Math 362: Mathematical Statistics II

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Chapter 11. Regression

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§ 11.4 Covariance and Correlation

§ 11.2 The Method of Least Squares

§ 11.3 The Linear Model

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§ 11.5 The Bivariate Normal Distribution

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§ 11.1 Introduction

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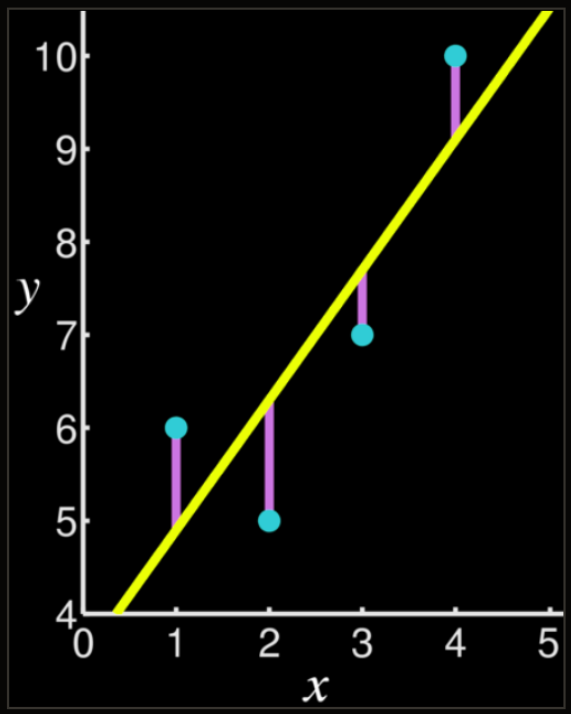
§ 11.5 The Bivariate Normal Distribution



In linear regression, the observations (**red**) are assumed to be the result of random deviations (**green**) from an underlying relationship (**blue**) between a dependent variable (y) and an independent variable (x).

Goal: Find a blue line that minimizes the sum of the square of the green lines

Thm. Given n points $(x_1, y_1), \cdots, (x_n, y_n)$, the straight line $y = a + bx$ minimizing

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

when

$$b = \frac{n \sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2}$$

and

$$a = \frac{\sum_{i=1}^{n} y_i - b \sum_{i=1}^{n} x_i}{n} = \bar{y} - b\bar{x}.$$

Proof.

$$\begin{cases} \dfrac{\partial}{\partial a} L(a, b) = \displaystyle\sum_{i=1}^{n} (-2) [y_i - (a + bx_i)] = 0 \\ \dfrac{\partial}{\partial b} L(a, b) = \displaystyle\sum_{i=1}^{n} (-2x_i) [y_i - (a + bx_i)] = 0 \end{cases}$$

(Normal equations)

$$\iff \quad \begin{cases} \sum_{i=1}^{n} y_i - na - b\sum_{i=1}^{n} x_i = 0 & (1) \\ \sum_{i=1}^{n} x_i y_i - a\sum_{i=1}^{n} x_i - b\sum_{i=1}^{n} x_i^2 = 0 & (2) \end{cases}$$

$$(1) \quad \Longrightarrow \quad a = \bar{y} - b\bar{x}$$

$$(1) \times \sum_{i=1}^{n} x_i - (2) \times n \quad \Longrightarrow \quad b = \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2}$$

□

(Moore-Penrose) Pseudoinverse

1. Well determined system

$$Ax = b \quad \Longrightarrow \quad x = A^{-1}y.$$

2. Overdetermined system

$$\begin{aligned} Ax &= y \\ A^T Ax &= A^T y \\ \underbrace{(A^T A)^{-1} A^T A}_{=I} x &= (A^T A)^{-1} A^T y \\ x &= \underbrace{(A^T A)^{-1} A^T}_{=:A^+} y \end{aligned}$$

3. Under determined system

$$Ax = y \quad \Longrightarrow \quad x = \underbrace{A^T (AA^T)^{-1}}_{=:A^+} y.$$

