Why Non-linear Activation Functions?

If the output function is also linear, it is analogously

$$\vec{\text{out}}_{U_2} = \mathbf{D}_{\text{out}} \cdot \vec{\text{act}}_{U_2} - \vec{\xi},$$

where

- $\vec{\text{out}}_{U_2} = (\text{out}_{u_1}, \ldots, \text{out}_{u_n})^T$ is the output vector,
- $\mathbf{D}_{\text{out}}$ is again an $n \times n$ diagonal matrix of factors, and
- $\vec{\xi} = (\xi_{u_1}, \ldots, \xi_{u_n})^T$ a bias vector.

Combining these computations we get

$$\vec{\text{out}}_{U_2} = \mathbf{D}_{\text{out}} \cdot \left(\mathbf{D}_{\text{act}} \cdot \left(\mathbf{W} \cdot \vec{\text{out}}_{U_1}\right) - \vec{\theta}\right) - \vec{\xi}$$

and thus

$$\vec{\text{out}}_{U_2} = \mathbf{A}_{12} \cdot \vec{\text{out}}_{U_1} + \vec{b}_{12}$$

with an $n \times m$ matrix $\mathbf{A}_{12}$ and an n-dimensional vector $\vec{b}_{12}$.

Why Non-linear Activation Functions?

Therefore we have

$$\vec{\text{out}}_{U_2} = \mathbf{A}_{12} \cdot \vec{\text{out}}_{U_1} + \vec{b}_{12}$$

and

$$\vec{\text{out}}_{U_3} = \mathbf{A}_{23} \cdot \vec{\text{out}}_{U_2} + \vec{b}_{23}$$

for the computations of two consecutive layers U_2 and U_3.

These two computations can be combined into

$$\vec{\text{out}}_{U_3} = \mathbf{A}_{13} \cdot \vec{\text{out}}_{U_1} + \vec{b}_{13},$$

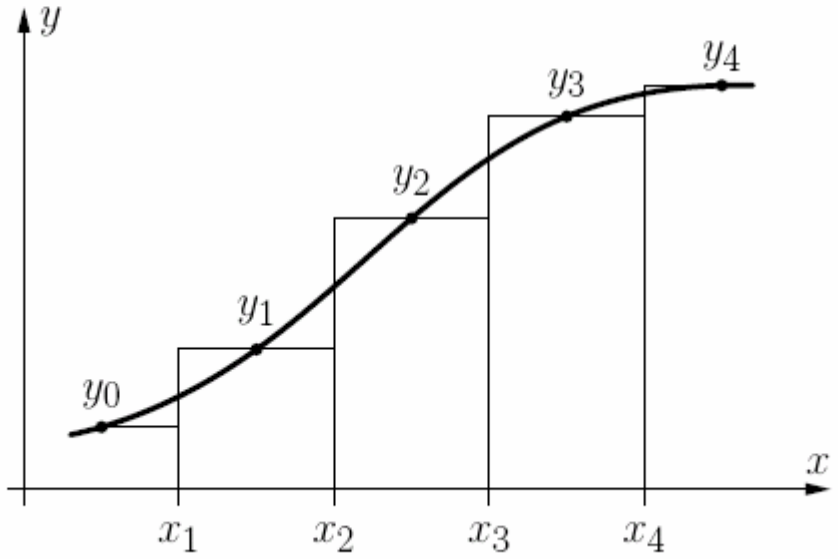
where $\mathbf{A}_{13} = \mathbf{A}_{23} \cdot \mathbf{A}_{12}$ and $\vec{b}_{13} = \mathbf{A}_{23} \cdot \vec{b}_{12} + \vec{b}_{23}$.

Result: With linear activation and output functions any multilayer perceptron can be reduced to a two-layer perceptron.

