Regression

Regression

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Regression

Also known as: **Method of Least Squares** (Carl Friedrich Gauß)

Given:
- A data set of data tuples (one or more input values and one output value).
- A hypothesis about the functional relationship between output and input values.

Desired:
- A parameterization of the conjectured function that minimizes the sum of squared errors ("best fit").

Depending on

- the hypothesis about the functional relationship and
- the number of arguments to the conjectured function

different types of regression are distinguished.

Reminder: Function Optimization

Task: Find values $\vec{x} = (x_1, \dots, x_m)$ such that $f(\vec{x}) = f(x_1, \dots, x_m)$ is optimal.

Often feasible approach:

- A necessary condition for a (local) optimum (maximum or minimum) is that the partial derivatives w.r.t. the parameters vanish (Pierre Fermat).
- Therefore: (Try to) solve the equation system that results from setting all partial derivatives w.r.t. the parameters equal to zero.

Example task: Minimize $f(x, y) = x^2 + y^2 + xy - 4x - 5y.$

Solution procedure:

1. Take the partial derivatives of the objective function and set them to zero:

$$\frac{\partial f}{\partial x} = 2x + y - 4 = 0, \qquad \frac{\partial f}{\partial y} = 2y + x - 5 = 0.$$

2. Solve the resulting (here: linear) equation system: $x = 1, \quad y = 2.$

Linear Regression

- Given: data set $((x_1, y_1), \dots, (x_n, y_n))$ of n data tuples
- Conjecture: the functional relationship is linear, i.e., $y = g(x) = a + bx$.

Approach: Minimize the sum of squared errors, i.e.

$$F(a,b) \;=\; \sum_{i=1}^{n} (g(x_i) - y_i)^2 \;=\; \sum_{i=1}^{n} (a + bx_i - y_i)^2.$$

Necessary conditions for a minimum:

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

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

Result of necessary conditions: System of so-called **normal equations**, i.e.

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

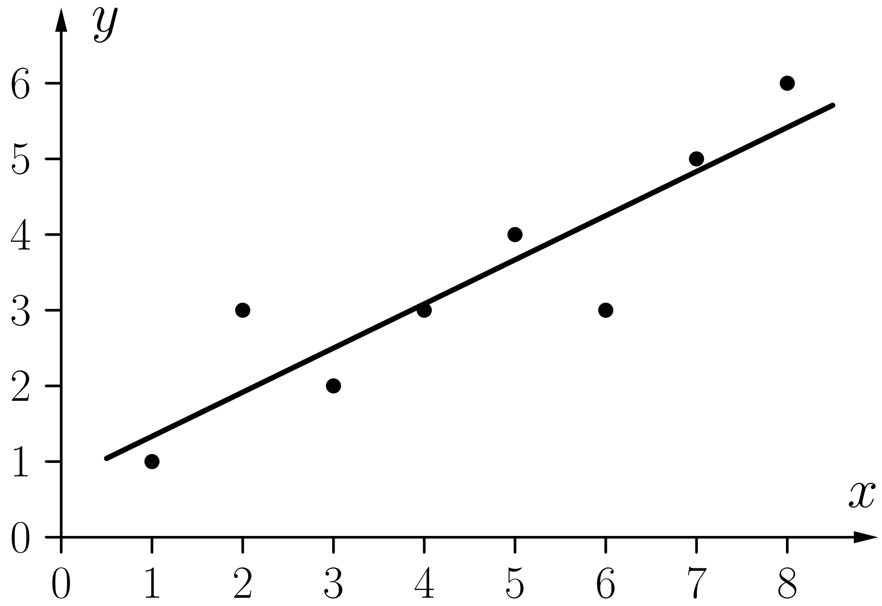
$$\left(\sum_{i=1}^{n} x_i\right) a + \left(\sum_{i=1}^{n} x_i^2\right) b = \sum_{i=1}^{n} x_i y_i.$$

- Two linear equations for two unknowns a and b.
- System can be solved with standard methods from linear algebra.
- Solution is unique unless all x-values are identical.
- The resulting line is called a **regression line**.

Linear Regression: Example

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

$$y = \frac{3}{4} + \frac{7}{12}x.$$



Least Squares and Maximum Likelihood

A regression line can be interpreted as a **maximum likelihood estimator:**

Assumption: The data generation process can be described well by the model

$$y = a + bx + \xi,$$

where ξ is normally distributed with mean 0 and (unknown) variance σ^2 (σ^2 independent of x, i.e. same dispersion of y for all x).

