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Business Analytics & Machine Learning
Tutorial sheet 3: Logistic Regression – Solution

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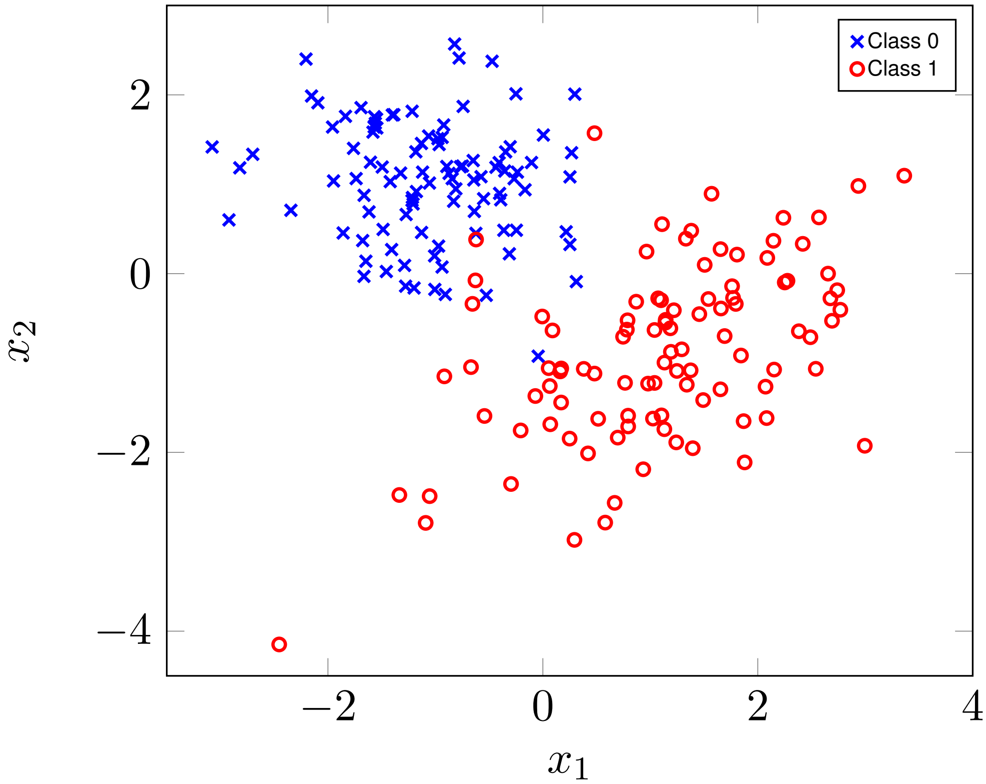
Exercise T3.1 *Logistic regression for a 2D classification problem*

You are given the data set in *2d-classification-data.csv* which is also visualized below. The data consists of two-dimensional points belonging to one of two classes: 0 or 1.



In this exercise, we are going to find a predicting model which can classify new data points.
Consider the logistic regression model:

$$\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$

$$\iff$$

$$p(y=1|x_1,x_2) = \sigma(\beta_0 + \beta_1 x_1 + \beta_2 x_2) = \frac{e^{\beta_0+\beta_1 x_1+\beta_2 x_2}}{1+e^{\beta_0+\beta_1 x_1+\beta_2 x_2}}$$

a) For which values $x = (x_1, x_2)$ does the logistic regression model output $p(y=1|x) = p(y=0|x)$? Derive a functional description $x_2 = f(x_1)$ which describes the corresponding decision boundary.

b) Without computation, draw a straight line which roughly separates the two classes. Consider this as a decision rule whether a sample belongs to class 0 or class 1: How many samples from the data set are miss-classified (attributed to the wrong class)?

c) Using Python and scikit-learn (or statsmodels), derive the optimal parameters for the logistic regression model. If you like, you may use the provided template notebook for this purpose.

d) Draw the decision boundary of the optimal model. How many samples are miss-classified? Can you explain why the model might perform worse (w.r.t the number of miss-classified samples) than your own decision boundary from b)?

