0	0	0	0	1	0	0	0
ALFA ROMEO 145 2.0 TS 16V Quadrifog.	800	121000	rot	ALFA ROMEO 145 2.0 TS 16V Quadrifog.	800	121000	0	0	0	0	1	0	0	0
ALFA ROMEO 145 2.0 TS 16V Quadrifog.	3200	156000	schwarz	ALFA ROMEO 145 2.0 TS 16V Quadrifog.	3200	156000	0	0	0	0	0	1	0	0
ALFA ROMEO 145 2.0 Ti 16V	770	158000	grau	ALFA ROMEO 145 2.0 Ti 16V	770	158000	0	0	1	0	0	0	0	0
ALFA ROMEO 145 2.0 Ti 16V	1200	119000	rot	ALFA ROMEO 145 2.0 Ti 16V	1200	119000	0	0	0	0	1	0	0	0
ALFA ROMEO 146 2.0 Ti 16V	4900	166000	schwarz	ALFA ROMEO 146 2.0 Ti 16V	4900	166000	0	0	0	0	0	1	0	0
ALFA ROMEO 146 2.0 Ti 16V	4900	102000	silber	ALFA ROMEO 146 2.0 Ti 16V	4900	102000	0	0	0	0	0	0	1	0
ALFA ROMEO 146 2.0 Ti 16V Kit Sport	5800	165000	schwarz	ALFA ROMEO 146 2.0 Ti 16V Kit Sport	5800	165000	0	0	0	0	0	1	0	0
ALFA ROMEO 147 1.6 16V Blackline	11500	46230	braun	ALFA ROMEO 147 1.6 16V Blackline	11500	46230	1	0	0	0	0	0	0	0

Figure 3.2: Turn categorical data into numerical data with the vector space model

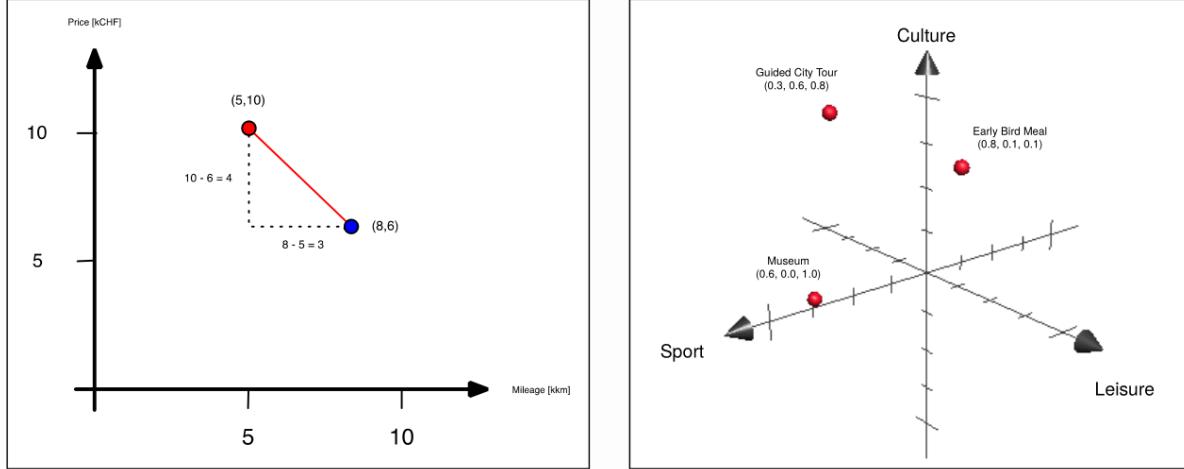


Figure 3.3: Transformed into vector space, data points can be interpreted as geometric points

3.3 Similarity of Data

The math we want to do is not even overly complicated: We just want to measure the distance between different points. Because **the smaller the distance between two points, the more similar they are**.

3.3.1 Euclidean Distance

The distance between two points is most easily calculated using the **euclidean distance**:

$$dist(X, Y) = \sqrt{\sum_{i=1}^n (x_i - y_i)^2} \quad (7)$$

So the distance between the points (5/10) and (8/6) can be calculated as

$$\sqrt{(5 - 8)^2 + (10 - 6)^2} \quad (8)$$

$$\sqrt{-3^2 + 4^2} \quad (9)$$

$$\sqrt{9 + 16} \quad (10)$$

$$\sqrt{25} = 5 \quad (11)$$

3.3.2 Cosine Similarity

If you want to compare two points that appear to be on a line (Pearson Correlation close to 1), but the euclidean distance is high, then the cosine similarity is probably pretty low.

The cosine similarity looks at the **angle** between point A and point B. However, it does also take the euclidean distance into consideration.

The cosine similarity is essentially just the scalar product of the two points.

$$sim(X, Y) = \frac{\sum_{i=1}^n x_i y_i}{\sqrt{\sum_{i=1}^n x_i^2} \sqrt{\sum_{i=1}^n y_i^2}} \quad (12)$$

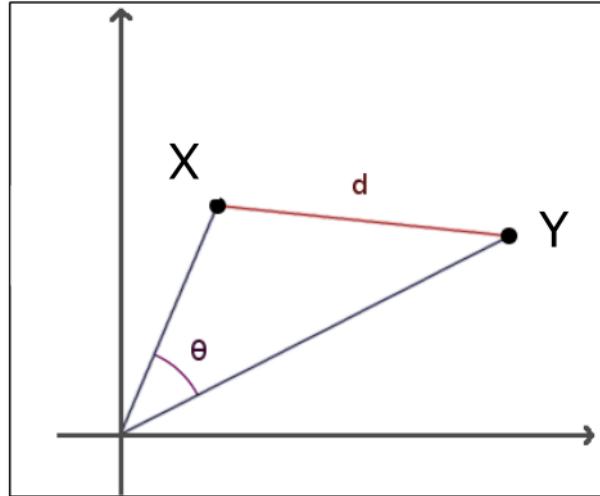


Figure 3.4: Cosine Similarity

$$dist(X, Y) = 1 - sim(X, Y) \quad (13)$$

3.3.3 Levenshtein / Edit Distance for Strings

Count the minimal number of changes necessary to turn one string into another:

- count +1 when deleting a character [d]
- count +1 when adding a character [a]
- count +2 when changing a character [c]

1. Word	2. Word	Levenshtein Distance
Hello	Yellow	1 [c] + 1 [a] = 3
MacDonald	McDonalds	1 [d] + 1 [a] = 2
banana	ananas	? d+a=2

Figure 3.5: Examples for Levenshtein Distance

4 Supervised Machine Learning

4.1 Regression and classification algorithms

Regression

- Linear Regression
- Polynomial Regression
- k-NN Regression
- Support Vector Regression
- Neural Networks
- Regression Trees

Classification

- Logistic Regression
- Naïve Bayes
- k-NN
- Support Vector Machines
- Neural Networks
- Decision Trees

4.2 Decision Boundaries

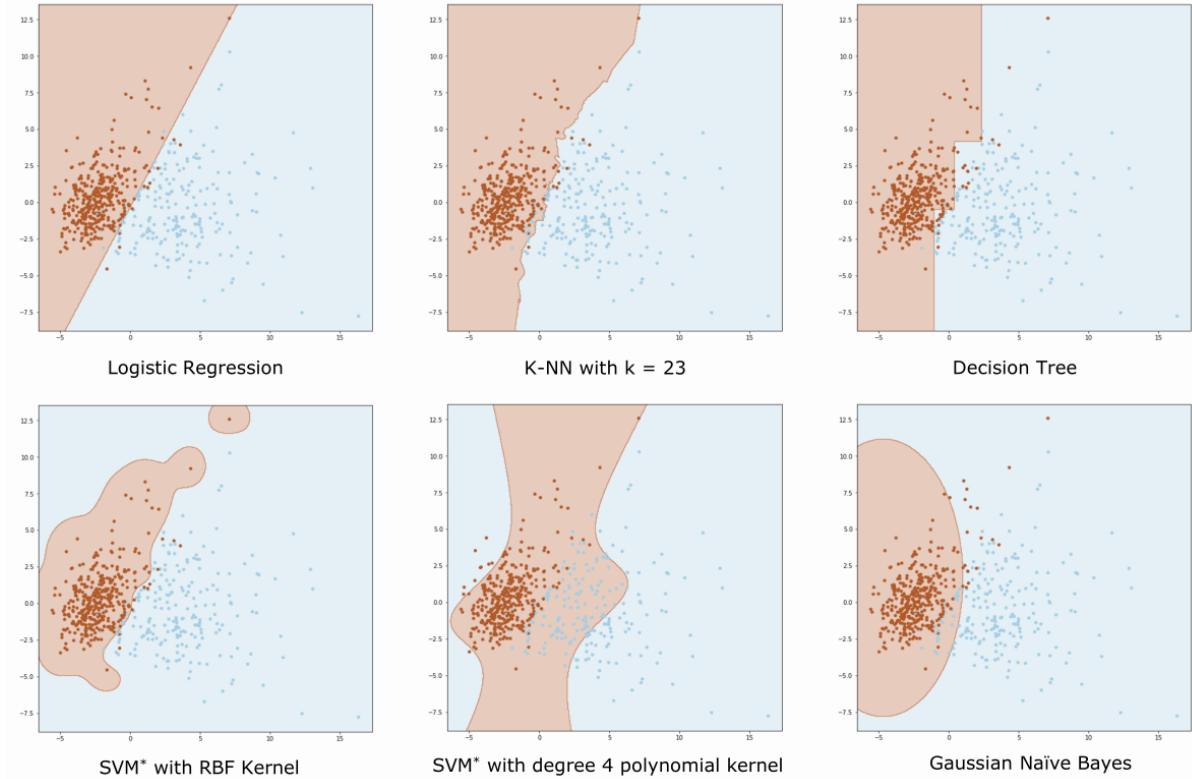


Figure 4.1: Decision Boundaries for different classification approaches

Classifications usually end in something like Figure 4.1. The example shows a classification whether a tumor is benign or cancerous. Brown means cancerous and blue means benign. Even though the data points are the same in all pictures, different approaches yield different results.

The goal of a 'good' classification-algorithm is to produce as few false-positive (algorithm says is cancer, but is actually not) and false-negatives (algorithm says its benign but is actually cancerous) as possible.

4.2.1 Kernel-Trick

The data in Fig. 4.1 is still theoretically linearly separable. But in case it is not, you could use the so-called 'kernel-trick', where you simply add a dimension and change your point of view (see Fig. 4.2)

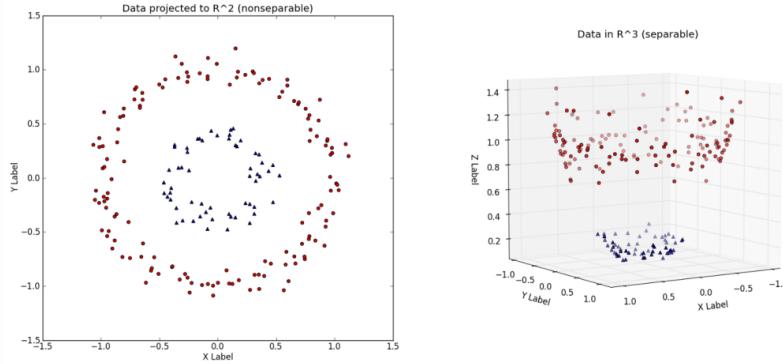


Figure 4.2: Kernel Trick to linearly separate data that is not linearly separable

4.3 k-Nearest-Neighbor

```

1   from sklearn.neighbors import
2     KNeighborsClassifier
3
4   knn = KNeighborsClassifier(n_neighbors=3)
5   knn.fit(X_train, y_train)
6   y_pred = knn.predict(X_test)
7   acc = accuracy_score(y_test, y_pred)
8
9   print("Test Set Accuracy for k=3" + ":
10    {:.2f}".format(acc))

```

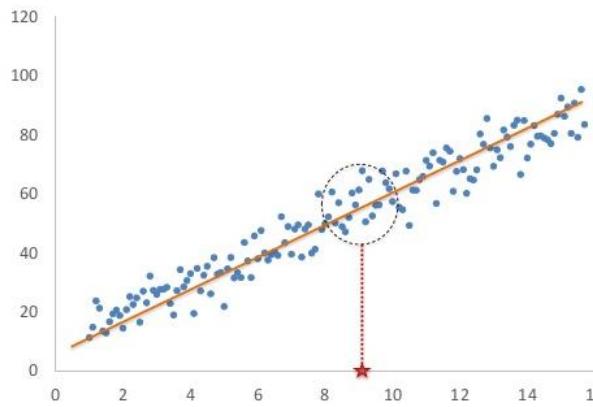
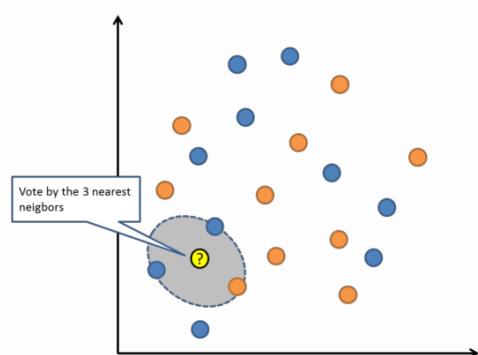


Figure 4.3: Regression with k-NN

especially useful if you want to use k-NN to e.g. form a regression line.

