AGH University of Science and Technology

Seminar in *Artificial Intelligence*

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1. Agenda

1. Intro, presentation plan.
2. What is regression?
3. What regression is used for?
4. Types of regression.
5. Simple Linear regression.
6. Multiple dimension extension.
7. Ordinary least squares.
8. Gradient descent in linear regression.
9. Regularization - Ridge and Lasso
10. Logistic regression.
11. Polynominal regression.
12. QA
13. Quiz.

2. What is regression?

- looks for the relationship between two or more variables.

3. What regression is used for?

- used in: forecasting, MS Excel :D, machine learning...

4. Types of regression

- linear regression
- logistic regression
- polynominal regression
- stepwise regression
- ridge regression
- lasso regression
- elasticNet regression

5. Linear regression

- First known research in this area — method of least squares published by Legendre in 1805 and by Gauss in 1809.
- The representation is a linear equation that combines a specific set of input values x the solution to which is the predicted output for that set of input values y. As such, both the input values x and the output value are numeric.

5. Simple Linear Regression

- Simple linear regression is a linear regression model with a single independent variable.
- Model for single dimension:

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i \tag{1}$$

- Naming:
  - The unknown parameters — β
  - The independent variables — X or x
  - The dependent variable — Y or y
  - Introduced error — ϵ

6. Multiple dimension extension

- When there is a single input variable x, the method is referred to as simple linear regression. When there are multiple input variables, literature from statistics often refers to the method as multiple linear regression.
- Model for n dimension:

$$y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + ... + \beta_n x_{i,n} + \epsilon_i \tag{2}$$

- To matrix representation:

$$y_i = x_i^T + \epsilon_i \tag{3}$$

$$Y = X\beta + \epsilon \tag{4}$$

7. Ordinary least squares

Method for estimating the unknown parameters in a linear regression model:

$$\hat{\beta} = argmin_{\beta} S(\beta) \tag{5}$$

$$S(\beta) = \sum_{i=1}^{n} \mid y_i - \sum_{j=1}^{p} X_{ij}\beta_j \mid^2 \tag{6}$$

$$\begin{bmatrix} n & \sum_{i=1}^{n} x_{2i} & \dots & \sum_{i=1}^{n} x_{ki} \\ \sum_{i=1}^{n} x_{2i} & \sum_{i=1}^{n} x_{2i}^2 & \dots & \sum_{i=1}^{n} x_{2i}x_{ki} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} x_{ki} & \sum_{i=1}^{n} x_{ki}x_{2i} & \dots & \sum_{i=1}^{n} x_{ki}^2 \end{bmatrix} \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_{2i}y_i \\ \vdots \\ \sum_{i=1}^{n} x_{ki}y_i \end{bmatrix}$$

7. Ordinary least squares (cont.)

Which leads to:

$$\begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_k \end{bmatrix} = \hat{\boldsymbol{\beta}} = \left[\mathbf{X}'\mathbf{X}\right]^{-1}\mathbf{X}'\mathbf{y}$$

8. Gradient descent in linear regression

Gradient descent is a first-order iterative optimization algorithm for finding the minimum of a function.
Denote E as squared mean error in example for linear regression:

$$E = 1/n \times \sum_{i=0}^{n} (y_i - \beta_1 \times x_i + \beta_0) \tag{7}$$

Let us assume that:

