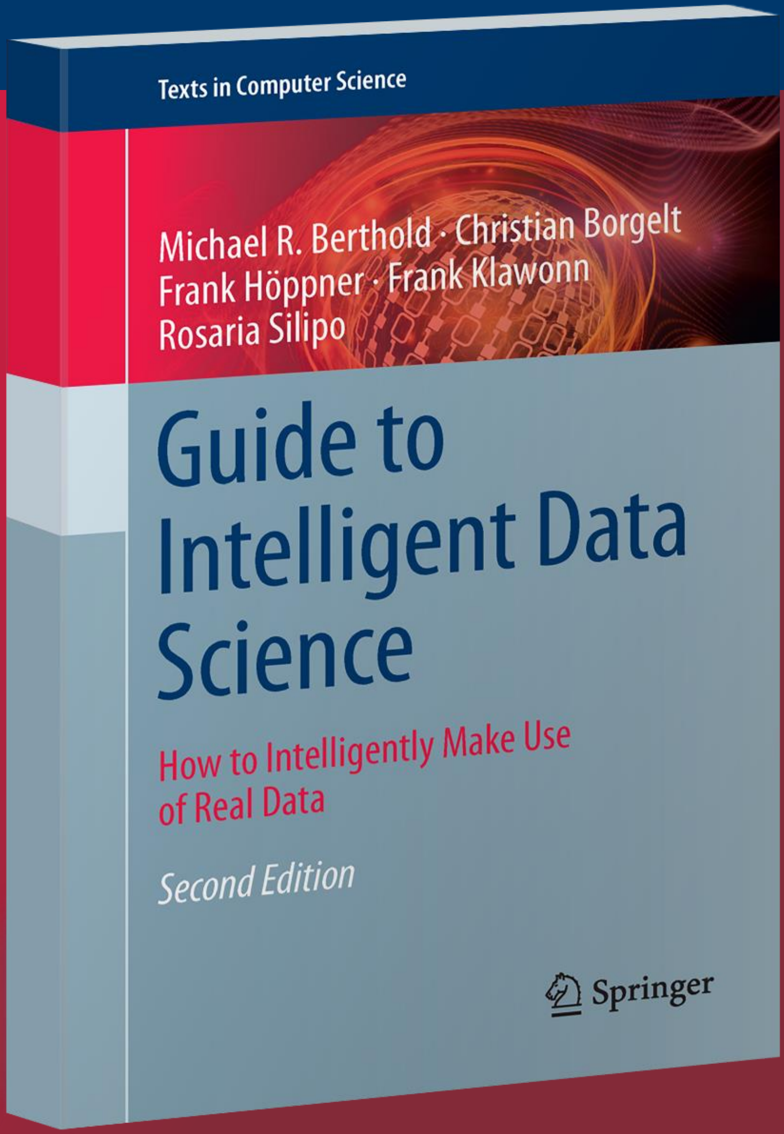
Regressions



"All models are approximations. Essentially, all models are wrong, but some are useful."
-George Box

How can we model the data?

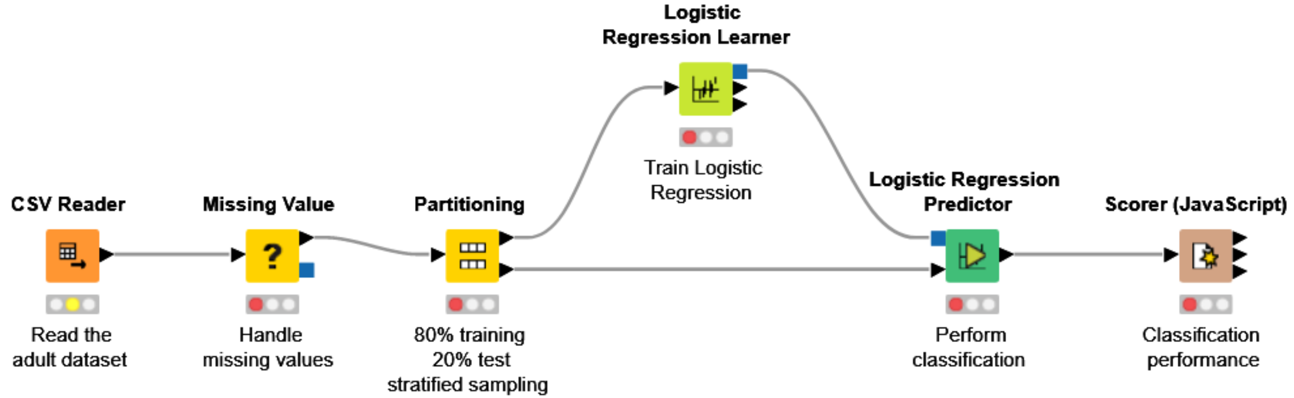
**This lesson refers to chapter 8 of the GIDS book*

Content of this Lesson

- Regression
  - The Regression Task
  - Linear Regression
  - Other Regressions
  - Logistic Regression
  - Robust Regression
  - Regression for Classification
  - Practical Example

Datasets

- Datasets used : adult dataset
- Example Workflow:
  - „Logistic regression“ https://kni.me/w/LWHdcrt_DFIepk0p
    - Missing value handling
    - Logistic regression



The Regression Task

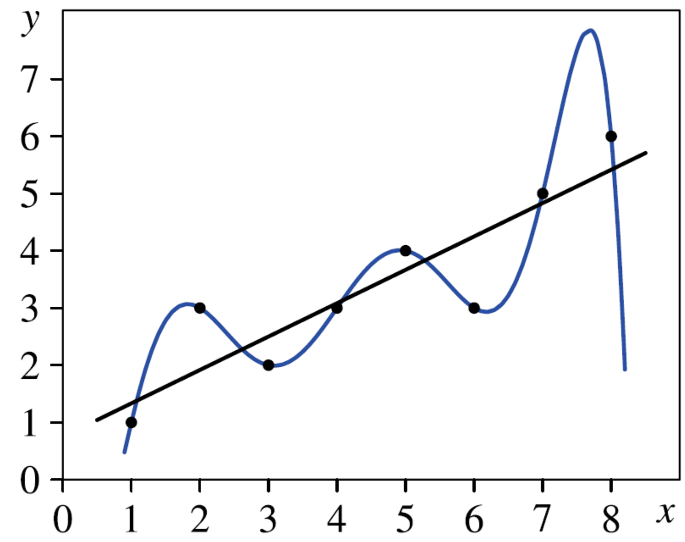
Note

- We are focusing on methods that find explanations for an unknown dependency within the data.

- **Supervised** (because we know the desired outcome)
- **Descriptive** (because we care about explanation)

- Goal: Explain how target attribute depends on descripitive attributes
  - Target attributes ➔ ***Response variable***
  - Descriptive attributes ➔ ***Regressor variables***

- As a parameterized function class *f*
  - Estimate parameters to describe the relationship
  - Must be simple enough for interpolation and extrapolation purposes
  - Example: Line (black) v.s. Polynomial (blue) with degree 7



Given a dataset $D = \{(\boldsymbol{x}_i, y_i) \mid i = 1, \dots, n\}$ with n tuples

- $\boldsymbol{x}$: Object description $[x_1, \dots, x_k]$
- y: Numerical target attribute

Find a function

$$f: \mathrm{dom}(x_1) \times \dots \times \mathrm{dom}(x_k) \rightarrow y \in \mathbb{R}$$

minimizing the error

$$E(f(x_1, \dots, x_k), y)$$

for all given n data objects $(\boldsymbol{x}_i, y_i)$.

Linear Regression

Regression Line

- Given a data set with two continuous attributes, x and y
- There is an approximate linear dependency between x and y

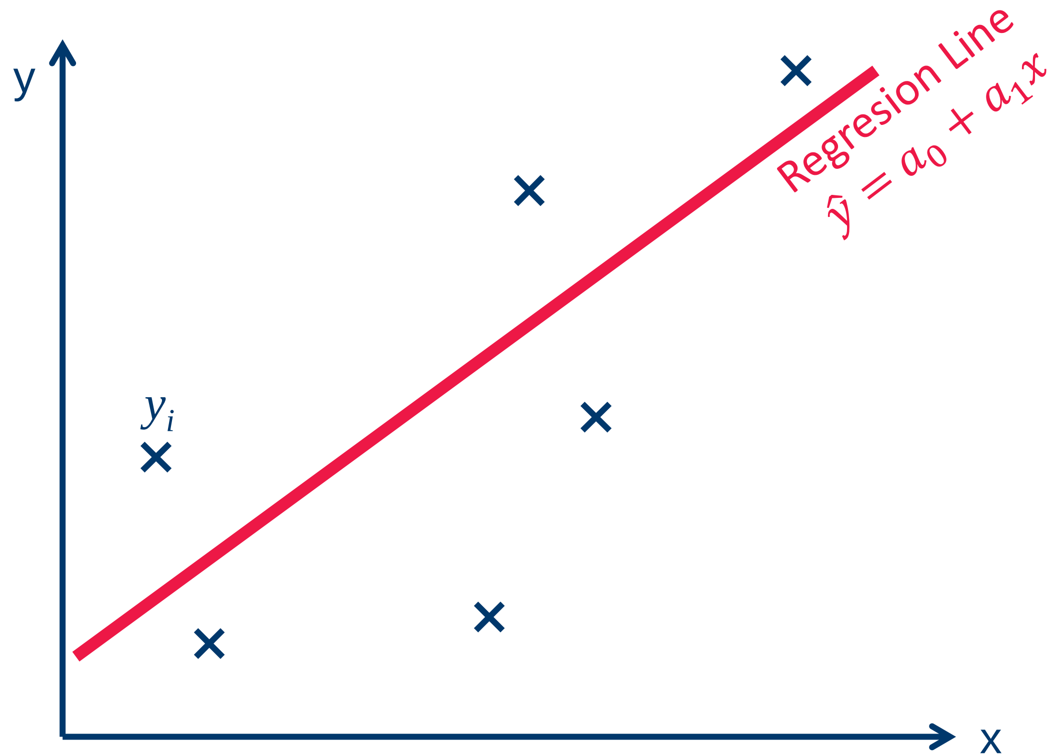
$$y \approx a + bx$$

- We find a **regression line** (i.e., determine the parameters a and b) such that the fits the data as well as possible