You can use k-NN for regression by simply assigning the mean of all k neighbors as label to the sample data.

4.4 Training- and Testdata

If you use the same data to train and test your algorithm, it might occur that the algorithm is 'memorizing' the data and gives you brilliant results. However, if you release it into the wild, where it encounters different data, it will perform really poorly. This is called **overfitting**

To counter overfitting, you usually split your data into **trainingdata** and **testdata**. You train the algorithm with the training data and test it with the testdata (who would've thought...).

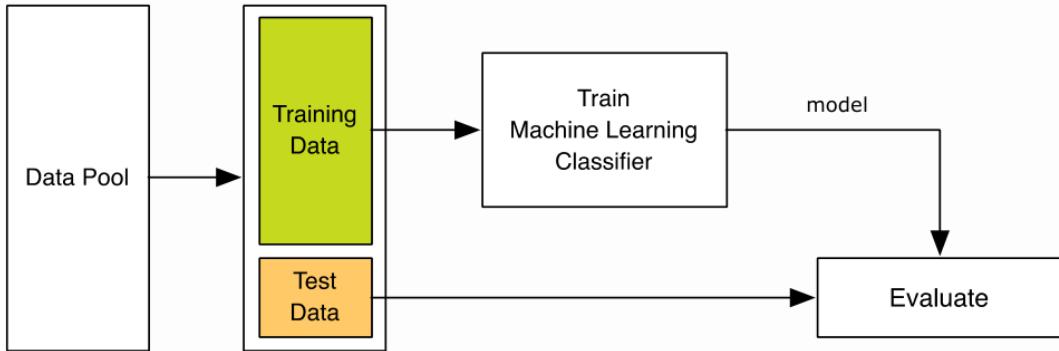


Figure 4.4: Split your data into training- and testdata

training means that you tweak the parameters of the algorithm to minimize the cost function.

testing means that you test the performance of the algorithm with those tweaked parameters on *yet unseen data*. If the algorithm has already seen the data, you might run into overfitting problems.

If you need to tweak your hyperparameters a lot (e.g. the 'k' in k-NN), you should probably use a more complex evaluation workflow. Because if you keep tweaking the hyperparameters and then testing them with the same data, you'll end up with the very same overfitting problem that I explained earlier (and will therefore probably get fired and have to live on the street).

Therefore, it is recommended that you add **validation data** to your workflow. You train your model with the training data, validate the results with the validation data, and if the result is satisfactory, you can test it on entirely different test data.



Figure 4.5: Add validation data to the mix

This method requires quite a lot of data. If you do not have the required amount of data, you could for example use **cross validation**. You still split your data into training- and testdata and then use a different 'slice' of your training data to validate the hyperparameter.

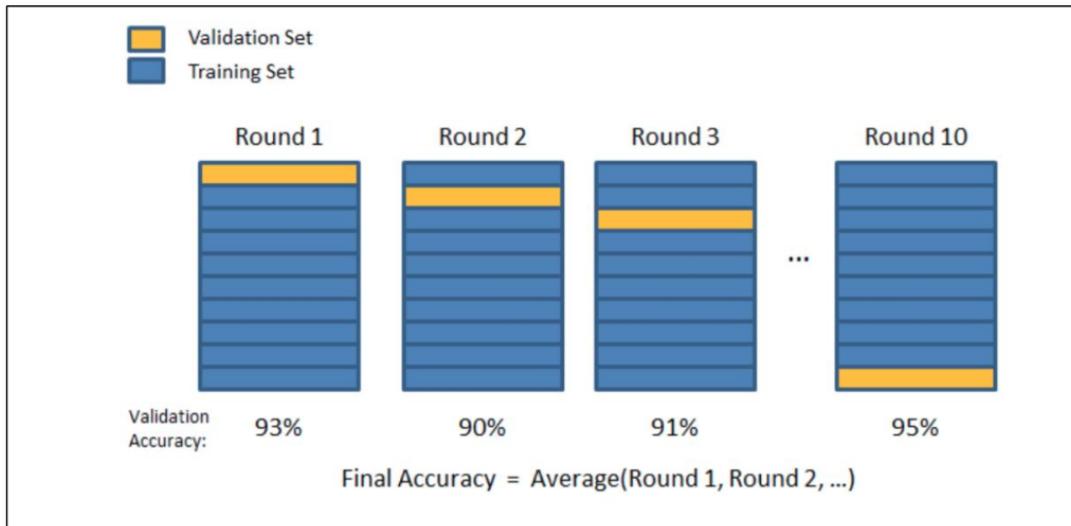


Figure 4.6: 10-fold cross validation

4.5 Measuring the performance of classification

To verify that your tweaked parameters are indeed within the margin that is acceptable, you need to do some quality assurance first.

4.5.1 Confusion Matrix

n=165	Predicted YES	Predicted NO
Actual No	50	10
Actual YES	5	100

True Positive: Predicted Yes, Actual Yes

True Negative: Predicted No, Actual No

False Positive: Predicted Yes, Actual No

False Negative: Predicted No, Actual Yes

The confusion matrix shows, how many true/false positives and true/false negatives the algorithm produced.

With these values, one can calculate the algorithms **Accuracy** and **Error Rate**

4.5.2 Accuracy and Error Rate

$$Accuracy = \frac{True\ Positive + True\ Negative}{Total} \quad (14)$$

$$Error\ Rate = \frac{False\ Positive + False\ Negative}{Total} = 1 - Accuracy \quad (15)$$

In our case the Accuracy would be $\frac{50+100}{50+100+5+10} = \frac{150}{165} = 0.91 = 91\%$ and the error rate therefore 9%

4.5.3 Sensitivity

Accuracy works great on balanced data, but it's not reliable on imbalanced data because Accuracy only checks how many times the classifier was right.

If there were 5000 NO instances and 20 YES instances, a classifier that only returns NO would have an accuracy of over 99%.

The **Sensitivity** (also called 'Recall') counts how many true positives there are.

$$Sensitivity = \frac{\text{True Positive}}{\text{Actual YES}} = \frac{\text{True Positive}}{\text{True Positive} + \text{False Negative}} \quad (16)$$

In our confusion matrix from earlier, the Sensitivity would be $\frac{100}{100+5} = \frac{100}{105} = 0.95 = 95\%$

4.5.4 Specificity

This is the inverse of the Sensitivity. It counts how many NO the algorithm correctly predicted.

$$Specificity = \frac{\text{True Negative}}{\text{Actual NO}} = \frac{\text{True Negative}}{\text{True Negative} + \text{False Positive}} \quad (17)$$

In our confusion matrix from earlier, the Specificity would be $\frac{50}{50+10} = \frac{50}{60} = 0.83 = 83\%$

4.5.5 Precision

Both of the preceding measures relied on the true negative. However, what would you do if you could not count the True Negatives? You use **Precision**. Precision shows how many times the algorithm is correct if it predicts YES.

$$Precision = \frac{\text{True Positive}}{\text{Predicted YES}} = \frac{\text{True Positive}}{\text{True Positive} + \text{False Positive}} \quad (18)$$

In our confusion matrix from earlier, the Precision would be $\frac{100}{100+10} = \frac{100}{110} = 0.91 = 91\%$

4.5.6 F1 Score

The F1 score is the harmonic mean between precision and recall/sensitivity

$$F1 = \frac{2 \cdot Precision \cdot Sensitivity}{Precision + Sensitivity} \quad (19)$$

In our confusion matrix from earlier, the Precision would be $\frac{2 \cdot 0.91 \cdot 0.95}{0.91 + 0.95} = \frac{1.73}{1.86} = 0.93 = 93\%$

Due to the fact that the F1 score does not take True Negatives into account, it tends to be strongly biased towards the worse score.

However, it is still one of the best methods to solve a classification problem with skewed data.

4.6 Measuring the performance of regression

4.6.1 Coefficient of Determination

$$R^2 = 1 - \frac{\frac{1}{m} \sum_{i=1}^m (y_i - f_i)^2}{\frac{1}{m} \sum_{i=1}^m (y_i - \bar{y})^2} = 1 - \frac{\sum_{i=1}^m (y_i - f_i)^2}{\sum_{i=1}^m (y_i - \bar{y})^2} \quad (20)$$

- The sum of errors does not make sense (positive and negative errors cancel out)

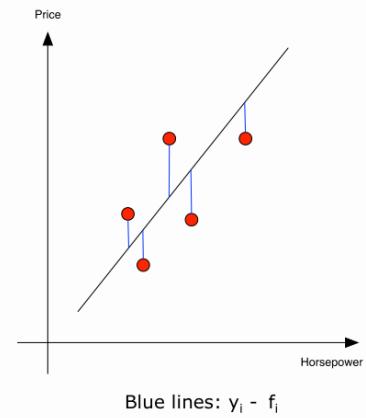
$$\frac{1}{m} \sum_{i=1}^m (y_i - f_i) \quad \text{✖}$$

- Mean Absolute Error

$$\frac{1}{m} \sum_{i=1}^m |y_i - f_i| \quad \text{✓}$$

- Mean Squared Error

$$\frac{1}{m} \sum_{i=1}^m (y_i - f_i)^2 \quad \text{✓}$$



R^2 is a staticstical measure of how well the predictions approximate the real data points. The top is the sum of squared errors (how much does the prediction deviate from the actual value) and the bottom is the deviation of the mean.

$R^3 = 1$ is a perfect prediction-line

$R^3 = 0.53$ means that 53% of the of the predictions are correct and can be explained by the model.

5 Linear Regression

Linear regression is a **supervised machine learning algorithm** to predict values based on previous variables.

It can also be used to verify whether two variables X and Y are **dependant** on each other.

Linear Regression produces a **straight line** (who would have thought) and each data point has a certain distance from that line. That distance is called **error** or **residual**.

These errors should cancel each other out, as the regression-line should be placed in the middle of all the points.

The equation for a 'normal' line is $g(x) = m \cdot x + q$, where m symbolizes the slope of the line and q tells you where the line crosses the y -axis.

The equation for the regression line is very much like the 'normal' line-equation, but we use greek symbols, because why not...

$$h_{\theta}(x) = \theta_0 + \theta_1 \cdot x \quad (21)$$

As mentioned before, deviation from that line are called errors. Therefore, the error of a given point i can be calculated from the difference of the actual y_i from the $h_{\theta}(x)$ (the y on the line)

$$e_i = y_i - (h_{\theta}(x_i)) \quad (22)$$

The goal of linear regression is to find the **optimal line**, ergo the line that **produces the smallest errors**.

However, as mentioned earlier, the errors usually cancel each other out, as sometimes the line lies above the data point (negative error) and sometimes it lies below it (positive error). To solve that problem, the parameter we will use to determine the quality of the produced line will be **the sum of squared error**. By squaring the errors, we can't have negative errors (because squared numbers cannot be negative). Therefore, the smaller the sum of squared errors, the better the line.

The sum of squared errors can be calculated as follows:

$$J(\theta_0, \theta_1) = \frac{1}{2n} \sum_{i=1}^n (e_i)^2 = \frac{1}{2n} \sum_{i=1}^n [y_i - (h_{\theta}(x_i))]^2 \quad (23)$$

To minimize $J(\theta_0, \theta_1)$, the **gradient** of J must be **minimized** or, ideally, zeroed.