$$a = \beta_1 \tag{8}$$

$$b = \beta_0 \tag{9}$$

$$D_a = \frac{\mathrm{d}}{\mathrm{d}a}(E) \tag{10}$$

$$D_b = \frac{\mathrm{d}}{\mathrm{d}b}(E) \tag{11}$$

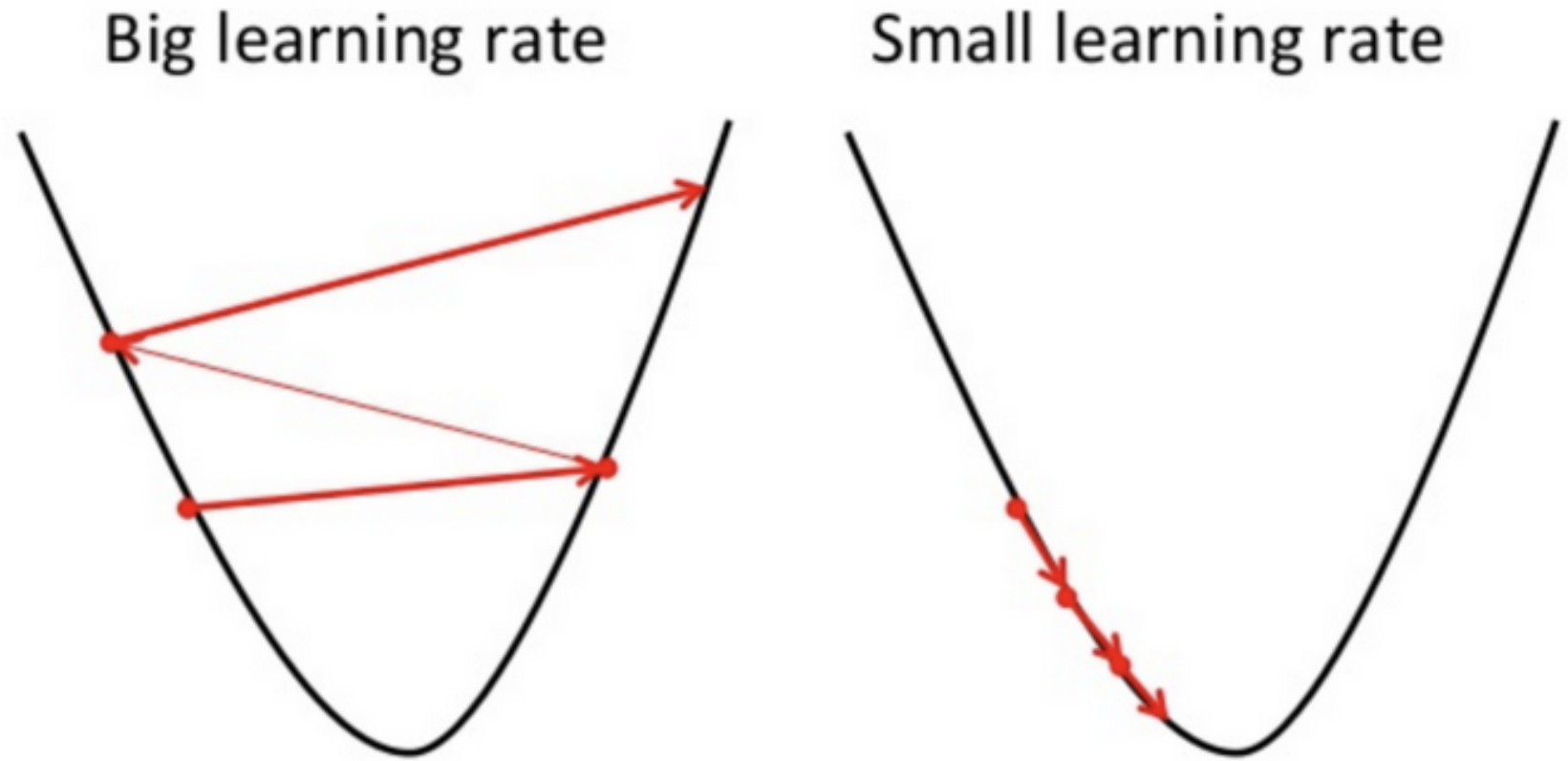
8. Gradient descent in linear regression (cont.)

Now find that a and b where function E will reach minimum or be small enough. Take some L as learning rate and iterative find values of a and b from equations:

$$a = a - L \times D_a \tag{12}$$

$$b = b - L \times D_b \tag{13}$$

8. Gradient descent in linear regression (cont.)



Training rate L has to be small enough to avoid skipping minimum.

9. Regularization

Regularization methods provide a means to control our regression coefficients, which can reduce the variance and decrease our of sample error.
Two popular examples of regularization procedures for linear regression are:

- Lasso Regression — called L1 regularization.
- Ridge Regression — called L2 regularization.

These methods are effective to use when there is collinearity in your input values and ordinary least squares would overfit the training data.

9. Regularization

Ridge Regression

Ridge should be used if we want to remain all parameters.