Solution

a) By inserting the definition of $p(y = 1|x)$ and the fact that $p(y = 1|x) + p(y = 0|x) = 1$, we find:

$$
\begin{aligned}
& & p(y=1|x) &= p(y=0|x) \\
&\Leftrightarrow & p(y=1|x) &= 1 - p(y=1|x) \\
&\Leftrightarrow & p(y=1|x) &= \frac{1}{2} \\
&\Leftrightarrow & \sigma(\beta_0 + \beta_1 x_1 + \beta_2 x_2) &= \frac{1}{2} \\
&\Leftrightarrow & \frac{e^{\beta_0 + \beta_1 x_1 + \beta_2 x_2}}{1 + e^{\beta_0 + \beta_1 x_1 + \beta_2 x_2}} &= \frac{1}{2} \\
&\Leftrightarrow & e^{\beta_0 + \beta_1 x_1 + \beta_2 x_2} &= \frac{1}{2} + \frac{1}{2} e^{\beta_0 + \beta_1 x_1 + \beta_2 x_2} \\
&\Leftrightarrow & e^{\beta_0 + \beta_1 x_1 + \beta_2 x_2} &= 1 \\
&\Leftrightarrow & \beta_0 + \beta_1 x_1 + \beta_2 x_2 &= \ln(1) = 0
\end{aligned}
$$

From the last equation, we can derive:

$$x_2 = f(x_1) = -\frac{\beta_0}{\beta_2} - \frac{\beta_1}{\beta_2} x_1$$

We observe that this is a linear function, represented by a straight.

This straight describes the decision boundary:

$$
\begin{aligned}
x_2 < f(x_1) &\implies & p(y=1|x) > p(y=0|x) \\
x_2 > f(x_1) &\implies & p(y=1|x) < p(y=0|x)
\end{aligned}
$$

(*Note*: The direction of the inequalities depend on the sign of β_2.)

b) See figure 1. We count 6 miss-classified samples.

c) Please have a look at the provided Jupyter Notebook for the solution.

The optimal parameter values are:

β_0	0.304
β_1	2.856
β_2	-2.685

Figure 2 shows the fitted regression model.

Note: If you use scikit-learn's `LogisticRegression` and don't specify that there is no penalty, you might end up with the following parameters:

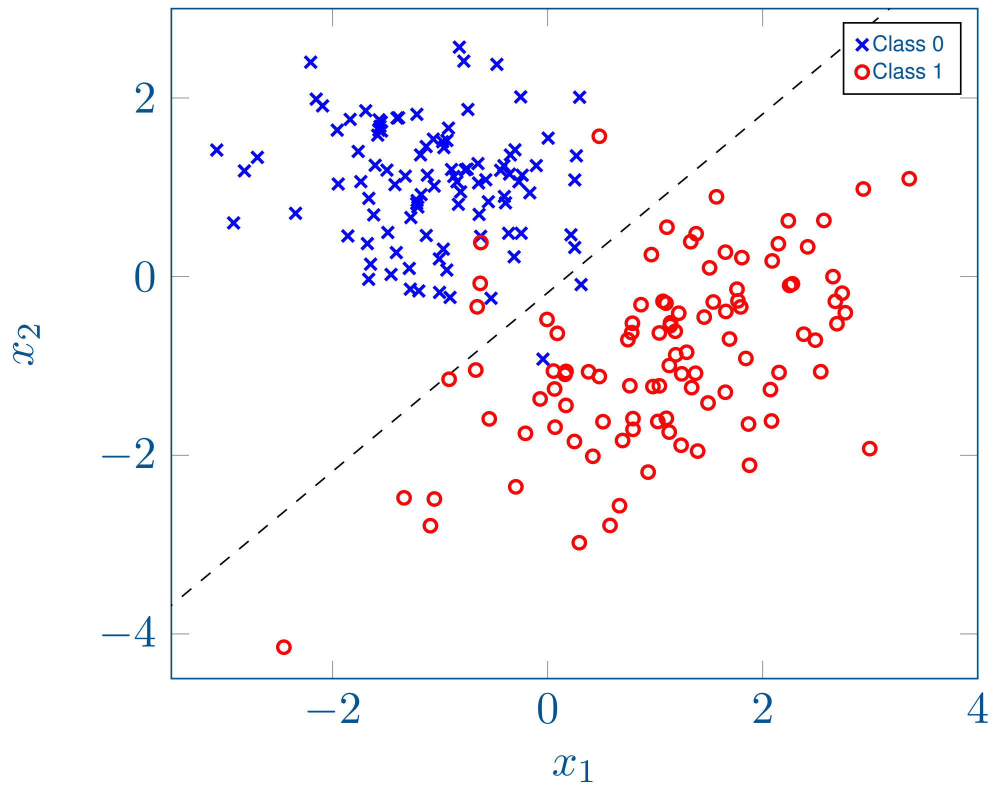


Figure 1 Human decision boundary to separate the two classes.

β_0	0.173
β_1	2.156
β_2	-2.082

They are the optimal (minimizing) values for the *regularized* loss

$$\hat{\mathcal{L}}(\beta) = -LL(\beta) + \frac{1}{2}\|\beta\|_2^2$$

where $LL(\beta)$ is the log-likelihood.

d) The fitted logistic regression model has 7 miss-classified samples. Note that the model thus has one more wrongly attributed sample than the self-drawn (human) boundary.

The reason for this is that the model does *not* minimize the number of miss-classified samples. Instead, it maximizes the (log-)likelihood ($LL(\beta)$) of the data

$$LL(\beta) = \sum_{i=1}^{n} y_i \ln \sigma(\beta^T x_i) + (1 - y_i) \ln(1 - \sigma(\beta^T x_i))$$

Values β^* which maximize $LL(\beta)$ not necessarily minimize the number of miss-classified data points! Still, this formulation makes sense since it helps us to explain the data from a probabilistic perspective and lets us use gradient-based optimization methods.

For a better intuition, we visualize the model-predicted probabilities in figure 3.

Note: If you used scikit-learn's `LogisticRegression` with a penalty term, the loss is modified further. This may also have a (minor) effect on the number of missclassified samples.

