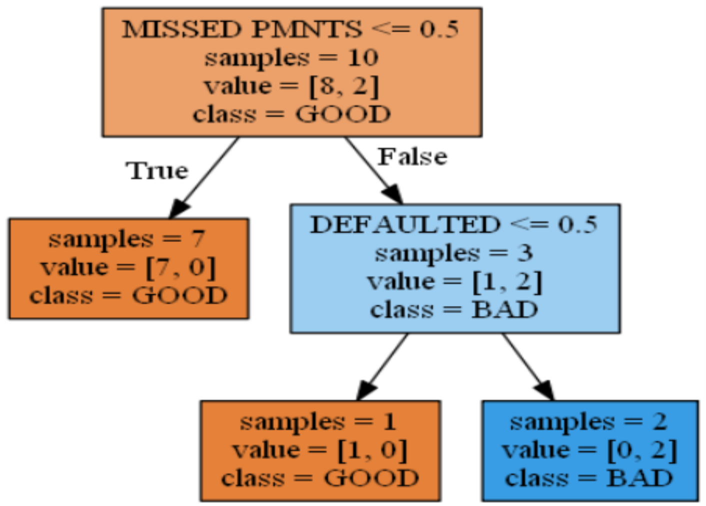
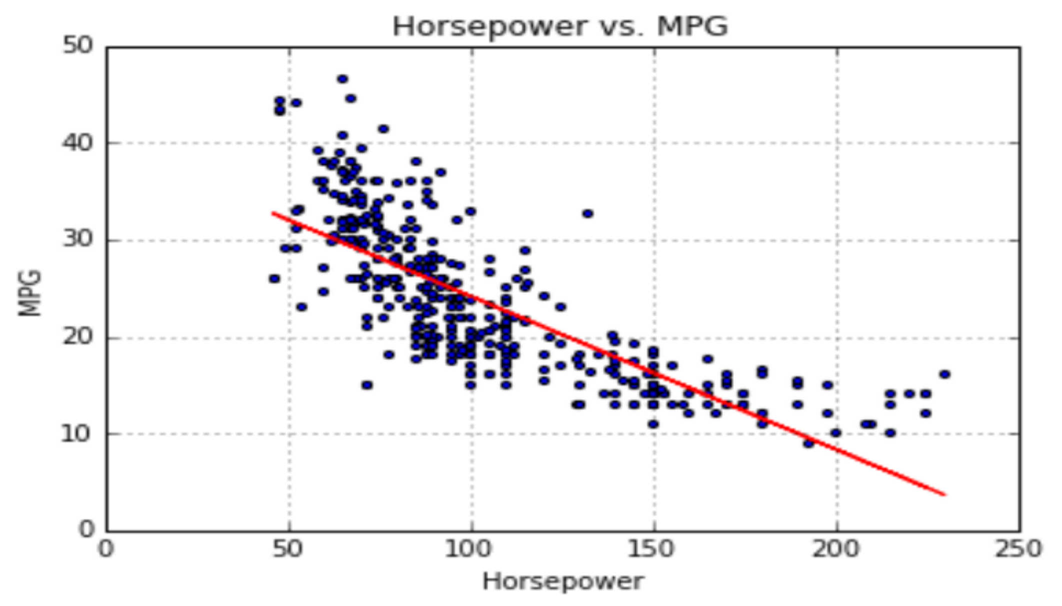
Logistic Regression with MLE

Machine Learning Models

Flach talks about three types of Machine Learning models [Fla12]