As a consequence we have

$$f(y \mid x) = \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{(y-(a+bx))^2}{2\sigma^2}\right).$$

With this expression we can set up the **likelihood function**

$$\begin{aligned} & L((x_1, y_1), \ldots (x_n, y_n); a, b, \sigma^2) \\ = & \prod_{i=1}^{n} f(x_i) f(y_i \mid x_i) \quad = \quad \prod_{i=1}^{n} f(x_i) \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{(y_i-(a+bx_i))^2}{2\sigma^2}\right). \end{aligned}$$

Least Squares and Maximum Likelihood

To simplify taking the derivatives, we compute the natural logarithm:

$$\begin{aligned}
&\ln L((x_1, y_1), \ldots (x_n, y_n); a, b, \sigma^2) \\
&= \ln \prod_{i=1}^{n} f(x_i) \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{(y_i - (a + bx_i))^2}{2\sigma^2}\right) \\
&= \sum_{i=1}^{n} \ln f(x_i) + \sum_{i=1}^{n} \ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - (a + bx_i))^2
\end{aligned}$$

From this expression it becomes clear that (provided $f(x)$ is independent of a, b, and σ^2) maximizing the likelihood function is equivalent to minimizing

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

Interpreting the method of least squares as a maximum likelihood estimator works also for the generalizations to polynomials and multilinear functions discussed next.

Polynomial Regression

Generalization to polynomials

$$y = p(x) = a_0 + a_1 x + \ldots + a_m x^m$$

Approach: Minimize the sum of squared errors, i.e.

$$F(a_0, a_1, \ldots, a_m) \;=\; \sum_{i=1}^{n} (p(x_i) - y_i)^2 \;=\; \sum_{i=1}^{n} (a_0 + a_1 x_i + \ldots + a_m x_i^m - y_i)^2$$

Necessary conditions for a minimum: All partial derivatives vanish, i.e.

$$\frac{\partial F}{\partial a_0} = 0, \quad \frac{\partial F}{\partial a_1} = 0, \quad \ldots, \quad \frac{\partial F}{\partial a_m} = 0.$$

System of normal equations for polynomials

$$
\begin{aligned}
n a_0 + \left(\sum_{i=1}^{n} x_i\right) a_1 + \ldots + \left(\sum_{i=1}^{n} x_i^m\right) a_m &= \sum_{i=1}^{n} y_i \\
\left(\sum_{i=1}^{n} x_i\right) a_0 + \left(\sum_{i=1}^{n} x_i^2\right) a_1 + \ldots + \left(\sum_{i=1}^{n} x_i^{m+1}\right) a_m &= \sum_{i=1}^{n} x_i y_i \\
\vdots \qquad\qquad & \qquad \vdots \\
\left(\sum_{i=1}^{n} x_i^m\right) a_0 + \left(\sum_{i=1}^{n} x_i^{m+1}\right) a_1 + \ldots + \left(\sum_{i=1}^{n} x_i^{2m}\right) a_m &= \sum_{i=1}^{n} x_i^m y_i,
\end{aligned}
$$

- $m + 1$ linear equations for $m + 1$ unknowns $a_0, \ldots, a_m$.
- System can be solved with standard methods from linear algebra.
- Solution is unique unless the points lie exactly on a polynomial of lower degree.

Generalization to more than one argument

$$z = f(x, y) = a + bx + cy$$

Approach: Minimize the sum of squared errors, i.e.

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

Necessary conditions for a minimum: All partial derivatives vanish, i.e.

$$\begin{aligned}
\frac{\partial F}{\partial a} &= \sum_{i=1}^{n} 2(a + bx_i + cy_i - z_i) &= 0, \\
\frac{\partial F}{\partial b} &= \sum_{i=1}^{n} 2(a + bx_i + cy_i - z_i)x_i &= 0, \\
\frac{\partial F}{\partial c} &= \sum_{i=1}^{n} 2(a + bx_i + cy_i - z_i)y_i &= 0.
\end{aligned}$$

Multilinear Regression

System of normal equations for several arguments

$$
\begin{aligned}
na + \left(\sum_{i=1}^{n} x_i\right) b + \left(\sum_{i=1}^{n} y_i\right) c &= \sum_{i=1}^{n} z_i \\
\left(\sum_{i=1}^{n} x_i\right) a + \left(\sum_{i=1}^{n} x_i^2\right) b + \left(\sum_{i=1}^{n} x_i y_i\right) c &= \sum_{i=1}^{n} z_i x_i \\
\left(\sum_{i=1}^{n} y_i\right) a + \left(\sum_{i=1}^{n} x_i y_i\right) b + \left(\sum_{i=1}^{n} y_i^2\right) c &= \sum_{i=1}^{n} z_i y_i
\end{aligned}
$$

- 3 linear equations for 3 unknowns a, b, and c.
- System can be solved with standard methods from linear algebra.
- Solution is unique unless all data points lie on a straight line.

