Fundaments of Machine learning for and with engineering applications

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Definition

Statistics is the science of acquiring and utilizing data

- It comprises tools for data collection, summarization, and interpretation.
- The aim is identifying the underlying structure, trends, and relationships inherent in the data.
- Is it all statistics then? Yes.
- Numbers to data, data to information

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Data properties

Before we talk about machine learning, we need to refresh some terminology.

Population

The universe of all possible outcomes and events.

Sample

A finite subset extracted from the population.

Exhaustivity

The samples covered the population spectra.

Representativity

The population is properly described by the samples.

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We speak of big data when dataset are very large: i.e. many instances and features Models have thus a large set of parameters (and often no one has a clue anymore of what is going on).

- Volume of data
- Variety different types of data sources with different length and scale.
- Frequency of data generation

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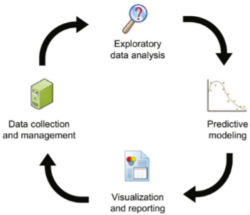
Sampling

Samples shall have no bias (to be randomly selected). If not, the bias has to be corrected for.

Cycle of data

1. Data is collected
2. Checked upon
3. Some modelling
4. Analysis and visualization



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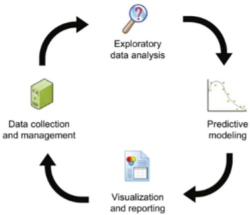

Data quality

1. Data has to be acquired and integrated
2. Data are passed to a quality analysis and control
3. Data cleaning, consistency check. Most of time goes here

Preliminary Modeling

Main tasks:

1. Hunt for redundancy
2. Reduce dimensionality
3. AnOmAlIes removal

- Descriptive modeling (unsupervised learning)
- Predictive modeling (supervised learning)
- The model can be used to guide data acquisition (risky!)

Visualization and reporting

- The data has to be condensed into a visualization to provide input for decisions.
- Depending on the goal, very very different visualizations are possible.
- Use a model to indicate what is undersampled or oversampled.

Summarizing and visualizing data as a starting point for more analysis later on.

- Computing summary statistics (e.g. means and variance)
- Determining conditional probabilities of cause+effect relationships
- Calculating correlation and rank correlation coefficient between two variables
- Visualizing univariate, bivariate and multivariate data
- ...

Exploratory data analysis

Summarizing and visualizing data as a starting point for more analysis later on.

- ...
- Estimating probability coverage levels for different distributions
- Analyzing behaviour of normal distributions
- Calculating confidence interval and sampling distribution for the mean
- Testing for significance of difference in means
- Comparing two different distributions for statistical equivalence
- Developing a nonparametric regression model from given data
- Reducing data dimensionality
- Grouping data

Random Variables

- A random variable is a real valued function that assigns a value to each outcome in the sample space
- A random variable (RV) can be either discrete or continuous
  - Discrete RV
  - Continuous RV

- The probability mass function (PMF),P, of a discrete RV, X, denotes the probability that the RV is equal to a specified value, a.

$$p(a) = p(X = a)$$

- The cumulative distribution function (CDF), F, denotes the sum

$$F(a) = P(X \leq a) = \sum_0^a f(x)dx$$

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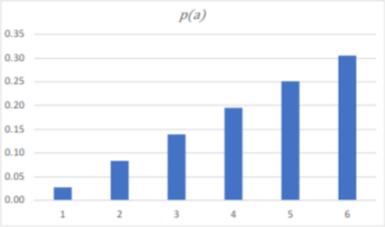
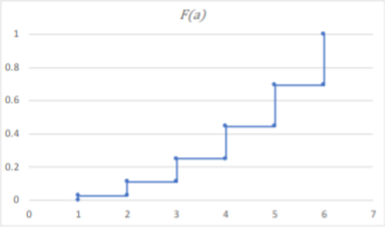
Random Variables

a	1	2	3	4	5	6
$p(a)$	1/36	3/36	5/36	7/36	9/36	11/36
$F(a)$	1/36	4/36	9/36	16/36	25/36	1





Sampling

- What are the effective sampling strategies? (Wind turbine example)
- Solar Panels to determine the efficiency of the source (Usage patterns, energy production forecast)
- Drilling (penetration rate)
- Corrosion extension
- Concrete Rigidity
- etc