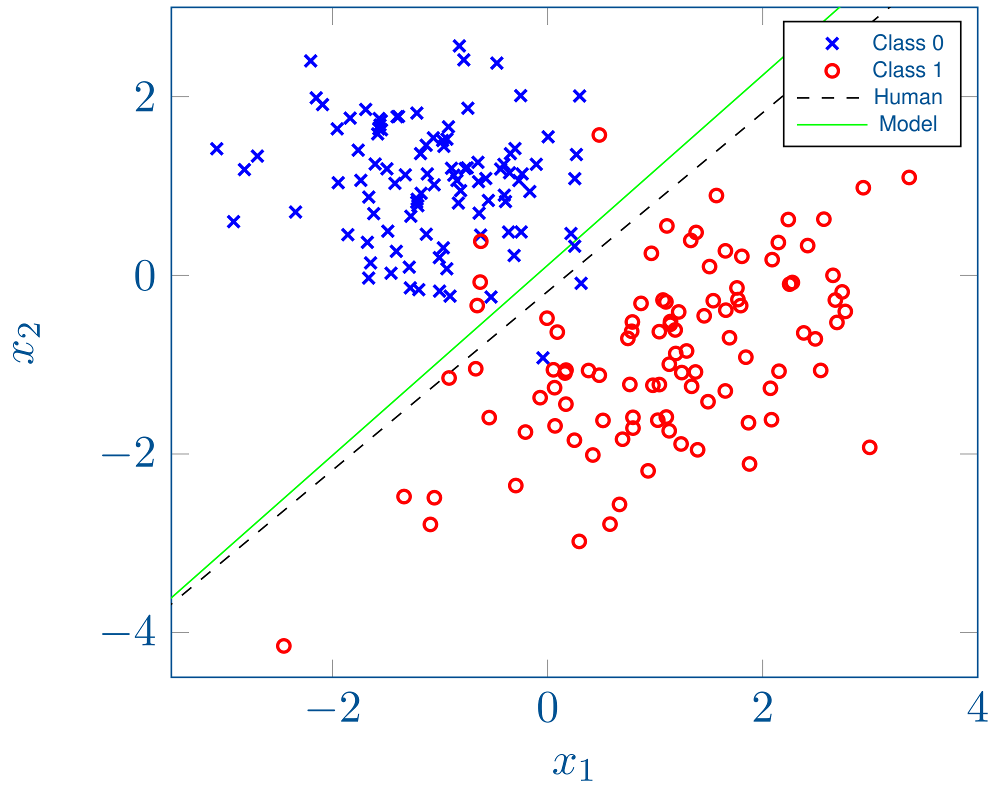


Figure 2 Decision boundary by logistic regression model (Model) and human (Human)

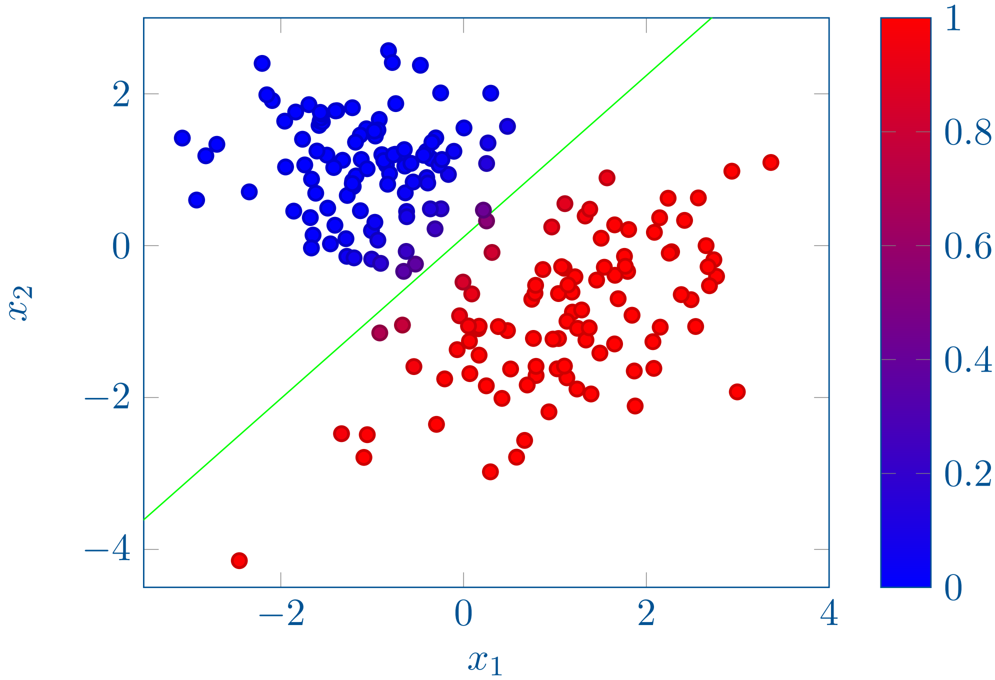


Figure 3 Predicted probabilities of class 1 for all samples.