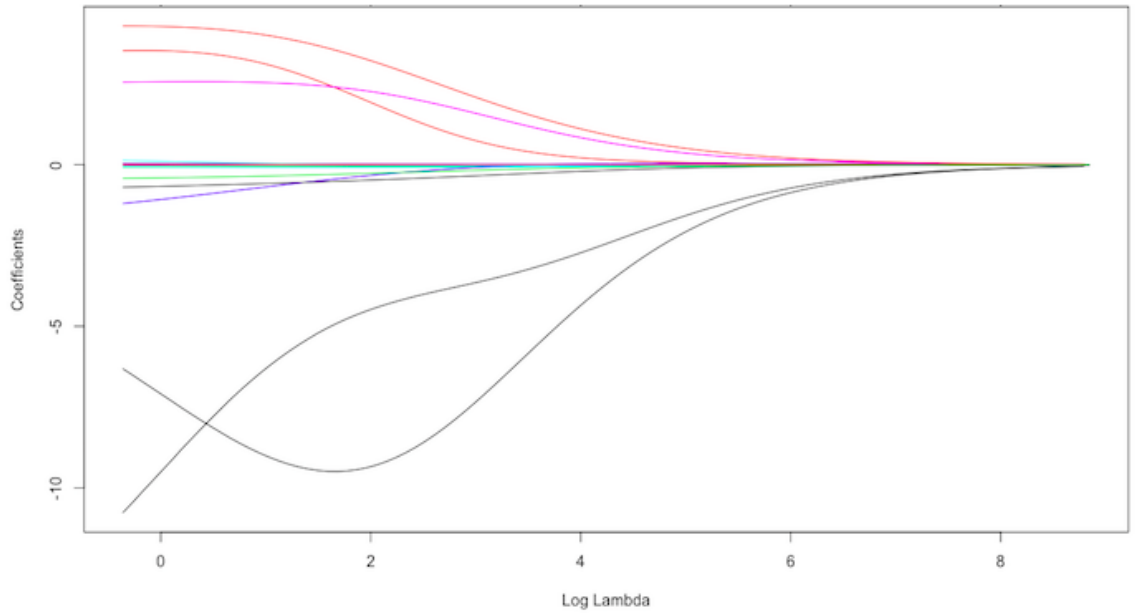
$$E = 1/n \times \sum_{i=0}^{n} (y_i - \beta_1 \times x_i + \beta_0) \tag{14}$$

Adding Ridge penalty:

$$\min(E + \lambda \sum_{j=1}^{p} \beta_j^2) \tag{15}$$

9. Regularization (cont.)

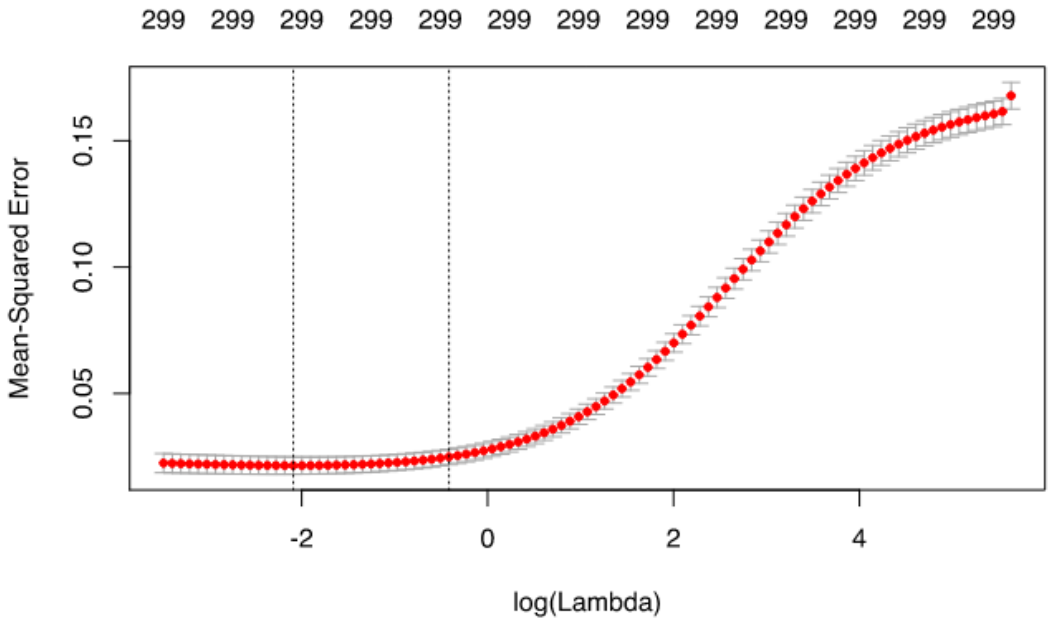
Ridge Regression



We see that Ridge remain all variables and with incrementing λ all are forced to 0. To find λ we can also perform CV.