This leads to the following formulas for θ_0 and θ_1

$$\theta_1 = \frac{S_{xy}}{S_{xx}} \quad (24) \qquad \theta_0 = \bar{y} - \theta_1 \cdot \bar{x} \quad (25)$$

Where \bar{x} and \bar{y} are the **mean** of the x and y values respectively

S_{xx} and S_{xy} are called **regression coefficients** and are calculated as follows:

$$S_{xy} = \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) \quad (26)$$

$$S_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2 \quad (27)$$

Example

$$X = [4, 6, 8, 10]$$

$$Y = [2.3, 4.1, 5.7, 6.9]$$

$$\bar{X} = \frac{1}{4}(4 + 6 + 8 + 10) = 7$$

$$\bar{Y} = \frac{1}{4}(2.3 + 4.1 + 5.7 + 6.9) = 7.25$$

$$S_{xx} = (4 - 7)^2 + (6 - 7)^2 + (8 - 7)^2 + (10 - 7)^2 = 20$$

$$S_{xy} = (4 - 7)(2.3 - 7.25) + (6 - 7)(4.1 - 7.25) + (8 - 7)(5.7 - 7.25) + (10 - 7)(6.9 - 7.25) = 15.4$$

$$\theta_1 = \frac{20}{15.4} = 0.77$$

$$\theta_0 = 4.75 - (0.77 - 7) = -0.64$$

From this follows that the regression line is:

$$h_\theta(x) = -0.64 + 0.77 \cdot x$$

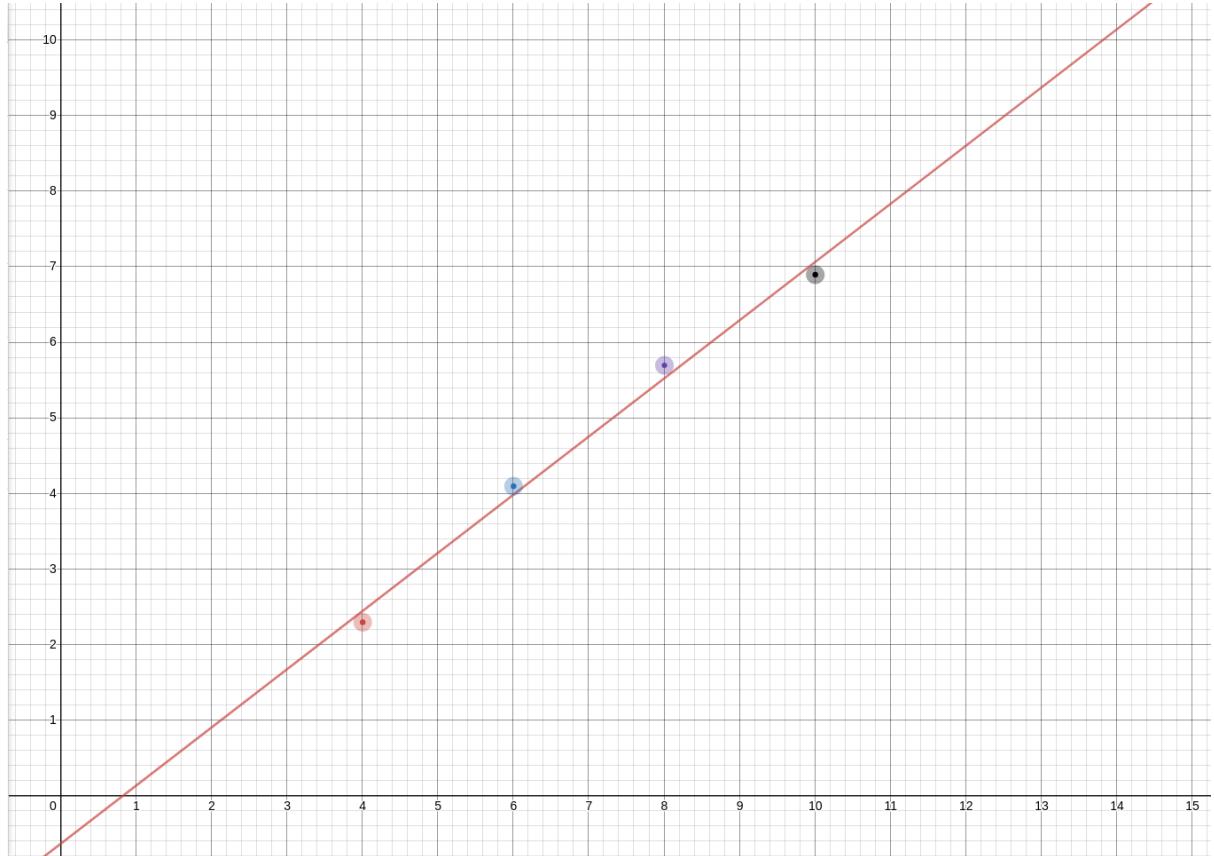


Figure 5.2: Regression line of the example

From figure 5.2 we can now see that for $x_i = 12$, y would most likely be at 8.6.

5.1 Coefficient of Determination

This coefficients was already mentioned in section 4.6.1 as 'way to measure how good a regression is'. But how does it even do that?

As mentioned earlier, the goal of a good regression is to **minimize the sum of squared errors**. However, there are three kinds of sum of squared Errors:

\bar{y} : Mean of all Y

\bar{x} : Mean of all X

\hat{y}_i : Expected value of y based on the regression line

y_i : Actual value of y

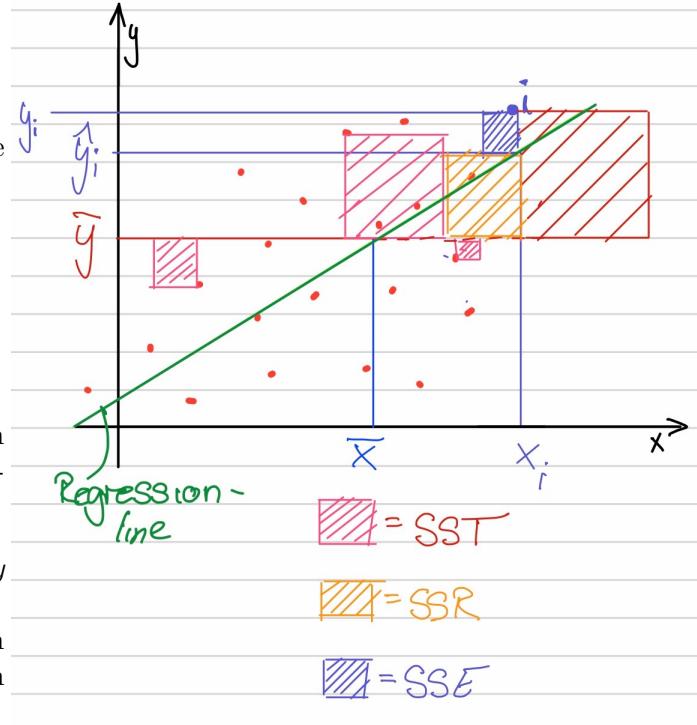
SST : Total sum of squares
Sum of SSE and SSR

SSE : Sum of squared Errors

The sum of the deviations from the predicted points to the regression line

SSR : Sum of squares explained by regression

The sum of all deviations from the mean (\bar{y}) to the regression line



As illustrated in the figure above, $SST = SSR + SSE$.

$$SST = \sum_{i=1}^n (y_i - \bar{y})^2 \quad (28)$$

$$SSE = \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (29)$$

$$SSR = \sum_{i=1}^n (\hat{y}_i - \bar{y})^2 \quad (30)$$

But how does the aforementioned Coefficient of Determination relate to all of this?

R^2 is the **fraction of the total error that can be explained by the regression**. If all errors can be explained by the regression ($R^2 = 1$), then the regression is perfect

$$R^2 = \frac{SSR}{SST} = \frac{SST - SSE}{SST} = 1 - \frac{SSE}{SST} \quad (31)$$

There's yet another error, the *Mean Squared Error* (MSE). MSE is basically the mean of SSE. It is calculated as

$$MSE = \frac{SSE}{n-2} = \frac{1}{n-2} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (32)$$

5.2 Correlation Analysis

So now that you have the regression parameters θ_0 and θ_1 , which make out the regression line. However, that regression line is only as good as your parameters. So how do you test how well you calculated the parameters?

Easy, you calculate the **standard deviation of these parameters**.

$$s_{\theta_0} = \sqrt{MSE} \cdot \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2}} \quad (33)$$

$$s_{\theta_1} = \sqrt{MSE} \cdot \sqrt{\frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2}} \quad (34)$$

Based on these standard deviations, you can calculate a **confidence interval**. This interval is a **degree of uncertainty**. Say we conducted a study and we publish our results with a **confidence level** of 95%.

This means that if we used the same sampling method to select different samples and computed an interval estimate for each sample, we would expect the true population parameter to fall within the interval estimates 95% of the time.

These intervals can be calculated with the aforementioned standard deviation of θ_0 and θ_1 and some *critical values*. These critical values depend on how high your confidence level and degrees of freedom are.

Kritische Grenzen der *t*-Verteilung

Kritische Grenzen $t_{1-\frac{\alpha}{2}}(\nu)$ der *t*-Verteilung mit ν Freiheitsgraden.

ν	1	2	3	4	5	6	7	8	9	10	11	12
$\alpha = 0.05$	12.71	4.30	3.18	2.78	2.57	2.45	2.36	2.31	2.26	2.23	2.20	2.18
$\alpha = 0.01$	63.66	9.92	5.84	4.60	4.03	3.71	3.50	3.36	3.25	3.17	3.11	3.05
ν	13	14	15	16	18	20	25	30	40	60	100	200
$\alpha = 0.05$	2.16	2.14	2.13	2.12	2.10	2.09	2.06	2.04	2.02	2.00	1.98	1.97
$\alpha = 0.01$	3.01	2.98	2.95	2.92	2.88	2.85	2.79	2.75	2.70	2.66	2.63	2.60

Für $\nu \rightarrow \infty$ konvergieren die Grenzen gegen die kritischen Grenzen 1.96 bzw. 2.58 der Normalverteilung.

Figure 5.3: Critical Values for Confidence Intervals

Degrees of freedom tell you how many regression parameters you already had to calculate. Take for example *SSE*, where both θ_0 and θ_1 are needed. Therefore, *SSE* has a degree of freedom of $n - 2$, given that you had to calculate 2 parameters.

