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

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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,

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

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

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

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

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

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

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 $\hat{X}$

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

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.

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 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

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