Data Analysis and Machine Learning: Linear Regression and more Advanced Regression Analysis

Morten Hjorth-Jensen[1,2]

[1]Department of Physics, University of Oslo

[2]Department of Physics and Astronomy and National Superconducting Cyclotron Laboratory, Michigan State University

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Regression analysis, overarching aims

Regression modeling deals with the description of the sampling distribution of a given random variable y varies as function of another variable or a set of such variables $\hat{x} = [x_0, x_1, \dots, x_p]^T$. The first variable is called the **dependent**, the **outcome** or the **response** variable while the set of variables $\hat{x}$ is called the independent variable, or the predictor variable or the explanatory variable.

A regression model aims at finding a likelihood function $p(y|\hat{x})$, that is the conditional distribution for y with a given $\hat{x}$. The estimation of $p(y|\hat{x})$ is made using a data set with

- n cases $i = 0, 1, 2, \dots, n-1$
- Response (dependent or outcome) variable y_i with $i = 0, 1, 2, \dots, n-1$
- p Explanatory (independent or predictor) variables $\hat{x}_i = [x_{i0}, x_{i1}, \dots, x_{ip}]$ with $i = 0, 1, 2, \dots, n-1$

The goal of the regression analysis is to extract/exploit relationship between y_i and $\hat{x}_i$ in or to infer causal dependencies, approximations to the likelihood functions, functional relationships and to make predictions .

General linear models

Before we proceed let us study a case from linear algebra where we aim at fitting a set of data $\hat{y} = [y_0, y_1, \dots, y_{n-1}]$. We could think of these data as a result of an experiment or a complicated numerical experiment. These data are functions of a series of variables $\hat{x} = [x_0, x_1, \dots, x_{n-1}]$, that is $y_i = y(x_i)$ with

$i = 0, 1, 2, \dots, n-1$. The variables x_i could represent physical quantities like time, temperature, position etc. We assume that $y(x)$ is a smooth function.

Since obtaining these data points may not be trivial, we want to use these data to fit a function which can allow us to make predictions for values of y which are not in the present set. The perhaps simplest approach is to assume we can parametrize our function in terms of a polynomial of degree $n-1$ with n points, that is

$$y = y(x) \to y(x_i) = \tilde{y}_i + \epsilon_i = \sum_{j=0}^{n-1} \beta_i x_i^j + \epsilon_i,$$

where ϵ_i is the error in our approximation.

Rewriting the fitting procedure as a linear algebra problem

For every set of values y_i, x_i we have thus the corresponding set of equations

$$\begin{aligned}
y_0 &= \beta_0 + \beta_1 x_0^1 + \beta_2 x_0^2 + \dots + \beta_{n-1} x_0^{n-1} + \epsilon_0 \\
y_1 &= \beta_0 + \beta_1 x_1^1 + \beta_2 x_1^2 + \dots + \beta_{n-1} x_1^{n-1} + \epsilon_1 \\
y_2 &= \beta_0 + \beta_1 x_2^1 + \beta_2 x_2^2 + \dots + \beta_{n-1} x_2^{n-1} + \epsilon_2 \\
\dots&\dots \\
y_{n-1} &= \beta_0 + \beta_1 x_{n-1}^1 + \beta_2 x_{n-1}^2 + \dots + \beta_1 x_{n-1}^{n-1} + \epsilon_{n-1}.
\end{aligned}$$

Rewriting the fitting procedure as a linear algebra problem, follows

Defining the vectors

$$\hat{y} = [y_0, y_1, y_2, \dots, y_{n-1}]^T,$$

$$\hat{\beta} = [\beta_0, \beta_1, \beta_2, \dots, \beta_{n-1}]^T,$$

$$\hat{\epsilon} = [\epsilon_0, \epsilon_1, \epsilon_2, \dots, \epsilon_{n-1}]^T,$$

and the matrix

$$\hat{X} = \begin{bmatrix}
1 & x_0^1 & x_0^2 & \dots & \dots & x_0^{n-1} \\
1 & x_1^1 & x_1^2 & \dots & \dots & x_1^{n-1} \\
1 & x_2^1 & x_2^2 & \dots & \dots & x_2^{n-1} \\
\dots & \dots & \dots & \dots & \dots & \dots \\
1 & x_{n-1}^1 & x_{n-1}^2 & \dots & \dots & x_{n-1}^{n-1}
\end{bmatrix}$$

we can rewrite our equations as

$$\hat{y} = \hat{X}\hat{\beta} + \hat{\epsilon}.$$

Generalizing the fitting procedure as a linear algebra problem

We are obviously not limited to the above polynomial. We could replace the various powers of x with elements of Fourier series, that is, instead of x_i^j we could have $\cos(jx_i)$ or $\sin(jx_i)$, or time series or other orthogonal functions. For every set of values y_i, x_i we can then generalize the equations to