Wind turbine example example

Turbine	Height	X	Y	Wind Speed	Air Density	Temperature	Power Output	Rotor Diameter	Hub Height	Air Pressure	Turbulence Intensity
WT-1	80	752.1	3945	7.5	1.225	15	1500	82	80	1013	0.1
WT-1	80	752.2	3945	8	1.223	15	1600	82	80	1012	0.12
WT-1	80	752.3	3945	7.8	1.224	16	1550	82	80	1013	0.11
WT-2	90	753.5	3946	6.5	1.226	14	1400	85	90	1012	0.15
WT-2	90	753.6	3946	7	1.225	14	1500	85	90	1011	0.13
WT-2	90	753.7	3946	7.2	1.227	14	1520	85	90	1012	0.14

Sampling approaches

Experimental design

Grid, parallel, series.

Sampling without replacement

SPR (single point representation).

Sampling with replacement

The number of the members of the population does not change.

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Univariate statistics

- Easy to displaying data:
  - histogram
  - frequency plots
  - cumulative

- Measures of Location
  - Mean, median, mode
  - Quartiles, Percentiles, Quantiles

- Measure of Dispersion (Spread)
  - Standard deviation (sd)
  - Variance (Var) or coefficient of variation

- Measures of shape
  - Skewness, modality

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Histograms

- Task 1: make a histogram from a 2d random distribution
- Task 2: make a 2d heat map from a 2d random distribution

Frequency plots and Histograms

Given a set of data

1. Look for min and max values
2. Divide the range of values into a number of sensible class intervals (bins)
3. Count
4. Make a frequency table (or percentage)
5. Plot (see jupyter notebook)

Does this histogram represent uncertainty?

No. It shows variability, but it can be used to quantify uncertainty.

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Class widths

- Class widths (bin sizes) are usually CONSTANT
  - the height of each bar is proportional to the number of values in it
- If class width are VARIABLE
  - the AREA of each bar is proportional to the number of values in it
- For small samples, the shape of the histogram can be very sensitive to the number and definition of the class intervals

Exercise

Plot a histogram from different random number distributions and bin sizes.

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Cumulative Histogram

- Cumulative frequency
- Each data point can be plotted individually
- It helps to read quantiles and compare distributions
- Practice with your jupyter notebook

Measure of Location: Central Tendency, MEAN

$$m_x = < x > = \bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

Each point weighted equally by $\frac{1}{n}$ (assumption)

- Every element is the data set contributes to the values of the mean
- An average provides a common measure for comparing one set of data to another
- The mean is influenced by the extreme values in the data set
- The mean may not be an actual element if the dataset
- The sum of all deviation from the mean is zero, and the sum of squared deviation is minimized when those deviations are measured from the mean

