Regression

Regression

- Analyze and understand relationships among several quantities
  - Build a model that that predicts the value of a variable (dependent variable) as a function of other variables (independent variables)
  - Supervised algorithm

Linear Regression / least-squares line

- The simplest relation between two variables x and y is the linear equation:

$$(x_1, y_1), \ldots, (x_n, y_n)$$

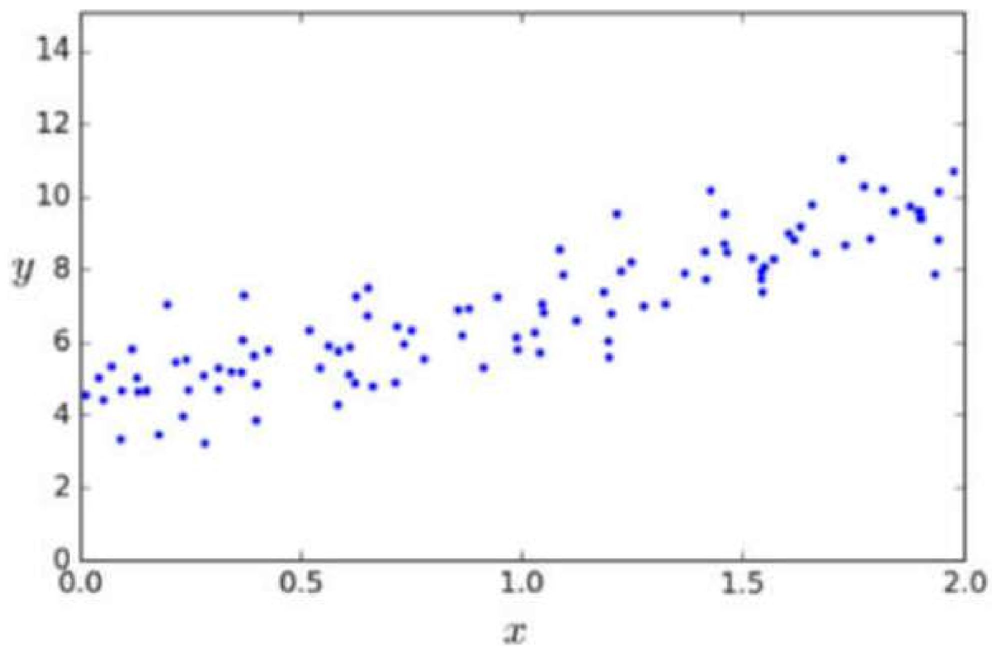
$$y = \beta_0 + \beta_1 x$$

  - The above notation is commonly used for least squares lines in stead of $y = mx + b$

Linear Regression (cont.)

$$(x_1, y_1), \ldots, (x_n, y_n)$$

$$y = \beta_0 + \beta_1 x$$



Linear Regression (cont.)

- If the data points were on a line, the parameters would satisfy the equations:

Predicted y-value		Observed y-value
$\beta_0 + \beta_1 x_1$	$=$	y_1
$\beta_0 + \beta_1 x_2$	$=$	y_2
$\vdots$		$\vdots$
$\beta_0 + \beta_1 x_n$	$=$	y_n