$$\begin{aligned}
y_0 &= \beta_0 x_{00} + \beta_1 x_{01} + \beta_2 x_{02} + \dots + \beta_{n-1} x_{0n-1} + \epsilon_0 \\
y_1 &= \beta_0 x_{10} + \beta_1 x_{11} + \beta_2 x_{12} + \dots + \beta_{n-1} x_{1n-1} + \epsilon_1 \\
y_2 &= \beta_0 x_{20} + \beta_1 x_{21} + \beta_2 x_{22} + \dots + \beta_{n-1} x_{2n-1} + \epsilon_2 \\
\dots & \dots \\
y_i &= \beta_0 x_{i0} + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_{n-1} x_{in-1} + \epsilon_i \\
\dots & \dots \\
y_{n-1} &= \beta_0 x_{n-1,0} + \beta_1 x_{n-1,2} + \beta_2 x_{n-1,2} + \dots + \beta_1 x_{n-1,n-1} + \epsilon_{n-1}.
\end{aligned}$$

Generalizing the fitting procedure as a linear algebra problem

We redefine in turn the matrix $\hat{X}$ as

$$\hat{X} = \begin{bmatrix} x_{00} & x_{01} & x_{02} & \dots & \dots & x_{0,n-1} \\ x_{10} & x_{11} & x_{12} & \dots & \dots & x_{1,n-1} \\ x_{20} & x_{21} & x_{22} & \dots & \dots & x_{2,n-1} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ x_{n-1,0} & x_{n-1,1} & x_{n-1,2} & \dots & \dots & x_{n-1,n-1} \end{bmatrix}$$

and without loss of generality we rewrite again our equations as

$$\hat{y} = \hat{X}\hat{\beta} + \hat{\epsilon}.$$

The left-hand side of this equation forms know. Our error vector $\hat{\epsilon}$ and the parameter vector $\hat{\beta}$ are our unknow quantities. How can we obtain the optimal set of β_i values?

Optimizing our parameters

We have defined the matrix $\hat{X}$

$$\begin{aligned} y_0 &= \beta_0 x_{00} + \beta_1 x_{01} + \beta_2 x_{02} + \cdots + \beta_{n-1} x_{0n-1} + \epsilon_0 \\ y_1 &= \beta_0 x_{10} + \beta_1 x_{11} + \beta_2 x_{12} + \cdots + \beta_{n-1} x_{1n-1} + \epsilon_1 \\ y_2 &= \beta_0 x_{20} + \beta_1 x_{21} + \beta_2 x_{22} + \cdots + \beta_{n-1} x_{2n-1} + \epsilon_1 \\ &\dots\dots \\ y_i &= \beta_0 x_{i0} + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_{n-1} x_{in-1} + \epsilon_1 \\ &\dots\dots \\ y_{n-1} &= \beta_0 x_{n-1,0} + \beta_1 x_{n-1,2} + \beta_2 x_{n-1,2} + \cdots + \beta_1 x_{n-1,n-1} + \epsilon_{n-1}. \end{aligned}$$

Optimizing our parameters, more details

We well use this matrix to define the approximation $\hat{\tilde{y}}$ via the unknown quantity $\hat{\beta}$ as

$$\hat{\tilde{y}} = \hat{X}\hat{\beta},$$

and in order to find the optimal parameters β_i instead of solving the above linear algebra problem, we define a function which gives a measure of the spread between the values y_i (which represent hopefully the exact values) and the parametrized values $\tilde{y}_i$, namely

$$Q(\hat{\beta}) = \sum_{i=0}^{n-1} (y_i - \tilde{y}_i)^2 = \left(\hat{y} - \hat{\tilde{y}}\right)^T \left(\hat{y} - \hat{\tilde{y}}\right),$$

or using the matrix $\hat{X}$ as

$$Q(\hat{\beta}) = \left(\hat{y} - \hat{X}\hat{\beta}\right)^T \left(\hat{y} - \hat{X}\hat{\beta}\right).$$

Interpretations and optimizing our parameters

The function

$$Q(\hat{\beta}) = \left(\hat{y} - \hat{X}\hat{\beta}\right)^T \left(\hat{y} - \hat{X}\hat{\beta}\right),$$

can be linked to the variance of the quantity y_i if we interpret the latter as the mean value of for example a numerical experiment. When linking below with the maximum likelihood approach below, we will indeed interpret y_i as a mean value

$$y_i = \langle y_i \rangle = \beta_0 x_{i,0} + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \cdots + \beta_{n-1} x_{i,n-1} + \epsilon_i,$$

where $\langle y_i \rangle$ is the mean value. Keep in mind also that till now we have treated y_i as the exact value. Normally, the response (dependent or outcome) variable y_i the outcome of a numerical experiment or another type of experiment and is thus only an approximation to the true value. It is then always accompanied by an error estimate, often limited to a statistical error estimate given by the standard deviation discussed earlier. In the discussion here we will treat y_i as our exact value for the response variable.