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Means

- Arithmetic
  - Mean of raw data

$$\frac{1}{n}\sum_{i=1}^{n} x_i$$

- Geometric
  - n^{th} root of product

$$\left(\prod_{i=1}^{n} x_i\right)^{\frac{1}{n}}$$

- Geometric

  * Mean of logarithms $exp\left(\frac{1}{n}\sum_{i=1}^{n} ln(x_i)\right)$

- Harmonic
  - Mean of inverses

$$\left(\frac{1}{n}\sum_{i=1}^{n} \frac{1}{x_i}\right)^{-1}$$

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Median

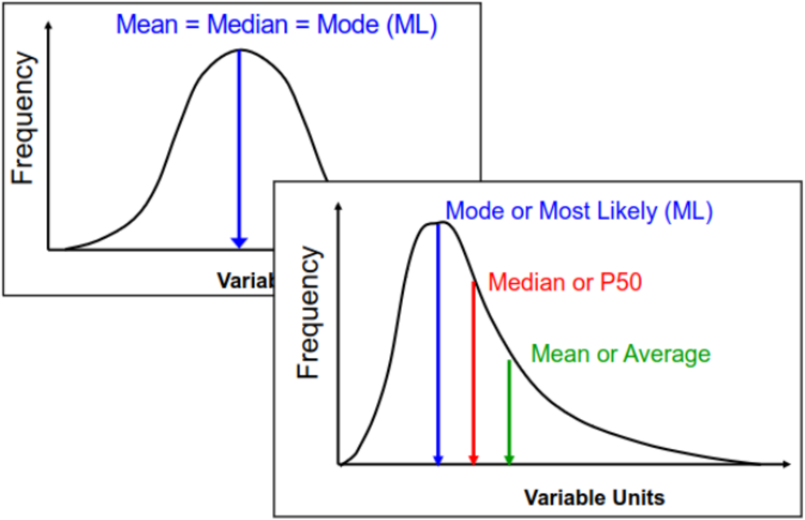
```
if n is odd:
    median = x[(n+1)/2]
else:
    median = x[n/2] + x[(n/2)+1]
```

- On a cumulative density plot, the value of the x-axis that corresponds to 50 % of the y-axis
- Not influenced by extreme values
- May not be contained in the dataset (if n is even)
- For a perfectly symmetrical dataset, means = median

Mode

- The mode is the most frequently occurring data element or the most likely or most probable value (for a pmf)
- A data set may have more than one mode and it thus called multimodal
- A mode is always a data element in the set
- For a perfectly symmetrical dataset, means = median = mode

Distribution Descriptors



Quantiles

Quartiles

The data split into quarters.

Deciles

The data are split into tenths. The fifth decile is also the median.

Percentiles

The data are split into hundredths. P10, P25, P50, P75 and P90 are the most commonly used.

Quantiles

A generalization of splitting data into any fraction

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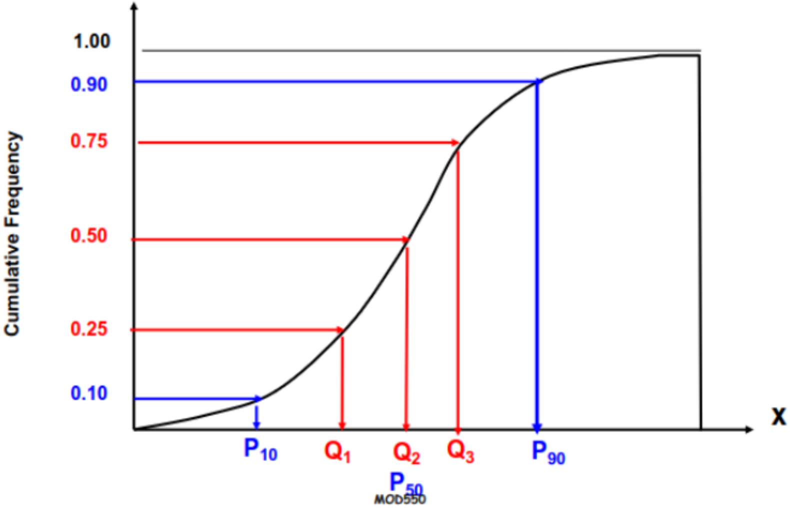


Dispersion (Spread)

Range

R = maximum - minimum

Inter-quantile Range

IQR = Q3 - Q1

Mean Deviation from the Mean

$$\text{MD} = \sum_{i=1}^{n}(x_i - \bar{x})/n$$

Mean Absolute Deviation

$$\text{MAD} = \sum_{i=1}^{n}|x_i - \bar{x}|/n$$

Variance

The variance is the average of squared differences between the sample data points and their mean

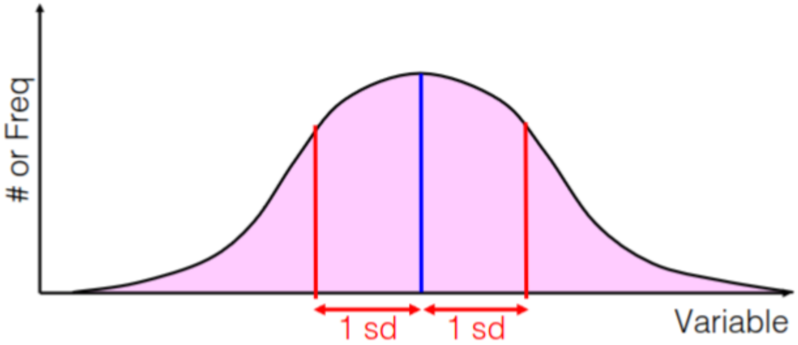
Variance

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

Standard Deviation (SD)