Confidence Intervals can be calculated with $[\theta_0 - (\text{critical value} \cdot s_{\theta_0}); \theta_0 + (\text{critical value} \cdot s_{\theta_0})]$

5.3 Linear Regression Example

$$X = [14, 16, 27, 42, 83, 50, 39]$$

$$Y = [2, 5, 7, 9, 20, 13, 10]$$

$$\bar{X} = \frac{1}{7} \sum_{i=1}^7 (x_i) = \frac{14 + 16 + 27 + 42 + 83 + 50 + 39}{7} = \frac{271}{7} = \underline{\underline{38.7}}$$

$$\bar{Y} = \frac{1}{7} \sum_{i=1}^7 (y_i) = \frac{2 + 5 + 7 + 9 + 20 + 13 + 10}{7} = \frac{66}{7} = \underline{\underline{9.4}}$$

$$S_{xy} = \sum_{i=1}^7 (x_i - \bar{x})(y_i - \bar{y}) = (14 - 38.7)(2 - 9.4) + (16 - 38.7)(5 - 9.4) + (27 - 38.7)(7 - 9.4) + (42 - 38.7)(9 - 9.4) + (83 - 38.7)(20 - 9.4) + (50 - 38.7)(13 - 9.4) + (39 - 38.7)(10 - 9.4) = \underline{\underline{819}}$$

$$S_{xx} = \sum_{i=1}^7 (x_i - \bar{x})^2 = (14 - 38.7)^2 + (16 - 38.7)^2 + (27 - 38.7)^2 + (42 - 38.7)^2 + (83 - 38.7)^2 + (50 - 38.7)^2 + (39 - 38.7)^2 = \underline{\underline{3363.4}}$$

$$\theta_1 = \frac{S_{xy}}{S_{xx}} = \frac{819}{3363.4} = \underline{\underline{0.24}}$$

$$\theta_0 = \bar{y} - \theta_1 \cdot \bar{x} = 9.4 - 0.24 \cdot 38.7 = \underline{\underline{-0.008}}$$

$$SSE = \sum_{i=1}^7 (y_i - \hat{y}_i)^2 = \sum_{i=1}^7 (y_i - (\theta_0 + \theta_1 \cdot x))^2 = \sum_{i=1}^7 (y_i - (-0.008 + 0.24 \cdot x))^2 = \sum_{i=1}^7 (y_i - (-0.232 \cdot x))^2 = \underline{\underline{5.87}}$$

$$SSR = \sum_i^7 (\hat{y}_i - \bar{y})^2 = \sum_i^7 ((\theta_0 + \theta_1 \cdot x) - 38.7)^2 = \sum_i^7 ((-0.008 + 0.24 \cdot x) - 38.7)^2 = \sum_i^7 ((-0.232 \cdot x) - 38.7)^2 = \underline{\underline{199.84}}$$

$$SST = SSE + SSR = 5.87 + 199.84 = \underline{\underline{205.71}}$$

$$R^2 = \frac{SSR}{SST} = \frac{199.84}{205.71} = \underline{\underline{0.97}}$$

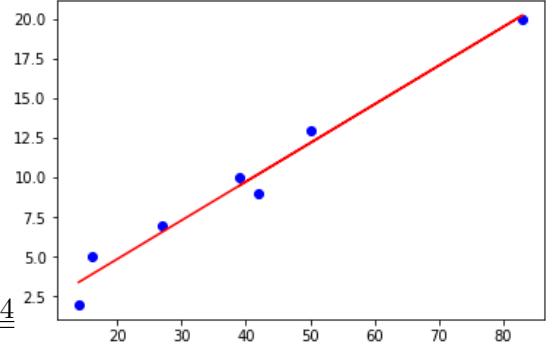
$$MSE = \frac{SSE}{n-2} = \frac{5.87}{7-2} = \underline{\underline{1.17}}$$

$$s_{\theta_0} = \sqrt{MSE} \cdot \sqrt{\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2}} = \sqrt{1.17} \cdot \sqrt{\frac{1}{7} + \frac{38.7^2}{\sum_{i=1}^n (x_i - 38.7)^2}} = \underline{\underline{-0.008}}$$

$$s_{\theta_1} = \sqrt{MSE} \cdot \sqrt{\frac{1}{\sum_{i=1}^n (x_i - \bar{x})^2}} = \sqrt{1.17} \cdot \sqrt{\frac{1}{\sum_{i=1}^n (x_i - 38.7)^2}} = \underline{\underline{0.019}}$$

$$Interval \theta_0 = [\theta_0 - 2.57 \cdot s_{\theta_0}; \theta_0 + 2.57 \cdot s_{\theta_0}] = \underline{\underline{[-2.14; 2.12]}}$$

$$Interval \theta_1[\theta_1 - 2.57 \cdot s_{\theta_1}; \theta_1 + 2.57 \cdot s_{\theta_1}] = \underline{\underline{[0.20; 0.29]}}$$



The results of the last page can also be achieved with the following python-code:

```

1 import matplotlib.pyplot as plt
2 import scipy.stats as st
3 import seaborn as sns
4 import pandas as pd
5 import numpy as np
6
7 %precision 10
8 %matplotlib inline
9
10 x=np.array([14, 16, 27, 42, 83, 50, 39])
11 y=np.array([2, 5, 7, 9, 20, 13, 10])
12
13 mean_x = np.mean(x)
14 mean_y = np.mean(y)
15
16 Sxx = np.sum((x-mean_x)**2)
17 Syy = np.sum((y-mean_y)**2)
18 Sxy = np.sum((x-mean_x)*(y-mean_y))
19
20 thet1 = Sxy/Sxx
21 thet0 = mean_y-thet1*mean_x
22
23 # To show the regression line
24 plt.plot(x,y, 'bo')
25 plt.plot(x,thet0+thet1*x, 'r')
26 plt.show()
27
28 hat_y = thet0+thet1*x
29
30 SSE=np.sum(((y-hat_y))**2)
31
32 SSR=np.sum((hat_y-mean_y)**2)
33
34 SST = SSE + SSR
35
36 R_sq = SSR/SST
37
38 MSE = SSE/(len(x)-2)
39
40 Sthet0 = np.sqrt(MSE)*np.sqrt((1/len(x))+(mean_x**2)/(np.sum((x-mean_x)**2)))
41
42 Sthet1 = (np.sqrt(MSE))*np.sqrt(1/(np.sum((x-mean_x)**2)))
43
44 print("theta_1: " + str(thet1))
45
46 print("Interval theta0: [" + str(thet0 - (2.57*Sthet0)) + " ; " + str(thet0 +
47 (2.57*Sthet0)) + "]")
48 print("Interval theta1: [" + str(thet1 - (2.57*Sthet1)) + " ; " + str(thet1 +
49 (2.57*Sthet1)) + "]")
```

5.4 Multple Linear Regression

Linear Regeression is great and all, but what if you wanted to predict an independent value based on **multiple** other values? In that case we would need **multilinear regression**. In

Muliple Linear Regression we try to fit a plane instead of a line. This plane is defined by

$$y = h_{\theta}(x_1, x_2) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 \quad (35)$$

And mapped to the sample with index i

$$y_i = \theta_0 + \theta_1 x_{1,i} + \theta_2 x_{2,i} + e_i$$

This can be transformed to matrices

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{1,1} & x_{2,1} \\ 1 & x_{1,2} & x_{2,2} \\ \vdots & \ddots & \vdots \\ 1 & x_{1,n} & x_{2,n} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$$

This can be solved as follows

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

In more than three dimensions our plane becomes a hyperplane, and the model is

$$y_i = \theta_0 + \theta_1 x_{1,i} + \theta_2 x_{2,i} + \cdots + \theta_m x_{m,i} + e_i = \sum_{k=0}^n \theta_k x_{k,i} + e_i$$

5.4.1 Example multilinear regression

Suppose we want to predict the weight of a weightlifter based on the training hours per week and the delivery of protein.

i	y	x_1	x_2
1	93	2	1.1
2	106	2	1.9
3	146	4	2
4	140	5	1.5
5	151	6	1.3
6	158	7	2.1
7	130	4	1.8
8	159	5	2.5

i : No. of observation

y : Weight in kg

x_1 : Training h/week

x_2 : Protein intake g/kg/day

We assume that the function to calculate the weight from training-hours and protein intake is as follows:

$$y = h_{\theta}(x_1, x_2) = \theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2$$

The following solution minimizes the sum of squared errors in this model (and therefore get a hella good regression).

$$\boldsymbol{\theta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} \rightarrow \begin{bmatrix} 55.7 \\ 11.1 \\ 17.5 \end{bmatrix}$$

According to this, the regression plane would be:

$$y = h_{\theta}(x_1, x_2) = 55.7 + 11.1 \cdot x_1 + 17.5 \cdot x_2$$

Motivation (cont.)

The model is

$$y^{(i)} = \theta_0 \cdot 1 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2 + e^{(i)}$$

$$\begin{bmatrix} 93 \\ 106 \\ 146 \\ 140 \\ 151 \\ 158 \\ 130 \\ 159 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 1.1 \\ 1 & 2 & 1.9 \\ 1 & 4 & 2 \\ 1 & 5 & 1.5 \\ 1 & 6 & 1.3 \\ 1 & 7 & 2.1 \\ 1 & 4 & 1.8 \\ 1 & 5 & 2.5 \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} + \begin{bmatrix} e^{(1)} \\ e^{(2)} \\ e^{(3)} \\ e^{(4)} \\ e^{(5)} \\ e^{(6)} \\ e^{(7)} \\ e^{(8)} \end{bmatrix}$$

abhl. Var. \rightarrow Beob. der Knalle. \leftarrow Fehler

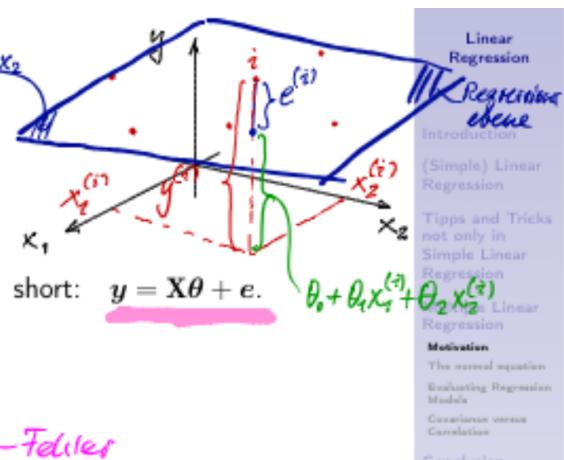


Figure 5.4: Model of the multilinear regression (©J. Bürgler, 2019)

Of course, this can also be done rather easily in Python:

```

1 import numpy as np
2
3 X = np.matrix([[2,1.1],[2,1.9],[4,2.0],[5,1.5],[6,1.3],[7,2.1],[4,1.8],[5,2.5]])
4
5 # Anzahl Reihen von X anhand der ersten Zeile (= Anzahl Beobachtungen)
6 n = X.shape[0]
7
8 y = np.matrix([93,106,146,140,151,158,130,159])
9
10 # Append a column of '1' in front of the X-matrix (to get the 'X'-matrix from the
11 # figure)
12 X_ext = np.c_[np.ones((n,1)),X]
13
14 theta = np.linalg.inv(X_ext.T.dot(X_ext)).dot(X_ext.T).dot(y)
15
16 print(theta)

```

6 Gradient Descent

The problem with Linear Regression is, that it does not scale well. For problems like these we can use Gradient Descent. The gradient (denoted with the Nabla Operator ∇) uses the properties of partial derivatives, which compute the slope in regards to an axis in a point a, b .

The gradient ∇f of the scalar function $f : \mathbb{R}^2 \rightarrow \mathbb{R}, (x, y) \mapsto f(x, y) = z$ is a vector, whose components are partial derivatives of f .

$$\nabla f(x, y) = \begin{bmatrix} \frac{\delta f}{\delta x}(x, y) \\ \frac{\delta f}{\delta y}(x, y) \end{bmatrix} = \begin{bmatrix} f_x(x, y) \\ f_y(x, y) \end{bmatrix} \quad (36)$$

6.0.1 Example of a gradient

Calculate the gradient of the function $f(x, y) = (3x + 2y)^2$ in general and in the point $(1, 2)$.

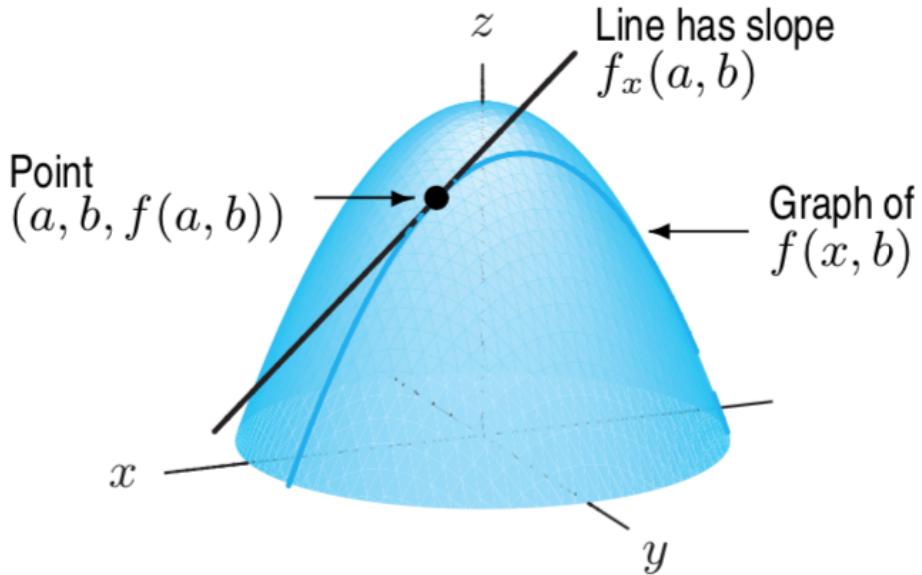


Figure 6.1: Partial derivative in regards to the x-axis in the point a,b (©J. Bürgler, 2019)

$$\nabla f(x, y) = \begin{bmatrix} 6(3x + 2y) \\ 4(3x + 2y) \end{bmatrix}$$

$$\nabla f(1, 2) = \begin{bmatrix} 42 \\ 28 \end{bmatrix}$$

6.1 Properties of the gradient

- The Gradient of a function f is a vector consisting of the partial derivatives of f with respect to all of its variables
- It points to the direction of maximal increase
- The negative Gradient points to the direction of maximal decrease
- The Gradient being a null-vector indicates a local extrema
- The Gradient is perpendicular to the contour lines of that function

6.2 Gradient descent

To find a local minima of a function f we follow the direction of the steepest descent, and thus the negative Gradient. As the Gradient is constantly changing, we have to take small steps.