- Geometric models
- Logical models
- Probabilistic models

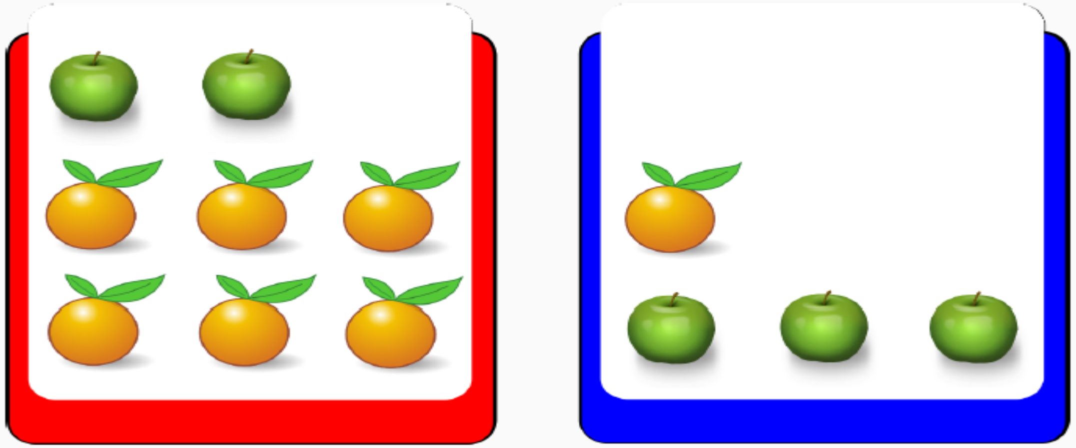




Definition

Simple example [Bis06]

1. We randomly pick one of the boxes (40% probability for the red and 60% for the blue box)
2. We randomly pick a fruit



$$p(B = r) = \frac{4}{10}, p(B = b) = \frac{6}{10}$$

- By definition probabilities lie in $[0; 1]$
- If the events include all possible outcomes and are mutually exclusive their probabilities must sum to one (eg. $\frac{4}{10} + \frac{6}{10} = 1$)

Definitions

- **Marginal probability** – the probability of an event occurring is not conditioned on any other event

$$p(B = r) = \frac{4}{10}$$

- **Joint probability** – probability of the events occurring together

$$p(B = r, F = a) =?$$

- **Conditional probability** – probability of an event occurring, given that another event occurs

$$p(B = a|B = r) = \frac{1}{4} \text{ (fraction of apples in the red box)}$$

Rules of Probability

- Sum rule – $p(X) = \sum_Y p(X, Y)$
- Product rule – $p(X, Y) = p(Y|X)p(X)$

Example 1 – $p(B = r, F = a) =?$

$$p(B = r, F = a) = p(F = a|B = r)\times p(B = r) = \frac{1}{4}\times\frac{4}{10} = \frac{1}{10}$$

Example 2 – $p(F = a) =?$

$$p(F = a) = \sum_{B\in\{r,b\}} p(F = a|B) = p(F = a|B = r)+$$

$$p(F = a|B = b) = p(F = a|B = r)p(B = r)+$$

$$p(F = a|B = b)p(B = b) = \frac{1}{4} \times \frac{4}{10} + \frac{3}{4} \times \frac{6}{10} = \frac{11}{20}$$

Binary Logistic Regression

Definition

Binary Logistic Regression

- We have a set of feature vectors $\boldsymbol{X}$ with corresponding binary outputs

$$\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}^\mathsf{T}$$
$$\boldsymbol{y} = \{y_1, y_2, \ldots, y_N\}^\mathsf{T}, \text{ where } y_i \in \{0, 1\}$$

- We want to model $p(y|\boldsymbol{x})$

$$p(y_i = 1|\boldsymbol{x_i}, \boldsymbol{w}) = \sum_j w_j x_{ij} = \boldsymbol{x_i}\boldsymbol{w}$$

By definition $p(y_i = 1|\boldsymbol{x_i}, \boldsymbol{w}) \in [0; 1]$. We want to transform the probability to remove the range restrictions, as $\boldsymbol{x_i}\boldsymbol{w}$ can take any real value.

Using odds

Odds

p – probability of an event occurring

$1 - p$ – probability of the event not occurring

The odds for event i are then defined as

$$\text{odds}_i = \frac{p_i}{1 - p_i}$$

Taking the log of the odds removes the floor and ceiling restrictions.

$$\log\left(\frac{p_i}{1 - p_i}\right) = \sum_j w_j x_{ij} = \boldsymbol{x_i w}$$

This way we map the probabilities from the $[0; 1]$ range to the entire number line.