- Examples:
  - Trend estimation (e.g., oil price over time)
  - Epidemiology (e.g., cigarette smoking vs. lifespan)
  - Finance (e.g., return on investment vs. return on all risky assets)
  - Economics (e.g., spending vs. available income)

Regression Line

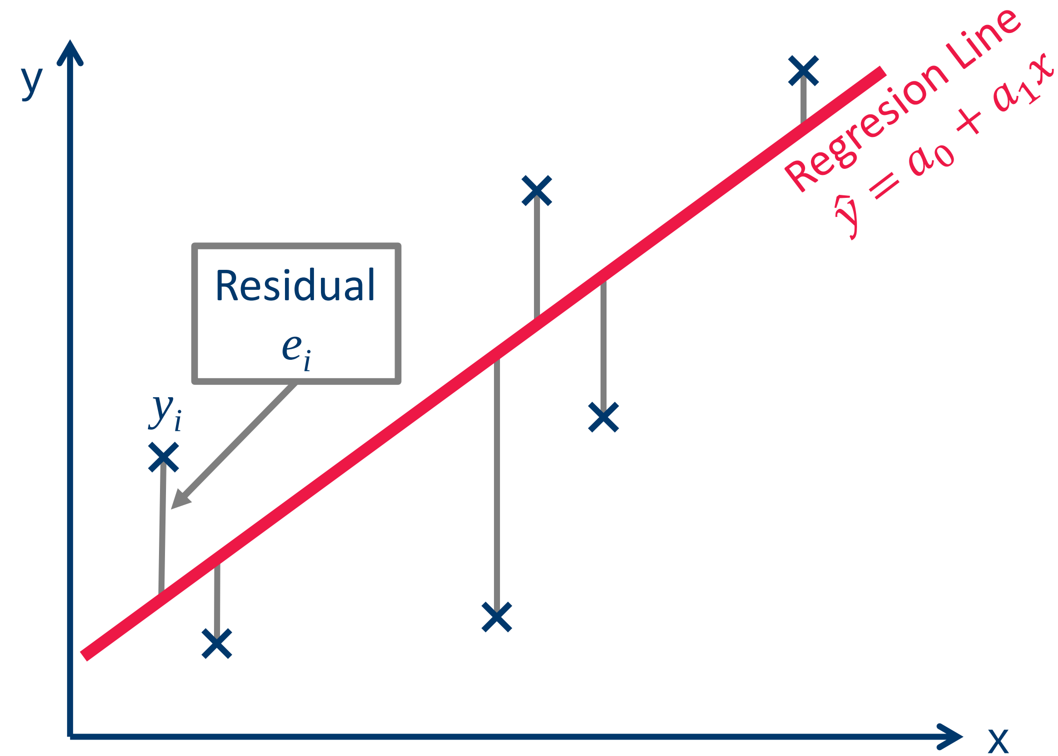
- What is a **good** fit?



- The error, or the ***residual***, is calculated at each data point
- The sum of square errors (SSE) is chosen as cost function (to be minimized)

$$\sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (\hat{y}_i - y_i)^2$$

- Referred as the ***least square method***



Cost Functions

- Sum of square errors

- Other reasonable cost functions
  - mean absolute distance
  - mean Euclidean distance
  - maximum absolute distance in y-direction (or equivalently: the
  - maximum squared distance in y-direction)
  - maximum Euclidean distance
  - . . .

Construction

- Think of a straight line $\hat{y} = f(x) = a + bx$
- Find a and b to model all observations (x_i, y_i) as close as possible
- ➔ SSE $F(a,b) = \sum_{i=1}^{n}(f(x) - y_i)^2 = \sum_{i=1}^{n}(a + bx_i - y_i)^2$ should be minimal
- **Goal**: The y-values that are computed with the linear equation should (squared and in total) deviate as little as possible from the measured values.

- SSE

$$F(a,b) = \sum_{i=1}^{n}(f(x) - y_i)^2 = \sum_{i=1}^{n}(a + bx_i - y_i)^2$$

is minimal if the partial derivatives w.r.t. a and b are 0

- That is:

$$\frac{\partial F}{\partial a} = \sum_{i=1}^{n} 2(a + bx_i - y_i) = 0$$

$$\frac{\partial F}{\partial b} = \sum_{i=1}^{n} 2(a + bx_i - y_i)\, x_i = 0$$

- As a consequence, we obtain the so-called **normal equations**

$$na + \left(\sum_{i=1}^{n} x_i\right) b = \sum_{i=1}^{n} y_i$$

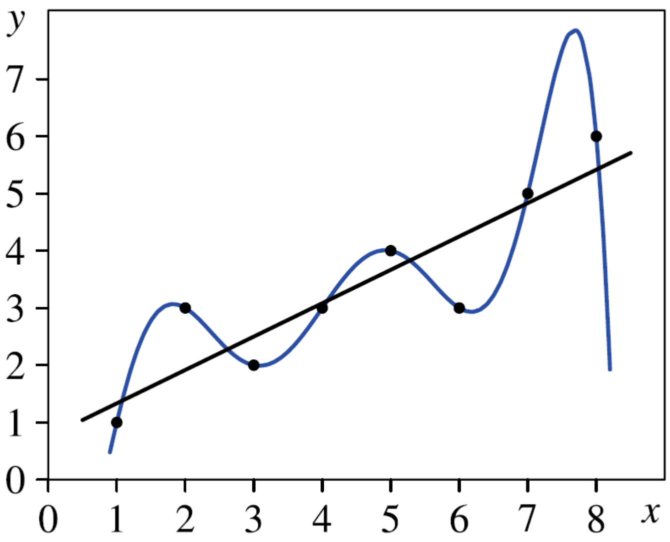
$$\left(\sum_{i=1}^{n} x_i\right) a + \left(\sum_{i=1}^{n} x_i^2\right) b = \sum_{i=1}^{n} x_i\, y_i$$

- that is, a two-equation system with two unknowns *a* and *b* which has a unique solution (if at least two different *x*-values exist).
- => A unique solution exists for a and b

- Example: data

x	1	2	3	4	5	6	7	8
y	1	3	2	3	4	3	5	6

- Resulting regression line: $y = \frac{3}{4} + \frac{7}{12}x$



- The straight line determined in this way is called **regression line** for the data set *D.*
- A regression line can be interpreted as a **maximum likelihood estimator** (MLE):
- **Assumption:** The data generation process can be described by the model

$$f(x) = a + bx + \xi$$

- where ξ is a normally distributed random variable with mean 0 and (unknown) variance σ^2.

- *The parameters that minimize the sum of squared deviations (in y-direction) from the data points maximizes the probability of the data given this model class.*

– Therefore:

$$f(y|x) = \frac{1}{2\pi\sigma^2}\,\exp\left(-\frac{\left(y-(a+bx)\right)^2}{2\sigma^2}\right)$$

– Leading to the likelihood function:

$$L\left((x_1,y_1),\ldots,(x_n,y_n);a,b,\sigma^2\right)$$

$$= \prod_{i=1}^{n} f(y_i|x_i)$$

$$= \prod_{i=1}^{n} \frac{1}{2\pi\sigma^2}\,\exp\left(-\frac{\left(y_i-(a+bx_i)\right)^2}{2\sigma^2}\right)$$

- To simplify the calculation of the derivatives to find the maximum, we compute the **logarithm**.

$$\ln\left(L\left((x_1,y_1),\dots,(x_n,y_n);a,b,\sigma^2\right)\right)$$
$$= \ln\left(\prod_{i=1}^{n}\frac{1}{2\pi\sigma^2}\exp\left(-\frac{\left(y_i-(a+bx_i)\right)^2}{2\sigma^2}\right)\right)$$
$$= \sum_{i=1}^{n}\ln\left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)-\frac{1}{2\sigma^2}\sum_{i=1}^{n}\left(y_i-(a+bx_i)\right)^2$$