Proof. (Another proof based on pseudoinverse)

$$A = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}_{n\times 2}, \qquad x = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}_{2\times 1}, \qquad y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}_{1\times n}$$

$$A^T A = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} = \begin{pmatrix} n & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \end{pmatrix}$$

$$(A^T A)^{-1} = \frac{1}{n\sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2} \begin{pmatrix} \sum_{i=1}^n x_i^2 & -\sum_{i=1}^n x_i \\ -\sum_{i=1}^n x_i & n \end{pmatrix}$$

$$A^T y = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \end{pmatrix}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = x = (A^T A)^{-1} A^T y$$

$$= \frac{1}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \begin{pmatrix} \sum_{i=1}^{n} x_i^2 & -\sum_{i=1}^{n} x_i \\ -\sum_{i=1}^{n} x_i & n \end{pmatrix} \begin{pmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i y_i \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{\left(\sum_{i=1}^{n} x_i^2\right)\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} x_i y_i\right)}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \\ \\ \dfrac{n \sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \end{pmatrix}$$

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

$$a = \frac{\left(\sum_{i=1}^{n} x_i^2\right)\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} x_i y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$= \frac{\left(\sum_{i=1}^{n} x_i^2\right)\left(\sum_{i=1}^{n} y_i\right) - \left(\sum_{i=1}^{n} x_i\right)\left[\left(\sum_{i=1}^{n} x_i y_i\right) - \frac{1}{n}\left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)\right]}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$- \frac{\frac{1}{n}\left(\sum_{i=1}^{n} x_i\right)^2\left(\sum_{i=1}^{n} y_i\right)}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$= \frac{1}{n}\sum_{i=1}^{n} y_i - b\frac{1}{n}\sum_{i=1}^{n} x_i = \bar{y} - b\bar{x}.$$

□

A probabilistic view ...

Def. The function $f(X)$ for which

$$\mathbb{E}\left[(Y - f(X))^2\right]$$

is minimized is called the **regression curve of Y on X**.

Thm. Let (X, Y) be two random variables such that $\mathrm{Var}(X)$ and $\mathrm{Var}(Y)$ both exist. Then the regression cure of Y on X is given (for all x) by

$$f(x) = \mathbb{E}\left[Y|X = x\right].$$

Proof. Let $f(x) = \mathbb{E}[Y|X = x]$ and let $\phi(x)$ be a general function. Then

$$\begin{aligned}\mathbb{E}\left[(Y - \phi(X))^2\right] =& \mathbb{E}\left[([Y - f(X)] + [f(X) - \phi(X)])^2\right] \\ =& \mathbb{E}\left[(Y - f(X))^2\right] + \mathbb{E}\left[(f(X) - \phi(X))^2\right] \\ &+ \mathbb{E}\left[(Y - f(X))\,(f(X) - \phi(X))\right].\end{aligned}$$

Let $\psi(x)$ be either $f(x)$ or $\phi(x)$. We claim that

$$\mathbb{E}\left[(Y - f(X))\,\psi(X)\right] = 0.$$

Indeed,

$$\begin{aligned}\mathbb{E}[Y\psi(X)] &= \iint_{\mathbb{R}^2} f_{X,Y}(x,y)\,y\,\psi(x)\mathrm{d}y\mathrm{d}x \\ &= \int_{\mathbb{R}} \mathrm{d}x\,\psi(x) f_X(x) \underbrace{\int_{\mathbb{R}} \mathrm{d}y\,\frac{f_{X,Y}(x,y)}{f_X(x)}\,y}_{=\mathbb{E}[Y|X=x]} \\ &= \mathbb{E}[f(X)\psi(X)].\end{aligned}$$

Hence,

$$\mathbb{E}\left[(Y - \phi(X))^2\right] = \mathbb{E}\left[(Y - f(X))^2\right] + \mathbb{E}\left[(f(X) - \phi(X))^2\right]$$

which is minimized when $\phi(x) = f(x)$. □

If one imposes that $f(x) = a + bx$, then

Thm. The following squared error:

$$\mathbb{E}\left[\{Y - (a + bX)\}^2\right]$$

is minimized at

$$b = \rho_{XY}\frac{\sigma_Y}{\sigma_X} = \frac{\sigma_{XY}}{\sigma_X^2} \quad \text{and} \quad a = \mathbb{E}[Y] - b\mathbb{E}[X]$$

with the mean squared error

$$\mathbb{E}\left[\{Y - (a + bX)\}^2\right] = \left(1 - \rho_{XY}^2\right)\sigma_Y^2.$$