6.2.1 Batch Gradient Descent

Elevating the strengths of vectors we can Gradient Descent along all columns of our data. For this we want to minimize the cost function

$$J(\theta) = \frac{1}{2n} \sum_{i=1}^n (h(bm\theta, \mathbf{x}^{(i)}) - y^{(i)})^2 \quad (37)$$

where $h(\theta, \mathbf{x}^{(i)})$ is

$$h(\boldsymbol{\theta}, \mathbf{x}^{(i)}) = \mathbf{x}^{(i)} \boldsymbol{\theta} = \theta_0 + \theta_1 x_1^{(i)} + \theta_2 x_2^{(i)} + \dots + \theta_m x_m^{(i)} \quad (38)$$

And calculate the next iteration with the learning rate α (usually $0 \leq \alpha \leq 0.1$)

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \alpha \nabla J(\boldsymbol{\theta}_k) \quad (39)$$

It can be shown that this yields

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \alpha \frac{1}{n} (h(\boldsymbol{\theta}, \mathbf{x}^{(i)}) - y^{(i)}) \cdot \mathbf{x}^{(i)} \quad (40)$$

6.3 Stochastic Gradient Descent

In Batch Gradient Descent the update to the parameter vector $\boldsymbol{\theta}$ is done all at once using the whole set of n training samples. If n is in the order of several 10^6 , this update process can become slow. One possible alternative is to update $\boldsymbol{\theta}$ for each training sample separately. This is done by randomly shuffling the training examples first and then updating $\boldsymbol{\theta}$ for each training sample.

6.3.1 Instructions

- Choose an initial parameter vector $\boldsymbol{\theta}$ and a learning rate α
- Repeat until an approximate minimum is obtained
 - Randomly shuffle the samples in the training set
 - For each sample $i \in 1, 2, \dots, n$ do

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \alpha \nabla J_i(\boldsymbol{\theta}_k) = \boldsymbol{\theta}_k - \alpha \frac{1}{n} (h(\boldsymbol{\theta}_k, \mathbf{x}^{(i)}) - y^{(i)}) \cdot \mathbf{x}^{(i)}$$

where $h(\boldsymbol{\theta}_k, \mathbf{x}^{(i)}) = \boldsymbol{\theta}_k^T \mathbf{x}^{(i)}$ and

$$J_i(\boldsymbol{\theta}) = \frac{1}{2n} (h(\boldsymbol{\theta}_k, \mathbf{x}^{(i)}) - y^{(i)})^2$$

is the cost for one data point $(x^{(i)}, y^{(i)})$

The difference to Batch Gradient Descent is that only one piece of data from the dataset is used to calculate the updated parameter and this piece of data is chosen randomly.

6.3.2 Stochastic Gradient Descent - Example

```

1 def parallel_cost(X,Y,x_data,y_data):
2     m = X.shape[0]; n = X.shape[1]
3     tot = np.zeros((m,n))
4     for i in range(1,len(x_data)):
5         tot += (X + Y * x_data[i] -
6                 y_data[i]) ** 2
7     return tot/(2 * len(x_data))
8
9     alpha = 0.03; epochs = 2000
10
11    for epoch in np.arange(0,epochs):
12        arr = np.arange(X.shape[0])
13        np.random.shuffle(arr)
14        for sample in np.arange(0,X.shape[0]):
15            i = arr[sample]
16            preds_i = X[i].dot(theta)
17            error_i = preds_i - y[i]
18            grad_i = X[i].dot(error_i)/X.shape[0]
19            theta = theta - alpha * grad_i
20            theta0_path.append(theta[0])
21            theta1_path.append(theta[1])

```

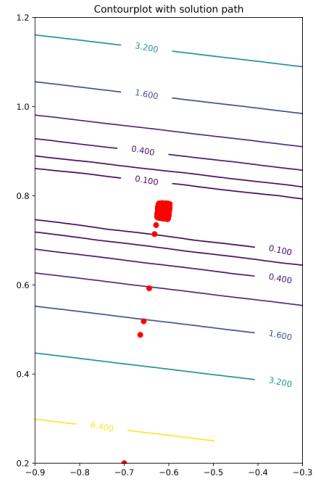


Figure 6.2: Stochastic Gradient Descent

6.4 Polynomial Regression, Feature Scaling and Checking Convergence

If we do not have a linear relationship, but a polynomial one between the features and estimated outcome, our equation is in the general form of

$$h(\boldsymbol{\theta}, \mathbf{x}) = \theta_0 + \theta_1 x^1 + \theta_2 x^2 + \cdots + \theta_n x^n \quad (41)$$

We could then use the features $x_1 = x$, $x_2 = x^2$ and $x_3 = x^3$, but if the features are not in the same range, we have a problem. To solve this we must use feature scaling:

1. Make sure the features are on a similar scale and get every feature into the range of $-1 \leq x_i \leq 1$
 - (a) Replace x_i with $x_i - \bar{x}_i$ to have features with an approximately zero mean. Does not apply to $x_0 = 1$
 - (b) Divide $x_i - \bar{x}_i$ by the range of $x_i = \max(x_i) - \min(x_i)$ or the standard deviation of x_i
2. Test if Gradient Descent is working correctly by plotting the cost function $J(\boldsymbol{\theta})$ versus the number of iterations
3. Declare convergence if $J(\boldsymbol{\theta})$ decreases by less than a given threshold (for example 10^{-3}) in one iteration

For sufficiently small α , $J(\boldsymbol{\theta})$ should decrease in every iteration, but a too small α leads to a slow convergence. Start with $\alpha = 0.001$, proceed with $0.003, 0.01, 0.03, 0.1, \dots$.

7 Regularisation

Under- and overfitting are common problems in machine learning. Underfitting occurs when the model is too general and can't aptly represent the data. Overfitting occurs, when the model is too precisely fitted to the training data.

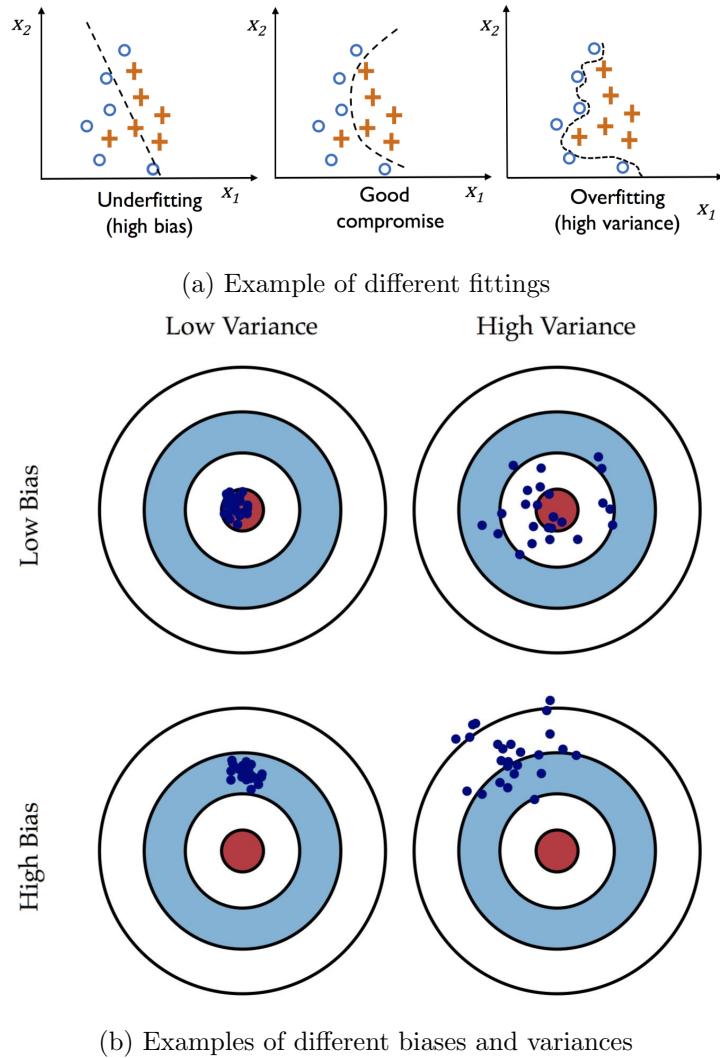


Figure 7.1: Under- and Overfitting, Biases and Variances

To address overfitting we can try these approaches

1. Reduce the number of features
 - Manually select which features to keep
 - Model selection algorithm
 2. Regularisation
 - Keep all features, but reduce magnitude of parameters θ_i
 - Works well with lots of features which each contribute just a bit to predict y

7.1 Ridge Regularisation

$$J(\theta) = \frac{1}{2n} \left[\sum_{i=1}^n (h(\theta, x_i) - y_i)^2 + \lambda \sum_{j=1}^m \theta_j^2 \right] \quad (42)$$

The second sum goes from 1 to the number of features m and it does not contain θ_0 . The regularisation hyperparameter λ controls the amount of regularisation. If $\lambda = 0$ there will be

no regularization, and if $\lambda = \infty$ there will be underfitting because only θ_0 will be different from zero. In Ridge regularised regression, we choose θ to minimize $J(\theta)$:

$$\hat{\theta} = \underset{\theta}{\operatorname{argmin}} J(\theta) \quad (43)$$

large λ	High Bias / Underfit
intermediate λ	Correct
small λ	High Variance / Overfit

7.2 How to choose the right model

7.2.1 Hold-out / Simple Cross Validation

1. Randomly split the Sample S into S_{train} and S_{cv} called the **hold-out cross validation set**. A standard split is 70% S_{train} and 30% S_{cv} .
2. For each degree of the polynomial k , train the model M_k on S_{train} to get the parameter vector θ_k
3. Select θ_k with the smallest error $\hat{\varepsilon}_{S_{cv}}(\theta_k)$

$$k = \underset{k \in 1, 2, \dots, 10}{\operatorname{argmin}} \hat{\varepsilon}_{S_{cv}}(\theta_k)$$

where $\hat{\varepsilon}_{S_{cv}}(\theta_k)$ is the empirical error, if we use θ_k as the parameter vector on the cross validation set S_{cv} .

The issue with **hold-out cross validation** is, that it wastes the amount of data used for the cross validation.

7.2.2 k-fold Cross Validation

To reduce the waste of data, we could hold out less data used per run: we use k-fold cross validation **k-fold cross validation**.

1. Randomly split S into l disjoint subsets S_1, S_2, \dots, S_l of $\frac{n}{l}$ training examples each
2. Evaluate each model $M_k, k \in 1, 2, \dots, 10$ as follows
 - For $j = 1, 2, \dots, l$ train M_k on all data, except the subset S_j to get θ_{kj} and test θ_{kj} on S_j to get the empirical error $\hat{\varepsilon}_{S_j}(\theta_{kj})$
 - The estimated generalisation of the model M_k is then calculated as the average of the $\hat{\varepsilon}_{S_j}(\theta_{kj})$

$$\frac{1}{l} \sum_{j=1}^l \hat{\varepsilon}_{S_j}(\theta_{kj}) \text{ where } \hat{\varepsilon}_{S_j}(\theta_{kj}) = \frac{1}{2n} \sum_{i=1}^n (h(\theta_k, \mathbf{x}^{(i)}) - y^{(i)})^2$$

3. Pick the model $M - K$ with the lowest estimated generalisation error and retrain that model on the entirety of the training set S .