- After computing the derivatives w.r.t. the parameters *a* and *b*, we realize that maximizing the likelihood function is equivalent to minimizing

$$F(a,b)=\sum_{i=1}^{n}(f(x)-y_i)^2=\sum_{i=1}^{n}(a+bx_i-y_i)^2$$

Other Regressions

- Least square method can be extended to **polynomials** of degree m

$$y = p(x) = a_0 + a_1 + a_2 x^2 + \cdots + a_m x^m$$

- Find a_i's that minimize the error function

$$\begin{aligned} F(a_0, a_1, \ldots, a_m) &= \sum_{i=1}^{n} (p(x) - y_i)^2 \\ &= \sum_{i=1}^{n} (a_0 + a_1 + a_2 x^2 + \cdots + a_m x^m - y_i)^2 \end{aligned}$$

- We form the partial derivatives of this function w.r.t. the parameters $a_k, k = 1, 2, \cdots, m$, and equate them to zero

Multivariate Regression

- Given a dataset $D = \{(\boldsymbol{x}_i, y_i) \mid i = 1, \dots, n\}$ with n tuples
  - Input vector $\boldsymbol{x}_i = (x_{i1}, x_{i2}, \dots, x_{im})$ with multiple regressors
  - And corresponding response y_i
- For which we want to determine the linear regression function

$$y = f(x_1, x_2, \dots, x_m) = a_0 + \sum_{k=1}^{m} a_k x_k$$

- Examples:
  - Price of a house (y) depending on its size (x_1) and age (x_2)
  - Ice cream consumption (y) based on the temperature (x_1), the price (x_2), and the family income (x_3)
  - Electric consumption (y) based on the number of flats with one (x_1), two (x_2), three (x_3) and four or more persons (x_4) living in them

– The cost function can be written as:

$$F(a_0, a_1, \dots, a_m) = \sum_{i=1}^{n} (f(\boldsymbol{x}_i) - y_i)^2$$

$$= \sum_{i=1}^{n} (a_0 + a_1 x_{i1} + a_2 x_{i2} + \cdots + a_m x_{im} - y_i)^2$$

- It is convenient to write in the matrix form:

$$F(\boldsymbol{a}) = (\boldsymbol{X}\boldsymbol{a} - \boldsymbol{y})^T(\boldsymbol{X}\boldsymbol{a} - \boldsymbol{y})$$

- where

$$\boldsymbol{a} = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{pmatrix} \qquad \boldsymbol{X} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1m} \\ 1 & x_{21} & \cdots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{nm} \end{pmatrix} = \begin{pmatrix} \boldsymbol{x}_1 \\ \boldsymbol{x}_2 \\ \vdots \\ \boldsymbol{x}_n \end{pmatrix} \qquad \boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$\boldsymbol{x}_i = (1, x_{i1}, x_{i2}, \cdots, x_{im})$$

- Find the minimum with the differential operator $\nabla_{\boldsymbol{a}}$

$$\nabla_{\boldsymbol{a}} = \left(\frac{\partial}{\partial a_0}, \frac{\partial}{\partial a_1}, \dots, \frac{\partial}{\partial a_m}\right)$$

- And find the solution to the equation

$$0 = \nabla_{\boldsymbol{a}} F(\boldsymbol{a}) = \nabla_{\boldsymbol{a}} (\boldsymbol{Xa} - \boldsymbol{y})^T (\boldsymbol{Xa} - \boldsymbol{y})$$

$$= \left(\nabla_{\boldsymbol{a}} (\boldsymbol{Xa} - \boldsymbol{y})\right)^T (\boldsymbol{Xa} - \boldsymbol{y}) + \left((\boldsymbol{Xa} - \boldsymbol{y})^T (\nabla_{\boldsymbol{a}} (\boldsymbol{Xa} - \boldsymbol{y}))\right)^{\boldsymbol{T}}$$

$$= \left(\nabla_{\boldsymbol{a}} (\boldsymbol{Xa} - \boldsymbol{y})\right)^T (\boldsymbol{Xa} - \boldsymbol{y}) + \left(\nabla_{\boldsymbol{a}} (\boldsymbol{Xa} - \boldsymbol{y})\right)^T (\boldsymbol{Xa} - \boldsymbol{y})$$

$$= 2\boldsymbol{X}^T (\boldsymbol{Xa} - \boldsymbol{y}) = 2\boldsymbol{X}^T \boldsymbol{Xa} - 2\boldsymbol{X}^T \boldsymbol{y}$$

- From which we obtain the system of normal equations:

$$\boldsymbol{X}^T \boldsymbol{Xa} = \boldsymbol{X}^T \boldsymbol{y}$$

$$\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{a} = \boldsymbol{X}^T\boldsymbol{y}$$

- The system is uniquely solvable iff $\boldsymbol{X}^T\boldsymbol{X}$ is invertible (nonsingular)
- In this case we have:

$$\boldsymbol{a} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\,\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{X}^{+}\boldsymbol{y}$$

- Moore-Penrose pseudo-inverse
  - The expression $(\boldsymbol{X}^T\boldsymbol{X})^{-1}\,\boldsymbol{X}^T = \boldsymbol{X}^{+}$ is also known as the (Moore-Penrose) pseudo-inverse of the matrix $\boldsymbol{X}$.
  - Pseudo-inverse matrices are used to compute the inverse of singular matrices.
  - They provide a least square solution to a system of linear equations without a unique solution.

Regression vs. Time Series Analysis

- **Regression**
  - Targets y & set of input features
  - No time order information
  - Describing the relationship between the target and input features
  - Model → interpolation

- **Time series analysis**
  - **Time** ordered sequence of observations
  - Predicting future observations from:
    - Past values in time series
    - Accompanying time series
  - Model → extrapolation

Solving equations based on partial derivatives of the cost function does not work in some cases with:

- Non-differentiable cost function (absolute value, maximum, etc)
- No analytical solution for equations

Example

- Nonlinear model $y = ae^{bx}$ (radioactive decay, growth of bacteria, …)
- Then the cost function and their partial derivatives are

$$F(a,b) = \sum_{i=1}^{n} \left(ae^{bx_i} - y_i\right)^2$$

$$\frac{\partial F}{\partial a} = 2\sum_{i=1}^{n} \left(ae^{bx_i} - y_i\right)e^{bx_i}$$

$$\frac{\partial F}{\partial b} = 2\sum_{i=1}^{n} \left(ae^{bx_i} - y_i\right)ax_i e^{bx_i}$$

Possible solutions:

- Iterative methods (e.g., gradient descent)
- Transformation of the regression function

Logistic Regression

- Nonlinear regression functions can be transformed, and solved as a linear regression
- Example:

$$y = ax^b$$

- Can be transformed by taking the natural log of the equation

$$\ln y = \ln a + b \cdot \ln x$$

- Notice the sum of squared error is minimized only in the log-transformed space (i.e., $x' = \ln x$, $y' = \ln y$)

Let's consider another transformation

- **Logistic functions** describe limited growth processes, and defined as

$$y = \frac{y_{max}}{1 + e^{a+bx}}$$

- The inverse of this function (**logit function**) produces a linear model

$$\frac{1}{y} = \frac{1 + e^{a+bx}}{y_{max}}$$

$$\frac{y_{max} - y}{y} = e^{a+bx}$$

$$\ln\left(\frac{y_{max} - y}{y}\right) = a + bx$$

- **logit function**

$$\ln\left(\frac{y_{max} - y}{y}\right) = a + bx$$

- We only need to transform the data points according to the left-hand side of the equation.

- Fitting the data to this model is often referred as **logistic regression**

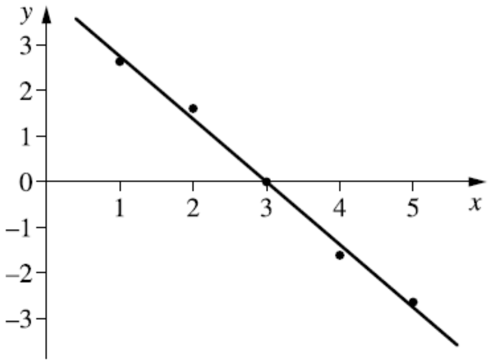
Example – Logit Transformation

– The data

x	1	2	3	4	5
y	0.4	1.0	3.0	5.0	5.6

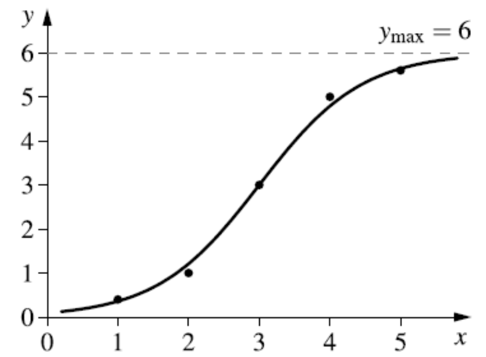
– Can be transformed with a logit-transformation, and the linear regression line is fitted to

$$z = logit(y) = 4.133 - 1.3775x$$



– We can transform y back with the logistic function, and obtain the logistic regression curve

$$y = \frac{6}{1 + e^{4.133 - 1.3775x}}$$



Model vs. Black-box

- When the principal functional dependency between the dependent variable Y and the predictor variables $x_1, \ldots, x_k$ is known, an explicit parameterized (possibly nonlinear) regression function can be specified.

