Linear Regression – Matrix Form

Consider the model

$$Y = X\beta + \epsilon$$

where $Y = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}$ $X = \begin{pmatrix} 1 & X_{11} & X_{12} & \dots & X_{1p} \\ 1 & X_{21} & X_{22} & \dots & X_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \dots & X_{np} \end{pmatrix}$ $\beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$ $\epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}$

Then using matrix calculus we find that the least squares estimate for β is given by

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

Hence, the least squares regression line is $\hat{Y} = X\hat{\beta}$.

Influence Matrix

Linear Regression – Matrix Form - Issues

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

Hence, the least squares regression line is $\hat{Y} = X\hat{\beta}$.

- N samples, p-dimensional (what if p > N ?)
- Complexity of matrix inversion (what if N very large ?)
- Collinearity

Gradient Descent

$$\hat{y} = \beta_0 + \beta_1 \mathbf{x}$$

$$\mathcal{L}(\mathbf{w}) = \mathcal{L}(\beta_0, \beta_1)$$

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

1. Initialize the parameters w to some random values.
2. Update the parameters using gradient descent rule

   $$\beta(t+1) = \beta(t) - \eta \nabla_{\beta} L\big(\beta(t)\big)$$

3. Repeat 2 until $|\nabla_{\beta} L\big(\beta(t)\big)|$ is close to 0

Gradient Descent

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2. Update the parameters using gradient descent rule

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3. Repeat 2 until $|\nabla_\beta L\big(\beta(t)\big)|$ is close to 0

$$\hat{y} = \beta_0 + \beta_1 \mathbf{x}$$

$$\begin{aligned}
\mathcal{L}(\beta_0, \beta_1) & \\
&= \frac{1}{n}\sum_{i=1}^{n}(\hat{y} - y)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}(\beta_0 + \beta_1\mathbf{x} - y)^2 \\
\implies \frac{\partial \mathcal{L}}{\partial \beta_0} &= \frac{1}{n}\sum_{i=1}^{n} 2(\beta_0 + \beta_1\mathbf{x} - y) \\
\implies \frac{\partial \mathcal{L}}{\partial \beta_1} &= \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}(\beta_0 + \beta_1\mathbf{x} - y)
\end{aligned}$$