In order to find the parameters β_i we will then minimize the spread of $Q(\hat{\beta})$ by requiring

$$\frac{\partial Q(\hat{\beta})}{\partial \beta_j} = \frac{\partial}{\partial \beta_j} \left[\sum_{i=0}^{n-1} \left(y_i - \beta_0 x_{i,0} - \beta_1 x_{i,1} - \beta_2 x_{i,2} - \dots - \beta_{n-1} x_{i,n-1}\right)^2 \right] = 0,$$

which results in

$$\frac{\partial Q(\hat{\beta})}{\partial \beta_j} = -2 \left[\sum_{i=0}^{n-1} x_{ij} \left(y_i - \beta_0 x_{i,0} - \beta_1 x_{i,1} - \beta_2 x_{i,2} - \dots - \beta_{n-1} x_{i,n-1}\right) \right] = 0,$$

or in a matrix-vector form as

$$\frac{\partial Q(\hat{\beta})}{\partial \hat{\beta}} = 0 = \hat{X}^T \left(\hat{y} - \hat{X}\hat{\beta} \right).$$

Interpretations and optimizing our parameters

We can rewrite

$$\frac{\partial Q(\hat{\beta})}{\partial \hat{\beta}} = 0 = \hat{X}^T \left(\hat{y} - \hat{X}\hat{\beta} \right),$$

as

$$\hat{X}^T \hat{y} = \hat{X}^T \hat{X} \hat{\beta},$$

and if the matrix $\hat{X}^T \hat{X}$ is invertible we have the solution

$$\hat{\beta} = \left(\hat{X}^T \hat{X} \right)^{-1} \hat{X}^T \hat{y}.$$

Interpretations and optimizing our parameters

The residuals $\hat{\epsilon}$ are in turn given by

$$\hat{\epsilon} = \hat{y} - \hat{\tilde{y}} = \hat{y} - \hat{X}\hat{\beta},$$

and with

$$\hat{X}^T \left(\hat{y} - \hat{X}\hat{\beta} \right) = 0,$$

we have

$$\hat{X}^T \hat{\epsilon} = \hat{X}^T \left(\hat{y} - \hat{X}\hat{\beta} \right) = 0,$$

meaning that the solution for $\hat{\beta}$ is the one which minimizes the residuals. Later we will link this with the maximum likelihood approach.

The χ^2 function

Normally, the response (dependent or outcome) variable y_i the outcome of a numerical experiment or another type of experiment and is thus only an approximation to the true value. It is then always accompanied by an error estimate, often limited to a statistical error estimate given by the standard deviation discussed earlier. In the discussion here we will treat y_i as our exact value for the response variable.

Introducing the standard deviation σ_i for each measurement y_i, we define now the χ^2 function as

$$\chi^2(\hat{\beta}) = \sum_{i=0}^{n-1}\frac{\left(y_i-\tilde{y}_i\right)^2}{\sigma_i^2} = \left(\hat{y}-\hat{\tilde{y}}\right)^T\frac{1}{\hat{\Sigma}^2}\left(\hat{y}-\hat{\tilde{y}}\right),$$

where the matrix $\hat{\Sigma}$ is a diagonal matrix with σ_i as matrix elements.

The χ^2 function

In order to find the parameters β_i we will then minimize the spread of $\chi^2(\hat{\beta})$ by requiring

$$\frac{\partial\chi^2(\hat{\beta})}{\partial\beta_j} = \frac{\partial}{\partial\beta_j}\left[\sum_{i=0}^{n-1}\left(\frac{y_i-\beta_0x_{i,0}-\beta_1x_{i,1}-\beta_2x_{i,2}-\dots-\beta_{n-1}x_{i,n-1}}{\sigma_i}\right)^2\right]=0,$$

which results in

$$\frac{\partial\chi^2(\hat{\beta})}{\partial\beta_j} = -2\left[\sum_{i=0}^{n-1}\frac{x_{ij}}{\sigma_i}\left(\frac{y_i-\beta_0x_{i,0}-\beta_1x_{i,1}-\beta_2x_{i,2}-\dots-\beta_{n-1}x_{i,n-1}}{\sigma_i}\right)\right]=0,$$

or in a matrix-vector form as

$$\frac{\partial\chi^2(\hat{\beta})}{\partial\hat{\beta}} = 0 = \hat{A}^T\left(\hat{b}-\hat{A}\hat{\beta}\right).$$

where we have defined the matrix $\hat{A}=\hat{X}/\hat{\Sigma}$ with matrix elements $a_{ij}=x_{ij}/\sigma_i$ and the vector $\hat{b}$ with elements $b_i=y_i/\sigma_i$.