$$s_x = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

Standard Deviation



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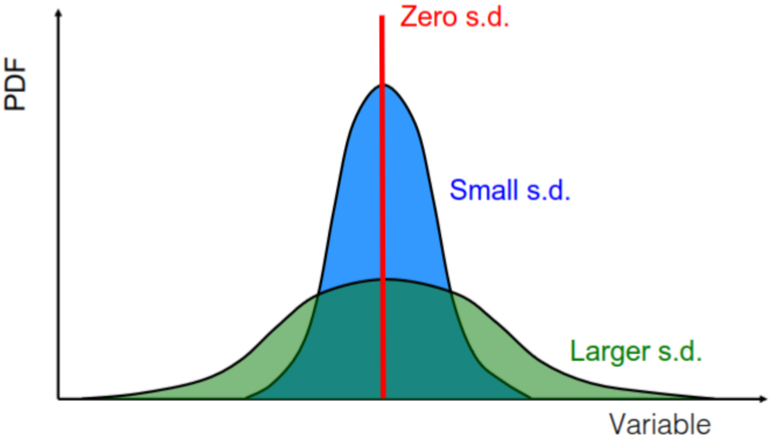


Measures of dispersion

Standard Deviation (SD)

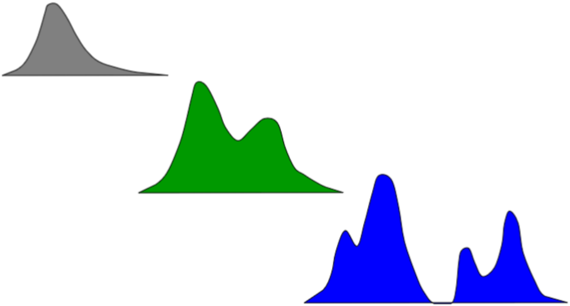
$$SE_x = \frac{s_x}{\sqrt{n}}$$

Coefficient of Variability

$$CV = \frac{s_x}{\bar{x}}$$

Modality

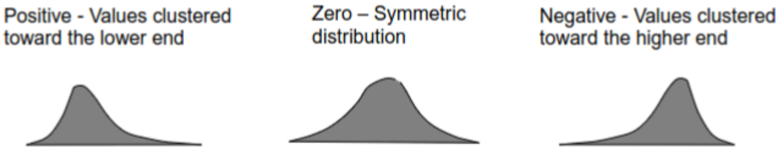
- Unimodal
- Bimodal
- Polymodal



Skewness

It measures the symmetry in a distribution

$$Sk = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^3}{s^3}$$



A bit out of fashion with ML

Distribution Models

Distribution

means of expressing uncertainty or variability

Models

- Uniform: useful when only upper and lower bounds are known
- Triangular: useful when estimates of min, max, mode [P10, P50, P90] are available
- Normal: symmetric model of random errors or unbiased uncertainties with mean of standard deviation specified
  - very common for observed data
  - additive processes tend to be normal as a result of the Central Limit Theorem
- log normal comes from multiplicative uncertainties with mean and standard deviation specified

Uniform Distribution

- The uniform distribution is useful as a rough model for representing low states of knowledge when only the upper and lower bounds are known.
- All possible values within the specified maximum and minimum values are equally likely (b=max, a=min):
- It can express maximum uncertainty