Multilinear Regression

General multilinear case:

$$\vec{y} = f(\vec{x}_1, \ldots, \vec{x}_m) = a_0 + \sum_{k=1}^{m} a_k \vec{x}_k$$

Approach: Minimize the sum of squared errors, i.e.

$$F(\vec{a}) = (\mathbf{X}\vec{a} - \vec{y})^\top (\mathbf{X}\vec{a} - \vec{y}),$$

where

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \ldots & x_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \ldots & x_{nm} \end{pmatrix}, \qquad \vec{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \qquad \text{and} \qquad \vec{a} = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{pmatrix}$$

Necessary condition for a minimum:

$$\nabla_{\vec{a}} F(\vec{a}) = \nabla_{\vec{a}} (\mathbf{X}\vec{a} - \vec{y})^\top (\mathbf{X}\vec{a} - \vec{y}) = \vec{0}$$

Multilinear Regression

- $\nabla_{\vec{a}}\, F(\vec{a})$ may easily be computed by remembering that the differential operator

$$\nabla_{\vec{a}} = \left(\frac{\partial}{\partial a_0}, \ldots, \frac{\partial}{\partial a_m}\right)$$

  behaves formally like a vector that is "multiplied" to the sum of squared errors.

- Alternatively, one may write out the differentiation componentwise.

Reminder: Vector Derivatives

- What is the derivative of $\vec{x}^\top\vec{x}$ w.r.t. $\vec{x}$?

$$\nabla_{\vec{x}}\vec{x}^\top\vec{x} = \left(\frac{\partial\vec{x}^\top\vec{x}}{\partial x_1}, \cdots, \frac{\partial\vec{x}^\top\vec{x}}{\partial x_m}\right)$$

- We get: $k = 1, \ldots, m$

$$\begin{aligned}\frac{\partial\vec{x}^\top\vec{x}}{\partial x_k} &= \frac{\partial}{\partial x_k}\sum_{i=1}^{m} x_i x_i \\ &= \frac{\partial}{\partial x_k}\left(x_1^2 + \cdots + x_k^2 + \cdots + x_m^2\right) \\ &= \frac{\partial}{\partial x_k}x_1^2 + \cdots + \frac{\partial}{\partial x_k}x_k^2 + \cdots + \frac{\partial}{\partial x_k}x_m^2 \\ &= 2x_k\end{aligned}$$

- Therefore we get:

$$\nabla_{\vec{x}}\vec{x}^\top\vec{x} = (2x_1, \ldots, 2x_k, \ldots, 2x_m) = 2\vec{x}$$

With the former method we obtain for the derivative:

$$\begin{aligned}
&\nabla_{\vec{a}} \, (\mathbf{X}\vec{a} - \vec{y})^\top (\mathbf{X}\vec{a} - \vec{y}) \\
&\quad = \; \left(\nabla_{\vec{a}} \, (\mathbf{X}\vec{a} - \vec{y})\right)^\top (\mathbf{X}\vec{a} - \vec{y}) + \left((\mathbf{X}\vec{a} - \vec{y})^\top \left(\nabla_{\vec{a}} \, (\mathbf{X}\vec{a} - \vec{y})\right)\right)^\top \\
&\quad = \; \left(\nabla_{\vec{a}} \, (\mathbf{X}\vec{a} - \vec{y})\right)^\top (\mathbf{X}\vec{a} - \vec{y}) + \left(\nabla_{\vec{a}} \, (\mathbf{X}\vec{a} - \vec{y})\right)^\top (\mathbf{X}\vec{a} - \vec{y}) \\
&\quad = \; 2\mathbf{X}^\top (\mathbf{X}\vec{a} - \vec{y}) \\
&\quad = \; 2\mathbf{X}^\top \mathbf{X}\vec{a} - 2\mathbf{X}^\top \vec{y} \; = \; \vec{0}
\end{aligned}$$