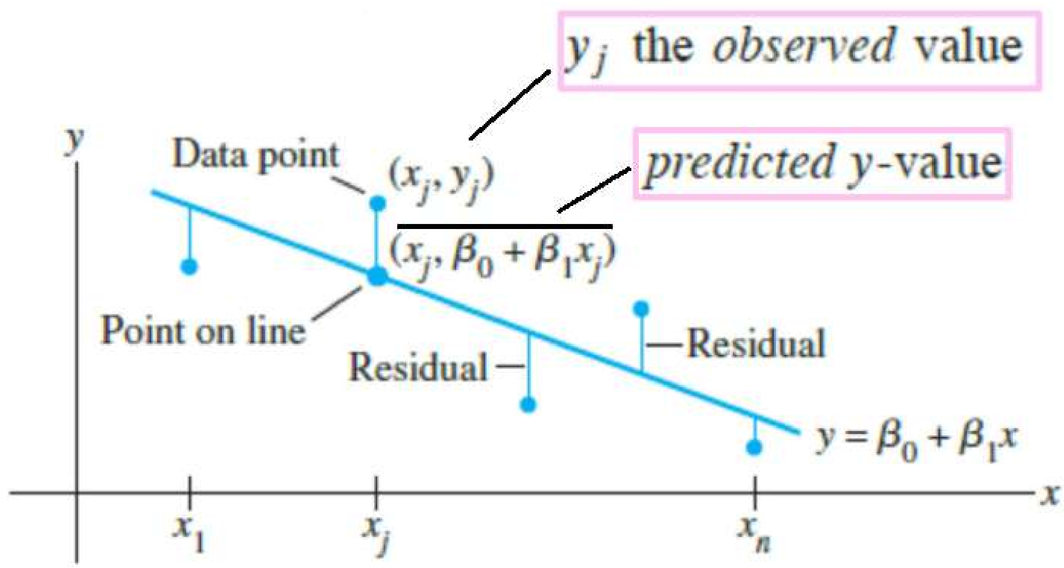
Linear Regression (cont.)

Predicted y-value		Observed y-value
$\beta_0 + \beta_1 x_1$	$=$	y_1
$\beta_0 + \beta_1 x_2$	$=$	y_2
$\vdots$		$\vdots$
$\beta_0 + \beta_1 x_n$	$=$	y_n

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \qquad \boxed{X\boldsymbol{\beta} = \mathbf{y}}$$

Linear Regression (cont.)

- If the data points do not lie on a line, then the are no parameters β_0, β_1 for which the predicted y-values in $X\beta$ equal the observed y-values.
  - Solution? Least squares line / line of regression



Linear Regression (cont.)

- There are several ways to measure how close the line is to the data.

- The usual choice is to add the squares of the residuals. The least-squares line is the line $y = \beta_0 + \beta_1 x$ that minimizes the sum of the squares of the residuals.

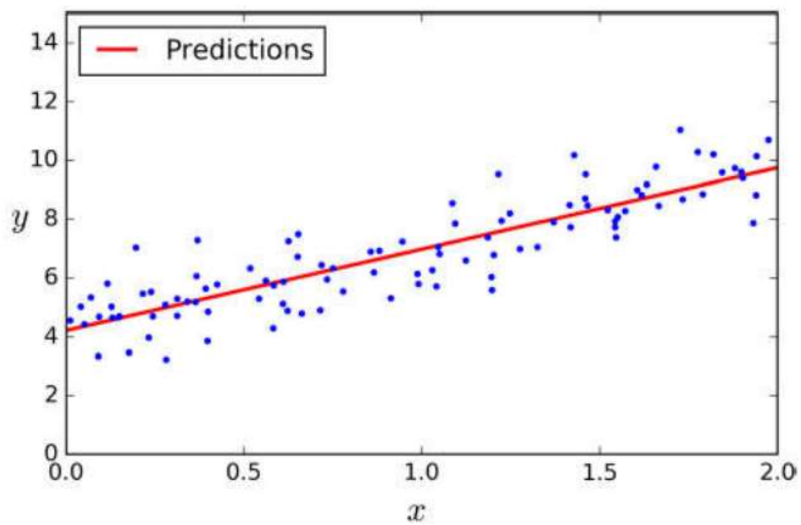
$$residual = \epsilon = y - X\beta$$

Cost Function

- Cost function = the sum of (squares of) the residuals

$$\epsilon^2 = (y - X\beta)^2$$

- The goal is to minimize the cost function



Cost Function (cont.)

$$\left|\left|\epsilon^2\right|\right| = (y - X\beta)^T(y - X\beta) = (X\beta)^T X\beta - (X\beta)^T y - y^T X\beta + y^T y$$

$$= (X\beta)^T X\beta - 2(X\beta)^T y + y^T y$$

$$\frac{\partial\left|\left|\epsilon^2\right|\right|}{\partial\beta} = 2X^T X\beta - 2X^T y = 0 \rightarrow \beta = (X^T X)^{-1}\, X^T y$$

Example

- Find the equation $y = \beta_0 + \beta_1 x$ of the least-squares line that best fits the data points $(2, 1)$, $(5, 2)$, $(7, 3)$, and $(8, 3)$.