- The coefficients a_i can be interpreted as weighting factors, at least when the predictor variables $x_1, \ldots, x_k$ have been normalised.
- They also provide information of a positive or negative correlation of the predictor variables with the dependent variable Y .
- Usually, complex regression functions yield black-box models, which might provide a good approximation of the data, but do not admit a useful interpretation (of the coefficients).

- Considering a data set as a collection of examples, describing the dependency between the predictor variables and the dependent variable, the regression function should “learn” this dependency from the data
- The same function should also be able to generalize it to make correct predictions on new data.

- The regression function “learns” a description of the data, not of the structure of the data.
- The prediction using a complex regression function can be worse than the prediction using a simpler regression function (overfitting).

Robust Regression

- Ordinary regression – sensitive to outliers
- Solution: ***robust regression***
- Let's re-write the cost function as

$$F(\boldsymbol{a}) = (\boldsymbol{X}\boldsymbol{a} - \boldsymbol{y})^T(\boldsymbol{X}\boldsymbol{a} - \boldsymbol{y}) = \sum_{i=1}^{n} \rho\,(e_i) = \sum_{i=1}^{n} \rho\left(\boldsymbol{x}_i^T\boldsymbol{a} - y_i\right)$$

- For the least square method, the function ρ is a square function
- (i.e., $\rho(e) = e^2$)

- More generally, the ρ function can be any function satisfying the following:

$$
\begin{aligned}
\rho(e) &\geq 0, \\
\rho(0) &= 0, \\
\rho(e) &= \rho(-e), \\
\rho(e_i) &\geq \rho(e_j) \quad \text{if } |e_i| \geq |e_j|.
\end{aligned}
$$

- Parameter estimation with a cost function with a ρ function satisfying these conditions are called an **M-estimator**.

- Calculate the derivatives w.r.t. the parameters a_i in

$$\sum_{i=1}^{n} \rho\left(e_i\right) = \sum_{i=1}^{n} \rho\left(\boldsymbol{x}_i^T \boldsymbol{a} - y_i\right)$$

- We find the solution to the system of linear equations

$$\sum_{i=1}^{n} \psi_i\left(\boldsymbol{x}_i^T \boldsymbol{a} - y_i\right)\boldsymbol{x}_i^T = 0$$

- Where $\psi = \rho'$. If we define $w(e) = \psi(e)/e$ and $w_i = w(e_i)$,

$$\sum_{i=1}^{n} \frac{\psi_i\left(\boldsymbol{x}_i^T \boldsymbol{a} - y_i\right)}{e_i} \cdot e_i \cdot \boldsymbol{x}_i^T = \sum\nolimits_{i=1}^{n} w_i e_i^2 \boldsymbol{x}_i^T = 0$$

- The solution is the same as the standard least squares problem with weights $\sum_{i=1}^{n} w_i e_i^2$

Problem in finding the solution:

- The weights w_i depend on the errors e_i
- The errors e_i depend on the weights w_i

Strategy: alternating optimization

1. Choose an initial solution $\boldsymbol{a}^{(0)}$, (e.g., standard least squares solution) and set all weights to $w_i = 1$
2. At step t, calculate the residuals $e^{(t-1)}$ and the corresponding weights $w^{(t-1)} = w(e^{(t-1)})$
3. Compute the solution to the weighted least squared problem

$$\boldsymbol{a}^{(0)} = \left(\boldsymbol{X}^T \boldsymbol{W}^{(t-1)} \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{W}^{(t-1)} \boldsymbol{y}$$

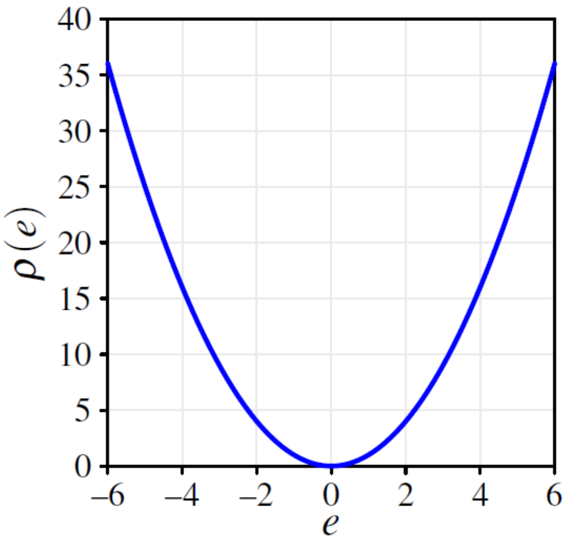
- Where $\boldsymbol{W}$ is a diagonal matrix with weights w_i on the main diagonal

Method	$\rho(e)$
Least squares	e^2
Huber	$\begin{cases} \frac{1}{2}e^2 & \text{if } \lvert e\rvert \leq k, \\ k\lvert e\rvert - \frac{1}{2}k^2 & \text{if } \lvert e\rvert > k. \end{cases}$
Tukey's bisquare	$\begin{cases} \frac{k^2}{6}(1-(1-(\frac{e}{k})^2)^3) & \text{if } \lvert e\rvert \leq k, \\ \frac{k^2}{6} & \text{if } \lvert e\rvert > k. \end{cases}$

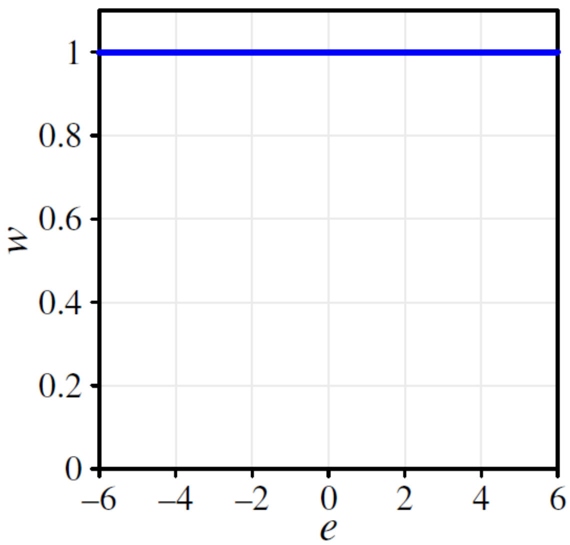
– Where parameter k needs to be chosen for Huber and Tukey's bisquare

– The error measure ρ increases in a quadratic manner with increasing deviation

→ Extreme outliers have full influence



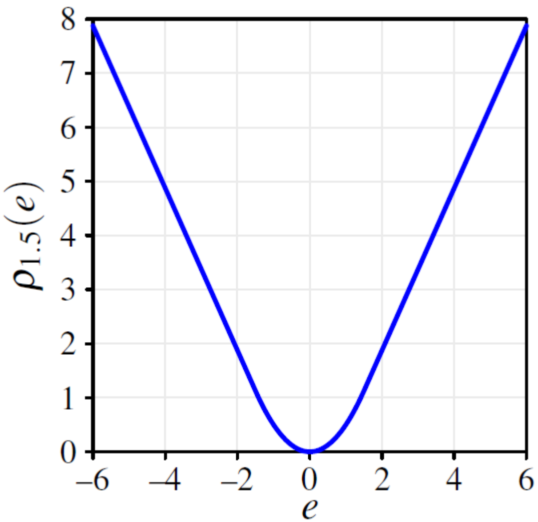
$\rho(e) = e^2$



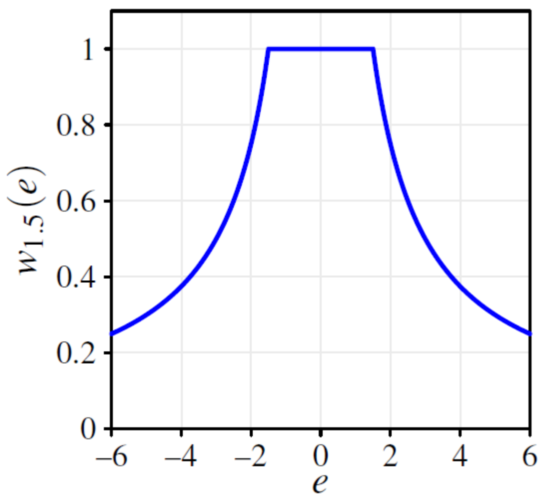
$\omega(e) = 1$

- The error measure ρ switches from quadratic (for small errors) to linear (for large errors)