Gradient Descent

1. Initialize the parameters w to some random values.
2. Update the parameters using gradient descent rule

$$w(t+1) = w(t) - \eta \nabla_w L(w(t))$$

3. Repeat 2 until $|\nabla_w L(w(t))|$ is close to 0

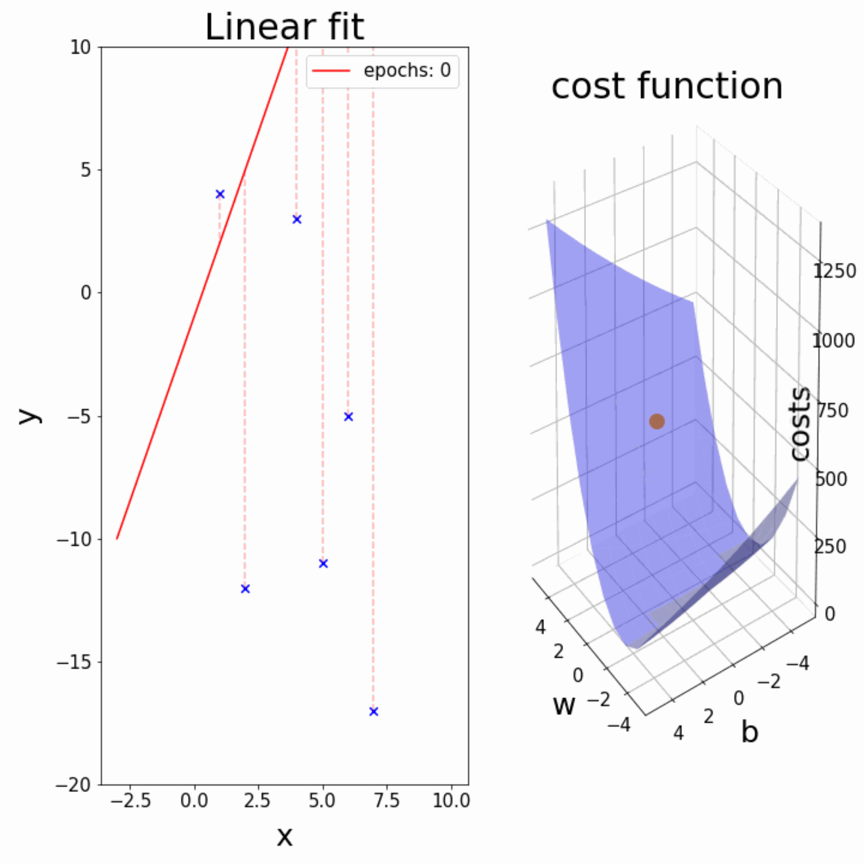
$$\mathbf{w} = [\beta_0 \ \ \beta_1]$$

$$\hat{y} = \beta_0 + \beta_1 \mathbf{x}$$

$$\begin{aligned}\mathcal{L}(\mathbf{w}) &= \mathcal{L}(\beta_0, \beta_1) \\ &= \frac{1}{n}\sum_{i=1}^{n}(\hat{y} - y)^2 \\ &= \frac{1}{n}\sum_{i=1}^{n}(\beta_0 + \beta_1\mathbf{x} - y)^2\end{aligned}$$

$$\Longrightarrow \frac{\partial \mathcal{L}}{\partial \beta_0} = \frac{1}{n}\sum_{i=1}^{n} 2(\beta_0 + \beta_1\mathbf{x} - y)$$

$$\Longrightarrow \frac{\partial \mathcal{L}}{\partial \beta_1} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}(\beta_0 + \beta_1\mathbf{x} - y)$$



Gradient Descent

1. Initialize the parameters w to some random values.
2. Update the parameters using gradient descent rule

$$w(t+1) = w(t) - \eta \, \nabla_w L(w(t))$$

3. Repeat 2 until $|\nabla_w L(w(t))|$ is close to 0

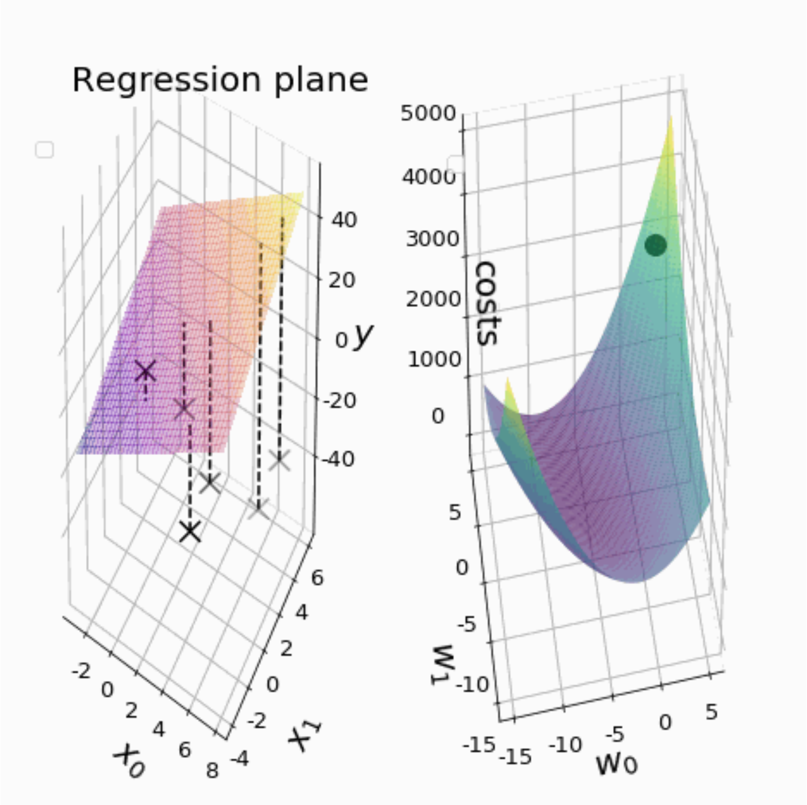
$$\mathbf{w} = [\beta_0 \;\; \beta_1]$$

$$\hat{y} = \beta_0 + \beta_1 \mathbf{x}$$

$$\begin{aligned}
\mathcal{L}(\mathbf{w}) &= \mathcal{L}(\beta_0, \beta_1) \\
&= \frac{1}{n} \sum_{i=1}^{n} (\hat{y} - y)^2 \\
&= \frac{1}{n} \sum_{i=1}^{n} (\beta_0 + \beta_1 \mathbf{x} - y)^2
\end{aligned}$$

$$\implies \frac{\partial \mathcal{L}}{\partial \beta_0} = \frac{1}{n} \sum_{i=1}^{n} 2(\beta_0 + \beta_1 \mathbf{x} - y)$$

$$\implies \frac{\partial \mathcal{L}}{\partial \beta_1} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}(\beta_0 + \beta_1 \mathbf{x} - y)$$