Logistic function

Logistic Regression Model

$$\log\left(\frac{p_i}{1-p_i}\right) = \boldsymbol{x_i w}$$

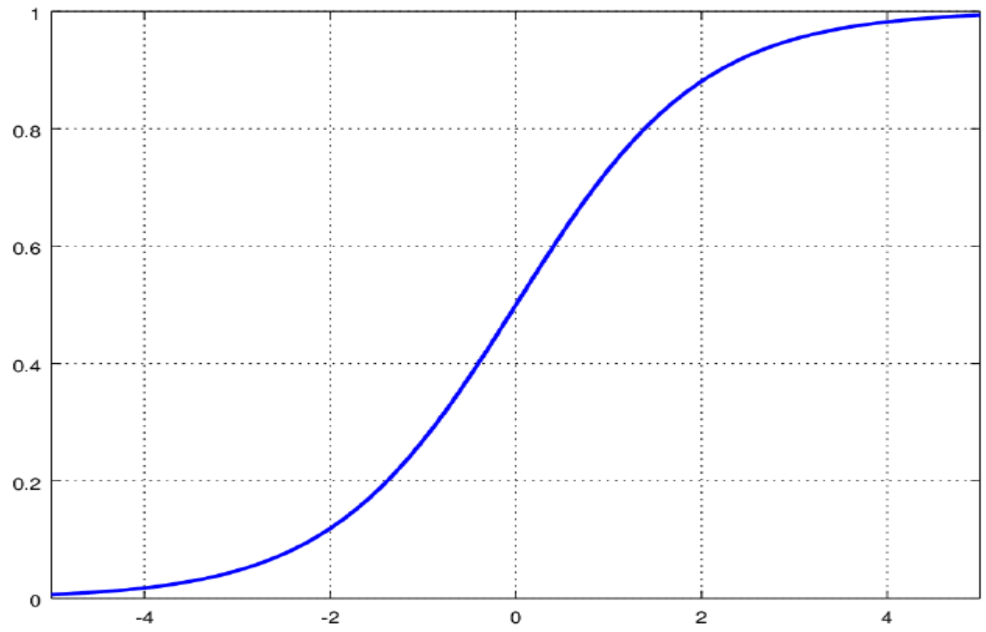
$$\frac{p_i}{1-p_i} = e^{\boldsymbol{x_i w}}$$

$$p_i = \frac{e^{\boldsymbol{x_i w}}}{1+e^{\boldsymbol{x_i w}}} = \frac{1}{1+e^{-\boldsymbol{x_i w}}}$$

$$p(y_i = 1|\boldsymbol{x_i};\boldsymbol{w}) = \frac{1}{1+e^{-\boldsymbol{x_i w}}}$$

$$p(y_i = 0|\boldsymbol{x_i};\boldsymbol{w}) = 1 - \frac{1}{1+e^{-\boldsymbol{x_i w}}}$$

$$p(y_i|\boldsymbol{x_i};\boldsymbol{w}) = \left(\frac{1}{1+e^{-\boldsymbol{x_i w}}}\right)^{y_i}\left(1 - \frac{1}{1+e^{-\boldsymbol{x_i w}}}\right)^{1-y_i}$$



Standard logistic sigmoid function

Estimation

$$\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N\}^\mathsf{T}, \text{ where } \boldsymbol{x}_i = \{x_{i1}, x_{i2}, \dots, x_{iD}\}$$
$$\boldsymbol{y} = \{y_1, y_2, \dots, y_N\}^\mathsf{T}, \text{ where } y_i \in \{0, 1\}$$
$$\boldsymbol{w} = \{w_1, w_2, \dots, w_D\}^\mathsf{T}$$

Maximum Likelihood Estimation (MLE)

1. **Step 1** – Specify the joint density function
$$p(\boldsymbol{y}|\boldsymbol{X}; \boldsymbol{w}) = \prod_{i=1}^{N} \left(\frac{1}{1+e^{-\boldsymbol{x}_i \boldsymbol{w}}}\right)^{y_i} \left(1 - \frac{1}{1+e^{-\boldsymbol{x}_i \boldsymbol{w}}}\right)^{1-y_i}$$
2. **Step 2** – Express this is a function of $\boldsymbol{w}$, where $\boldsymbol{X}$ and $\boldsymbol{y}$ are fixed parameters – $L(\boldsymbol{w}) = p(\boldsymbol{y}|\boldsymbol{X}; \boldsymbol{w})$
3. **Step 3** – Maximize $L(\boldsymbol{w})$
$$\boldsymbol{w}_{\text{MLE}} = \text{argmax}_{\boldsymbol{w}} L(\boldsymbol{w})$$

Likelihood Maximization

$$L(\boldsymbol{w}) = \prod_{i=1}^{N} \left(\frac{1}{1+e^{-\boldsymbol{x}_i\boldsymbol{w}}}\right)^{y_i} \left(1 - \frac{1}{1+e^{-\boldsymbol{x}_i\boldsymbol{w}}}\right)^{1-y_i}$$