Multilinear Regression

Necessary condition for a minimum therefore:

$$\begin{aligned}\nabla_{\vec{a}} F(\vec{a}) &= \nabla_{\vec{a}} (\mathbf{X}\vec{a} - \vec{y})^\top (\mathbf{X}\vec{a} - \vec{y}) \\ &= 2\mathbf{X}^\top \mathbf{X}\vec{a} - 2\mathbf{X}^\top \vec{y} \stackrel{!}{=} \vec{0}\end{aligned}$$

As a consequence we get the system of **normal equations**:

$$\mathbf{X}^\top \mathbf{X}\vec{a} = \mathbf{X}^\top \vec{y}$$

This system has a unique solution if $\mathbf{X}^\top \mathbf{X}$ is not singular. Then we have

$$\vec{a} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \vec{y}.$$

$(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$ is called the (Moore–Penrose) **pseudoinverse** of the matrix $\mathbf{X}$.

With the matrix-vector representation of the regression problem an extension to **multipolynomial regression** is straighforward:
Simply add the desired products of powers to the matrix $\mathbf{X}$.

Generalization to non-polynomial functions

Idea: Find transformation to linear/polynomial case.

Simple example: The function $y = ax^b$

can be transformed into $\ln y = \ln a + b \cdot \ln x$.

Special case: **logistic function**

$$y = \frac{Y}{1 + e^{a+bx}} \quad \Leftrightarrow \quad \frac{1}{y} = \frac{1 + e^{a+bx}}{Y} \quad \Leftrightarrow \quad \frac{Y - y}{y} = e^{a+bx}.$$

Result: Apply so-called **Logit Transformation**

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

Logistic Regression: Example

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

Transform the data with

$$z = \ln\left(\frac{Y - y}{y}\right), \qquad Y = 6.$$

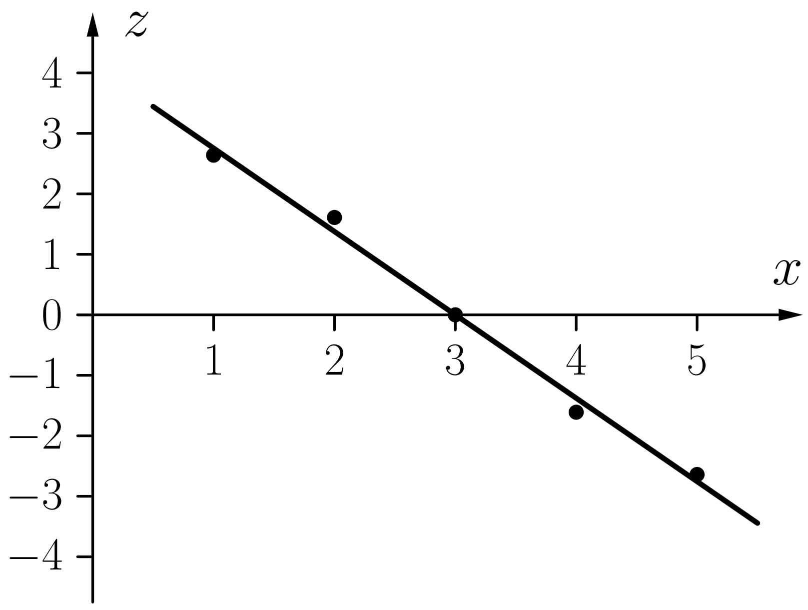
The transformed data points are

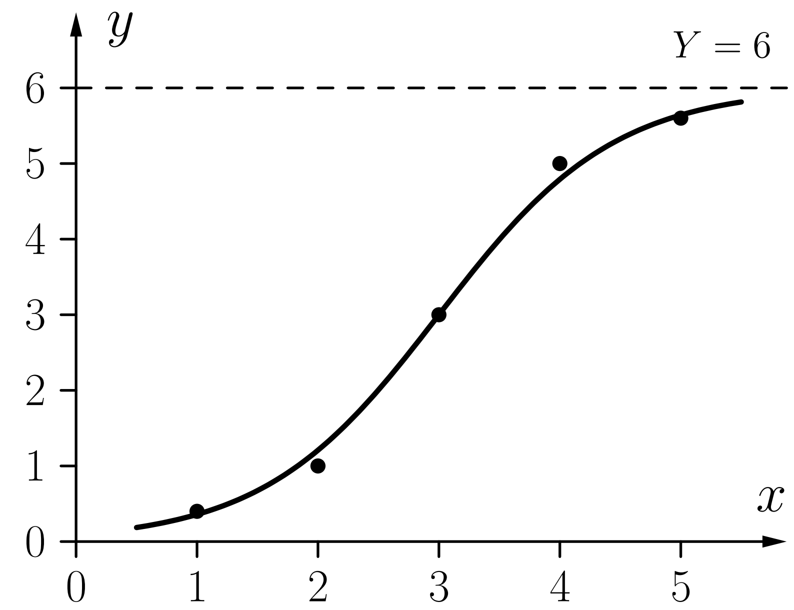
x	1	2	3	4	5
z	2.64	1.61	0.00	-1.61	-2.64