Linear Regression

- Linear Regression → Linear in coefficients and NOT variables

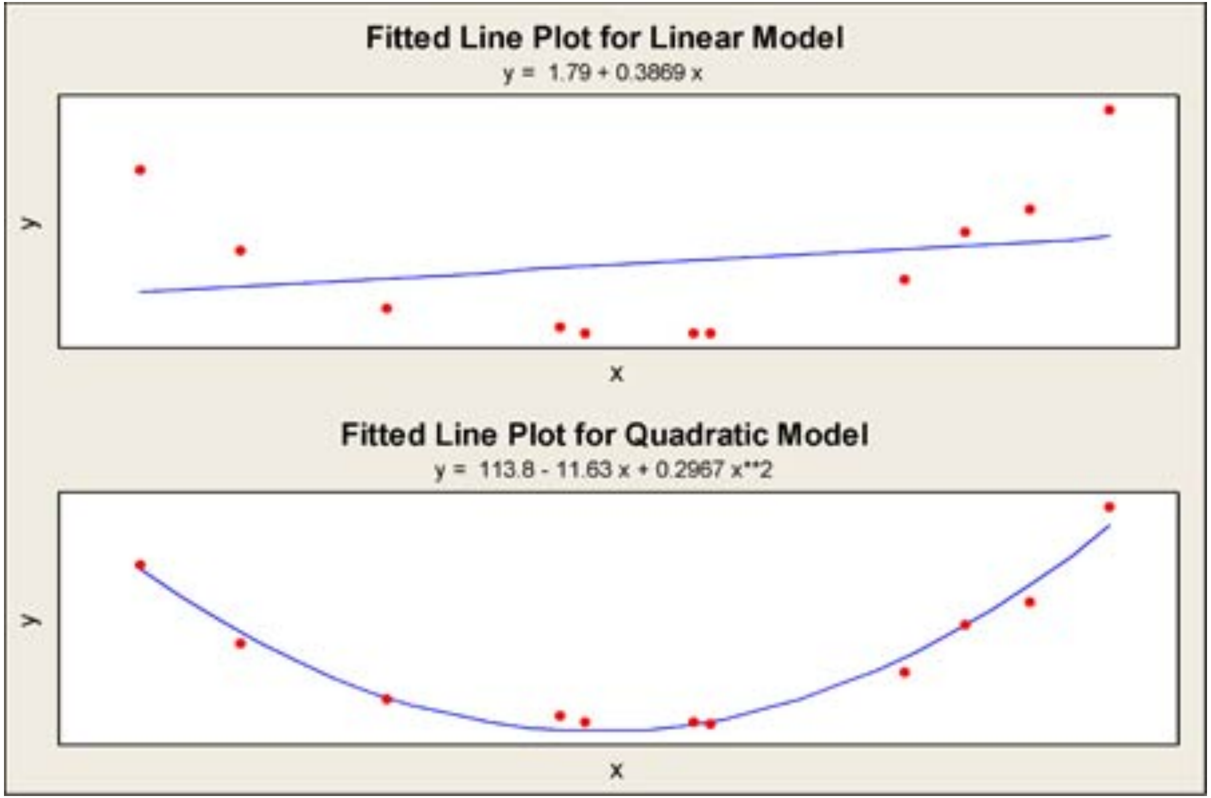
- A second-order model (quadratic model):

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

- β_1: Linear effect parameter.
- β_2: Quadratic effect parameter.

kth order polynomial model in one variable

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_k x^k + \epsilon$$



Fitted Line Plot for Linear Model
y = 1.79 + 0.3869 x
y
x
Fitted Line Plot for Quadratic Model
y = 113.8 - 11.63 x + 0.2967 x**2
y
x