We can simplify $L(\boldsymbol{w})$ by taking its log and then differentiate to get the gradient.

$$\ell(\boldsymbol{w}) = \sum_{i=1}^{N} \left[y_i \log\left(\frac{1}{1+e^{-\boldsymbol{x}_i\boldsymbol{w}}}\right) + (1-y_i)\left(1+\frac{1}{1+e^{-\boldsymbol{x}_i\boldsymbol{w}}}\right)\right]$$

$$\nabla_w \ell(\boldsymbol{w}) = \nabla_w \sum_{i=1}^{N} \left[y_i \log\left(\frac{1}{1+e^{-\boldsymbol{x}_i\boldsymbol{w}}}\right) + (1-y_i)\left(1+\frac{1}{1+e^{-\boldsymbol{x}_i\boldsymbol{w}}}\right)\right]$$

Derivative of the sigmoid

Let $\sigma(x) = \frac{1}{1+e^{-x}}$

$$\frac{d}{dx}\sigma(x) = \frac{d}{dx}\frac{1}{1+e^{-x}} = \frac{d}{dx}(1+e^{-x})^{-1} =$$

$$-(1+e^{-x})^{-2}(-e^{-x}) = \frac{e^{-x}}{(1+e^{-x})^2} =$$

$$\frac{1}{(1+e^{-x})}\frac{-e^{-x}}{(1+e^{-x})} = \frac{1}{(1+e^{-x})}\frac{(1+e^{-x})-1}{(1+e^{-x})} =$$

$$\frac{1}{(1+e^{-x})}\left(1 - \frac{1}{(1+e^{-x})}\right) = \sigma(x)(1-\sigma(x))$$

Derivative of the log likelihood

$$\nabla_w \ell(\boldsymbol{w}) = \nabla_w \sum_{i=1}^{N} \left[y_i \log\left(\frac{1}{1+e^{-\boldsymbol{x_i w}}}\right) + (1-y_i)\left(1+\frac{1}{1+e^{-\boldsymbol{x_i w}}}\right)\right] =$$

$$\nabla_w \sum_{i=1}^{N} \left[y_i \log(\sigma(\boldsymbol{x_i w})) + (1-y_i)\log(1-\sigma(\boldsymbol{x_i w}))\right] =$$

$$\sum_{i=1}^{N} \left(y_i \frac{1}{\sigma(\boldsymbol{x_i w})}\sigma(\boldsymbol{x_i w})(1-\sigma(\boldsymbol{x_i w})\boldsymbol{x_i} + (1-y_i)\frac{1}{\sigma(\boldsymbol{x_i w})}(-1)\sigma(\boldsymbol{x_i w})\boldsymbol{x_i}\right) =$$

$$\sum_{i=1}^{N} \left(y_i(1-\sigma(\boldsymbol{x_i w}))\boldsymbol{x_i} + (1-y_i)(-1)\sigma(\boldsymbol{x_i w}))\boldsymbol{x_i}\right) =$$

$$\sum_{i=1}^{N} \left(y_i\boldsymbol{x_i} - y_i\sigma(\boldsymbol{x_i w})\boldsymbol{x_i} - \sigma(\boldsymbol{x_i w})\boldsymbol{x_i} + y_i\sigma(\boldsymbol{x_i w})\boldsymbol{x_i}\right) =$$

$$\sum_{i=1}^{N} (y_i\boldsymbol{x_i} - \sigma(\boldsymbol{x_i w})\boldsymbol{x_i}) = \sum_{i=1}^{N}\left(y_i - \frac{1}{(1+e^{-\boldsymbol{x_i w}})}\right)\boldsymbol{x_i}$$

Likelihood Maximization

We can now use gradient ascent to maximize $\ell(\boldsymbol{w})$

The update rule will be:

repeat until convergence {

$$w_j := w_j + \alpha \sum_{i=1}^{N} \left(y_i - \frac{1}{(1 + e^{-\boldsymbol{x}_i \boldsymbol{w}})} \right) x_{ij}$$