Solution

- Find the equation $y = \beta_0 + \beta_1 x$ of the least-squares line that best fits the data points $(2, 1), (5, 2), (7, 3)$, and $(8, 3)$.

- **Solution**:

$$X = \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}$$

- For the least-squares solution of $X\boldsymbol{\beta} = \boldsymbol{y}$, obtain the following normal equation.

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

Solution (cont.)

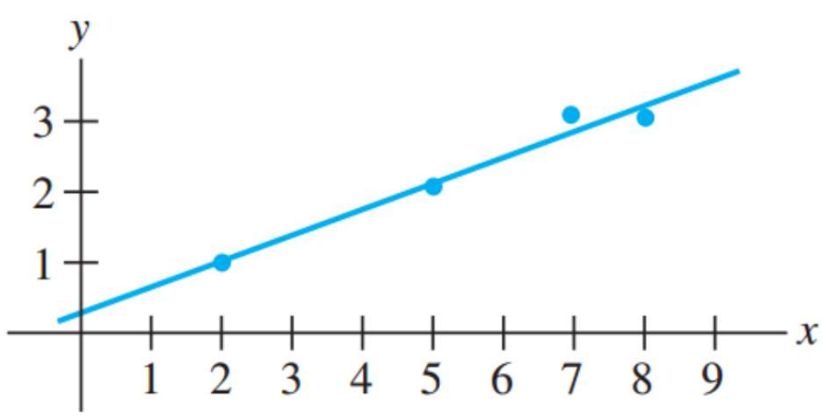
$$X^TX = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} = \begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix}$$

$$X^T\mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$$

Solution (cont.)

$$\begin{bmatrix}\beta_0\\ \beta_1\end{bmatrix}=\begin{bmatrix}4 & 22\\ 22 & 142\end{bmatrix}^{-1}\begin{bmatrix}9\\ 57\end{bmatrix}=\frac{1}{84}\begin{bmatrix}142 & -22\\ -22 & 4\end{bmatrix}\begin{bmatrix}9\\ 57\end{bmatrix}=\frac{1}{84}\begin{bmatrix}24\\ 30\end{bmatrix}=\begin{bmatrix}2/7\\ 5/14\end{bmatrix}$$

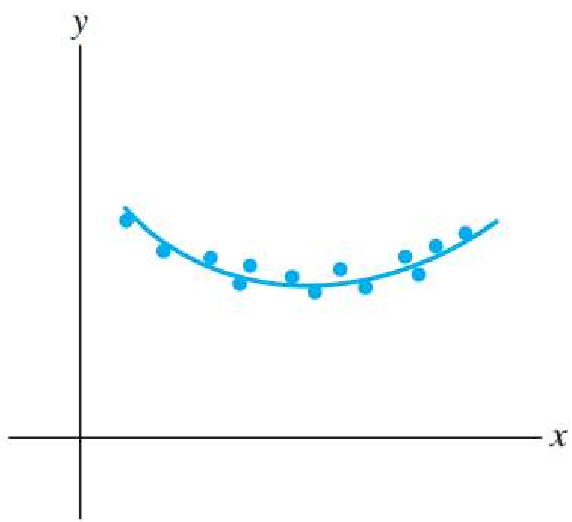
$$\boxed{y=\frac{2}{7}+\frac{5}{14}x}$$

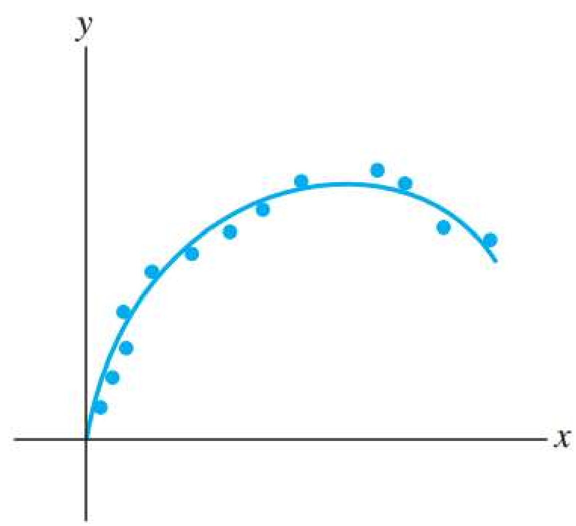


Non-linear Regression / Curve fitting

- When data points $(x_1, y_1), \ldots, (x_n, y_n)$ on a scatter plot do not lie close to any line, some other functional relationship between x and y may be tried:

$$y = \beta_0 f_0(x) + \beta_1 f_1(x) + \cdots + \beta_k f_k(x)$$





Example

- Suppose data points appear to lie along some sort of parabola. More precisely, we wish to approximate the data by an equation of the form:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2$$