9. Regularization

Ridge Regression - Example



In this case Ridge is not providing improvements. What about Lasso?

9. Regularization

Lasso Regression

Lasso allows to get rid of some parameters.

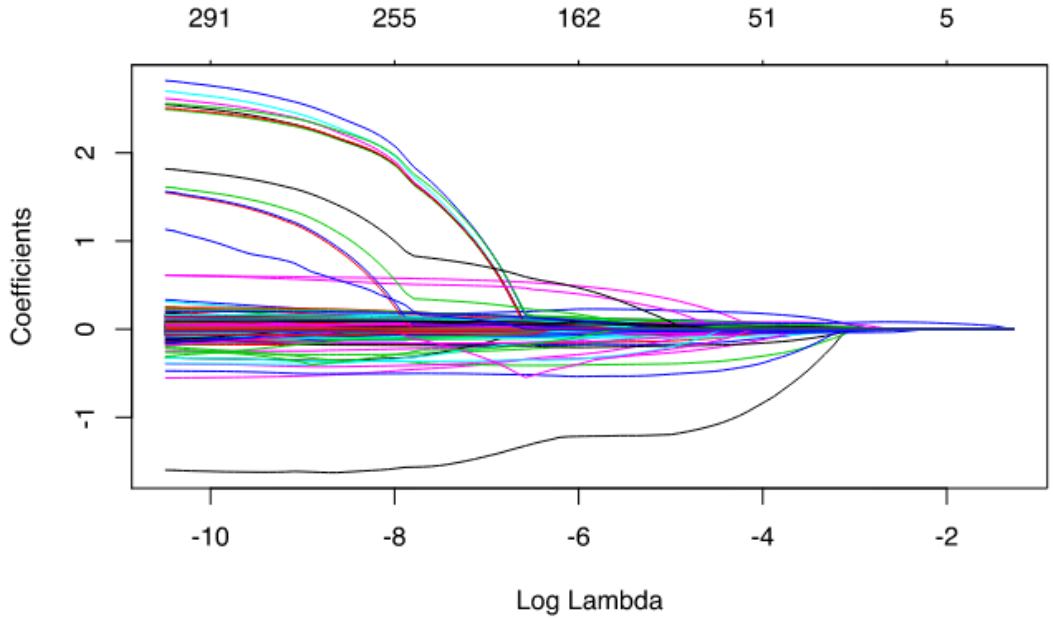
$$E = 1/n \times \sum_{i=0}^{n} (y_i - \beta_1 \times x_i + \beta_0) \tag{16}$$

Adding Lasso penalty:

$$minimize(E + \lambda \sum_{j=1}^{p} |\beta_j|) \tag{17}$$

9. Regularization (cont.)

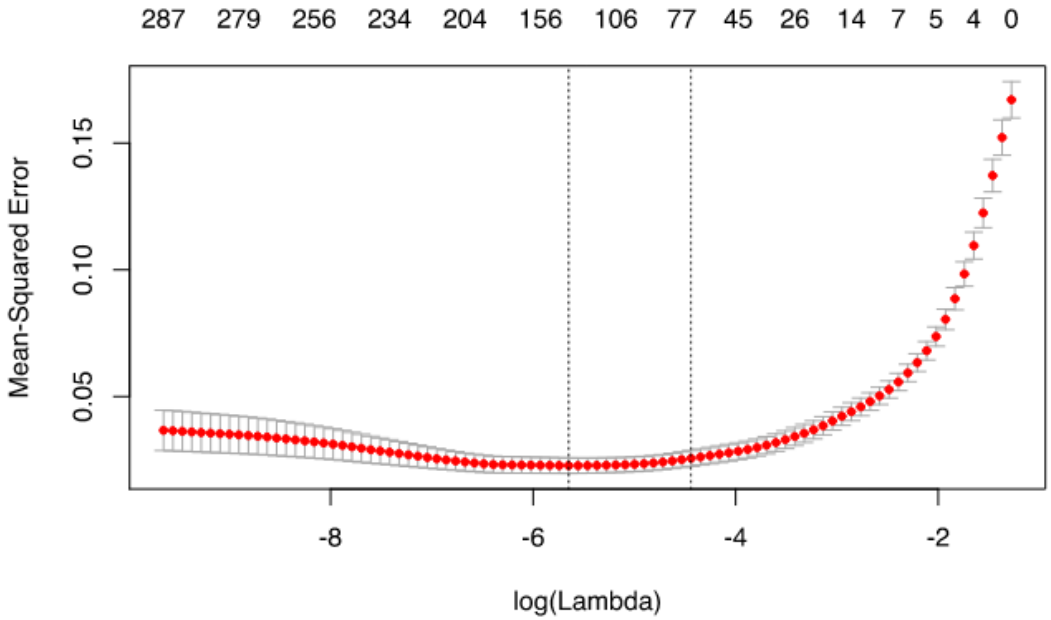
Lasso Regression



How to find λ? We can perform cross-validation. Example:

9. Regularization (cont.)

Lasso Regression



There is improvement but some coefficients are equals to 0 which indicades that some parameters will not be taken into consideration.

10. Logistic regression

- Logistic regression was developed by statistician David Cox in 1958
- Logistic Regression is one of the basic and the most popular algorithm to solve a classification problem.
- The main idea of logistic regression is to find a relationship between features and probability of particular outcome.

10. Logistic regression

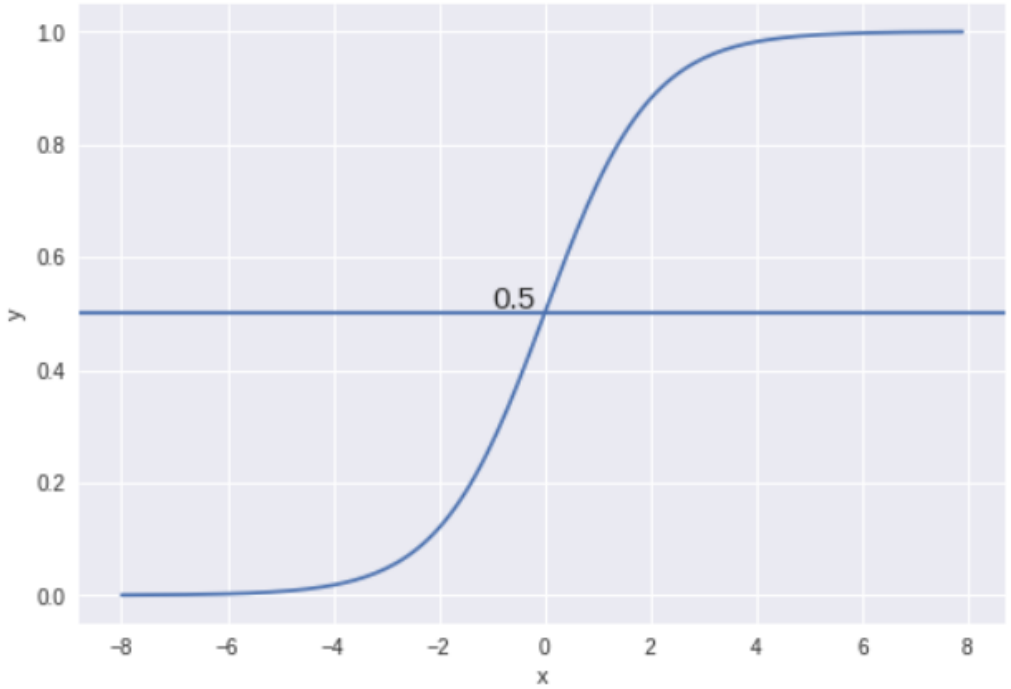
- In logistic regression, the dependent variable is binary or dichotomous, i.e. it only contains data coded as 1 (TRUE, success, etc.) or 0 (FALSE, failure, etc.).
- Linear regression predicts values outside the acceptable range (e.g. predicting probabilities outside the range 0 to 1).

10. Logistic regression

Function graph:

- For the begining arguments values are nearly 0 or 1.
- After reaching critical value we see dynamically increase/decrease of function value.
- For the final arguments values are nearly 1 or 0 (opposite to the begining).