The resulting regression line is

$$z \approx -1.3775x + 4.133.$$

Logistic Regression: Example



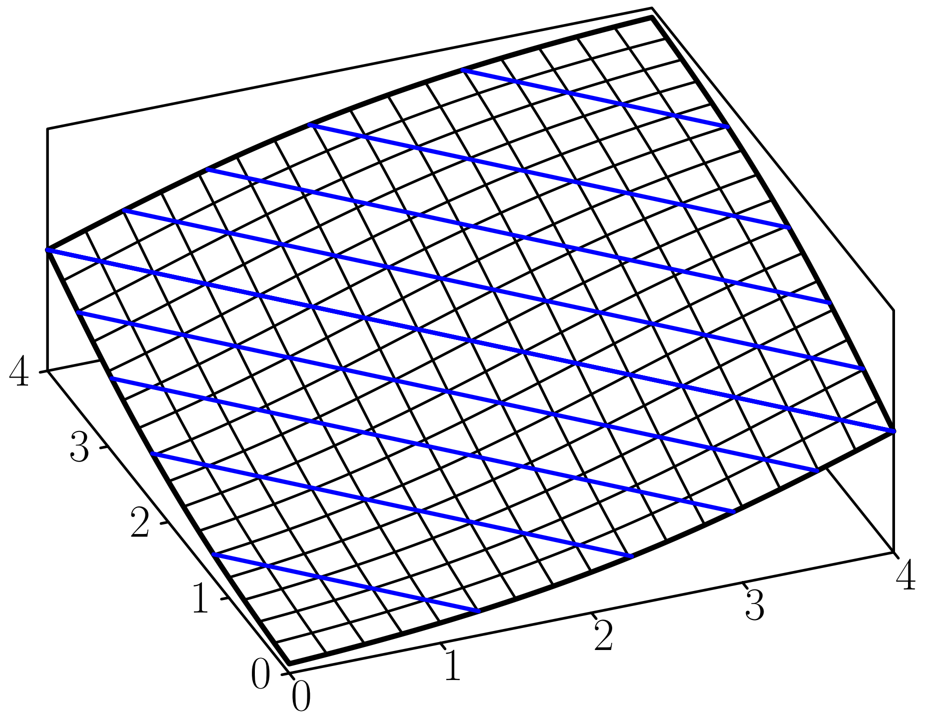


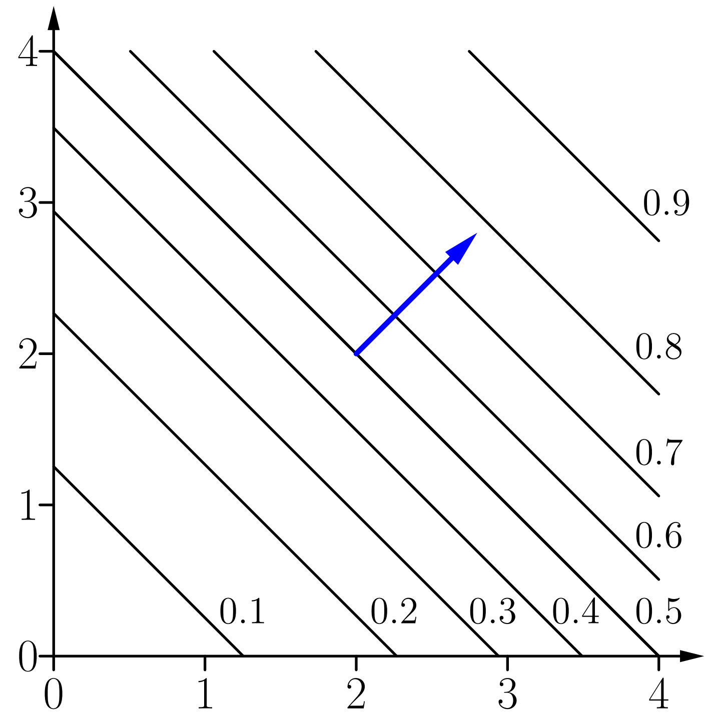
- **Attention:** The sum of squared errors is minimized only in the space the transformation maps to, not in the original space.
- Nevertheless this approach usually leads to very good results.
  The result may be improved by a gradient descent in the original space.