Exercise T3.2 *Maximum likelihood estimation*

You are given the following dataset with the dependent binary variable y and the independent variable x.

x	y
1	0
2	0
2.5	1
4	1

Based on these data points we want to create a logistic regression model with the logistic function σ (or more broadly a sigmoid function):

$$\Pr[Y|X] = p(x) = \sigma(\beta_0 + \beta_1 x) = \frac{e^{\beta_0+\beta_1 x}}{1 + e^{\beta_0+\beta_1 x}}.$$

To estimate the logistic regression coefficients, we will use *maximum likelihood estimation*.
To simplify notation, let $p_i = p(x_i) = \sigma(z_i)$ and $z_i = \beta_0 + \beta_1 x_i$.

a) Determine the likelihood function $L(\beta)$.
Hint: To keep everything simple, it is sufficient to formulate L in terms of p_i (which includes the dependency on β).

b) Find the gradient for the log of the likelihood function $LL(\beta)$. The gradient is defined as:

$$\nabla LL(\beta) = \begin{pmatrix} \frac{\partial LL(\beta)}{\partial \beta_0} \\ \frac{\partial LL(\beta)}{\partial \beta_1} \end{pmatrix}.$$

Hint: Use the chain rule: $\frac{\partial LL}{\partial \beta_j} = \sum_{i=1}^{n} \frac{\partial LL}{\partial p_i} \frac{\partial p_i}{\partial z_i} \frac{\partial z_i}{\partial \beta_j}$ with $z_i = \beta_0 + \beta_1 x_i$. You may use the following derivative of the logistic function σ without proof: $\sigma'(z_i) = \sigma(z_i)(1 - \sigma(z_i))$.

c) Given the initial values $\beta^{(0)} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and a learning rate $\alpha = 0.2$, calculate the coefficients after the first iteration of gradient ascent.

d) If a linear regression model was fitted to a logistic regression dataset, what could be the problems w.r.t. the Gauss Markov properties?

Solution

a) The likelihood function is the probability that the dependent variables are observed, assuming the data set is produced by the logistic model. For a single data point, its likelihood is p_i if $y_i = 1$ and $1 - p_i$ if $y_i = 0$. Therefore,

$$L(y \mid x, \beta) = \prod_{i=1}^{n} p_i^{y_i} (1 - p_i)^{1-y_i} = p_3 p_4 (1 - p_1)(1 - p_2). \tag{1}$$

b) Simply taking the logarithm of the likelihood function gives us

$$\begin{aligned} LL &= \sum_{i=1}^{n} y_i \ln p_i + (1-y_i)\ln(1-p_i) \\ &= \ln(p_3) + \ln(p_4) + \ln(1-p_1) + \ln(1-p_2). \end{aligned} \tag{2}$$

Now,

$$\nabla_\beta LL = \begin{pmatrix} \frac{\partial LL}{\partial \beta_0} \\ \frac{\partial LL}{\partial \beta_1} \end{pmatrix}, \quad \text{where } \frac{\partial LL}{\partial \beta_j} = \sum_{i=1}^{n} \frac{\partial}{\partial p_i} LL(y_i, p_i) \frac{\partial}{\partial z_i} p_i(z_i) \frac{\partial}{\partial \beta_j} z_i.$$

Further,

$$\frac{\partial z_i}{\partial \beta_0} = 1, \qquad \frac{\partial z_i}{\partial \beta_1} = x_i, \qquad \frac{\partial p_i}{\partial z_i} = p_i(1-p_i), \qquad \frac{\partial LL}{\partial p_i} = \frac{y_i}{p_i} - \frac{1-y_i}{1-p_i}.$$

Calculate partial derivative for β_0:

$$\begin{aligned} \frac{\partial}{\partial \beta_0} LL(\beta) &= \sum_{i=1}^{n} \frac{\partial LL}{\partial p_i} \frac{\partial p_i}{\partial z_i} \frac{\partial z_i}{\partial \beta_0} = \sum_{i=1}^{n} \left(\frac{y_i}{p_i} - \frac{1-y_i}{1-p_i} \right) \cdot (p_i(1-p_i)) \cdot 1 \\ &= \sum_{i=1}^{n} y_i(1-p_i) - p_i(1-y_i) \\ &= -p_1 - p_2 + (1-p_3) + (1-p_4). \end{aligned} \tag{3}$$