}

or using matrix notation

repeat until convergence {

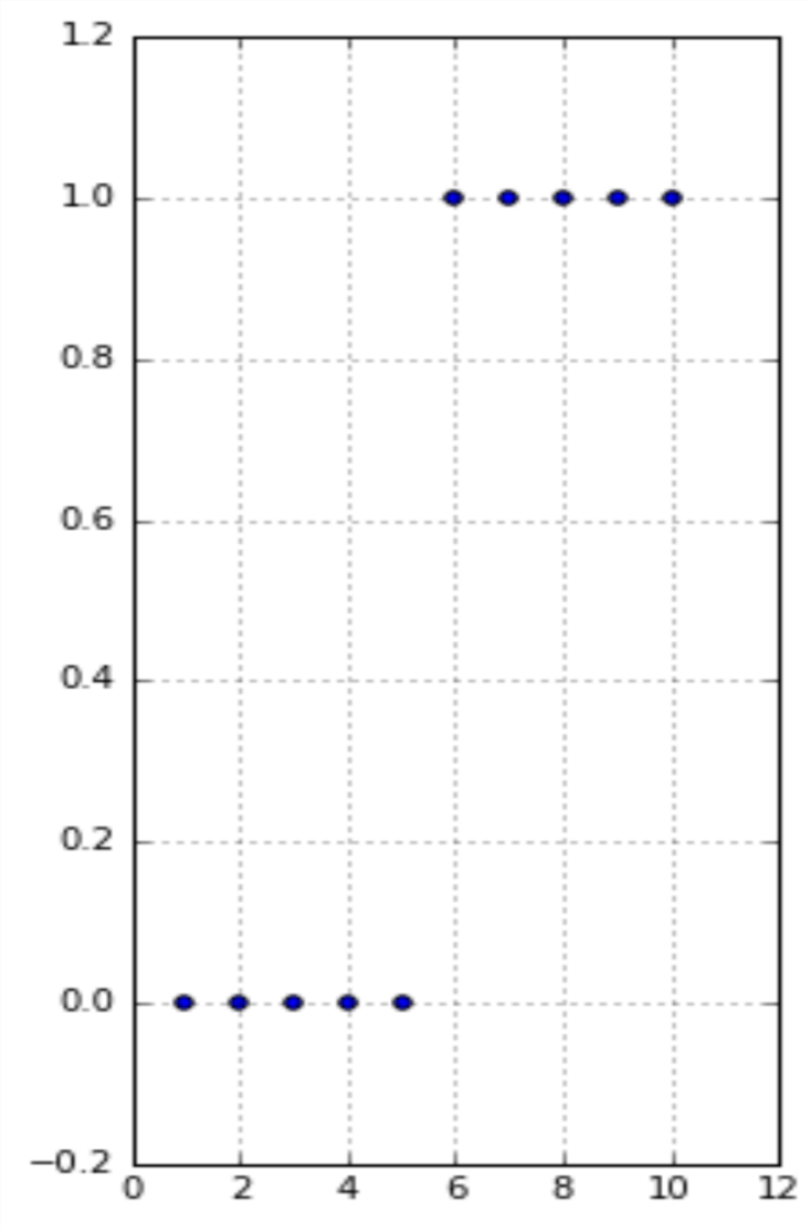
$$\boldsymbol{w} := \boldsymbol{w} + \alpha \boldsymbol{X}^\top \left(\boldsymbol{y} - \frac{1}{1 + e^{-\boldsymbol{X}\boldsymbol{w}}} \right)$$

}

Example

Simple example

$$\boldsymbol{X} = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}^\mathsf{T}$$
$$\boldsymbol{y} = \{0, 0, 0, 0, 0, 1, 1, 1, 1, 1\}^\mathsf{T}$$