Logistic Regression: Two-dimensional Example

Example logistic function for two arguments x_1 and x_2:

$$y = \frac{1}{1 + \exp(4 - x_1 - x_2)} = \frac{1}{1 + \exp\left(4 - (1,1)(x_1, x_2)^\top\right)}$$





Logistic Regression: Two Class Problems

- Let C be a class attribute, $\text{dom}(C) = \{c_1, c_2\}$, and $\vec{X}$ an m-dim. random vector.
  Let $P(C = c_1 \mid \vec{X} = \vec{x}) = p(\vec{x})$ and $P(C = c_2 \mid \vec{X} = \vec{x}) = 1 - p(\vec{x})$.
- **Given:** A set of data points $\mathbf{X} = \{\vec{x}_1, \ldots, \vec{x}_n\}$ (realizations of $\vec{X}$), each of which belongs to one of the two classes c_1 and c_2.
- **Desired:** A simple description of the function $p(\vec{x})$.
- **Approach:** Describe p by a logistic function:

$$p(\vec{x}) = \frac{1}{1 + e^{a_0 + \vec{a}\vec{x}}} = \frac{1}{1 + \exp\left(a_0 + \sum_{i=1}^{m} a_i x_i\right)}$$

Apply logit transformation to $p(x)$:

$$\ln\left(\frac{1 - p(\vec{x})}{p(\vec{x})}\right) = a_0 + \vec{a}\vec{x} = a_0 + \sum_{i=1}^{m} a_i x_i$$

The values $p(\vec{x}_i)$ may be obtained by kernel estimation.

Kernel Estimation

- **Idea:** Define an "influence function" (kernel), which describes how strongly a data point influences the probability estimate for neighboring points.

- Common choice for the kernel function: **Gaussian function**

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

- Kernel estimate of probability density given a data set $\mathcal{X} = \{\vec{x}_1, \ldots, \vec{x}_n\}$:

$$\hat{f}(\vec{x}) \quad = \quad \frac{1}{n}\sum_{i=1}^{n} K(\vec{x}, \vec{x}_i).$$

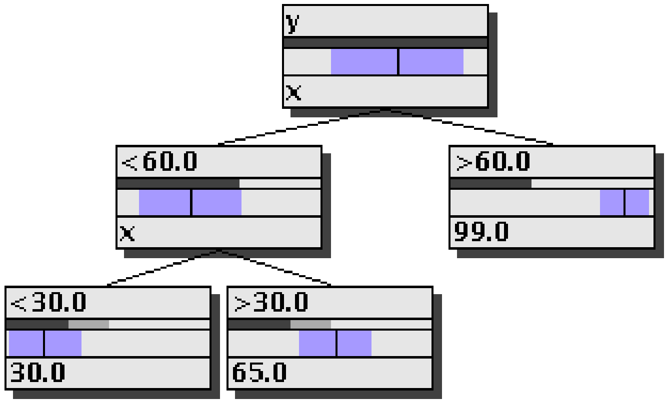
- Kernel estimation applied to a two class problem:

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

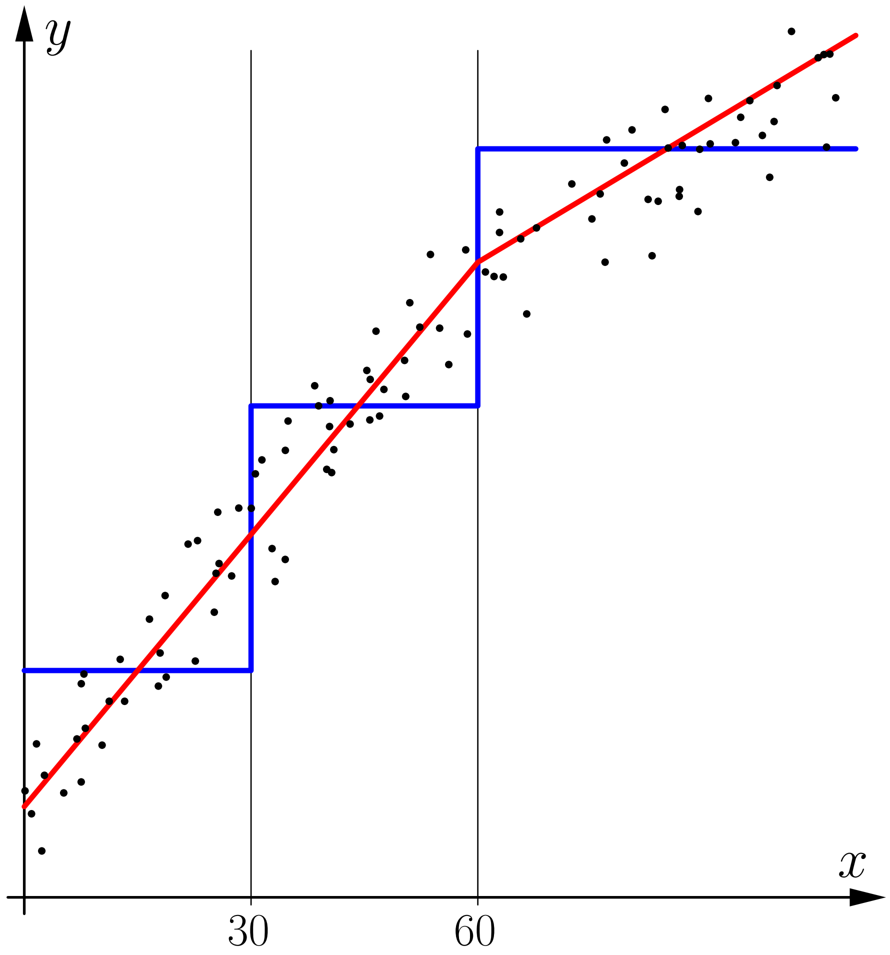
(It is $c(\vec{x}_i) = 1$ if x_i belongs to class c_1 and $c(\vec{x}_i) = 0$ otherwise.)

Regression Trees

- Target variable is not a class, but a numeric quantity.
- Simple regression trees: predict constant values in leaves. (blue lines)

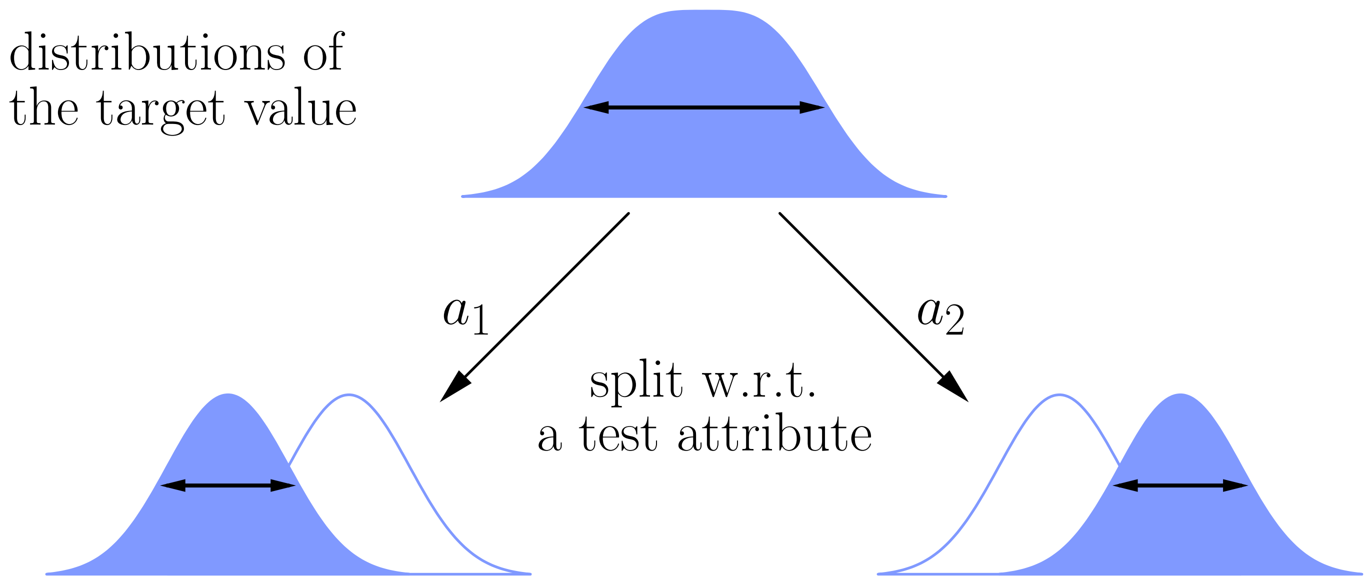


- More complex regression trees: predict linear functions in leaves. (red line)