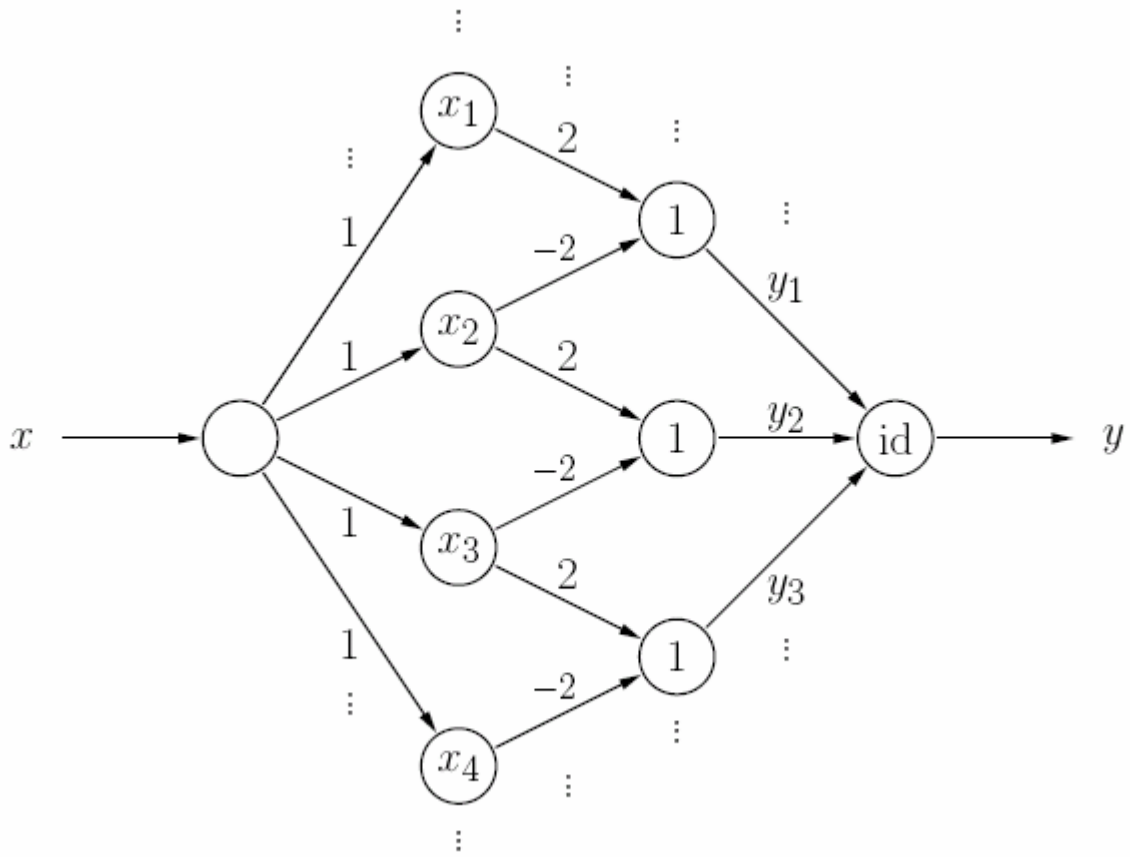
Multilayer Perceptrons: Function Approximation

General idea of function approximation

- Approximate a given function by a step function.
- Construct a neural network that computes the step function.



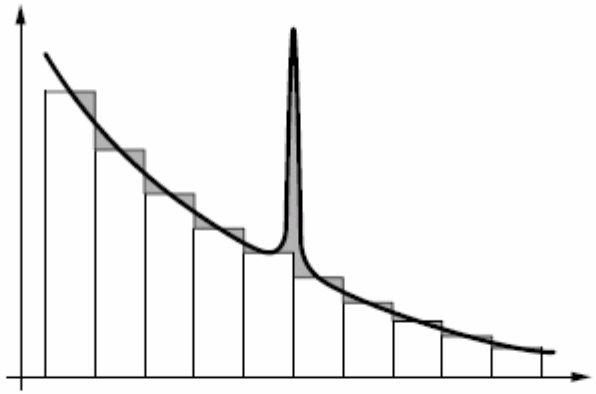
Multilayer Perceptrons: Function Approximation