8 Support Vector Machines

8.1 Scalar Product

The scalar product between two vectors \vec{a}, \vec{b} is defined as

$$\vec{a} \cdot \vec{b} = \sum_{i=1}^n a_i b_i = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n \quad (44)$$

The following rules hold true for the scalar product

symmetry $\vec{a} \cdot \vec{b} = \vec{b} \cdot \vec{a}$

distributivity $\vec{a} \cdot (\vec{b} + \vec{c}) = \vec{a} \cdot \vec{b} + \vec{a} \cdot \vec{c}$

multiplication by scalars $\lambda(\vec{a} \cdot \vec{b}) = (\lambda\vec{a}) \cdot \vec{b} = \vec{a} \cdot (\lambda\vec{b})$

Using the scalar product we can define the length of a vector, also called the L²-Norm

$$\|\vec{a}\| = \sqrt{a_1^2 + a_2^2 + \cdots + a_n^2} = \sqrt{\vec{a} \cdot \vec{a}} \quad (45)$$

Two vectors are orthogonal if and only if their scalar product is zero:

$$\vec{a} \cdot \vec{b} = 0 \Leftrightarrow \vec{a} \perp \vec{b} \quad (46)$$

Example of scalar product

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 4 \end{bmatrix} = 1 \cdot 3 + 2 \cdot 4 = 11$$

8.1.1 The Hessian normal form of a straight line

The straight line g is defined by some point x_0 and the normal vector \vec{n} with length 1 (refer to figure 8.1).

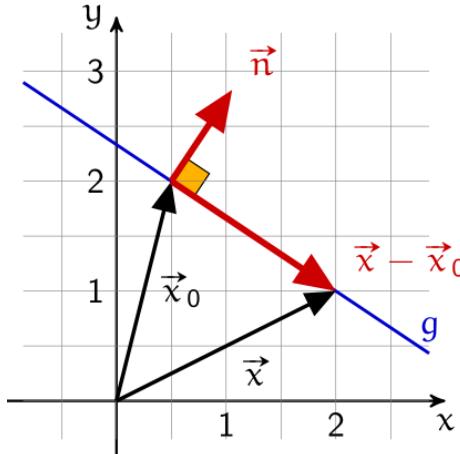


Figure 8.1: Plot of g and the relevant vectors \vec{x}_0 and \vec{n}

For any point x on the line we have

$$\vec{n} \cdot (\vec{x} - \vec{x}_0) = 0$$

And find

$$\Rightarrow n_x x + n_y y - (n_x x_0 n_y y_0) = n_x x + n_y y + d = 0$$

With $d = -(n_x x_0 + n_y y_0)$ the signed distance $-\vec{n} \cdot \vec{x}_0$ from the origin

The generalisation of the Hessian normal form to a plane in 3D-space is straight forward:

$$\vec{n} \cdot (\vec{x} - \vec{x}_0) = 0 \text{ or } \vec{n} \cdot \vec{x} + d = 0 \text{ with } d = -\vec{n} \cdot \vec{x}_0 \quad (47)$$

Example of the Hessian Normal Form The line g is taken from figure 8.2

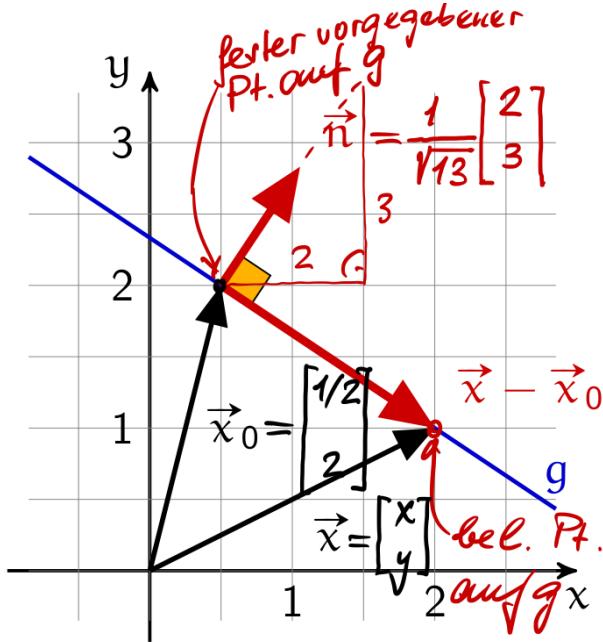


Figure 8.2: Annotated figure 8.1

$$\begin{aligned}\vec{n} &= \frac{1}{\sqrt{13}} \begin{bmatrix} 2 \\ 3 \end{bmatrix} \\ 0 &= \vec{n} \cdot (\vec{x} - \vec{x}_0) \\ &= \frac{1}{\sqrt{13}} \begin{bmatrix} 2 \\ 3 \end{bmatrix} \cdot \left(\begin{bmatrix} x \\ y \end{bmatrix} - \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \right) \\ &= \frac{1}{\sqrt{13}} \begin{bmatrix} 2 \\ 3 \end{bmatrix} \cdot \begin{bmatrix} x - 0.5 \\ y - 0.5 \end{bmatrix}\end{aligned}$$

8.1.2 Motivation for Support Vector Machines

- Classifying data means splitting it up
- There are many ways to split the data, even using only a linear function
- We want the best possible split

The line in the middle of figure 8.3 is called the hyperplane (a line in two dimensions, a plane in three). We know that this is the best possible split, because it is the furthest from both clusters. The data points (samples) closest to the hyperplane are called support vectors.

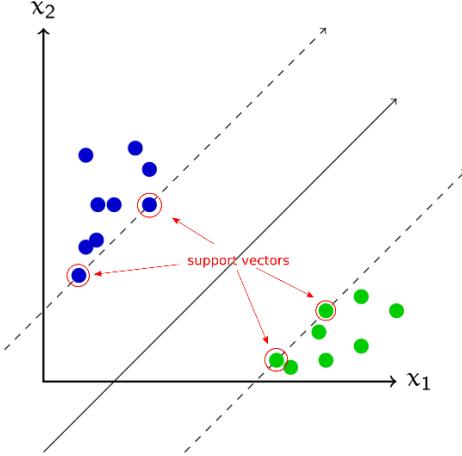


Figure 8.3: Support Vector Machine

8.2 Basic ideas and features

- Finds optimal hyperplane for linearly separable patterns
- Extended patterns which are not linearly separable are transformed into another (possibly higher dimensional) feature space
- Not affected by the local minima problem
- No dimensionality problem
- Modular design allows separate implementation of various components
- Support vectors are the data points or samples closest to the decision hyperplane
- Support vectors are the most difficult to classify
- Support vectors directly influence the position of the decision hyperplane and are the critical elements in the training set
- Problem of finding an optimal separating hyperplane can be solved using standard optimisation techniques

8.2.1 Linear Classifier

A linear classifier has the form

$$f(\vec{x}) = \theta_0 + \theta_1 x_1 + \cdots + \theta_m x_m = b + w_1 x_1 + w_2 x_2 + \cdots + w_m x_m = b + \vec{w}^T \vec{x}_b \quad (48)$$

where $\vec{w} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_m \end{bmatrix}$ is the normal vector on the hyperplane and $b = \theta_0$ is the bias.

8.2.2 How to determine optimality

In figure 8.4 \vec{w} is the normal vector on the decision hyperplane, its length depends on the margin which is maximised through the Support Vector Machine. Maximising the margin $\frac{2}{\|\vec{w}\|}$

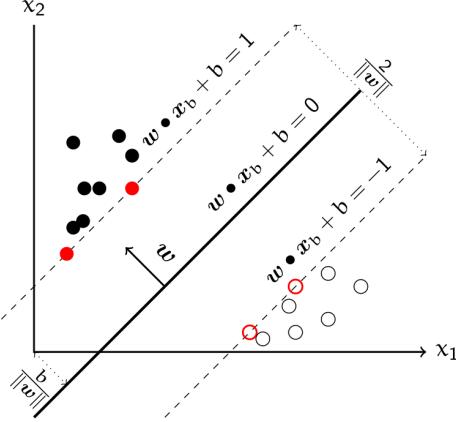


Figure 8.4: Hyperplane with support vectors in red

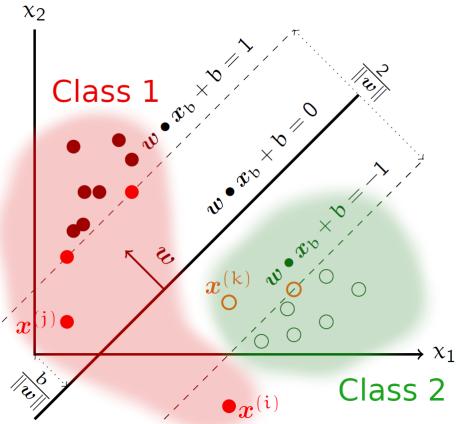


Figure 8.5: Support Vector Machine with soft margins

is equivalent to minimising $\frac{\vec{w}^T \vec{w}}{2}$, therefore we

$$\underset{\vec{w}, b}{\text{minimise}} \frac{1}{2} \vec{w}^T \vec{w} \quad (49)$$

subject to $y^{(i)}(\vec{w}^T \vec{x}^{(i)} + b) \geq 1$ for $i = 1, 2, \dots, n$

8.3 From the hard margin to the soft margin problem

So far we have discussed the hard margin problem (see equation 49), which fails if the problem is not separable. To address this we could introduce a **slack variable** ζ_i for each data point $x^{(i)}$ and solve the **soft margin problem**

$$\underset{\vec{w}, b}{\text{minimise}} \frac{1}{2} \vec{w}^T \vec{w} + C \sum_{i=1}^n \zeta_i \text{ subject to } y^{(i)}(\vec{w}^T \vec{x}^{(i)} + b) \geq 1 - \zeta_i \quad (50)$$

with $\zeta_i \geq 0$ for $i = 1, 2, \dots, n$. The slack variable ζ_i measures how much the i -th instance $\vec{x}^{(i)}$ is allowed to violate the margin.

8.3.1 The slack variable explained

The margin can be less than 1, by setting $\zeta_i > 0$, but then this gets factored in as a penalty $C\zeta_i$ in the minimisation. Thus the sum $\sum_{i=1}^n \zeta_i$ gives an upper bound on the number of training errors. With this soft margin Support Vector Machines minimise training error traded off against better margins. The parameter C is the *regularisation parameter*, which provides a way to control overfitting:

- small C ($C \rightarrow 0$) Constraints are easily ignored, we obtain a large margin
- large C ($C \rightarrow \infty$) Constraints are hard to ignore, we obtain a narrow margin
- $C = \infty$ All constraints enforced, we have a hard margin

Therefore we still have a quadratic optimisation problem with a unique minimum and we only have to deal with the parameter C .

8.4 The Kernel Trick

The kernel transforms a problem to another coordinate system, where the problem may be linearly separable.