→ Only data points with small error have full influence



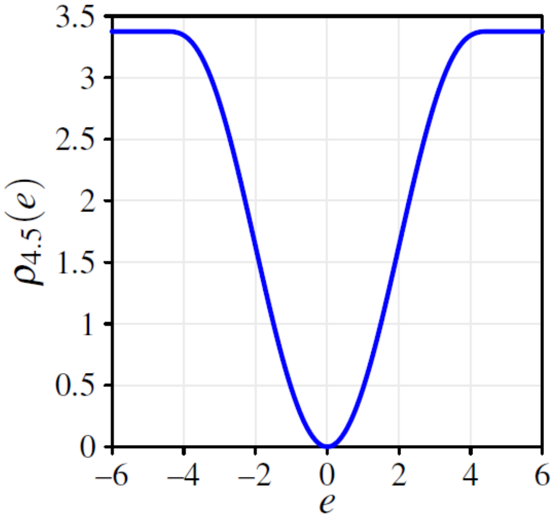
$\rho(e)$	
$\frac{1}{2}e^2$	if $\lvert e\rvert \le k$
$k\lvert e\rvert - \frac{1}{2}k^2$	if $\lvert e\rvert > k$

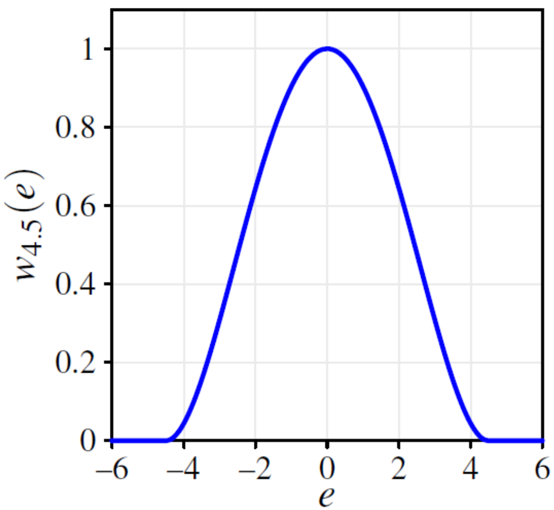


$\omega(e)$	
1	if $\lvert e\rvert \le k$
$\frac{k}{\lvert e\rvert}$	if $\lvert e\rvert > k$

- The error measure ρ does not increase for large errors

→ Weights of extreme outliers drop to zero

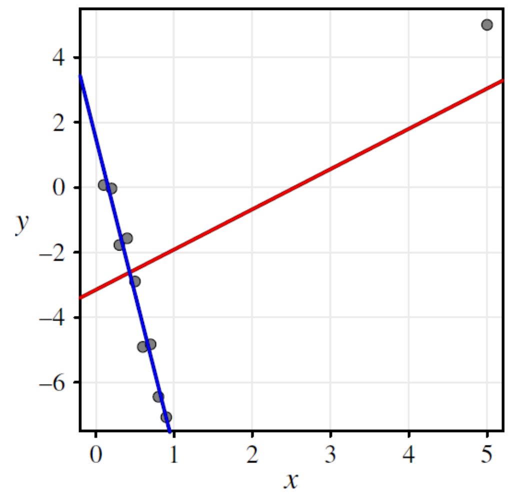




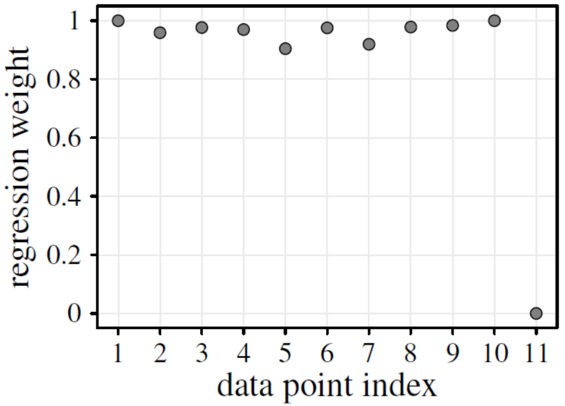
$\rho(e)$	
$\frac{k^2}{6}\left(1-\left(1-\left(\frac{e}{k}\right)^2\right)^3\right)$	if $\|e\| \leq k$
$\frac{k^2}{6}$	if $\|e\| > k$

$\omega(e)$	
$(1-(\frac{e}{k})^2)^2$	if $\|e\| \leq k$
0	if $\|e\| > k$

- An extreme outlier influences the regression line in least squares
- The influence of the outlier is attenuated in robust regression



- Reduced weight is apparent in a plot of regression weights in robust regression



Regression for Classification

Regression and nominal attributes

If:

- most of the predictor variables are numerical,
- and the few nominal attributes have small domains, and
- the data set is sufficiently large and covers all combinations.

then we can construct a regression function for each possible combination of the values of the nominal attributes.

Example:

Attribute	Type / Domain
sex	F/M
vegetarian	yes/no
Age	numerical
Height	numerical
Weight	numerical

Possible solution to predict weight: four regression functions for (F,Yes),(F,No),(M,Yes),(M,No) using only age and height as predictor variables.

Alternative approach:

- Encode the nominal attributes as numerical attributes.
- Binary attributes can be encoded as 0/1 or −1/1
- For nominal attributes with more than two values, a 0/1 or −1/1 numerical attribute should be introduced for each possible value of the nominal attribute (1-of-*n* coding).
- Do not encode nominal attributes with more than two values in one numerical attribute, unless the nominal attribute is actually ordinal.

- A two-class classification problem (classes 0 vs. 1) can be viewed as a regression problem

Challenges:

- A regression function usually cannot produce outcomes 0 or 1
- The cost functions aim to reduce the numerical error (measured as squared residuals, for example), not misclassification

Solution:

- A regression model for the probability of belonging to a certain class
- A probability cut-off (e.g, probability > 0.5) can be used for classification

Classification as Regression: Example

- 1000 data objects, 500 belonging to class 0, 500 to class 1.
- Regression function f yields 0.1 for all data from class 0 and 0.9 for all data from class 1.
- Regression function g always yields the exact and correct values 0 and 1, except for 9 data objects where it yields 1 instead of 0 and vice versa.

Regression function	Mis-classifications	MSE
f	0	0.01
g	9	0.009

- From the viewpoint of regression g is better than f (smaller MSE), from the viewpoint of misclassifications f should be preferred.

- Two-Class Problem:
- If Y belongs to one of two classes $\{c_1, c_2\}$, then we can model the probability for one class only

$$P(Y = c_1 \mid X = \boldsymbol{x}) = p(\boldsymbol{x})$$

$$P(Y = c_2 \mid X = \boldsymbol{x}) = 1 - p(\boldsymbol{x})$$

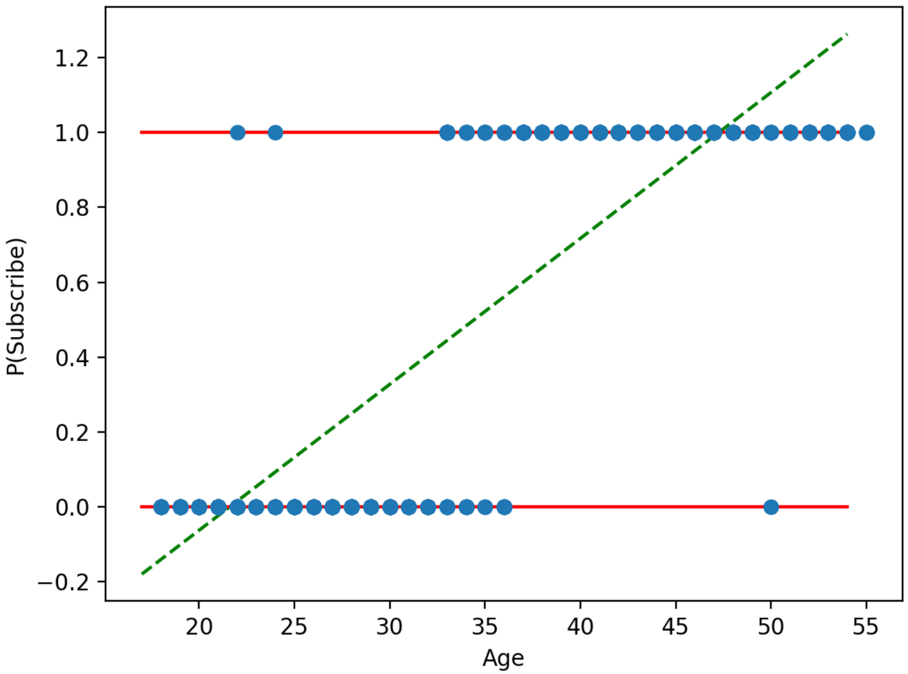
- **Given**: A set of data points $\{\boldsymbol{x}_1, .., \boldsymbol{x}_n\}$ each assigned to one of the two classes c_1 and c_2.
- **Desired:** Train a function, which gives us the probability $p(\boldsymbol{x})$ for each class (0 and 1) based on the input features for the given dataset.