PDF: $f(x) =$

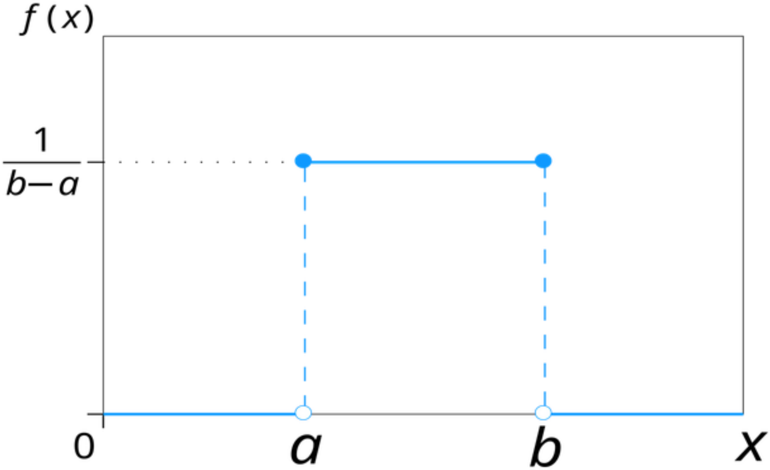
$/frac1b - a, a \leq x \leq b$

CDF: $F(x) =$

$/fracx - ab - a$

Notation: $X \sim U(a, b)$

Uniform Distribution



Triangular distribution

- The triangular distribution can be used for modeling situations, where non extremal (central) values are more likely than the upper and lower bounds.
- Take min, mode and max as inputs. Typically on the basis of subjective judgement:

PDF: $f(x) =$

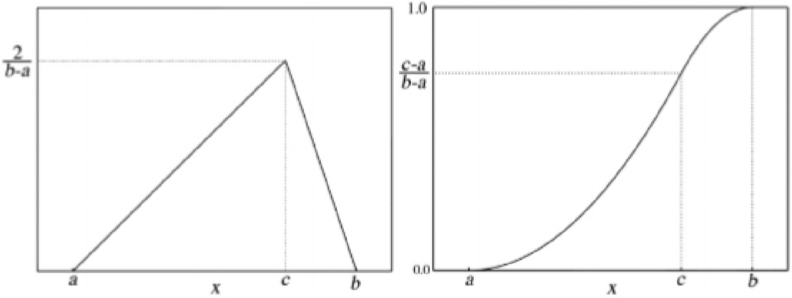
$\frac{2(x-a)}{(b-a)(c-a)}$; if $a \leq x \leq c$
$\frac{2(b-x)}{(b-a)(c-a)}$; if $c \leq x \leq b$

CDF: $F(x) =$

$\frac{(x-a)^2}{(b-a)(c-a)}$; if $a \leq x \leq c$
$1 - \frac{(b-x)^2}{(b-a)(c-a)}$; if $c \leq x \leq b$

Triangular Distribution

Notation: $X \sim T(a, b, c)$



It can be symmetric or asymmetric

Normal Distribution

- The normal distribution ('bell curve' or Gaussian) for modeling unbiased uncertainties and random errors of the additive kind of symmetrical distributions of many material processes and phenomena.
- A commonly cited rational for assuming normal distribution is the central limit theorem, which states that the sum of independent observations asymptotically approaches a normal distribution regardless of the shape of the underlying distributions(s=

PDF:

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} exp\left\{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right\};\ -\infty \leq x \leq \infty$$

CDF: $F(x) =$

has no closed form solution but is often presented using the complementary error function solution

Normal Distribution

Notation: $X \sim G(\mu, \sigma)$

It is a Symmetric distribution around the mean

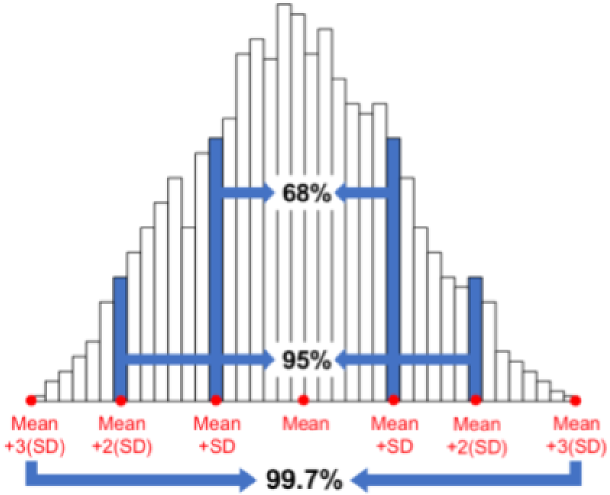
μ is the mean, σ is the standard deviation