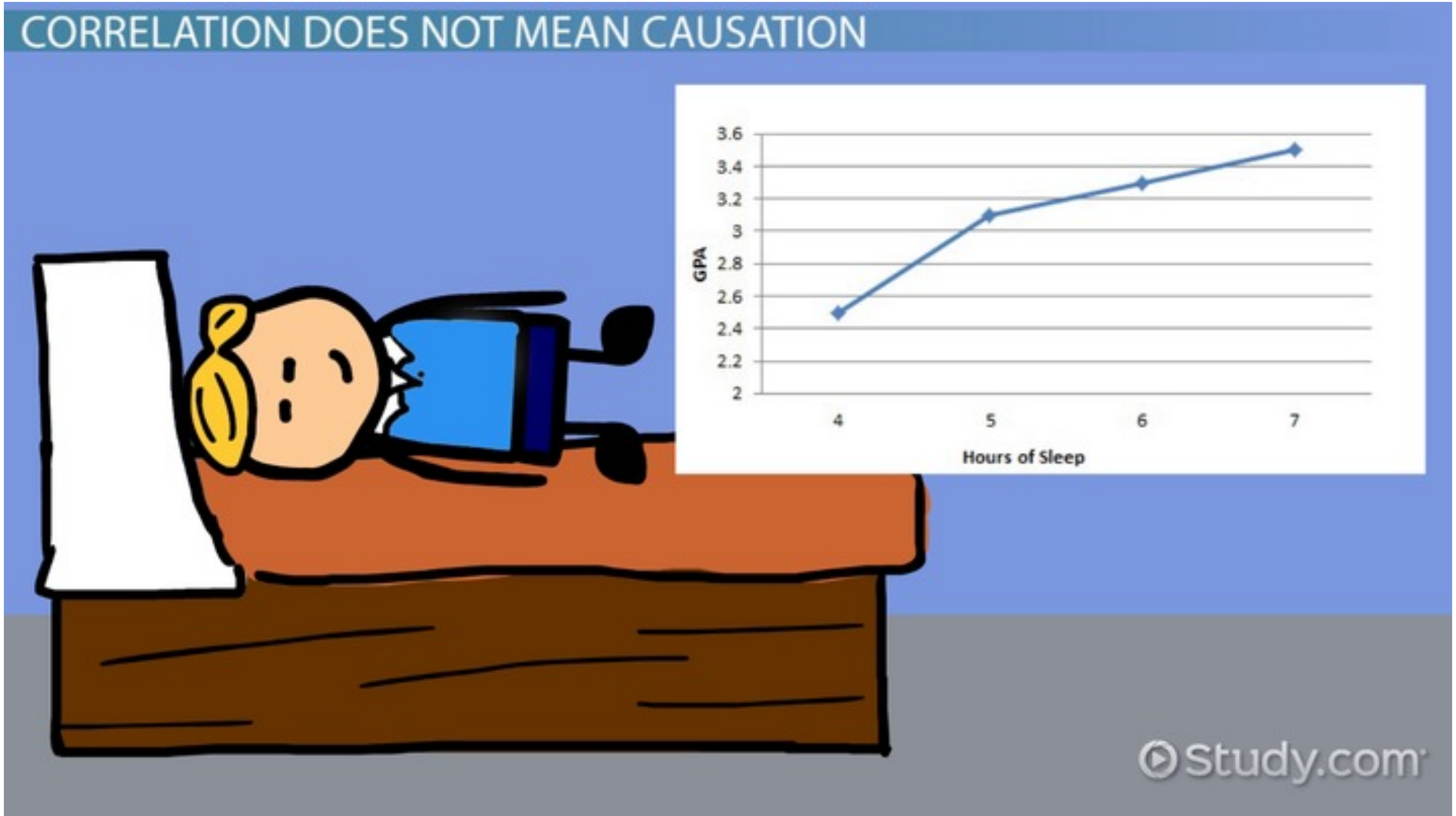
A quadratic polynomial regression function

$$Y_i = \beta_0 + \beta_1 X_i + \beta_{11} X_i^2 + \varepsilon_i$$

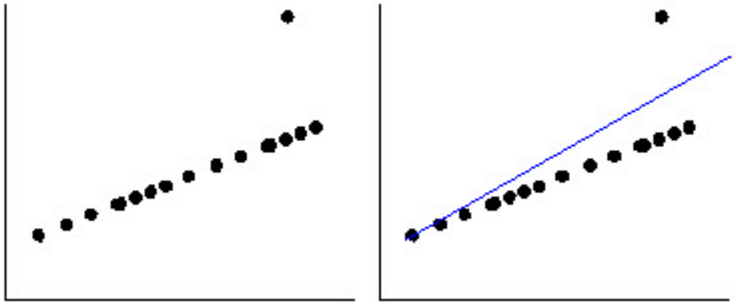
where:

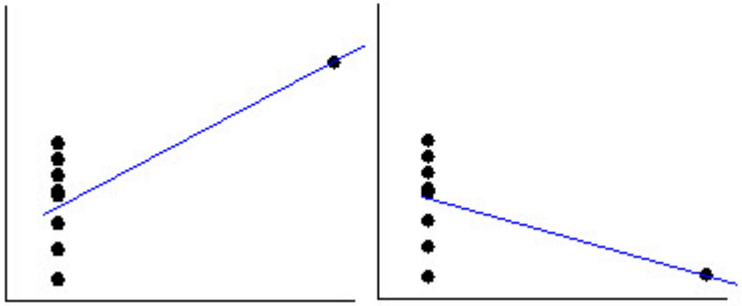
- Y_i = amount of immunoglobin in blood (mg)
- X_i = maximal oxygen uptake (ml/kg)
- typical assumptions about error terms ("INE")

Careful: X may not be causing y !

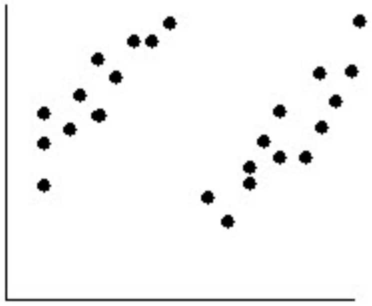


Linear Regression – Outliers





Linear Regression is problematic in many other cases



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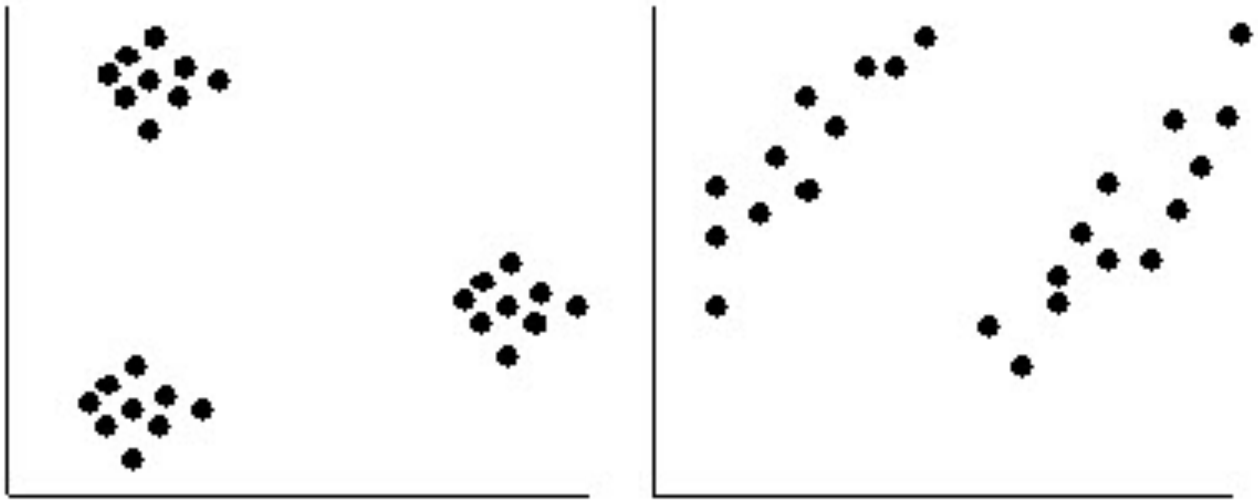