Linear Regression vs. Logistic Regression

	Linear Regression	**Logistic Regression**
Target variable y	Numeric $y \in (-\infty, \infty)/[a, b]$	***Nominal*** $y \in \{0, 1, 2, 3\}/\{red, white\}$
Functional relationship between features and…	… target value y $y = f(x_1, \dots, x_n, \beta_0, \dots, \beta_n)$ $y = \beta_0 + \beta_1 x_1 + \cdots + \beta_n x_n$	… ***class probability P (y = class i)*** $P(y = c_i) = f(x_1, \dots, x_n, \beta_0, \dots, \beta_n)$

Goal: Find the regression coefficients $\beta_0, \dots, \beta_n$

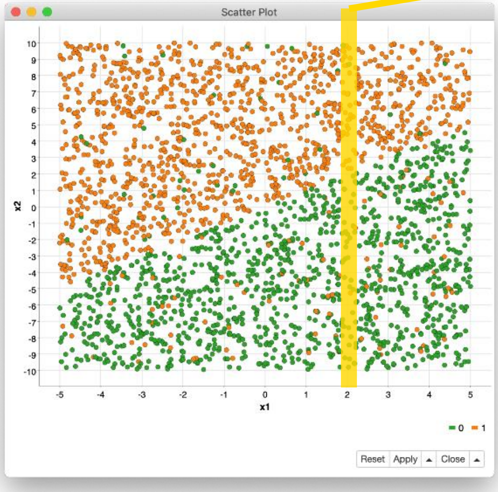
- **Result:** $p(subscribe) = -0.84 + 0.04\ age$
- **Problem:** $p(subscribe) < 0$ for age $= 20$ and $p(subscribe) > 1\ for\ age = 50$

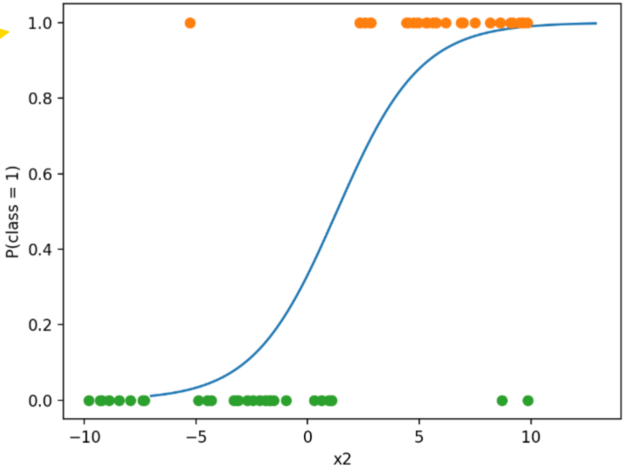


Probability function given $x_1 = 2$

$$P(y=1) = f(x_1, x_2; \beta_0, \beta_1, \beta_2) := \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1 + \beta_2 x_2)}}$$

Feature space





- **Approach:** Describe the probability *p* by the logistic function:

$$p(\boldsymbol{x}) = \frac{1}{1 + \exp(a_0 + \sum_{j=1}^{m} a_j x_j)}$$

- By applying the logit-transformation, we have a multivariate regression problem

$$\ln\left(\frac{1 - p(\boldsymbol{x})}{p(\boldsymbol{x})}\right) = a_0 + \sum_{j=1}^{m} a_j x_j$$

- that is, a multilinear regression problem, which can be solved with the introduced techniques.

How do we determine class probability $p(\boldsymbol{x})$ for this regression problem?

– If we have sufficiently *many* realizations for all possible data points

→ $p(\boldsymbol{x})$ can be estimated by the relative frequencies of the classes

– If there aren’t many realizations, we rely on ***kernel estimation***

- **Idea**: Define an “influence function” (kernel), which describes how strongly a data point influences the probability estimate for neighboring points.
- The “influence” is stronger from a closer point, weaker for a distant point
- The “influence” is modeled by a kernel function
- Example: **Gaussian kernel**

$$K(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{(2\pi\sigma^2)^{\frac{m}{2}}} \exp\left(-\frac{(\boldsymbol{x}-\boldsymbol{y})^T(\boldsymbol{x}-\boldsymbol{y})}{2\sigma^2}\right)$$

- Where $\boldsymbol{y}$ is a neighbor of $\boldsymbol{x}$
- Higher (or lower) influence if $\boldsymbol{x}$ and $\boldsymbol{y}$ are closer (or farther)
- Variance σ^2 has to be chosen by the user.

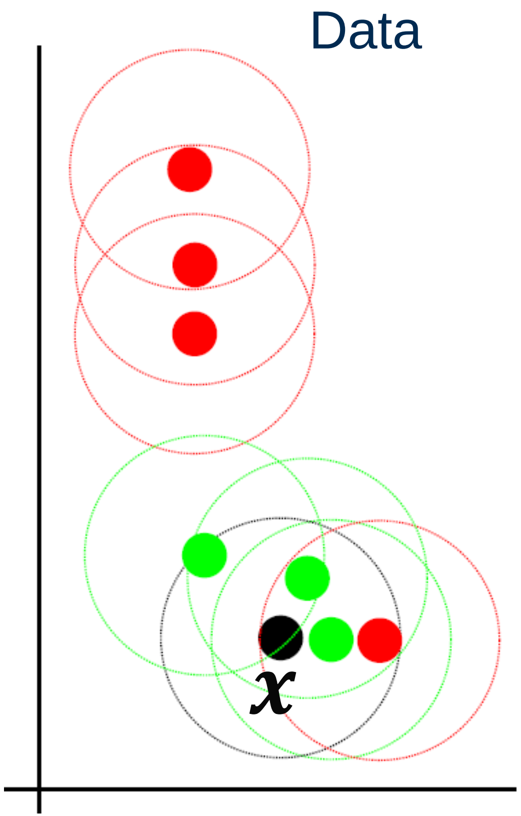
– Kernel estimation for a two-class problem

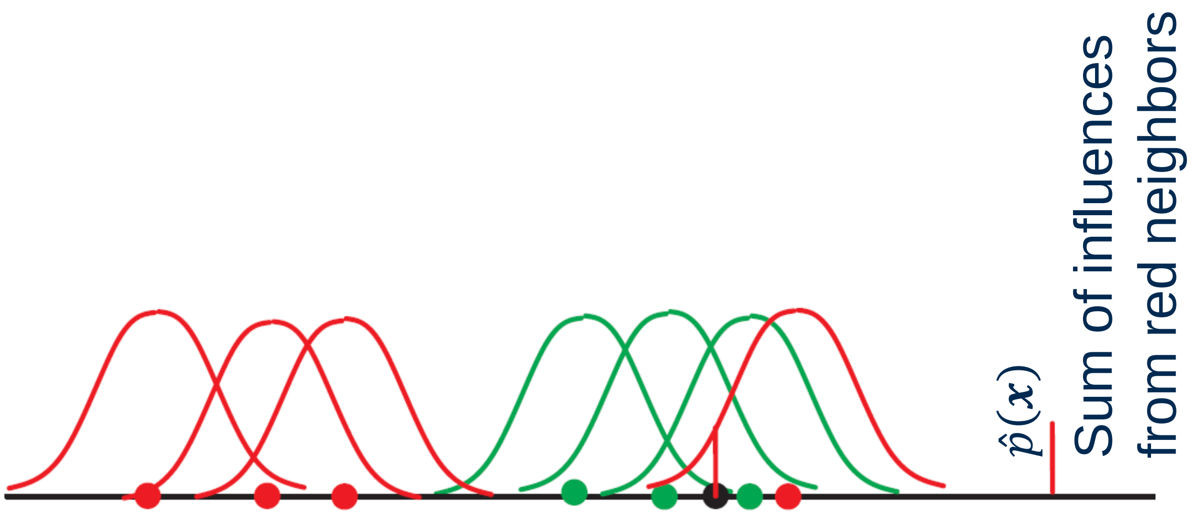
→ $p(\boldsymbol{x})$ is estimated as the sum of $k(\cdot,\cdot)$ between $\boldsymbol{x}$ and all other data points belonging to class c_1

$$\hat{p}(\boldsymbol{x}) = \frac{\sum_{i=1}^{n} c(\boldsymbol{x}_i) K(\boldsymbol{x}, \boldsymbol{x}_i)}{\sum_{i=1}^{n} K(\boldsymbol{x}, \boldsymbol{x}_i)}$$

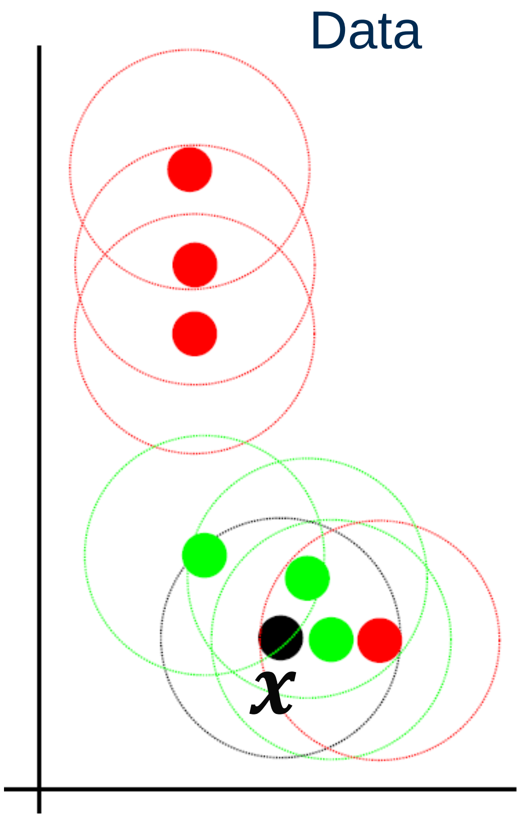
$$c(\boldsymbol{x}_i) = \begin{cases} 1 & \text{if } \boldsymbol{x}_i \text{ belongs to class } c_1 \\ 0 & \text{otherwise} \end{cases}$$