$\mu \pm \sigma : 68.3\% probability$

$\mu \pm 2\sigma : 95.4\% probability$

$\mu \pm 3\sigma : 99.7\% probability$

Normal Distribution

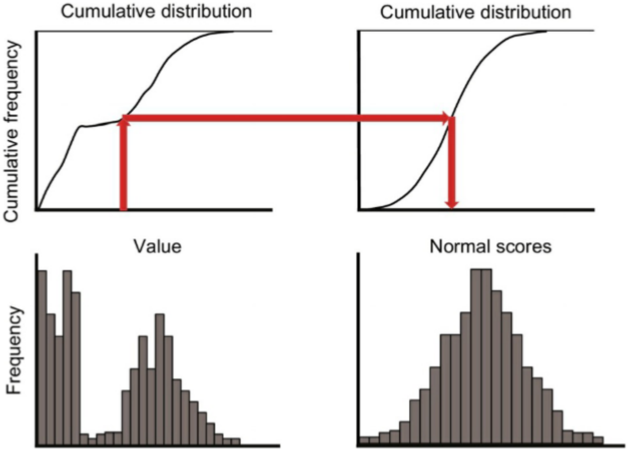


Data transformations

- Often, it is useful to transform a sample distribution into the space of an equivalent normal distribution, where many statistical operations can be easily performed and visualized
- The approach involves a rank-preserving one-to-one transformation.
- Transforming the data so that their distribution matches a prescribed (target) distribution.
- Sometimes we must transform the data...

Normal Score Transformation

1. From data to cumulative distribution.
2. From cumulative distribution and map back.



Match Quantiles

A **linear model**

Considering a univariate case, we have:

$$q = f(x)$$

which relates the **independent variable** x to the **true dependent variable** q.

Assuming a linear model

$$q = \beta_0 + \beta_1 x$$

where β_i are the arbitrary selected coefficients.

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Model set-up

For a given x we do not know the true response q, only the measurementa y_i for experiment i.

We have that:

$$y_i = q_i + \epsilon_i$$

NOTE: do not proceed if you do not fully understand this equation.

which is

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

Discussion point

Does ϵ_i matter? And why so?

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$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

Discussion point

Does ϵ_i matter? And why so?

Estimated model paramters

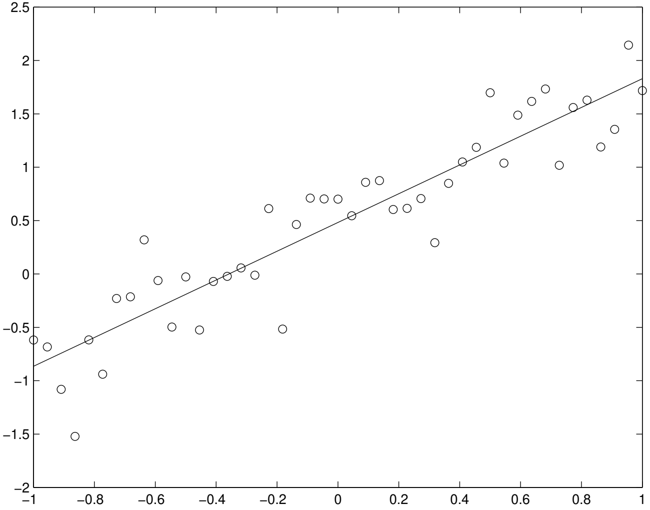
The model parameters β_0, β_1 are unknown, but they can be **estimated**. To distinguish estimates from true model parameters we call them b_0, b_1. These estimates are calculated such that the model

$$\hat{y} = b_0 + b_1 x$$

fits the n different experimental observations as well as possible.

Linear model example

We would like to find the TRUTH (What it it?)