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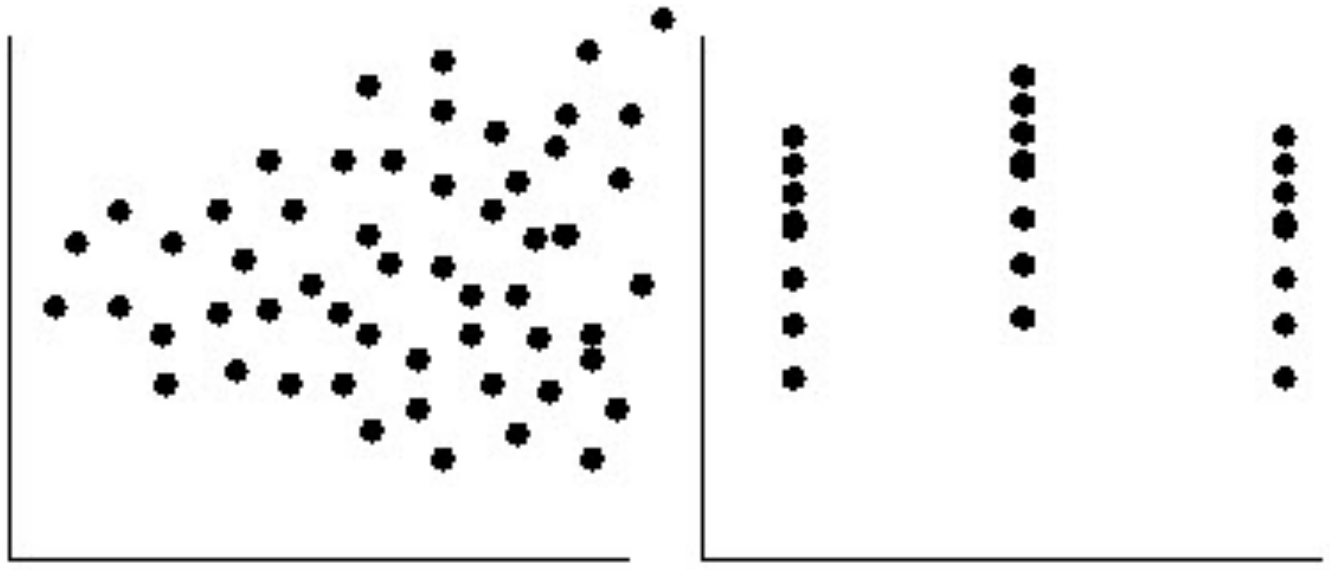
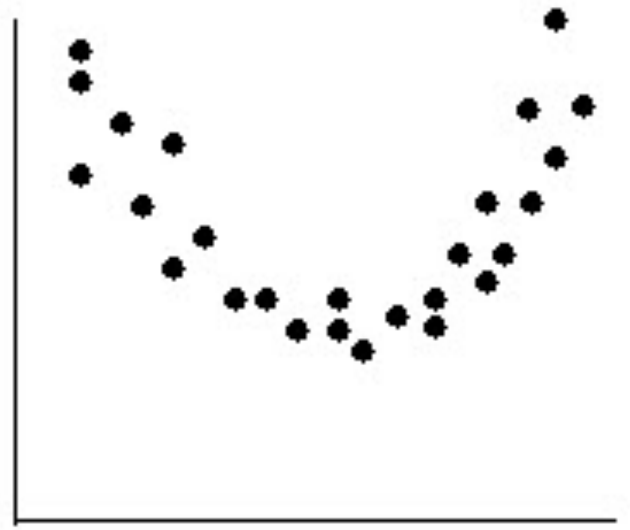
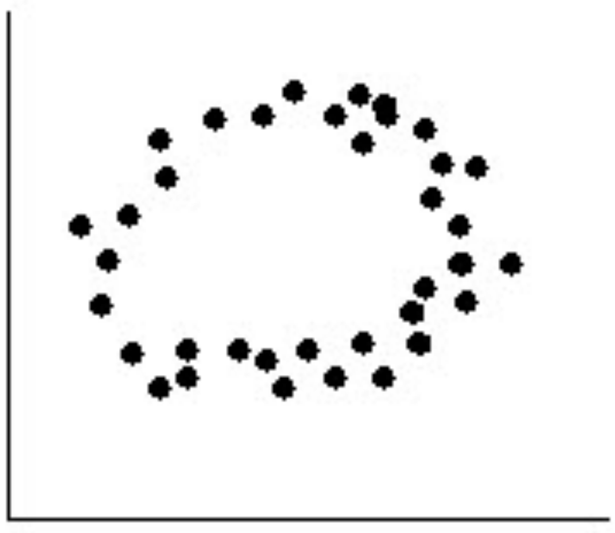
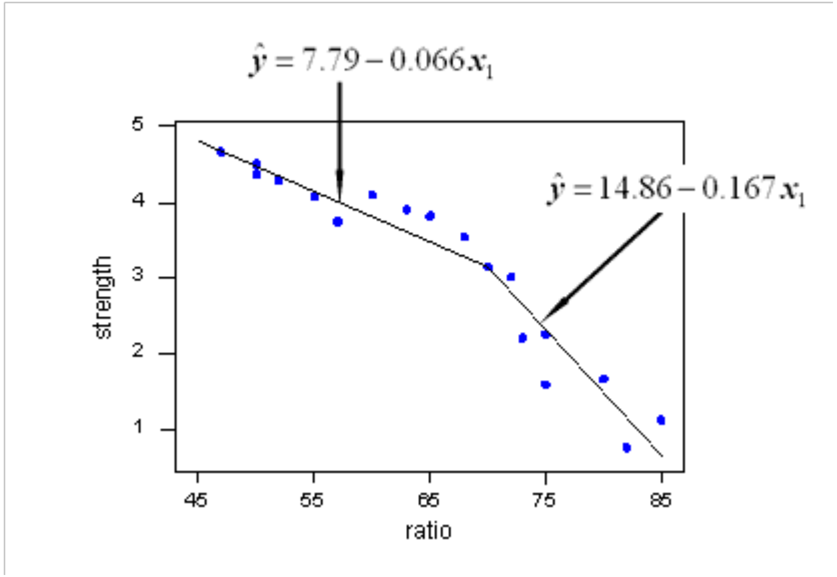