10. Logistic regression (cont.)

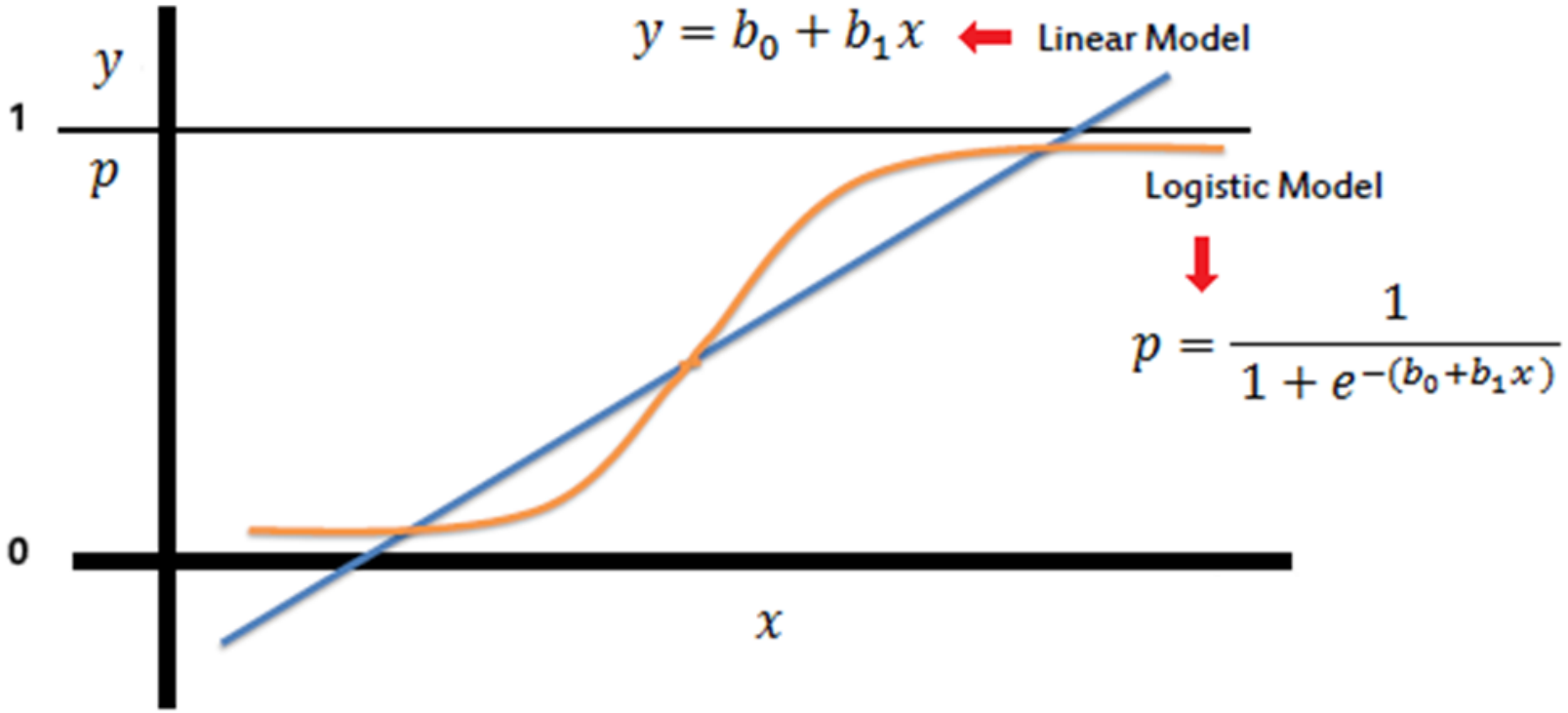


sigmoid function

10. Logistic regression

- The biggest difference between linear and logistic regrresion is how the line is fit to the data.
- Logistic regression uses maximum likelihood estimation (MLE) to get the model coefficients.

10. Logistic regression (cont.)



10. Logistic regression

Why should we use logistic regression instead of linear?