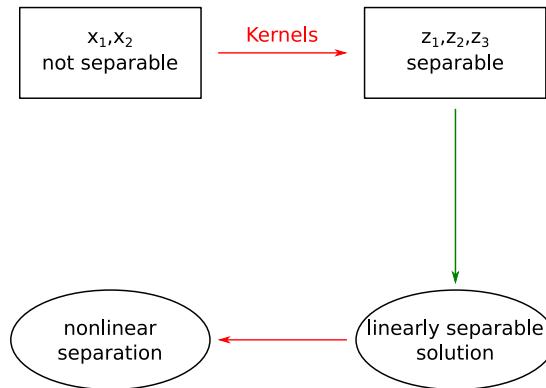


Figure 8.6: Course of action for the kernel method

8.4.1 Kernel Functions Examples

polar coordinates $\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^2, \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \mapsto \begin{bmatrix} r \\ \theta \end{bmatrix} = \begin{bmatrix} \sqrt{x_1^2 + x_2^2} \\ \arctan(\frac{x_2}{x_1}) \pm \pi \end{bmatrix}$ (refer to figure 8.7)

polynomial mapping $\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^3, (x_1, x_2) \mapsto (z_1, z_2, z_3) = (x_1^2, \sqrt{2} \cdot x_1 \cdot x_2, x_2^2) = \Phi(x_1, x_2)$
(refer to figure 8.8)

radial $\Phi(x_1, x_2) = e^{-\frac{\|x_1 - x_2\|^2}{2\sigma^2}}$

Kernel function Φ satisfy:

- positive semidefinite $\forall x_1, x_2 (\Phi(x_1, x_2) \geq 0)$
- symmetric $\Phi(x_1, x_2) = \Phi(x_2, x_1)$

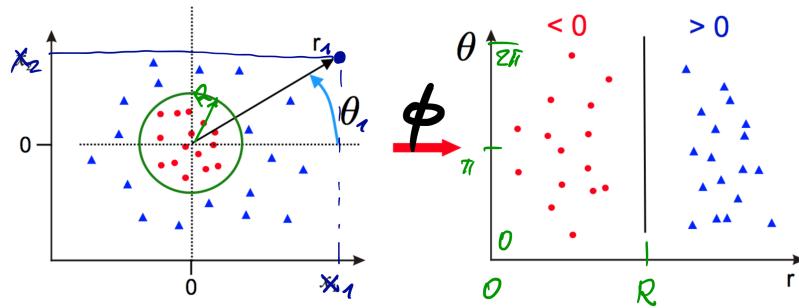


Figure 8.7: Transformation from cartesian to polar coordinate system

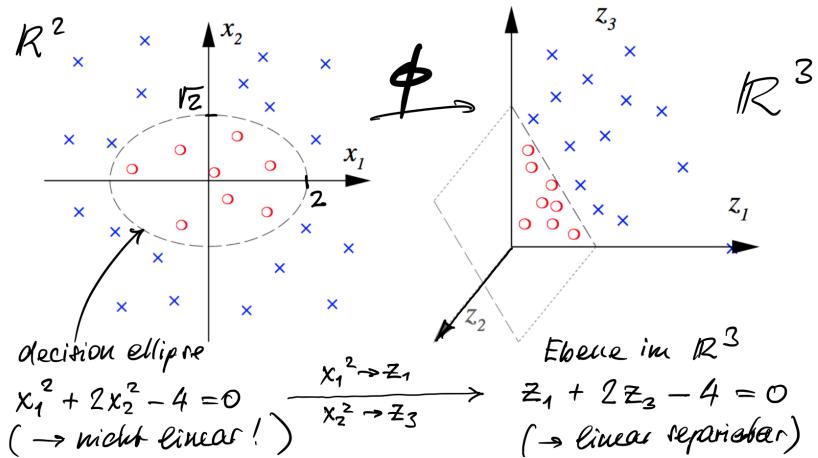


Figure 8.8: Transformation to higher dimension

9 Clustering and Association Rules

9.1 k-Means Algorithm

The k-Means algorithm is an algorithm that automatically identifies cluster centers. One has to specify the amount of clusters one wants before it can start though. The algorithm functions as follows:

1. Input: Number of clusters $k > 0$ and data points $x_1, \dots, x_n \in \mathbb{R}^m$
2. Randomly choose k cluster centers $\mu_1, \dots, \mu_k \in \mathbb{R}^m$
3. Repeat until convergence
 - (a) Assign each data point x_i to its nearest cluster center μ_j

$$c_i = \underset{j \in \{1, \dots, k\}}{\operatorname{argmin}} \|x_i - \mu_j\|^2$$

- (b) Update each cluster center to the mean of all assigned data points

$$\mu_j := \frac{\sum_{i:c_i=j} x_i}{|\{i : c_i = j\}|}$$

9.1.1 A note on the Euclidean Distance between two points

$$\begin{aligned}
x &= (x_1, x_2) \\
\|x\| &= \sqrt{x_1^2 + x_2^2} \\
\|x\|^2 &= x_1^2 + x_2^2 \\
y &= (y_1, y_2) \\
\|x - y\| &= \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}
\end{aligned}$$

9.1.2 Clustering Distortion

The total distortion can be measured by summing up the squared distance between each point and it's cluster center

$$\sum_{i=1}^n \|x_i - \mu_{c_i}\|^2 \quad (51)$$

The average distortion per data point is

$$\frac{1}{n} \sum_{i=1}^n \|x_i - \mu_{c_i}\|^2 \quad (52)$$

Average distortion allows to compare clusterings over different data sets

9.1.3 Convergence and Optimality

Optimal clustering minimises the total distortion, which is a NP-hard problem for $x > 1$. Therefore k-Means only approximates the optimal solution, but always converges, albeit not necessarily to a global minimum. In practice k-Means is executed several time and the clustering with minimum distortion is chosen.

9.1.4 Choose the Number of Clusters

The choice of clusters balances between low distortion and fewest number of clusters. The elbow method finds a good compromise in general (see figure 9.1).

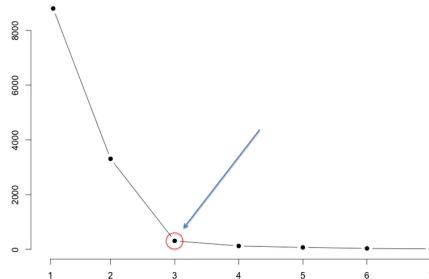


Figure 9.1: The elbow method to find the best number of clusters

9.2 Association

An **association rule** is an implication $X \rightarrow Y$, where X and Y are disjoint item sets (refer to 9.2).

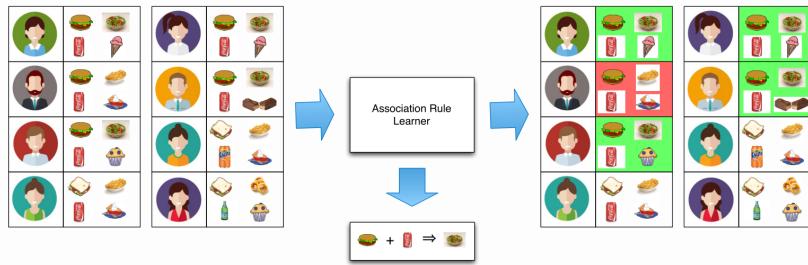


Figure 9.2: A graphical representation of an Association Rule Learner

9.2.1 Support of a Set of Items

Support is the proportion of transactions which contains a specific item set, and thus measures how frequently items are bought together.

$$\text{support}(\{i_1, \dots, i_n\}) = \frac{\#\text{purchases of } \{i_1, \dots, i_n\}}{\#\text{transactions}}$$

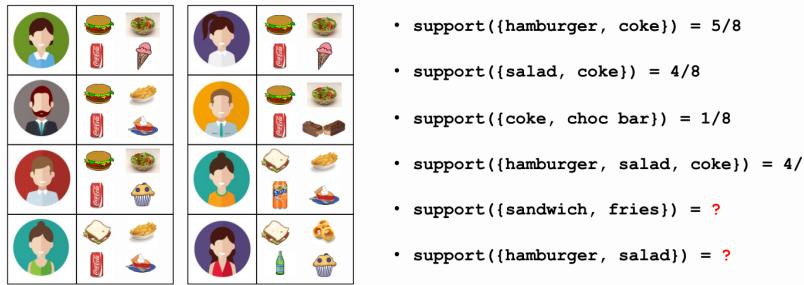


Figure 9.3: Examples of support

9.2.2 Support of an Association Rule

The support of an association rule is defined as

$$\text{support}(X \rightarrow Y) = \text{support}(X \cup Y)$$

The support is *direction invariant* and therefore cannot measure the quality of a directed rule

$$\text{support}(X \rightarrow Y) = \text{support}(Y \rightarrow X)$$



Figure 9.4: Support of association rules

The support measures how frequently an item set occurs in the data. Rules with low support may occur simply by chance, while **good association rules have a high support**.

Theorem 1 *Support = Interestingness*

9.2.3 Confidence of an Association Rule

The **confidence** of an association rule is defined as

$$\text{confidence}(X \rightarrow Y) = \frac{\text{support}(X \cup Y)}{\text{support}(X)}$$

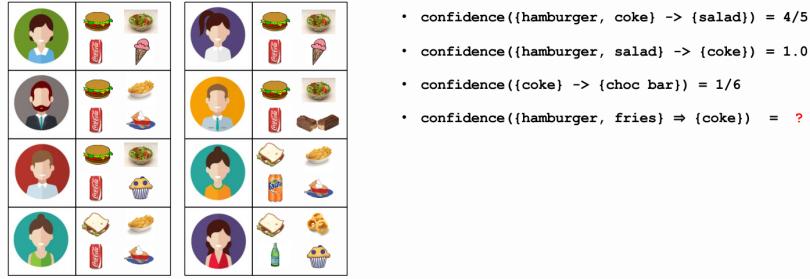


Figure 9.5: Examples of confidence

For a given rule $X \rightarrow Y$, the higher the confidence, the more likely it is for Y to be present in transactions that contain X . Confidence therefore measures reliability or trustworthiness of a rule, and a **good association rule has high confidence**.

Theorem 2 *Confidence = Trustworthiness*

9.2.4 Apriori Algorithm

Given a set of transactions we want to find all rules having a minimum support $\geq \min_s$ and a minimum confidence $\geq \min_c$. The Apriori Algorithm finds such association rules in two steps:

1. Generate frequent item sets satisfying the support threshold
2. Extract rules from frequent item sets satisfying the confidence threshold

The Apriori Algorithm has the following two properties, the second one allows for efficient pruning (refer to figure 9.6):

1. If an item set is **frequent** (has high support), all of its subsets must be frequent too
2. If an item set is **infrequent** (has low support), all of its super-sets must be infrequent too

After the pruning we generate Rules from the Frequent Item Sets and prune this tree as well. The method for pruning is based on the fact that if a rule $[X \rightarrow Y - X]$ violates the confidence threshold, then any rule $[X' \rightarrow Y - X']$ with X' being a subset of X violates the confidence threshold as well (refer to figure 9.7)

9.2.5 Lift of an Association Rule

The **lift** of an association rule is defined as and measures how many times more often X and Y show up together than expected if they were statistically independent.

$$\text{lift}(X \rightarrow Y) = \frac{\text{support}(X \cup Y)}{\text{support}(X) \cdot \text{support}(Y)}$$

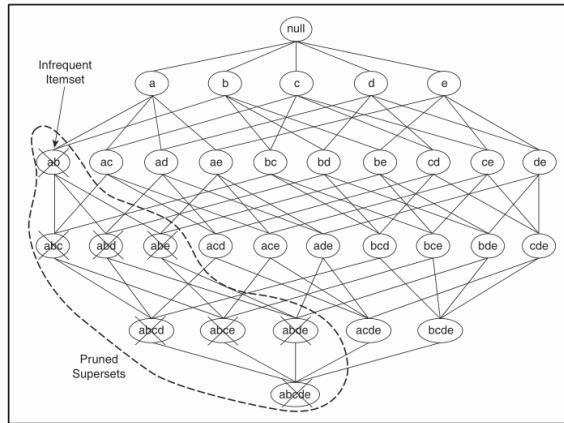


Figure 9.6: Pruning of supersets of sets with low support

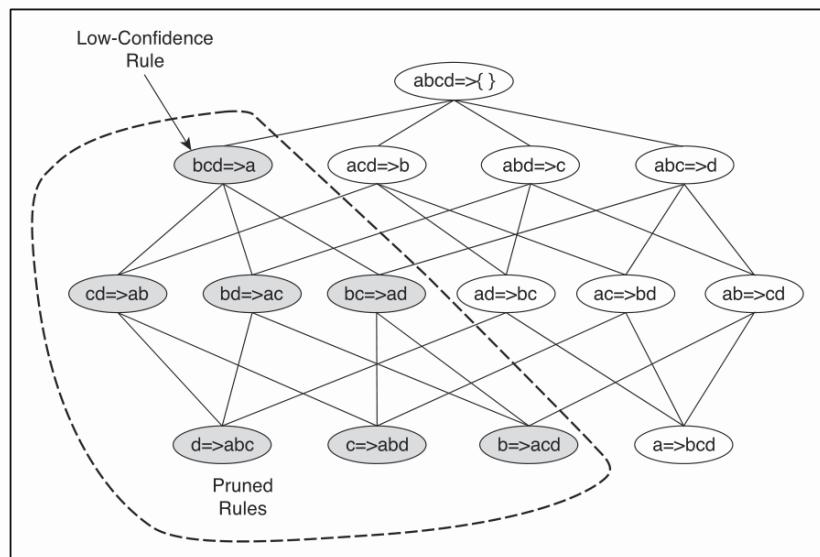


Figure 9.7: Pruning of subset of a low confidence set

- confidence({hamburger, salad} \rightarrow {coke}) = 1.0
- support({hamburger, salad, coke}) = 4/8
- support({hamburger, salad}) = 4/8
- support({coke}) = 6/8
- lift({hamburger, salad} \rightarrow {coke}) = 8/6 > 1

Figure 9.8: Example of lift

lift = 1 X and Y are statistically independent

lift \downarrow 1 indicates that X and Y appear less often together than expected, the occurrence of X has a negative effect on the occurrence of Y and vice-versa, X and Y are **anti-correlated**

lift \uparrow 1 indicates that X and Y appear more often together than expected,

the occurrence of X has a positive effect on the occurrence of Y and vice-versa, X and Y are **correlated**

In general, the larger the lift value, the stronger the association between X and Y . A good rule has high lift.