The χ^2 function

We can rewrite

$$\frac{\partial\chi^2(\hat{\beta})}{\partial\hat{\beta}} = 0 = \hat{A}^T\left(\hat{b}-\hat{A}\hat{\beta}\right),$$

as

$$\hat{A}^T\hat{b}=\hat{A}^T\hat{A}\hat{\beta},$$

and if the matrix $\hat{A}^T\hat{A}$ is invertible we have the solution

$$\hat{\beta}=\left(\hat{A}^T\hat{A}\right)^{-1}\hat{A}^T\hat{b}.$$

The χ^2 function

If we then introduce the matrix

$$\hat{H} = \hat{A}^T\hat{A},$$

we have then the following expression for the parameters β_j (the matrix elements of $\hat{H}$ are h_{ij})

$$\beta_j = \sum_{k=0}^{p-1} h_{jk}\sum_{i=0}^{n-1}\frac{y_i}{\sigma_i}\frac{x_{ik}}{\sigma_i} = \sum_{k=0}^{p-1} h_{jk}\sum_{i=0}^{n-1} b_i a_{ik}$$

We state without proof the expression for the uncertainty in the parameters β_j as

$$\sigma^2(\beta_j) = \sum_{i=0}^{n-1}\sigma_i^2\left(\frac{\partial\beta_j}{\partial y_i}\right)^2,$$

resulting in

$$\sigma^2(\beta_j) = \left(\sum_{k=0}^{p-1} h_{jk}\sum_{i=0}^{n-1} a_{ik}\right)\left(\sum_{l=0}^{p-1} h_{jl}\sum_{m=0}^{n-1} a_{ml}\right) = h_{jj}!$$

The χ^2 function

The first step here is to approximate the function y with a first-order polynomial, that is we write

$$y = y(x) \rightarrow y(x_i) \approx \beta_0 + \beta_1 x_i.$$

By computing the derivatives of χ^2 with respect to β_0 and β_1 show that these are given by

$$\frac{\partial\chi^2(\hat{\beta})}{\partial\beta_0} = -2\left[\sum_{i=0}^{1}\left(\frac{y_i - \beta_0 - \beta_1 x_i}{\sigma_i^2}\right)\right] = 0,$$

and

$$\frac{\partial\chi^2(\hat{\beta})}{\partial\beta_0} = -2\left[\sum_{i=0}^{1} x_i\left(\frac{y_i - \beta_0 - \beta_1 x_i}{\sigma_i^2}\right)\right] = 0.$$

The χ^2 function

We define then

$$\gamma = \sum_{i=0}^{1}\frac{1}{\sigma_i^2},$$

$$\gamma_x = \sum_{i=0}^{1}\frac{x_i}{\sigma_i^2},$$

$$\gamma_y = \sum_{i=0}^{1} \left(\frac{y_i}{\sigma_i^2}\right),$$

$$\gamma_{xx} = \sum_{i=0}^{1} \frac{x_i x_i}{\sigma_i^2},$$

$$\gamma_{xy} = \sum_{i=0}^{1} \frac{y_i x_i}{\sigma_i^2},$$

and show that

$$\beta_0 = \frac{\gamma_{xx}\gamma_y - \gamma_x\gamma_y}{\gamma\gamma_{xx} - \gamma_x^2},$$

$$\beta_1 = \frac{\gamma_{xy}\gamma - \gamma_x\gamma_y}{\gamma\gamma_{xx} - \gamma_x^2}.$$

The LSM suffers often from both being underdetermined and overdetermined in the unknown coefficients β_i. A better approach is to use the Singular Value Decomposition (SVD) method discussed below.

The singular value decompostion

How can we use the singular value decomposition to find the parameters β_j? More details will come. We first note that a general $m \times n$ matrix $\hat{A}$ can be written in terms of a diagonal matrix $\hat{\Sigma}$ of dimensionality $n \times n$ and two orthognal matrices $\hat{U}$ and $\hat{V}$, where the first has dimensionality $m \times n$ and the last dimensionality $n \times n$. We have then

$$\hat{A} = \hat{U}\hat{\Sigma}\hat{V}$$