Fundaments of Machine learning for and with engineering applications

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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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Estimated model paramters

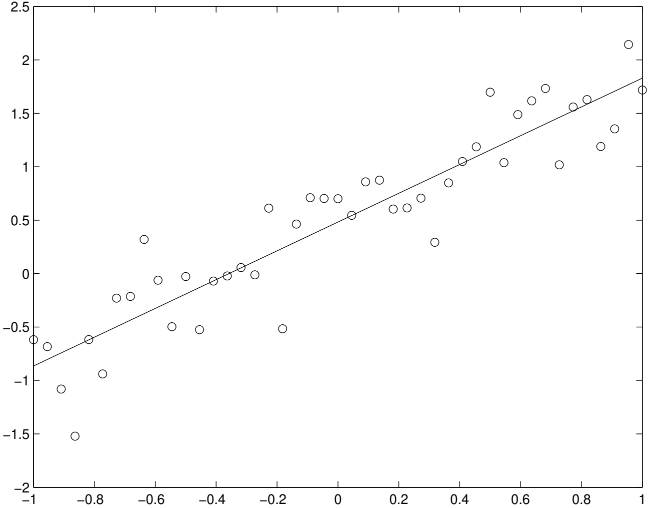
The model parameters β_0, β_1 are unknown, but they can be **estimated**. To distinguish estimates from true model parameters we call them b_0, b_1. These estimates are calculated such that the model

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

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

```python
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

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

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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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where:

$$R = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 =$$
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Skipping the math (but you are more than welcome to try), here are the results:

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\begin{aligned}
b_0 &= \bar{y} - b_1 \bar{x} \\
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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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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.

Many variable equation

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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 $\mathbf{e}$:

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

thus

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

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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:

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

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

Residual

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

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

$$y^T Xb = b^T X^T y$$

This gives

$$R = y^T y - 2y^T Xb + b^T X^T Xb$$

Residual

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

Vector differentiation ! Let

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

If

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

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

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

General solution

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

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

if **A** is symmetric
(check *Matrix calculus* for more properties)

We can use this to compute

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

General solution

We have from above:

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

Vector differentiation gives

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

Solving this for b we get:

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

Multiple linear regression

Previous equation make the solution of MLR rather obvious!

When we have a matrix of y-variables **Y**:

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

in the equation:

$$Y = XB.$$

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

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Model evaluation

We can measure the accuracy of a prediction only when we have a 'truth' to compare with.

Model outcome

The accuracy of a prediction is limited by the available data set (not an universal quantity).

Given a dataset, we split the data in a train and a test set.

One has to be extremely careful to not introduce a **bias** in each of them when splitting. (or to introduce a bias properly, when for example, working with time series.

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Train

A train dataset is a subset of the original data. Generally it is circa a 70 % (common practice, not a rule) of the *INSTANCES*.

For each selected instance, all the features are kept, as their labels.

Random measurements

Some models are able to also consider the sequence of instances; the selection of the train dataset has to be randomised.

The opposite consideration shall be done for time series, where each data point is correlated to the previous.

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Train-Validation-Test

1. Data is split into train, validation and test dataset
2. A model is trained on the train dataset
3. The model (hyper)parameters are improved on the validation dataset
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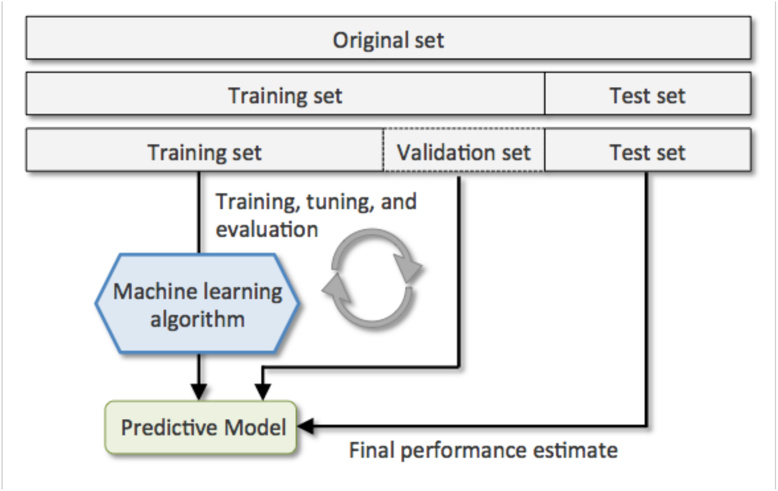

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1. Data is split into train and test.
2. Train dataset is then split into k-folds (different subsets, usually 5 to 10)
3. A model is trained on all k subset but one, sequentially
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