– If red≡c_1, we calculate the sum of kernel functions between $\boldsymbol{x}$ and all red neighbors

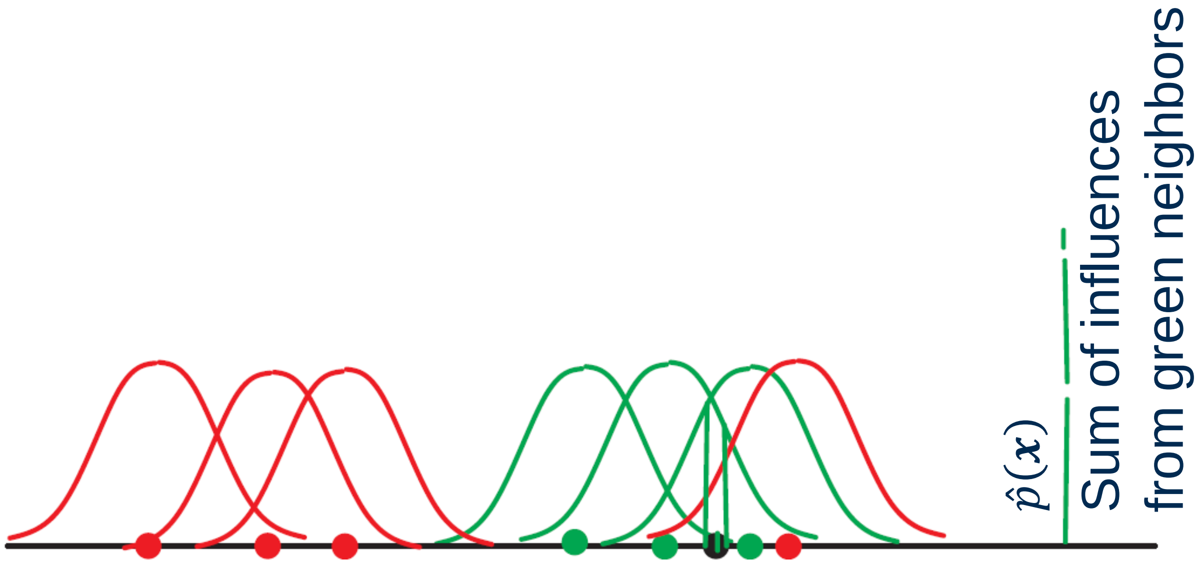




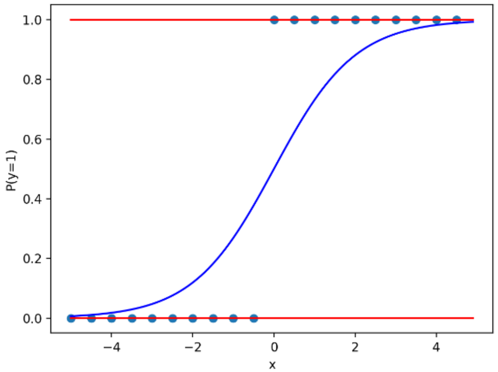
Example – Kernel Estimation



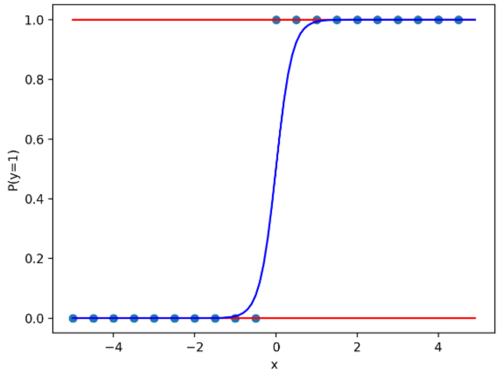
– If green≡c_1, we calculate the sum of kernel functions between $\boldsymbol{x}$ and all green neighbors



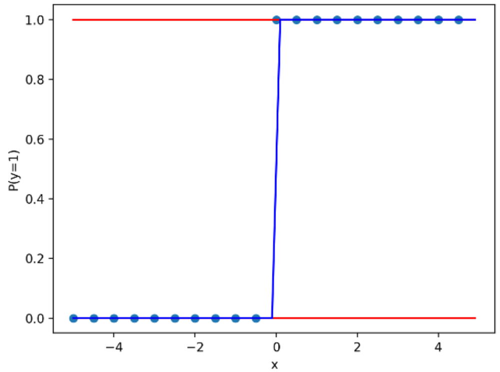
– Is there a way to handle overfitting?



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



$$P(y=1) = \frac{1}{1+e^{-5x}}$$



$$P(y=1) = \frac{1}{1+e^{-100x}}$$

– If data are linearly separable, coefficients becomes extremely large

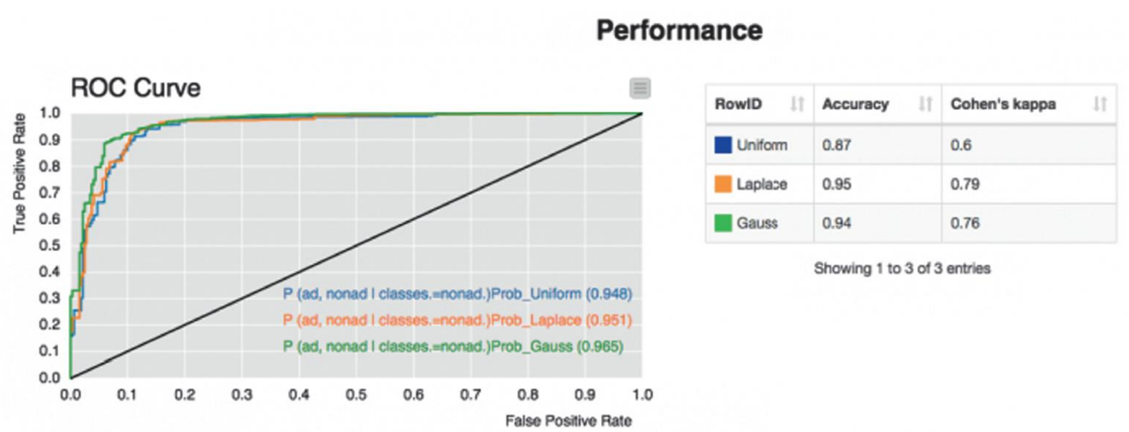
→ *Overfitting*

- The parameters in a logistic regression model is determined by maximizing the likelihood function
- Or equivalently, minimizing the (negative) log-likelihood function
- To avoid overfitting: add regularization by penalizing large coefficients
- Estimate of coefficient vector β obtained by:

$$\hat{\beta} = \min_{\beta}\{-LL(\beta, y, \boldsymbol{x}) + \lambda R(\beta)\}$$

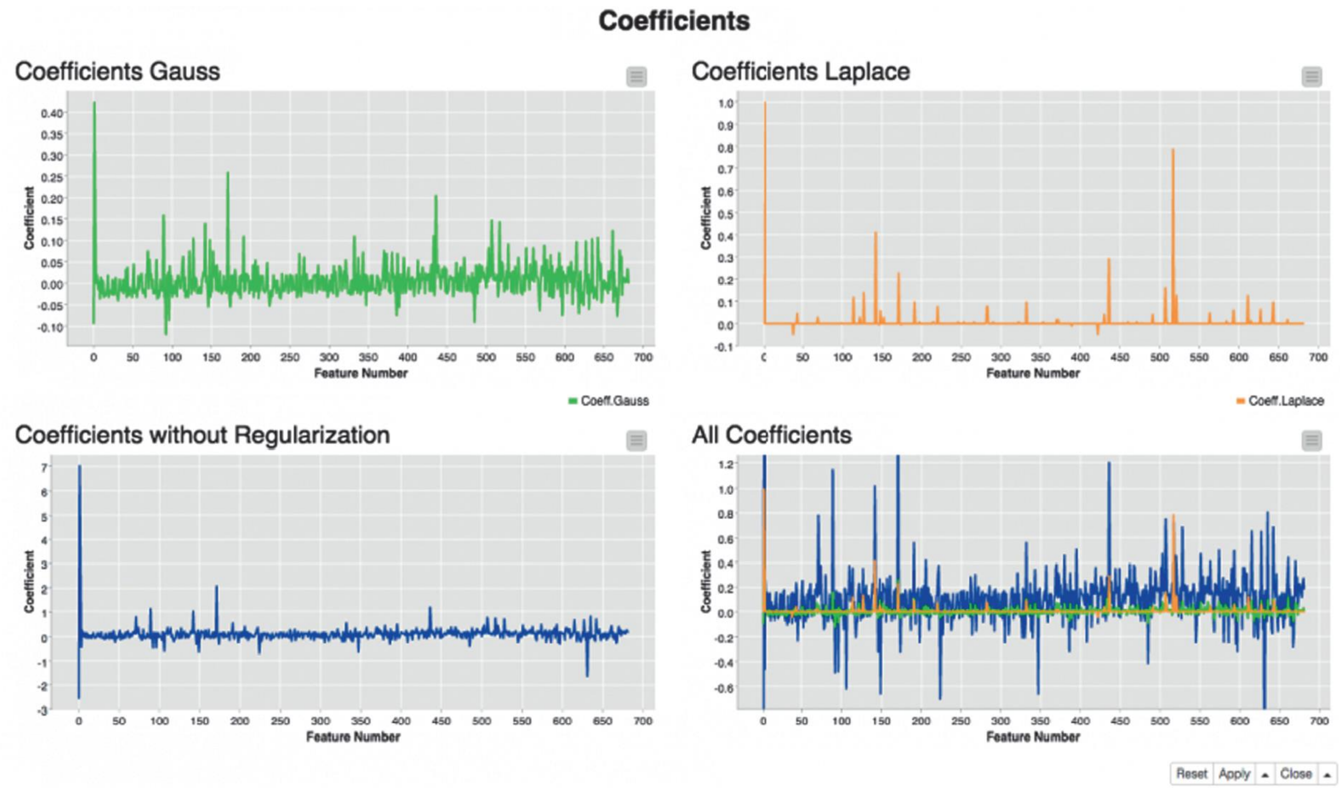
- The choice of the regularization term $R(\beta)$: **Gauss**, **Laplace**, **L1**, **L2**, etc.