Theorem 3 $Lift = \text{Association Strength}$

10 Anomaly or Outlier Detection

Anomaly or Outlier Detection is an important topic in unsupervised learning. Anomaly and outlier are used as synonyms. Anomalies are patterns in data that do not conform to a well-defined notion of normal behavior.

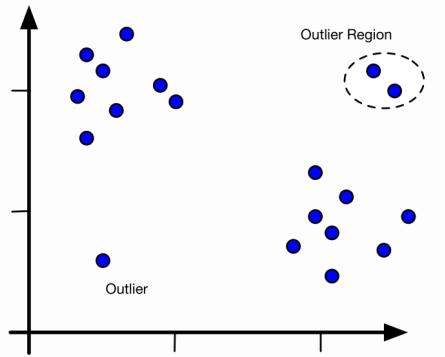


Figure 10.1: Example of an outlier and outlier region

We differentiate between three types of outliers

1. **Global outliers** deviate significantly from the rest of the dataset
2. **Contextual outliers** deviate significantly with respect to a specific context
3. **Collective outliers** deviate as a group from the entire dataset but not necessarily as individuals

We can solve the problem of outlier detection with machine learning:

Supervised Learning Outlier detection can be considered a classification problem with categories *normal* and *outlier*.

When outliers are rare events, collecting enough training data becomes a severe issue, and special measures must be taken because the two classes are extremely imbalanced

Unsupervised Learning These methods assume that outliers deviate from the structural pattern of normal data objects.

1. Statistical Methods
2. Proximity-based Methods
3. Clustering Methods

10.1 Statistical Methods

Statistical methods assume that normal data objects are generated by a stochastic model, and that data not following that model are outliers.

1. Assumption: The data follows a normal distribution with parameters μ and σ^2
2. Method: Find best parameters with Maximum Likelihood method
3. Conclusion: Find threshold where most of the data is located, for example $\mu \pm 3\sigma$ and classify all data outside of this range as outliers

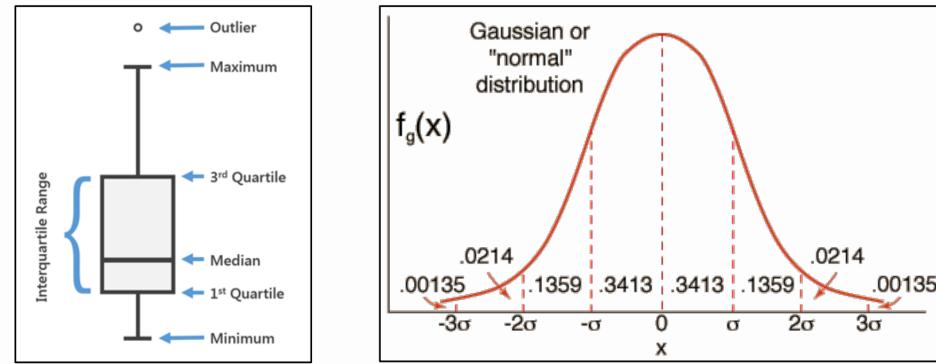


Figure 10.2: Comparison of BoxPlots to Normal Distribution

Observe that these techniques for anomaly detection consider only single variables.

10.2 Proximity-based Methods

In proximity-based methods, records that are far from others are considered outliers. There are two types of proximity-based methods:

1. **Distance based methods** find outliers with respect to the global dataset
2. **Density-based methods** find outliers with respect to local neighbourhood

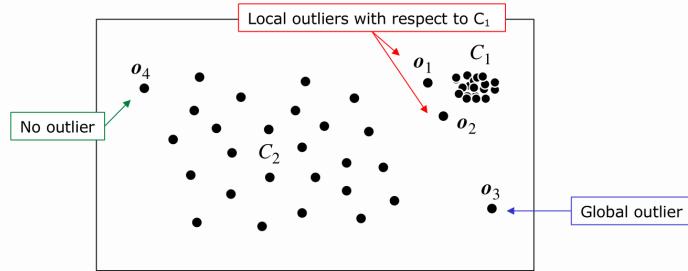


Figure 10.3: Outliers classified by proximity-based methods

10.2.1 Distance-Based Outliers

- Specify a distance threshold $r > 0$ and a fraction threshold $0 < \pi \leq 1$
- For each record count the numbers of other records in the r -neighbourhood
- Consider a record as outlier if $\frac{|\{o' \in D : o \neq o' \text{ and } dist(o, o') \leq r\}|}{|D|} \leq \pi$

10.2.2 Density-Based Outliers

The density around a non-outlier is similar to the density around its neighbours, while the density around an outlier is significantly different from its neighbours (refer to figure 10.4).

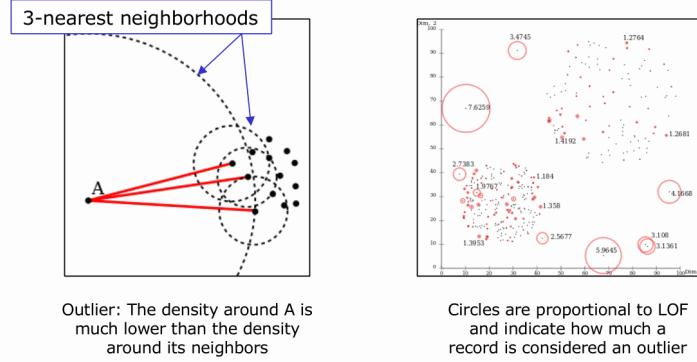


Figure 10.4: Graphical representation of density-based outlier detection

The local outlier factor (LOF) is a score that indicates how likely it is that a certain data point is an outlier. A $\text{LOF} \approx 1$ means no outlier, while $\text{LOF} \gg 1$ means outlier. The k-Distance is the distance of a point to its k-th neighbour.

Reachability Distance The reachability distance is the maximum of the distance between two points and the k-distance of the second point. Consider it as a smoothing term, as a lower distance bound that depends on the neighbourhood density.

$$\text{reachability distance}_k(A, B) = \max\{\text{k-distance}(B), d(A, B)\} \quad (53)$$

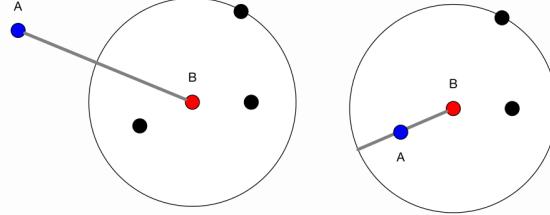


Figure 10.5: Reachability distance visualised

Local Reachability Density (lrd) Calculate the reachability distance of A to all its k-nearest neighbours and take the average of that number, then get the density by taking the inverse. Intuitively, the local reachability density tells how far we have to travel to reach the next point or cluster of points, the lower the local reachability density of a point, the less dense its region, the longer we have to travel.

$$\text{lrd}_k(A) := \frac{1}{\left(\frac{\sum_{B \in N_k(A)} \text{reachability distance}_k(A, B)}{|N_k(A)|} \right)} \quad (54)$$

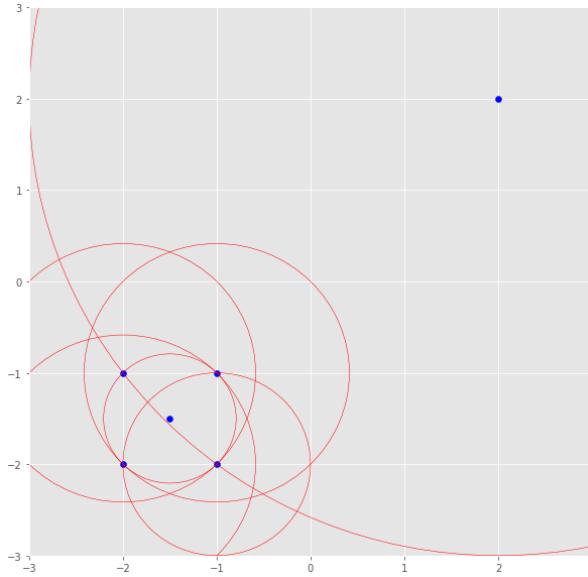


Figure 10.6: The local reachability density is not symmetric

Local Outlier Factor The local outlier factor is the local reachability density of a point in comparison to its k neighbours, more specifically, k ratios of the local reachability distance of each point to its neighbouring points are calculated and averaged.

$$\text{LOF}_k(A) := \frac{\sum_{B \in N_k(A)} \text{lrd}(B)}{\text{lrd}(A)} = \frac{\sum_{B \in N_k(A)} \text{lrd}(B)}{|N_k(A)|} \quad (55)$$

$\text{LOF}(k) \approx 1$ similar density as neighbors : **Normal**

$\text{LOF}(k) < 1$ higher density than neighbors : **Inlier**

$\text{LOF}(k) > 1$ lower density than neighbors : **Outlier**

10.3 Clustering Methods

Clustering-based approaches detect outliers by examining the relationship between records and clusters.

1. Records not belonging to any cluster are outliers
2. Records with a large distance to their closest cluster center are outliers
3. All records in a small and sparse cluster are considered outliers

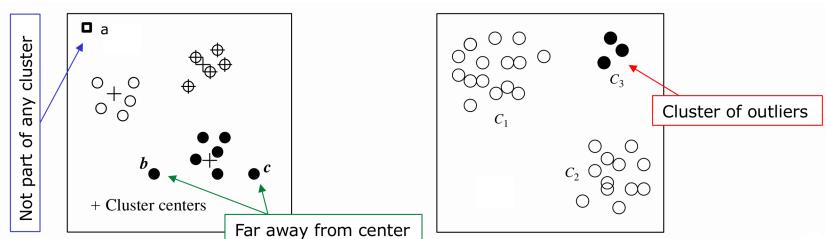


Figure 10.7: Different kind of cluster outliers

Classification-based Approaches Train a classifier, a Support Vector Machine for example, to distinguish normal data from anomalies and generate the decision boundary of the normal class. New objects outside the decision boundary are considered outliers

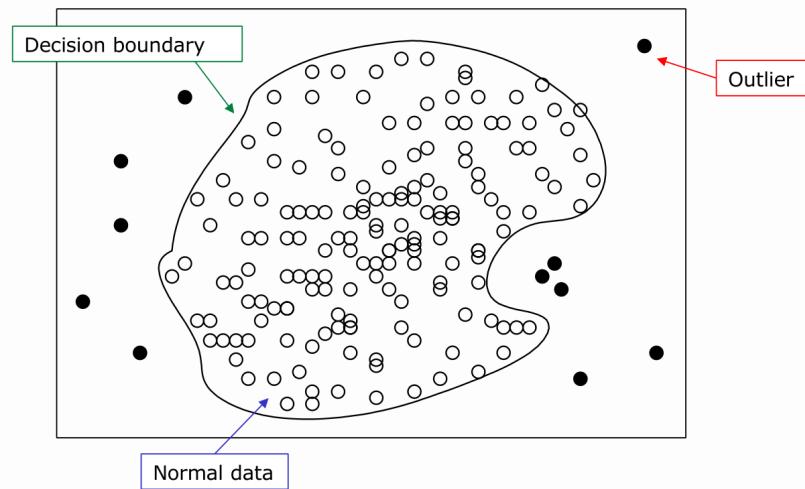


Figure 10.8: Example of a classifier for outlier detection