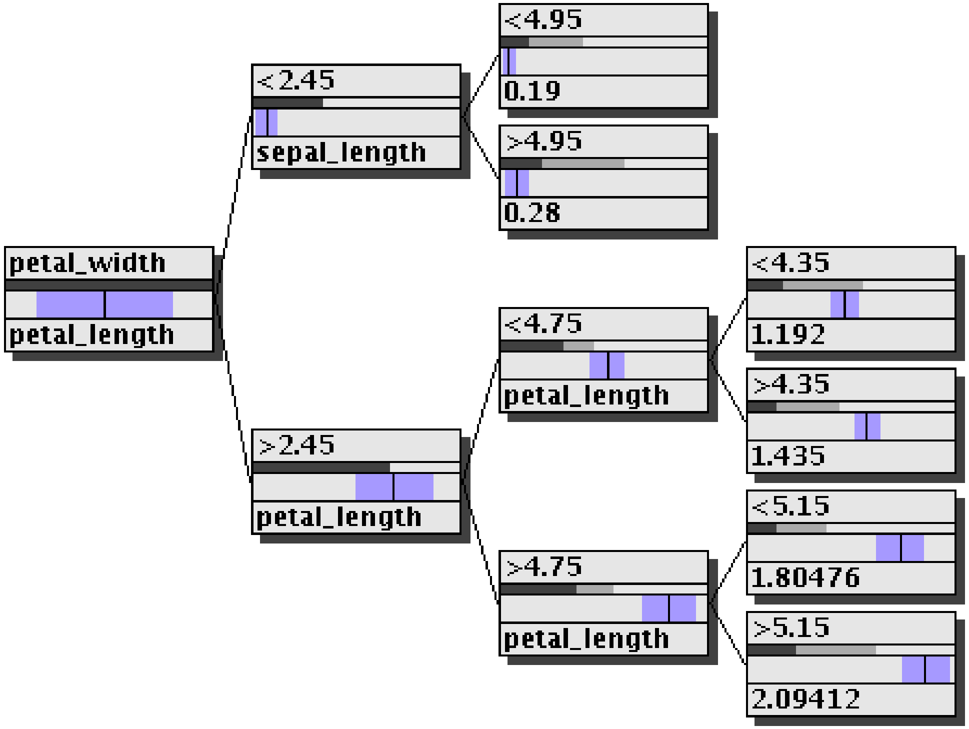
x: input variable, y: target variable

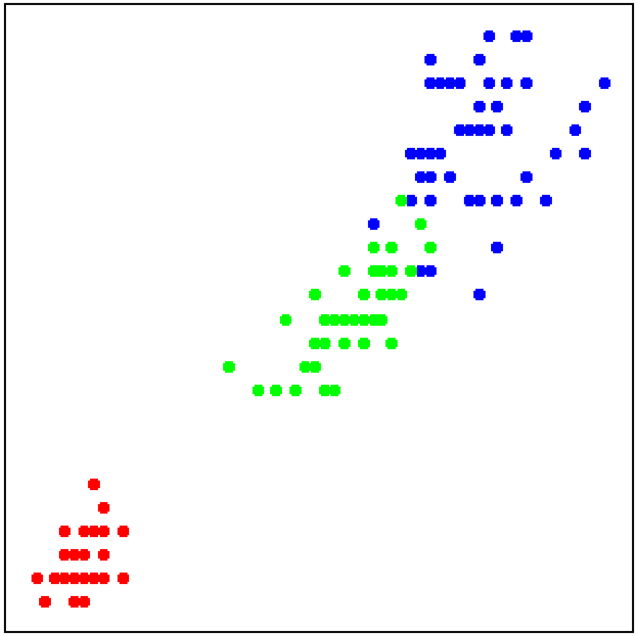
Regression Trees: Attribute Selection



- The variance / standard deviation is compared to the variance / standard deviation in the branches.
- The attribute that yields the highest reduction is selected.

A regression tree for the Iris data (petal width)
(induced with reduction of sum of squared errors)





Summary Regression

- **Minimize the Sum of Squared Errors**
  - Write the sum of squared errors
    as a function of the parameters to be determined.
- **Exploit Necessary Conditions for a Minimum**
  - Partial derivatives w.r.t. the parameters to determine must vanish.
- **Solve the System of Normal Equations**
  - The best fit parameters are the solution of the system of normal equations.
- **Non-polynomial Regression Functions**
  - Find a transformation to the multipolynomial case.
  - Logistic regression can be used to solve two class classification problems.