Calculate partial derivative for β_1:

$$\begin{aligned} \frac{\partial}{\partial \beta_1} LL(\beta) &= \sum_{i=1}^{n} \frac{\partial LL}{\partial p_i} \frac{\partial p_i}{\partial z_i} \frac{\partial z_i}{\partial \beta_1} = \sum_{i=1}^{n} \left(\frac{y_i}{p_i} - \frac{1-y_i}{1-p_i} \right) \cdot (p_i(1-p_i)) \cdot x_i \\ &= \sum_{i=1}^{n} (y_i(1-p_i) - (1-y_i))\, x_i \\ &= -p_1 - 2p_2 + 2.5(1-p_3) + 4(1-p_4). \end{aligned} \tag{4}$$

c) Here, for $\beta^{(0)} = (0,0)^T$, one calculates $z_i = \beta_0 + \beta_1 x_i = 0$ and

$$p_i(z_i) = \frac{\exp(0)}{1+\exp(0)} = 0.5 \quad \text{for all } i = 1, \ldots, 4.$$

Plugging these values into the calculated partial derivatives, we obtain

$$\begin{aligned} \frac{\partial}{\partial \beta_0} LL(\beta^{(0)}) &\overset{\text{Equation 3}}{=} -0.5 - 0.5 + 0.5 + 0.5 = 0, \\ \frac{\partial}{\partial \beta_1} LL(\beta^{(0)}) &\overset{\text{Equation 4}}{=} -0.5 - 2 \cdot 0.5 + 2.5 \cdot 0.5 + 4 \cdot 0.5 = \frac{7}{4}. \end{aligned}$$

Finally, the update step is given by

$$\begin{aligned} \beta_0^{(1)} &= \beta_0^{(0)} + \alpha \frac{\partial LL}{\partial \beta_0} = 0 + 0.2 \cdot 0 = 0, \\ \beta_1^{(1)} &= \beta_1^{(0)} + \alpha \frac{\partial LL}{\partial \beta_1} = 0 + 0.2 \cdot \frac{7}{4} = 0.35, \end{aligned}$$

which lets us conclude that $\beta^{(1)} = \begin{pmatrix} 0 \\ 0.35 \end{pmatrix}$.

d) First, if a linear regression model were fitted to this data, the predicted values of $\hat{y}$ could be outside $[0, 1]$, which in a binary logistic setting would not be a good prediction since the interpretation as a probability would not make sense.

   Second, the properties of *autocorrelation* and *homoscedasticity* would be violated.

   - Autocorrelation: It can be noted that the residuals of a linear model fitted to a setting with a binary dependent variable would result in positive residuals on one side, negative on the other and in the range of $\hat{y} = [0, 1]$ they would be in the interval $[-1, 1]$. This would form a pattern that indicates autocorrelation.
   - Homoscedasticity: Error terms do not have constant variance, because true y values take on only two values from the set $\{0, 1\}$, therefore they are heteroscedastic.

Exercise T3.3 *Poisson regression*

You are provided the following numbers from the result of a *Poisson regression model*.

Variable	Estimate	Std. Error
Intercept	1.5499	0.0503
Age	-0.0047	0.0009

a) According to the model above, what *qualitative* effect does a change in the independent variable age (+1) have on the dependent variable dv.

b) According to the model above, what *quantitative* effect (on the incidence rate and log-incidence rate) does a change in the independent variable age (+1) have on the dependent variable dv.

Solution

a) Given the coefficients in the result, we can write the equation

$$\ln(dv) = 1.5499 + (-0.0047)\text{age}.$$

   As can be seen, an increase in age will decrease the dependent variable dv.

b) The log-incidence rate decreases by 0.0047 with an increase of 1 in the variable age:

$$\Delta(\text{log incidence rate}) = \beta_1 = -0.0047.$$

   The incidence rate decreases by a factor of 0.9953 when the variable age increases by 1 unit:

$$\Delta(\text{incidence rate}) = e^{\beta_1} = 0.9953.$$

   This means that there is an approximate 0.5% reduction for each increase in the age by 1 unit.