Proof.

$$\mathbb{E}\left[\{Y-(a+bX)\}^2\right]$$

$$=\mathbb{E}\left[\left\{[Y-\mathbb{E}(Y)]-b[X-\mathbb{E}(X)]-[a-\mathbb{E}[Y]+b\mathbb{E}(X)]\right\}^2\right]$$

$$\begin{array}{c} || \\ \mathbb{E}\left[[Y-\mathbb{E}(Y)]^2\right] \\ +b^2\mathbb{E}\left[[X-\mathbb{E}(X)]^2\right] \\ +\left[a-\mathbb{E}[Y]+b\mathbb{E}(X)\right]^2 \\ -2b\mathbb{E}\Big[[Y-\mathbb{E}(Y)][X-\mathbb{E}(X)]\Big] \\ -2\Big[a-\mathbb{E}[Y]+b\mathbb{E}(X)\Big]\mathbb{E}\left[Y-\mathbb{E}(Y)\right] \\ +2b\Big[a-\mathbb{E}[Y]+b\mathbb{E}(X)\Big]\mathbb{E}\left[X-\mathbb{E}(X)\right] \end{array} \quad = \quad \begin{array}{c} \mathrm{Var}(Y) \\ +b^2\mathrm{Var}(X) \\ +\left[a-\mathbb{E}[Y]+b\mathbb{E}(X)\right]^2 \\ -2b\,\mathrm{Cov}(X,Y) \\ +0 \\ +0 \end{array}$$

$$\Downarrow$$

$$\mathbb{E}\left[\{Y-(a+bX)\}^2\right]$$

$$||$$

$$\mathrm{Var}(Y)+b^2\mathrm{Var}(X)+\Big[a-\mathbb{E}[Y]+b\mathbb{E}(X)\Big]^2-2b\,\mathrm{Cov}(X,Y)$$

The best a, called a^*, should be such that

$$\Big[a^*-\mathbb{E}[Y]+b\mathbb{E}(X)\Big]^2=0 \quad\Longleftrightarrow\quad a^*=\mathbb{E}[Y]-b\mathbb{E}[X]$$

$$\Downarrow$$

$$\mathbb{E}\left[\{Y-(a^*+bX)\}^2\right]$$

$$||$$

$$\mathrm{Var}(Y)+b^2\mathrm{Var}(X)-2b\,\mathrm{Cov}(X,Y)$$

$$||$$

$$\sigma_Y^2+b^2\sigma_X^2-2b\rho_{XY}\sigma_X\sigma_Y$$

$$||$$

$$\left(1-\rho_{XY}^2\right)\sigma_Y^2+\left(b\sigma_X-\rho_{XY}\sigma_Y\right)^2$$

The best b, called b^*, should be

$$\left(b^*\sigma_X-\rho_{XY}\sigma_Y\right)^2=0 \quad\Longleftrightarrow\quad b^*=\rho_{XY}\frac{\sigma_Y}{\sigma_X}$$

$$\Downarrow$$

$$\mathbb{E}\left[\{Y-(a^*+b^*X)\}^2\right]$$

$$||$$

$$\left(1-\rho_{XY}^2\right)\sigma_Y^2$$

with

$$b^*=\rho_{XY}\frac{\sigma_Y}{\sigma_X}=\frac{\sigma_{XY}}{\sigma_X^2} \qquad \text{and} \qquad a^*=\mathbb{E}[Y]-b\mathbb{E}[X]$$

□

Remark In practice, we have data $(x_1, y_1), \cdots, (x_n, y_n)$ instead of the joint law of (X, Y)

$$\Downarrow$$

Replace

$$\mu_X, \mu_Y, \sigma_X^2, \sigma_Y^2, \rho_{XY}, \sigma_{XY}$$

by their maximum likelihood estimates

$$\bar{x}, \bar{y}, \hat{\sigma}_X^2, \hat{\sigma}_Y^2, r_{XY}, \hat{\sigma}_{XY}$$

1. $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$, $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$