– Internet Advertisement Data – UCI Machine Learning Repository
– More features (680) than samples (n=120)
→ Prone to overfitting
– Logistic regression with no regularization (uniform) (blue), Laplace (orange), and Gauss (green)

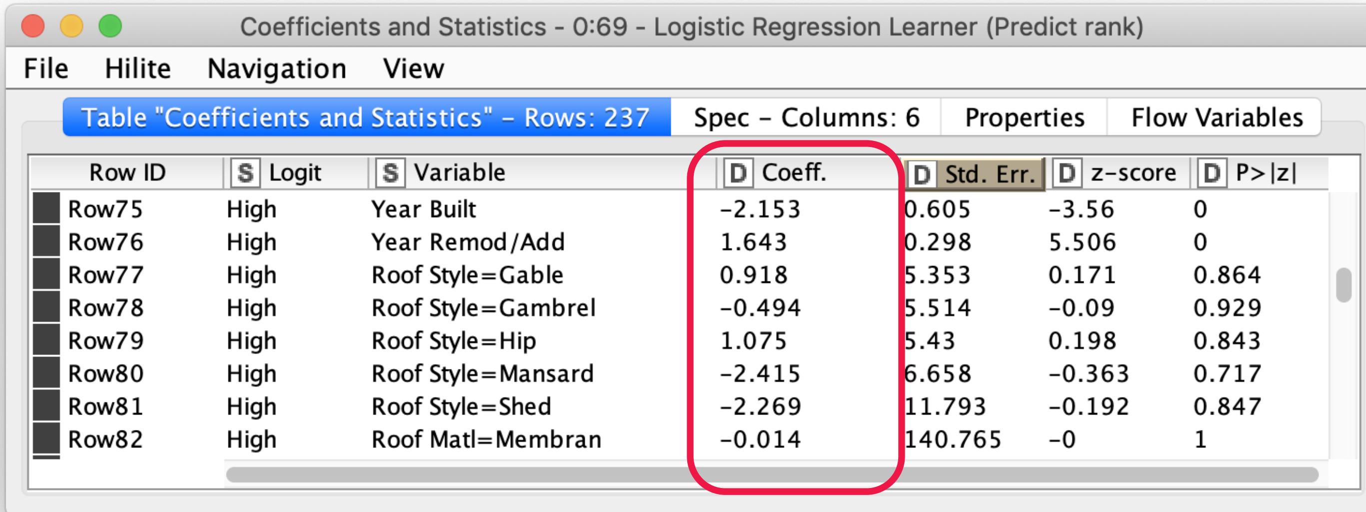


RowID	Accuracy	Cohen's kappa
Uniform	0.87	0.6
Laplace	0.95	0.79
Gauss	0.94	0.76

– Without regularization → large regression coefficients



Interpretation of the Coefficients


Coefficients and Statistics - 0:69 - Logistic Regression Learner (Predict rank)

File Hilite Navigation View

Table "Coefficients and Statistics" – Rows: 237 | Spec – Columns: 6 | Properties | Flow Variables

Row ID	S Logit	S Variable	D Coeff.	D Std. Err.	D z-score	D P>|z|
Row75	High	Year Built	-2.153	0.605	-3.56	0
Row76	High	Year Remod/Add	1.643	0.298	5.506	0
Row77	High	Roof Style=Gable	0.918	5.353	0.171	0.864
Row78	High	Roof Style=Gambrel	-0.494	5.514	-0.09	0.929
Row79	High	Roof Style=Hip	1.075	5.43	0.198	0.843
Row80	High	Roof Style=Mansard	-2.415	6.658	-0.363	0.717
Row81	High	Roof Style=Shed	-2.269	11.793	-0.192	0.847
Row82	High	Roof Matl=Membran	-0.014	140.765	-0	1

- Interpretation of the sign
  - $\beta_i > 0$: Bigger x_i lead to higher probability
  - $\beta_i < 0$: Bigger x_i lead to smaller probability

Interpretation of the p Value

Coefficients and Statistics - 0:69 - Logistic Regression Learner (Predict rank)

File Hilite Navigation View

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– p- value < α: input feature has a significant impact on the dependent variable.

Pros:

- Strong mathematical foundation
- Simple to calculate and to understand (for a moderate number of dimensions)
- High predictive accuracy

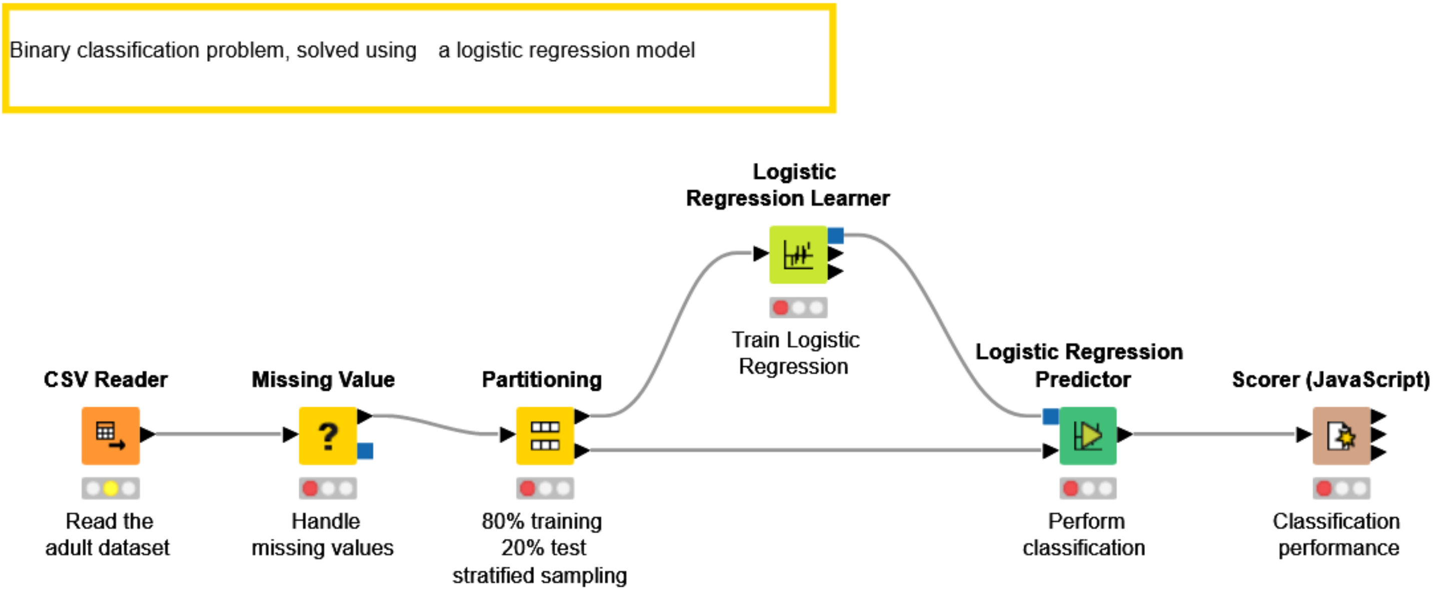
Cons:

- Many dependencies are non-linear
- Global model does not adapt to locally different data distributions

Summary - Regression

- Logistic regression is used for classification problems
- The regression coefficients are calculated by maximizing the likelihood function, which has no closed form solution, hence iterative methods are used.
- Regularization can be used to avoid overfitting.
- The p-value shows us whether an independent variable is significant

Practical Example with KNIME Analytics Platform



- Training and application of a logistic regression model. Notice the Missing Value node to fix possible missing values in the data

Thank you

For any questions please contact: education@knime.com