Multilayer Perceptrons: Function Approximation

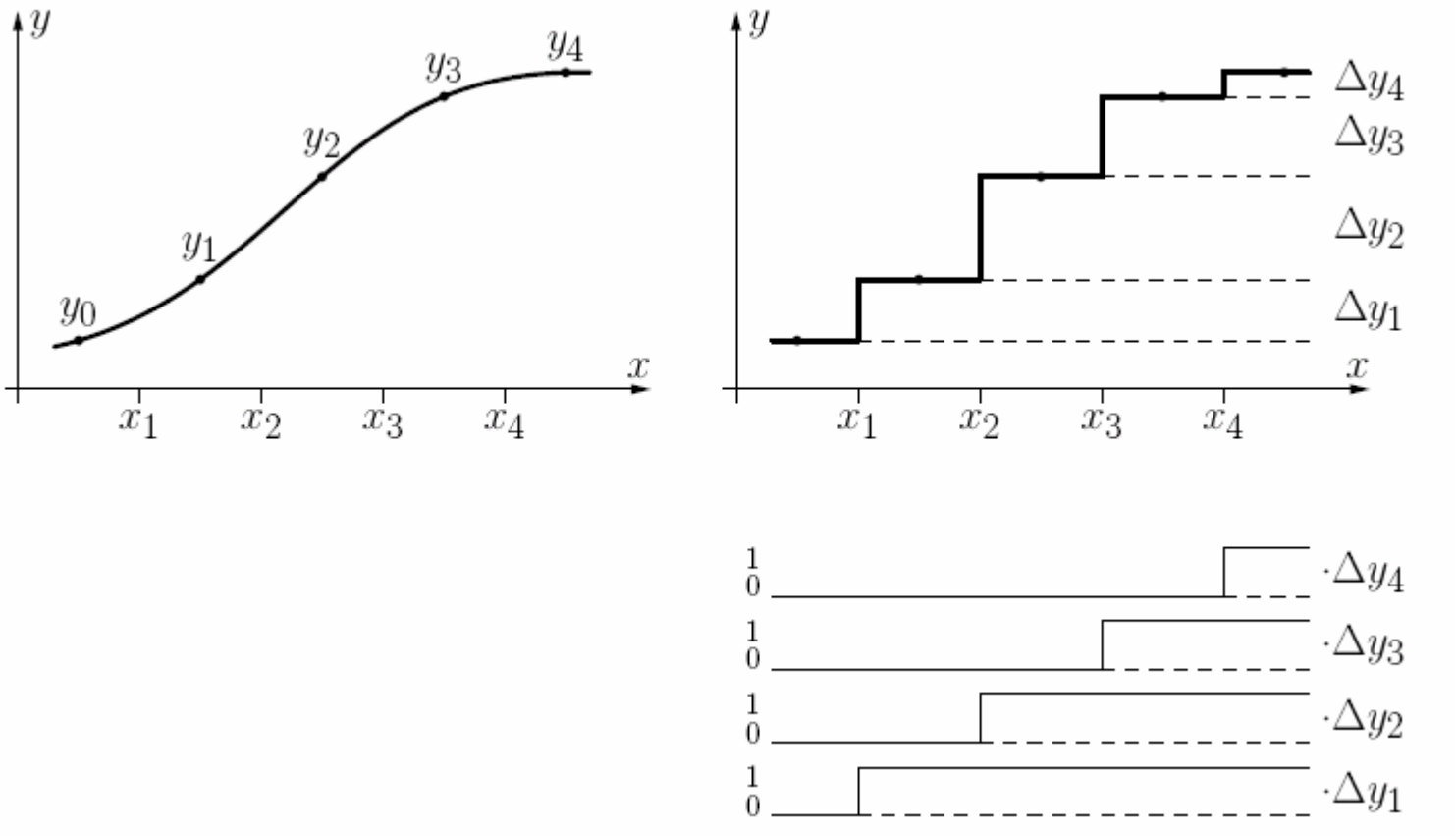
Theorem: Any Riemann-integrable function can be approximated with arbitrary accuracy by a four-layer perceptron.