2. $$\hat{\sigma}_X^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{1}{n}\sum_{i=1}^{n} x_i^2 - \bar{x}^2 = \frac{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}{n^2}$$
$$\hat{\sigma}_Y^2 = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2 = \frac{1}{n}\sum_{i=1}^{n} y_i^2 - \bar{y}^2 = \frac{n\sum_{i=1}^{n} y_i^2 - \left(\sum_{i=1}^{n} y_i\right)^2}{n^2}$$

3. $$\hat{\sigma}_{XY} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) = \frac{1}{n}\sum_{i=1}^{n} x_i y_i - \bar{x}\bar{y}$$
$$= \frac{n\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} y_i\right)}{n^2}$$

4. $r_{XY} = \frac{\hat{\sigma}_{XY}}{\hat{\sigma}_X \hat{\sigma}_Y}$

$$\Downarrow$$

$$\boxed{b = r_{XY}\frac{\hat{\sigma}_Y}{\hat{\sigma}_X} = \frac{\hat{\sigma}_{XY}}{\hat{\sigma}_X^2}, \qquad a = \bar{y} - b\bar{x}}$$

Maximum likelihood estimates

$$\hat{\sigma}_X^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

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

$$\hat{\sigma}_{XY} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

Sample (co)variances

$$s_X^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

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

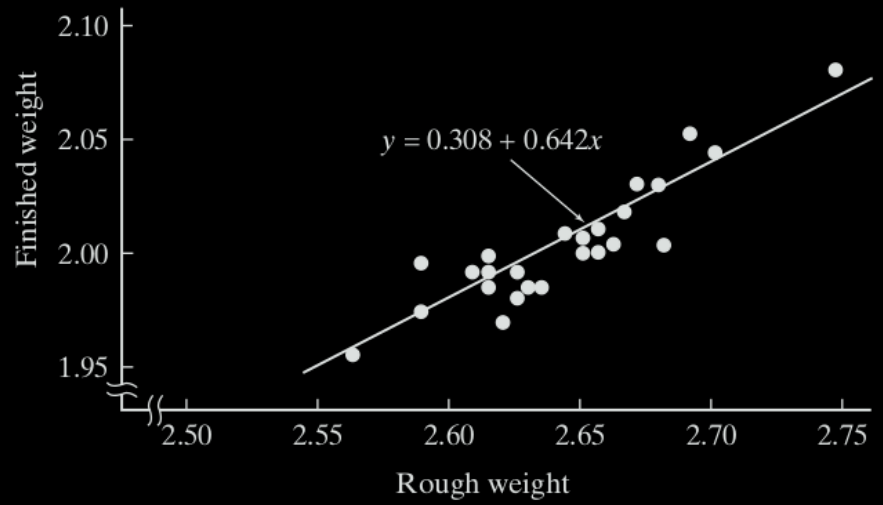
$$s_{XY} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

E.g. 1 Producing air conditioners. x = rough weight of a rod. y = finished weight. Find the best linear approximation of xy-relationship. Predict the weight when $x = 2.71$

Table 11.2.1

Rod Number	Rough Weight, x	Finished Weight, y	Rod Number	Rough Weight, x	Finished Weight, y
1	2.745	2.080	14	2.635	1.990
2	2.700	2.045	15	2.630	1.990
3	2.690	2.050	16	2.625	1.995
4	2.680	2.005	17	2.625	1.985
5	2.675	2.035	18	2.620	1.970
6	2.670	2.035	19	2.615	1.985
7	2.665	2.020	20	2.615	1.990
8	2.660	2.005	21	2.615	1.995
9	2.655	2.010	22	2.610	1.990
10	2.655	2.000	23	2.590	1.975
11	2.650	2.000	24	2.590	1.995
12	2.650	2.005	25	2.565	1.955
13	2.645	2.015			

Sol. …


2.10
2.05
2.00
1.95
Finished weight
$y = 0.308 + 0.642x$
2.50
2.55
2.60
2.65
2.70
2.75
Rough weight

…

□

Def. Let a and b be the least squares coefficients with the sample $(x_1, y_1), \cdots, (x_n, y_n)$.