- Let **x** be some feature and **y** be the output which can be either 0 or 1.
- The probability that the output is 1 can be represented as:

$$P = (y = 1|x) \tag{18}$$

- Using linear regression we will get:

$$p(X) = \beta_0 + \beta_1 X \tag{19}$$

- Logistic regression is expressed by logit function, therefore:

$$p(X) = e^{\beta_0+\beta_1 X}/1 + e^{\beta_0+\beta_1 X} \tag{20}$$

10. Logistic regression

Different types of logistic regression:

- 1. Binary: The categorical response has only two 2 possible outcomes (e.g.: Spam or Not).
- 2. Multinomial: Three or more categories without ordering. (e.g.: Predicting which food is preferred more (Veg, Non-Veg, Vegan)).
- 3. Ordinal: Three or more categories with ordering. (e.g.: Movie rating from 1 to 5).

10. Logistic regression

Summing up

- Logistic regression's ability to provide probabilities and classify new samples using continuous and discrete measurements makes it a popular machine learning method.

11. Polynominal Regression

- Occurs when regression equation has independent variable in power higher than 1.
- General equation:

$$y = \beta_0 + \beta_1 \times x_i + \beta_2 \times x_i^2 + \beta_3 \times x_i^3 + ... + \beta_m \times x_i^m + E, i = 1, 2, 3... \tag{21}$$

- Example (variable in 2 power):

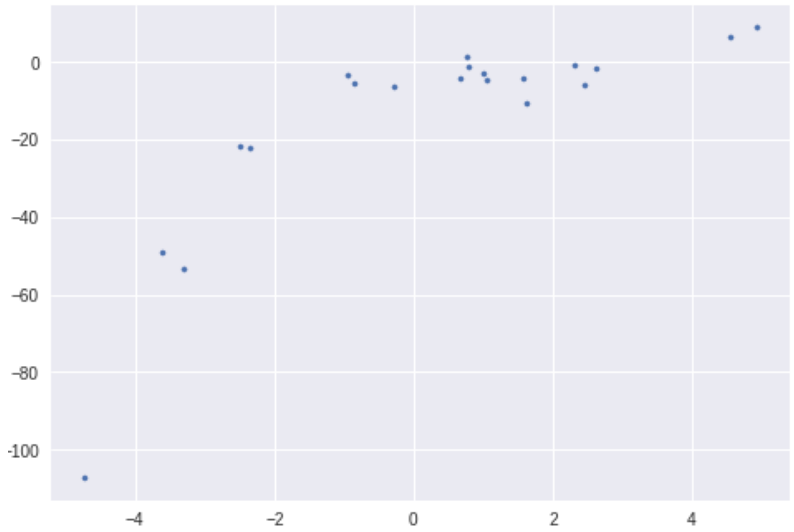
$$y = a + b \times x^2 \tag{22}$$

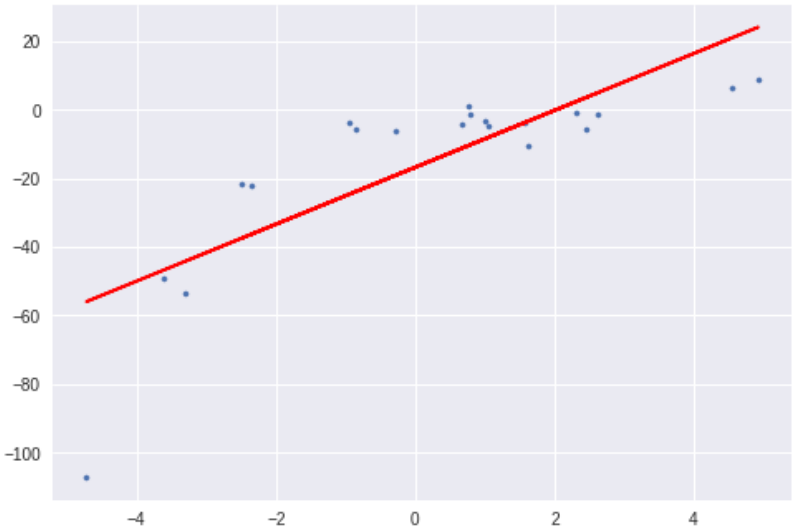
- the best fit is rather curve not a straight line.