- But: Error is measured as the **area** between the functions.

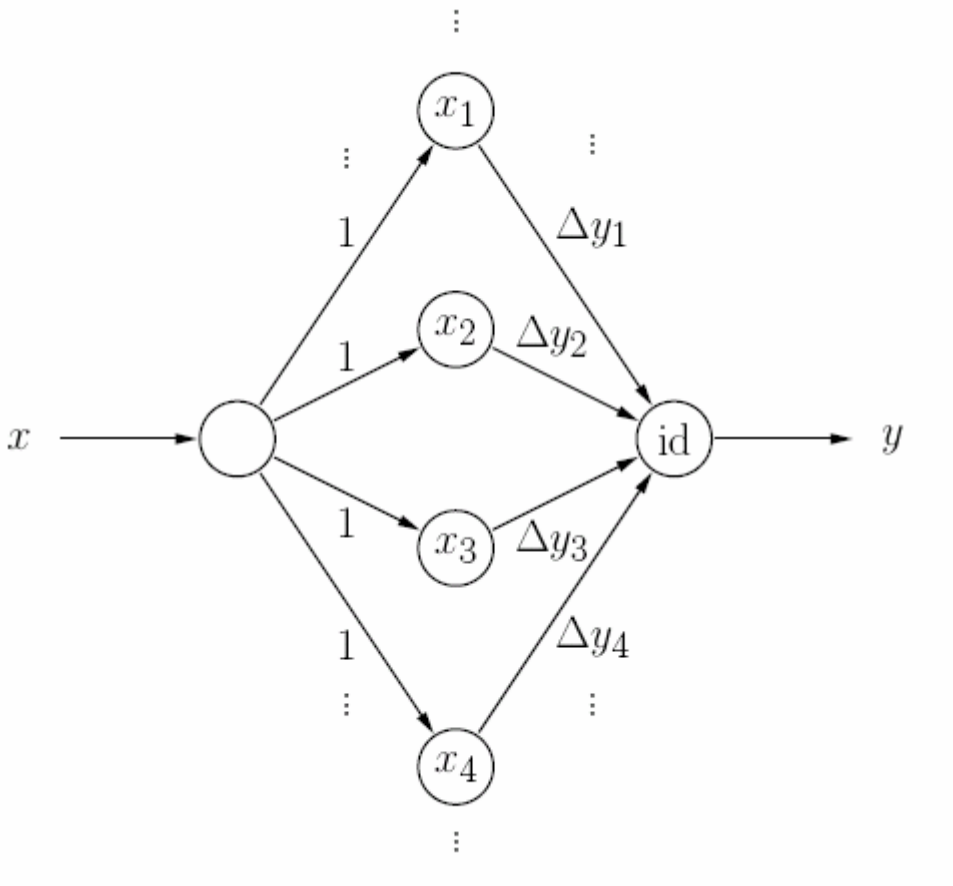


- More sophisticated mathematical examination allows a stronger assertion: With a three-layer perceptron any continuous function can be approximated with arbitrary accuracy (error: maximum function value difference).