Python Example

```
import numpy as np
import matplotlib.pyplot as plt

def generate_linear_data(n_random_points, noise=16):
    x = np.random.rand(n_random_points) * 10

    # Make 'perfect' data
    true_slope,  true_intercept = 2, 5
    y = true_slope * x + true_intercept

    # Add noise
    y += np.random.randn(n_random_points)*noise

    return x, y, true_slope, true_intercept

# Use the function to generate data
x, y, true_slope, true_intercept = generate_linear_data(
        n_random_points=166,
        noise=3)

# Plot all
plt.plot(x, true_slope*x + true_intercept,
         color='red', label='Truth Line')
plt.scatter(x, y, color='blue', label='Data Points')
plt.show()
```

Estimation of linear regression parameters

For the 1-dimensional problem, we have

$$\hat{y} = b_0 + b_1 x$$

where $\hat{y}$ is the estimated y-value from the approximate model that has been generated from a set of measurements (x_i, y_i). We aim to find the b_i parameters such that the regression line fits the observed data as well as possible.

This means we want to minimise the residuals

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$$e_i = y_i - \hat{y}_i$$

Estimation of linear regression parameters

- Cannot sum e_i values since they might be positive and negative and thus cancel
- Could use e.g. $\sum_{i=1}^{n} |e_i|$, but is mathematically more difficult to handle
- Residual"smallness" measured by $\sum_{i=1}^{n} e_i^2$.

Thus, we find the linear regression coefficients by *minimising*

$$R = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

How?

Regression!

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Let's recaps

Before to continue, let's make sure to have all the main elements clear:

1. Splitting the data in dependent and independent variables
2. Assumption of a linear model between them
3. Recognise the difference between the truth and the estimation
4. Aiming to *minimize* the residuals

Discussion

What happen when the sum of residual is 0 ?

What happens where the data is heavily correlated?

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Regression

To minimize the sum of the square residuals, we can try to solve the following equations:

$$\frac{\partial R}{\partial b_0} = 0$$
$$\frac{\partial R}{\partial b_1} = 0$$

where:

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

$$\sum_{i=1}^{n} (y_i - (b_0 + b_1 x_i))^2 = \sum_{i=1}^{n} u_i^2$$

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Regression

Skipping the math (but you are more than welcome to try), here are the results:

$$\begin{aligned} b_0 &= \bar{y} - b_1\bar{x} \\ b_1 &= \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \end{aligned}$$

Straightforward derivation becomes very cumbersome for multiple variables. Thus, a different approach must be used. Yet, it is important to understand that there is an analytical solution (even if not all the time).

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Linear model(s)

Does a linear model mean only straight lines (or hyperplanes in general)?

That answer to this is *no*. different. In general for a model f to be defined linear, it has to be linear with respect to the unknown parameters $\beta_0, \cdots, \beta_n$. The general linear model is

$$q = \beta_0 + \beta_1 f_1(x_1) + \beta_2 f_2(x_2) + \cdots + \beta_n f_n(x_n)$$

where $f_i(x_i)$ may be non-linear functions. It is the **form** of the equation which makes it linear, i.e. that $f_i(x_i)$ does not depend on the parameters β_i.

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Consider the following model example - is it linear?

$$q = \beta_0 + \beta_1 x_1^2 + \beta_2 x_2^{-1} + \beta_3 \log x_3$$

The answer is *yes* because by simple substitution it is possible to convert this formula into a linear form.

With $h_1 = x_1^2$, $h_2 = x_2^{-1}$ and $h_3 = \log x_3$, then we can formulate the new model:

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Curvilinear models

A special class of linear models which we will investigate later are those which are expressed in terms of *polynomials* (here in only 1D):

$$q = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_m x^m = \sum_{i=0}^{n} \beta_i x^i$$

For n-D case there are a wide range of interaction terms and combinations, that can still be converted to standard linear form.

Such models are sometimes referred to as **curvilinear** instead of non-linear

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Nonlinear models

But there are many other models that cannot be substituted to such a form. For instance:

$$q = \beta_0 + \log(x - \beta_1)$$

No substitution can transform this equation to the linear form.

That is the case for all the model that:

$$q \sim f(x, \beta)$$

Another example is:

$$f(x, \beta) = \frac{x\beta}{x + \beta}$$

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Many variable equation

The general equation would look like:

$$\hat{y} = b_0 + b_1 x_1 + b_2 x_2 + \cdots + b_n x_n = \sum_{j=0}^{m} x_{ij} b_j$$

where we will have to solve all the $n+1$ equations (called the **normal equations**) of the form:

$$\frac{\partial R}{\partial b_j} = 0 \quad \forall j \in [0, n]$$

Is there a way for us to simplify this?