$\hat{y} = a + bx$: **predicted value** of y

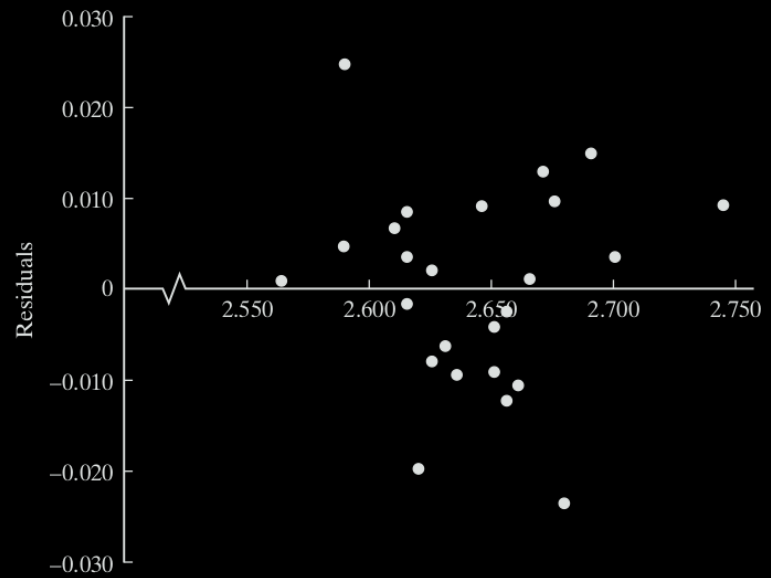
$y_i - \hat{y}_i = y_i - (a + bx_i)$: ***i*th residual**

Remark Use the residual plots to assessing the model.

E.g. 1’ Here are the residues and their plots:

Table 11.2.2

x_i	y_i	$\hat{y}_i$	$y_i - \hat{y}_i$
2.745	2.080	2.070	0.010
2.700	2.045	2.041	0.004
2.690	2.050	2.035	0.015
2.680	2.005	2.029	−0.024
2.675	2.035	2.025	0.010
2.670	2.035	2.022	0.013
2.665	2.020	2.019	0.001
2.660	2.005	2.016	−0.011
2.655	2.010	2.013	−0.003
2.655	2.000	2.013	−0.013
2.650	2.000	2.009	−0.009
2.650	2.005	2.009	−0.004
2.645	2.015	2.006	0.009
2.635	1.990	2.000	−0.010
2.630	1.990	1.996	−0.006
2.625	1.995	1.993	0.002
2.625	1.985	1.993	−0.008
2.620	1.970	1.990	−0.020
2.615	1.985	1.987	−0.002
2.615	1.990	1.987	0.003
2.615	1.995	1.987	0.008
2.610	1.990	1.984	0.006
2.590	1.975	1.971	0.004
2.590	1.995	1.971	0.024
2.565	1.955	1.955	0.000



E.g. 2 Predict the Social Security expenditures.