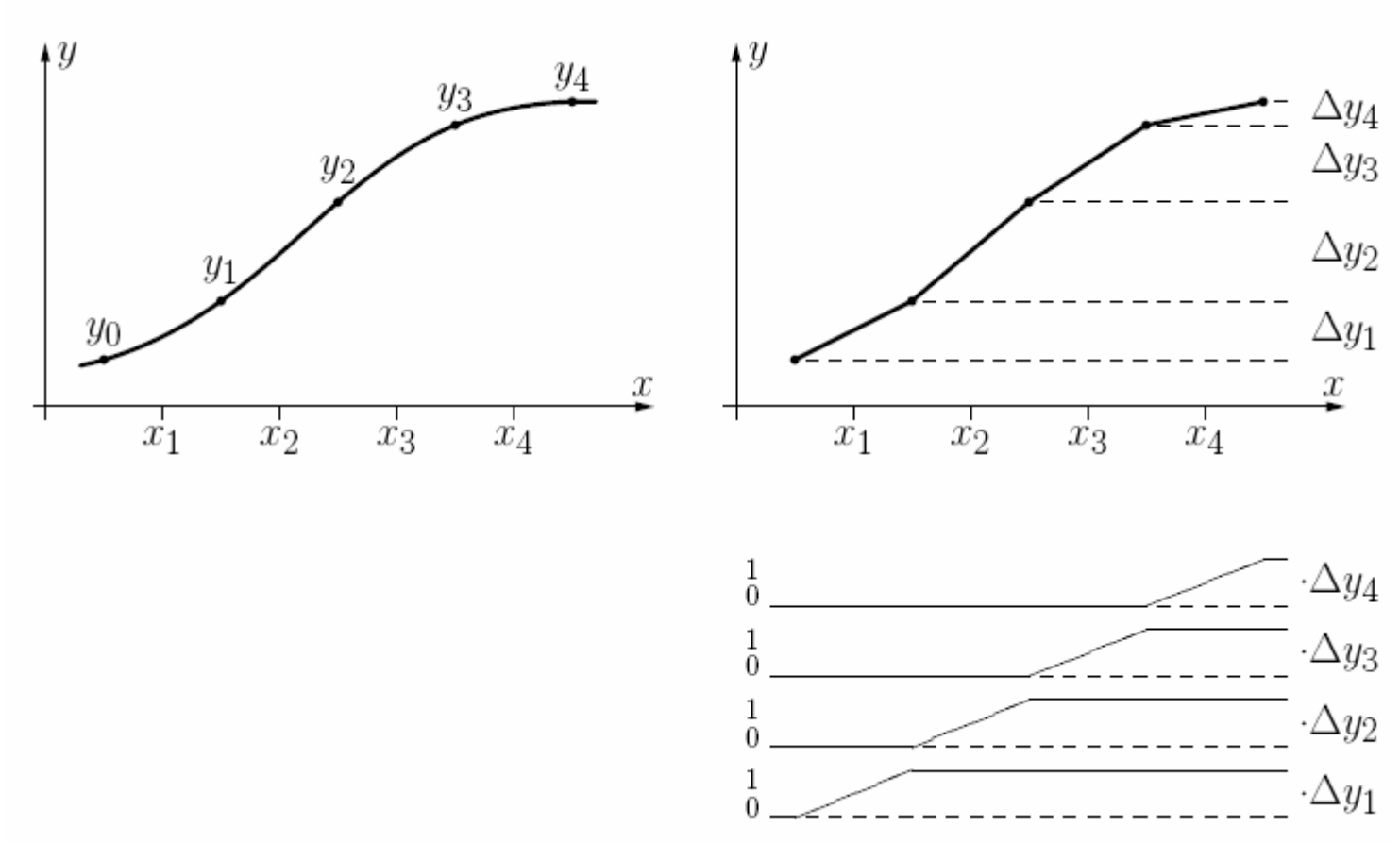
Multilayer Perceptrons: Function Approximation