We can use vector and matrix algebra.

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Regression via Matrix operation

Remember that

$$R = \sum_{i=1}^{N} (y_i - \hat{y}_i)^2$$

then we can define the vector **e**:

$$\boldsymbol{e} = \boldsymbol{y} - \hat{\boldsymbol{y}}$$

thus

$$\boldsymbol{e}^T = [(y_1 - \hat{y}_1)\ (y_2 - \hat{y}_2) \cdots\ (y_N - \hat{y}_N)]$$

and can then write

$$R = \boldsymbol{e}^T \boldsymbol{e}$$

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From the following equation:

$$\hat{y}_i = b_0 + \sum_{j=1}^{m} x_{ij} b_j = \sum_{j=0}^{m} x_{ij} b_j$$

where $x_{i0} = 1$
we make the matrix equation:

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{b}$$

where the first column in **X** consists of ones only.

Residual

$$
\begin{aligned}
R &= \boldsymbol{e}^T \boldsymbol{e} \\
&= (\boldsymbol{y} - \hat{\boldsymbol{y}})^T (\boldsymbol{y} - \hat{\boldsymbol{y}}) \\
&= (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{b})^T (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{b}) \\
&= (\boldsymbol{y}^T - \boldsymbol{b}^T \boldsymbol{X}^T)(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{b}) \\
&= \boldsymbol{y}^T \boldsymbol{y} - \boldsymbol{y}^T \boldsymbol{X}\boldsymbol{b} - \boldsymbol{b}^T \boldsymbol{X}^T \boldsymbol{y} \\
&+ \boldsymbol{b}^T \boldsymbol{X}^T \boldsymbol{X}\boldsymbol{b}
\end{aligned}
$$

All the parts of this equation are scalar values. This means e.g. that

$$\boldsymbol{y}^T \boldsymbol{X}\boldsymbol{b} = \boldsymbol{b}^T \boldsymbol{X}^T \boldsymbol{y}$$

This gives

$$R = \boldsymbol{y}^T \boldsymbol{y} - 2\boldsymbol{y}^T \boldsymbol{X}\boldsymbol{b} + \boldsymbol{b}^T \boldsymbol{X}^T \boldsymbol{X}\boldsymbol{b}$$

Residual

But how can we now compute $\frac{\partial R}{\partial b_j}$ more efficiently in matrix form?

Vector differentiation ! Let

$$y = \boldsymbol{a}^T \boldsymbol{x} = a_1 x_1 + \cdots + a_n x_n$$

If

$$\frac{\partial y}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_n} \end{bmatrix} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix} = \boldsymbol{a}$$

and $y = \boldsymbol{x}^T \boldsymbol{a}$, then:

$$\frac{\partial y}{\partial \boldsymbol{x}} = \boldsymbol{a}$$

General solution

In general, when $y = \boldsymbol{x}^T \boldsymbol{A}\boldsymbol{x}$, then

$$\frac{\partial y}{\partial \boldsymbol{x}} = 2\boldsymbol{A}\boldsymbol{x}$$

if $\mathbf{A}$ is symmetric
(check *Matrix calculus* for more properties)

We can use this to compute

$$\frac{\partial R}{\partial \boldsymbol{b}}$$

General solution

We have from above:

$$\begin{aligned} R &= \boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{y}^T\boldsymbol{X}\boldsymbol{b} \\ &+ \boldsymbol{b}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{b} \end{aligned}$$

Vector differentiation gives

$$\frac{\partial R}{\partial \boldsymbol{b}} = 0 - 2\boldsymbol{X}^T\boldsymbol{y} + 2\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{b} = 0$$

Solving this for $\boldsymbol{b}$ we get:

$$\begin{aligned} \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{b} &= \boldsymbol{X}^T\boldsymbol{y} \\ (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{b} &= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ \boldsymbol{b} &= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \end{aligned}$$

Multiple linear regression

Previous equation make the solution of MLR rather obvious!

When we have a matrix of y-variables $\mathbf{Y}$:

$$\boldsymbol{B} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}$$

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These equations give us the **multiple linear regression** (MLR) solution.

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