11. Polynominal Regression

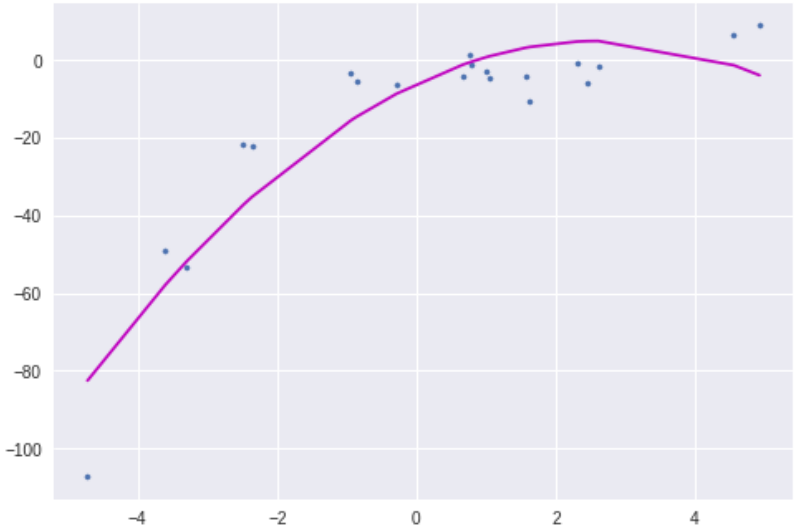
- polynominal with higher degree can give us lower error rate.
- if degree will be too high then overfitting will occur.
- curve sholud fit the nature of the problem (trend) not every single sample.
- nonlinear "relationship" of variables, but it is considered as linear model due to the coefficients/weights associated with the features are still linear.

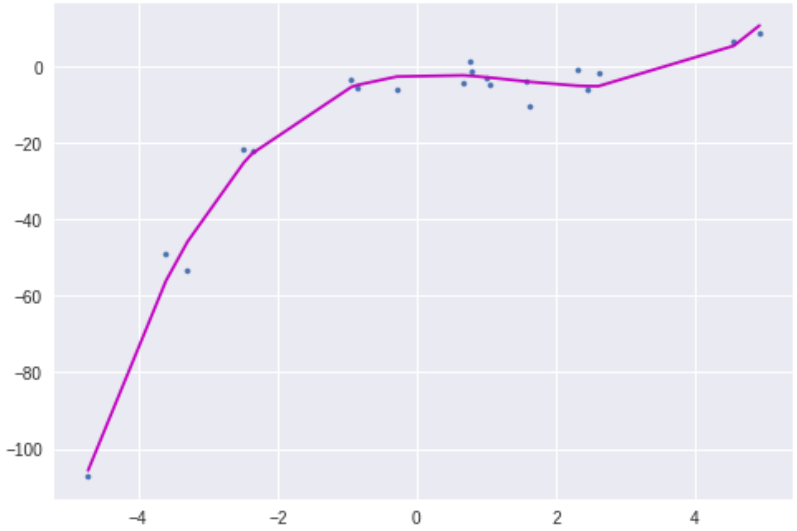
11. Polynominal Regression



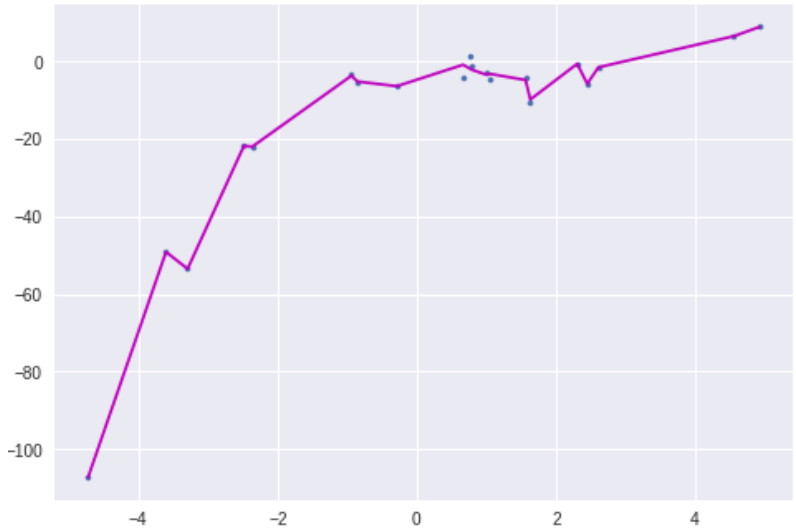


11. Polynominal Regression





11. Polynominal Regression



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Thank you for your attention!

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Q & A