Describe the model that produces a least-squares fit of the data.

Solution

$$
\begin{aligned}
y_1 &= \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \epsilon_1 \\
y_2 &= \beta_0 + \beta_1 x_2 + \beta_2 x_2^2 + \epsilon_2 \\
&\vdots \\
y_n &= \beta_0 + \beta_1 x_n + \beta_2 x_n^2 + \epsilon_n
\end{aligned}
$$

where ϵ_i is the residual error between the observed value y_i and the predicted y-value.

Solution (cont.)

$$\mathbf{y} \quad = \quad X \quad \boldsymbol{\beta} \quad + \quad \boldsymbol{\epsilon}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

Multiple Regression

- Suppose we have two independent variables, say u and v, and we wish to predict y (dependent variable). A simple (linear) equation for predicting y from u and v:

$$y = \beta_0 + \beta_1 u + \beta_2 v$$

- A more general prediction equation:

$$y = \beta_0 + \beta_1 u + \beta_2 v + \beta_3 u^2 + \beta_4 uv + \beta_5 v^2$$

Multiple Regression (cont.)

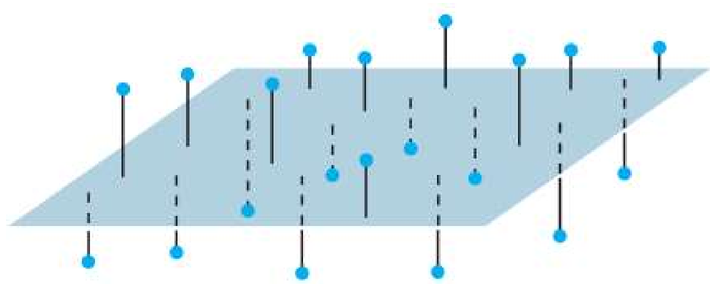
- In general, a linear model will arise whenever y is to be predicted by an equation of the form:

$$y = \beta_0 f_0(u, v) + \beta_1 f_1(u, v) + \cdots + \beta_k f_k(u, v)$$

with $f_0, \dots, f_k$ any sort of known functions & $\beta_0, \dots, \beta_k$ unknown parameters.

Example

- Suppose we have training data of the form: $(u_1, v_1, y_1), \ldots, (u_n, v_n, y_n)$
- Describe the linear model that gives a least-square fit to such data. The solution is called the least-squares plane.



Solution

- We expect the data to satisfy the following equations:

$$
\begin{aligned}
y_1 &= \beta_0 + \beta_1 u_1 + \beta_2 v_1 + \epsilon_1 \\
y_2 &= \beta_0 + \beta_1 u_2 + \beta_2 v_2 + \epsilon_2 \\
&\vdots \qquad\qquad \vdots \\
y_n &= \beta_0 + \beta_1 u_n + \beta_2 v_n + \epsilon_n
\end{aligned}
$$

- The system has the matrix form $\boldsymbol{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where

$$
\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad X = \begin{bmatrix} 1 & u_1 & v_1 \\ 1 & u_2 & v_2 \\ \vdots & \vdots & \vdots \\ 1 & u_n & v_n \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}
$$

Solution (cont.)

- This example shows that the linear model for multiple regression has the same abstract form as the model for the simple regression in the earlier examples.

- Once X is defined properly, the normal equations for β have the same matrix form, no matter how many variables are involved.

➢ For any linear model where $X^T X$ is invertible, the least squares β is given by $(X^T X)^{-1} X^T \boldsymbol{y}$.

Source

- D. Lay, J. McDonald, S. Lay, Linear Algebra and Its Applications, Chapter 6, 2020