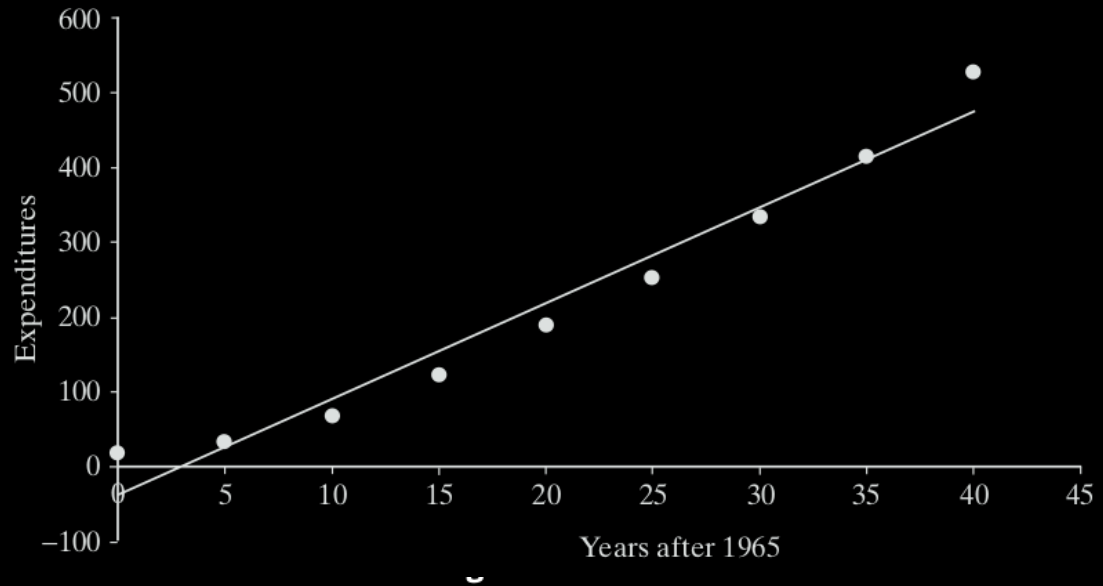
Table 11.2.3

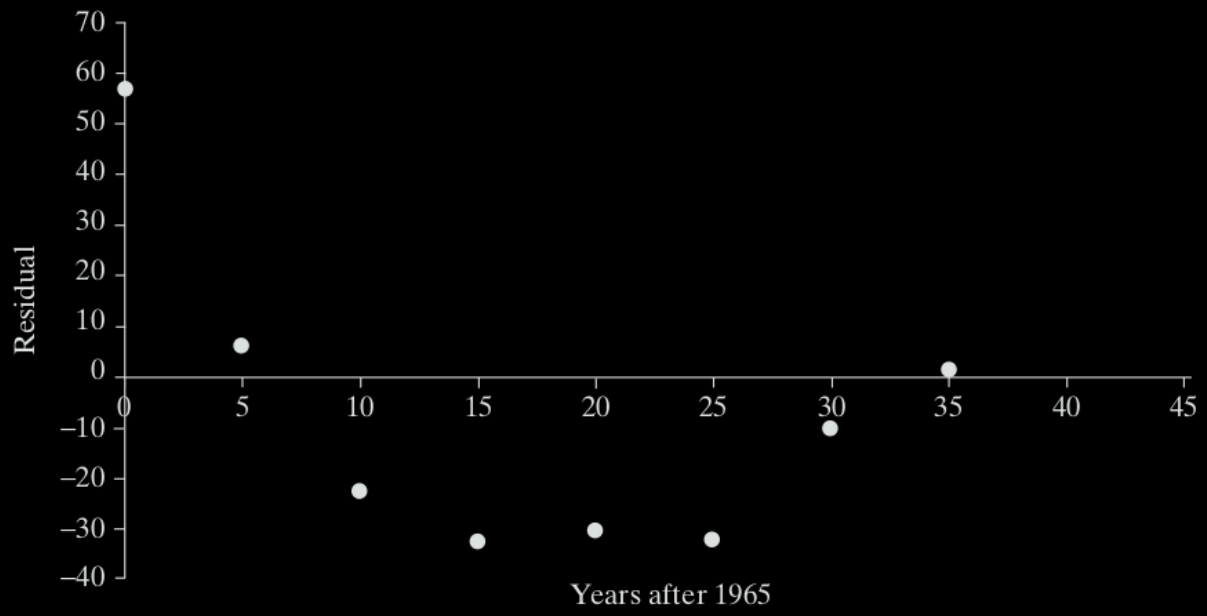
Year	Years after 1965, x	Social Security Expenditures ($ billions), y
1965	0	19.2
1970	5	33.1
1975	10	69.2
1980	15	123.6
1985	20	190.6
1990	25	253.1
1995	30	339.8
2000	35	415.1
2005	40	529.9