Non linear decision boundary

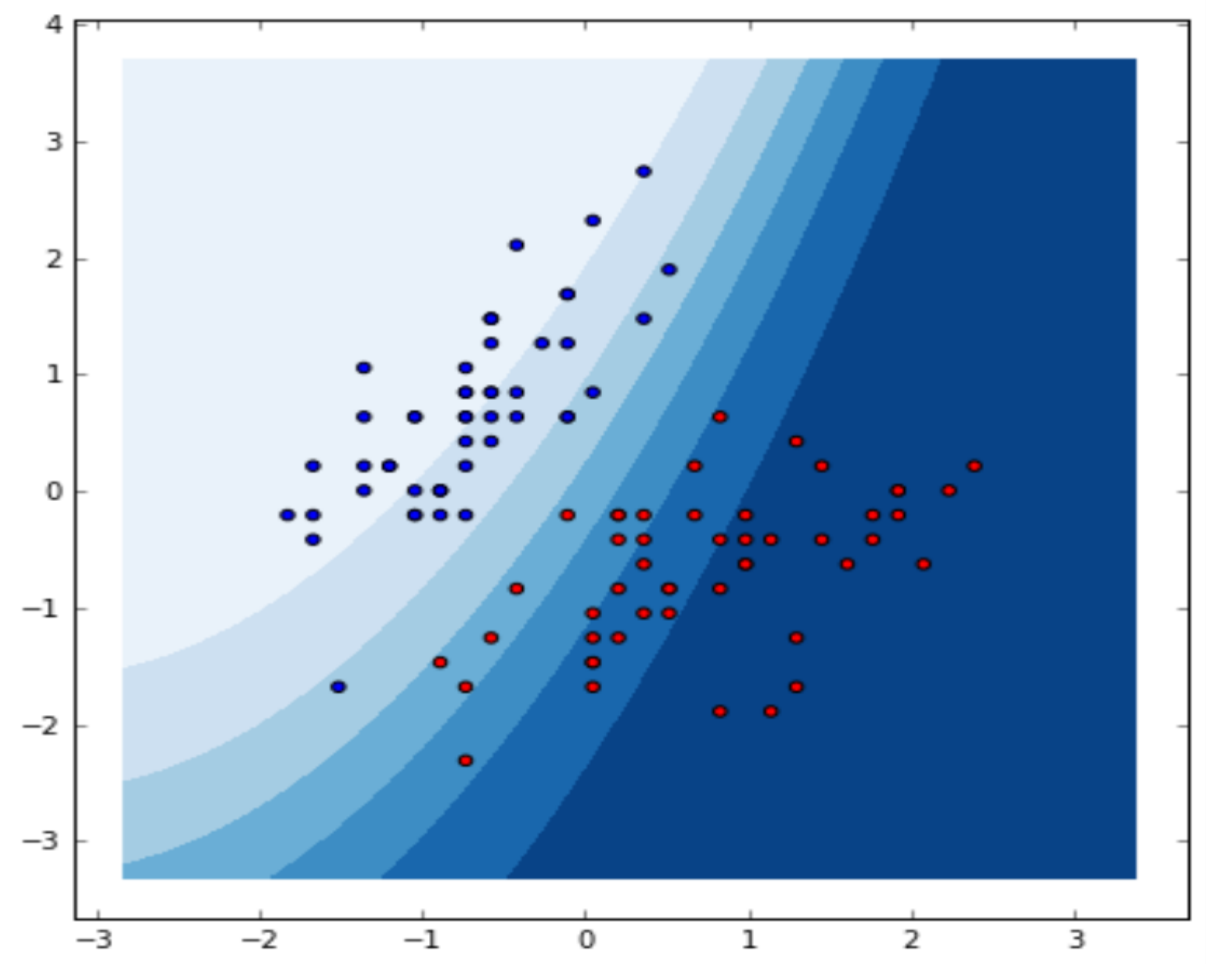
Polynomial predictors

- Relationship is modelled using a k^{th} degree polynomial
- The hypothesis is then

$$\hat{y}(x_i) = \left(\frac{1}{1 + e^{-\boldsymbol{x_i w}}}\right)$$

where

$$\boldsymbol{x_i w} = w_0 + w_1 x_i + w_2 x_i^2 + \cdots + w_k x_i^k$$



Final remarks

No analytical solution

Assumptions

- Not as strict as Linear Regression (e.g. no assumption on homoscedasticity, no linear relationship between dependent and independent variables, residual do not need to be normally distributed etc.)
- There are still certain assumptions
    - Linear relationship between the $logit$ of the independent variables and the dependent variable
    - Binary dependent variable
    - Independent error terms
    - The sample is sufficiently large – check [Hsi89]

References I

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- Christopher M. Bishop, *Pattern recognition and machine learning (information science and statistics)*, Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2006.
- Peter Flach, *Machine learning: The art and science of algorithms that make sense of data*, Cambridge University Press, New York, NY, USA, 2012.
- F. Y. Hsieh, *Sample size tables for logistic regression*, Statistics in Medicine **8** (1989), no. 7, 795–802.