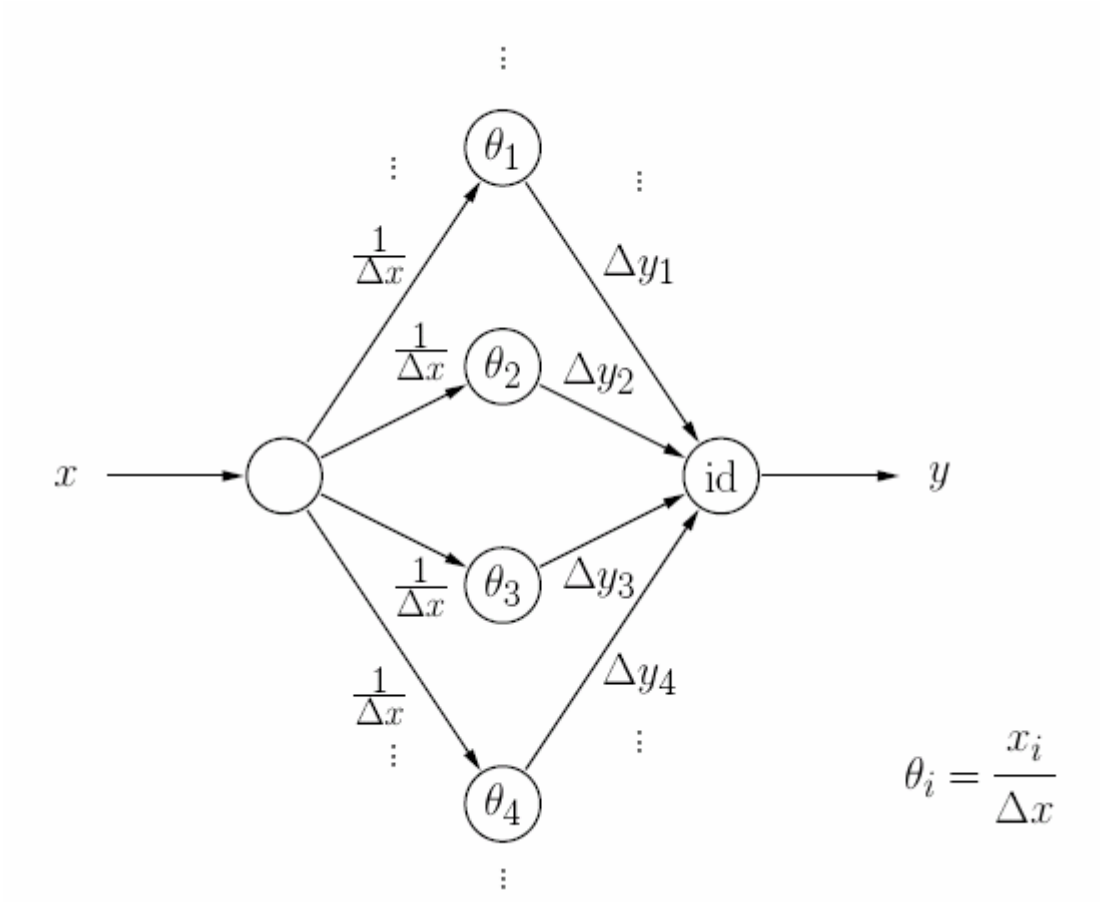
Multilayer Perceptrons: Function Approximation



Multilayer Perceptrons: Function Approximation



Multilayer Perceptrons: Function Approximation



Mathematical Background: Linear Regression

Training neural networks is closely related to regression

Given:
- A dataset $((x_1, y_1), \ldots, (x_n.y_n))$ of n data tuples and
- a hypothesis about the functional relationship, e.g. $y = g(x) = a + bx$.

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:

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

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

Mathematical Background: Linear Regression

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

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

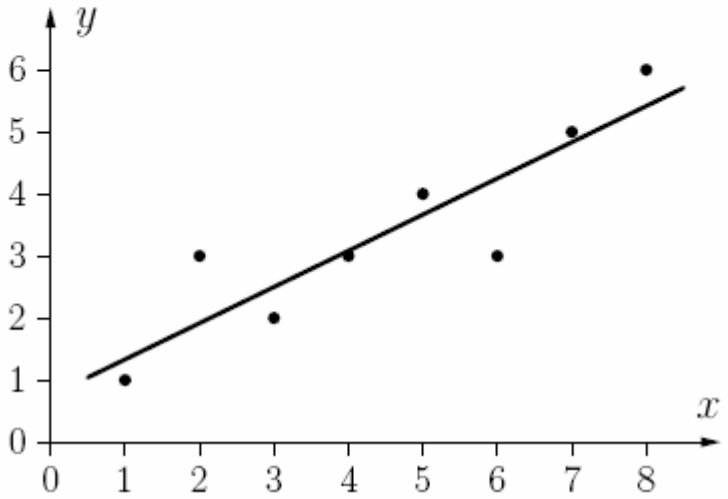
$$\left(\sum_{i=1}^{n} x_i\right) a + \left(\sum_{i=1}^{n} x_i^2\right) b = \sum_{i=1}^{n} x_i y_i.$$

- 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

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



Mathematical Background: 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.

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

Mathematical Background: Polynomial Regression

System of normal equations for polynomials

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

- $m+1$ 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 all x-values are identical.

Mathematical Background: Multilinear Regression

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.

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

Mathematical Background: 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 x- or all y-values are identical.

Mathematical Background: Logistic Regression

Generalization to non-polynomial functions

$$y = ax^b$$

Idea: Find transformation to linear/polynomial case.

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

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

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

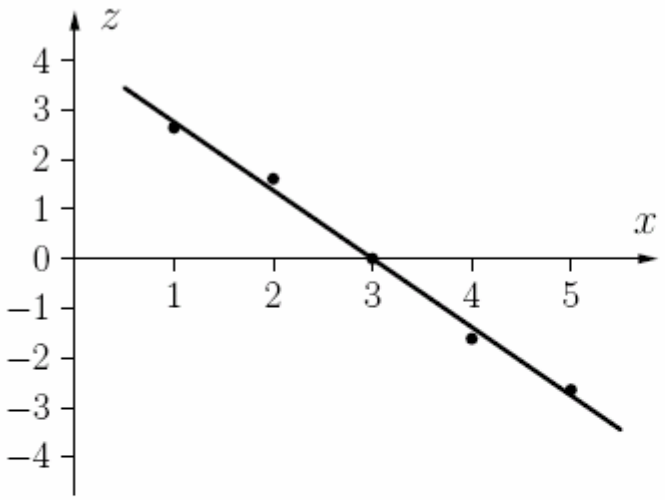
The transformed data points are

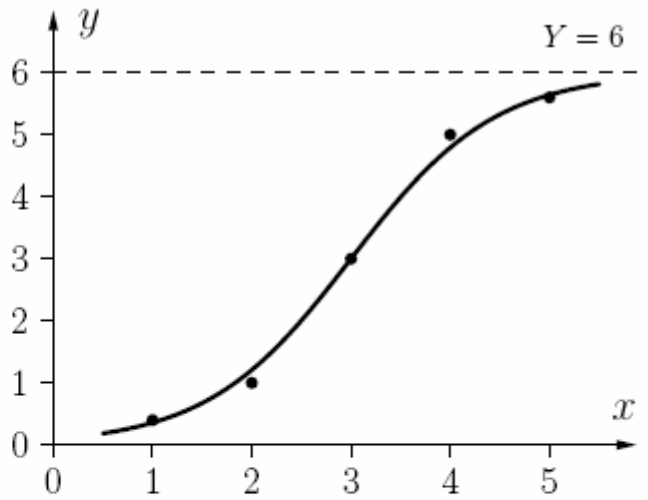
x	1	2	3	4	5
z	2.64	1.61	0.00	-1.61	-2.64

The resulting regression line is

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

Logistic Regression: Example





The logistic regression function can be computed by a single neuron with

- network input function $f_{\text{net}}(x) \equiv wx$ with $w \approx -1.3775$,
- activation function $f_{\text{act}}(\text{net}, \theta) \equiv (1 + e^{-(\text{net} - \theta)})^{-1}$ with $\theta \approx 4.133$ and
- output function $f_{\text{out}}(\text{act}) \equiv 6\,\text{act}$.