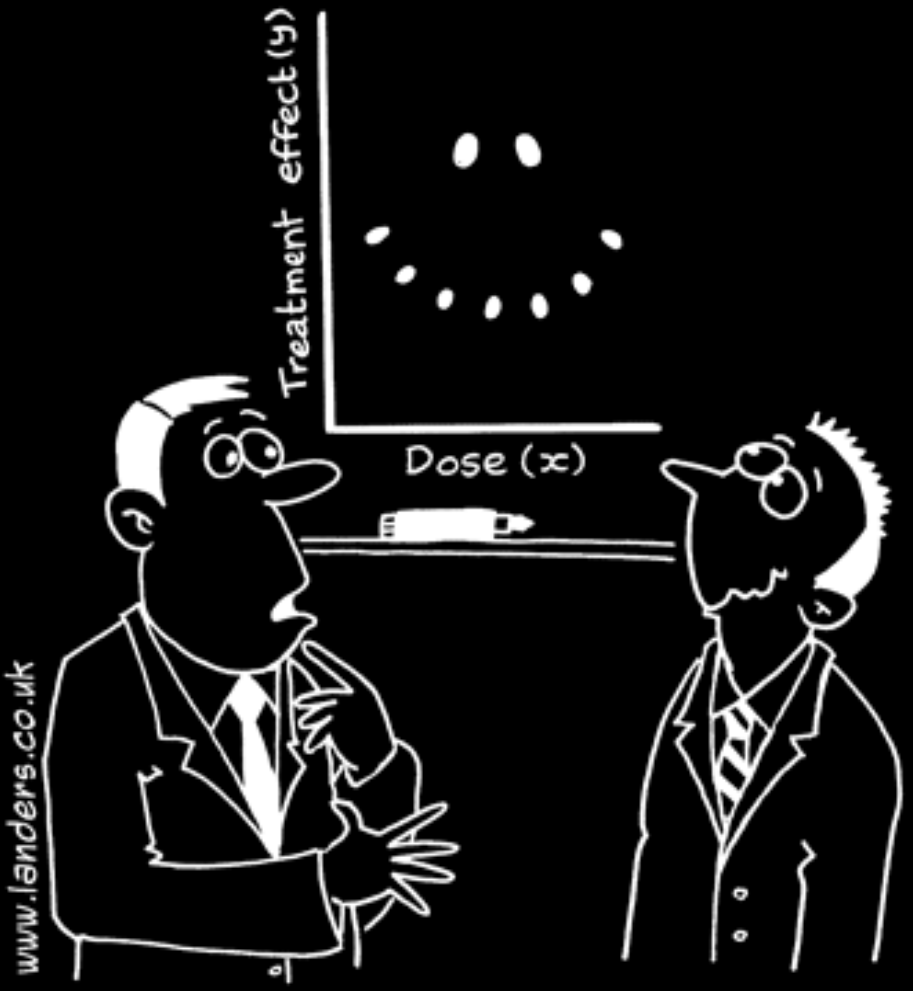
Source: www.socialsecurity.gov/history/trustfunds.html.

Does the the least squares line $y = -38.0 + 12.9x$ a good model to predict the cost in 2010 would be \$543, i.e., the case $x = 45$?

Sol.

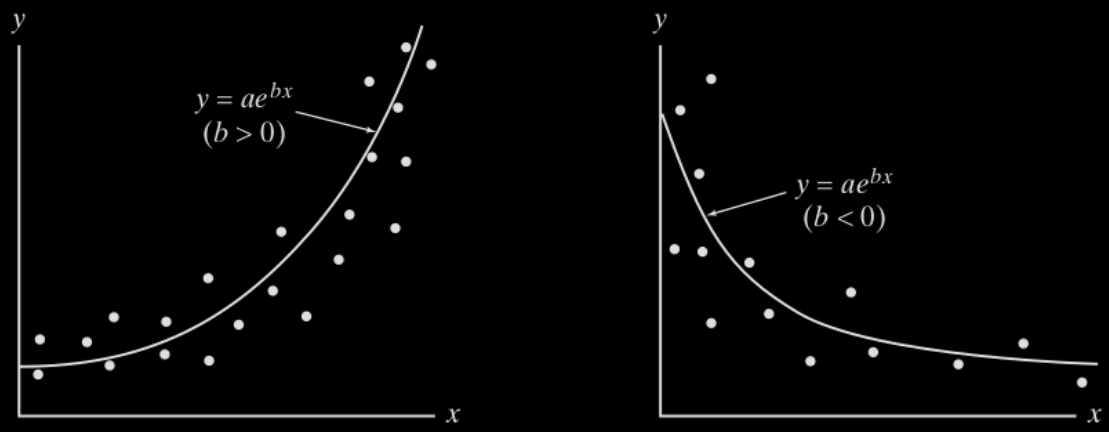

600
500
400
300
200
100
0
–100
Expenditures
0
5
10
15
20
25
30
35
40
45
Years after 1965


70
60
50
40
30
20
10
0
–10
–20
–30
–40
Residual
0
5
10
15
20
25
30
35
40
45
Years after 1965



"It's a non-linear pattern with outliers.....but for some reason I'm very happy with the data."