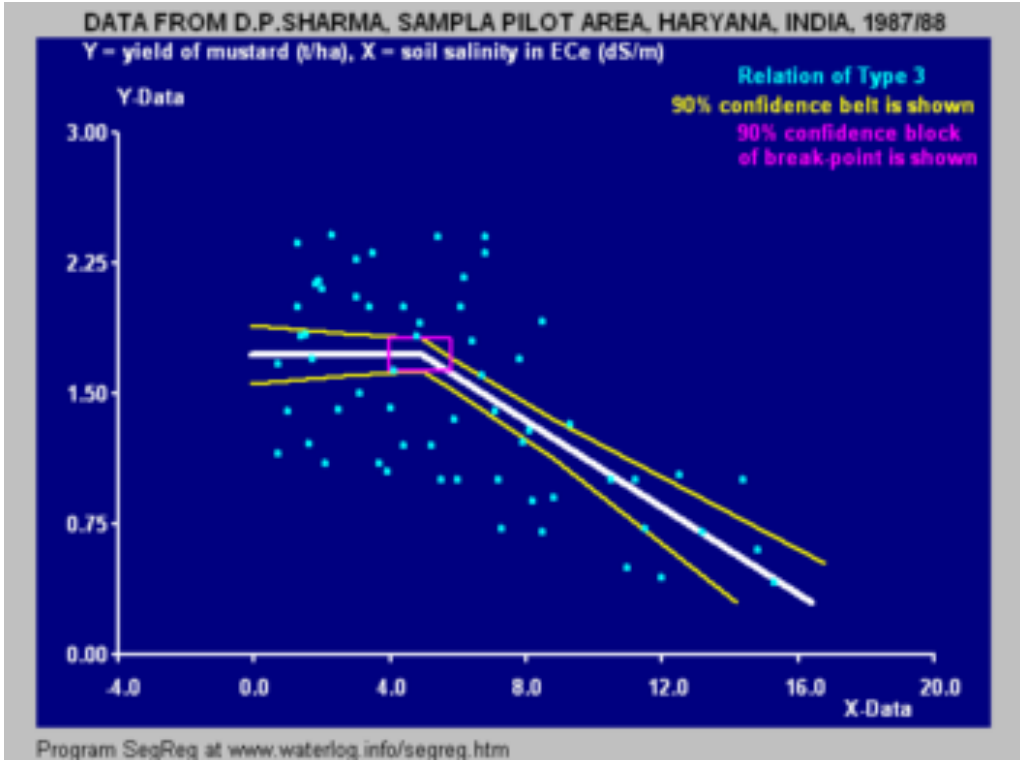
Linear Regression is problematic in many other cases





Piecewise Linear Regression





Also ref: Multivariate Adaptive Regression Splines (MARS)

Bivariate and multivariate models

Bivariate or simple regression model

(Education) $x \longrightarrow y$ (Income)

Multivariate or multiple regression model

(Education) x_1

(Gender) x_2

(Experience) x_3

(Age) x_4

$\longrightarrow$ y (Income)

Model with simultaneous relationship

Price of wheat $\longleftrightarrow$ Quantity of wheat produced

Types of Regression Models