Exponential Regression



$$y = ae^{bx} \iff \ln y = \ln a + bx$$

$$b = \frac{n\sum_{i=1}^{n} x_i \ln y_i - \left(\sum_{i=1}^{n} x_i\right)\left(\sum_{i=1}^{n} \ln y_i\right)}{n\left(\sum_{i=1}^{n} x_i^2\right) - \left(\sum_{i=1}^{n} x_i\right)^2} \qquad \ln a = \frac{\sum_{i=1}^{n} \ln y_i - b\sum_{i=1}^{n} x_i}{n}$$

E.g. Moore's law:

Gordon Moore predicted in 1965 that the number of transistors per chip would double every 18 months.

Based on the real data, check:

1) Whether is the chip capacity doubling at a fixed rate?

2) Find out the rate.

Table 11.2.5

Chip	Year	Years after 1975, x	Transistors per Chip, y
8080	1975	0	4,500
8086	1978	3	29,000
80286	1982	7	90,000
80386	1985	10	229,000
80486	1989	14	1,200,000
Pentium	1993	18	3,100,000
Pentium Pro	1995	20	5,500,000

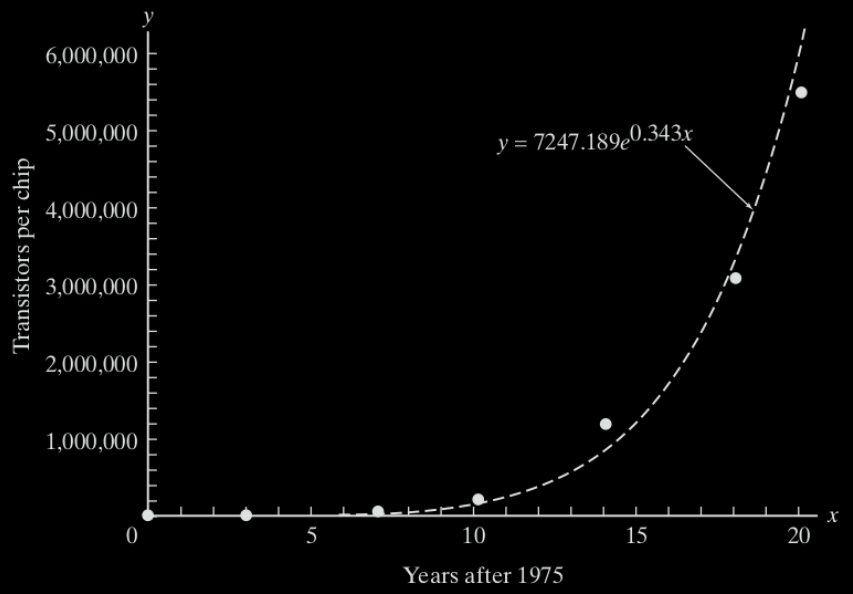
Source: en.wikipedia.org/wiki/Transistor—count.

Sol. To check whether chip capacity doubles in a fixed rate, one needs to carry out exponential regression:

Table 11.2.6

Years after 1975, x_i	x_i^2	Transistors per Chip, y_i	$\ln y_i$	$x_i \cdot \ln y_i$
0	0	4,500	8.41183	0
3	9	29,000	10.27505	30.82515
7	49	90,000	11.40756	79.85292
10	100	229,000	12.34148	123.41480
14	196	1,200,000	13.99783	195.96962
18	324	3,100,000	14.94691	269.04438
20	400	5,500,000	15.52026	310.40520
72	1078		86.90093	1009.51207

$$\Longrightarrow \quad b = \cdots = 0.342810, \quad a = \cdots = e^{\ln a} = e^{8.89} = 7247.189.$$



Finally, to find out the rate:

$$e^{0.343x} = e^{\ln 2 \times \frac{0.343}{\ln 2} x} = 2^{\frac{0.343}{\ln 2} x}$$

$$\frac{0.343}{\ln 2} x = 1 \quad \Longrightarrow \quad x = \frac{\ln 2}{0.343} = 2.020837.$$

□

Other curvilinear models

Table 11.2.10

a. If $y = ae^{bx}$, then $\ln y$ is linear with x.

b. If $y = ax^b$, then $\log y$ is linear with $\log x$.

c. If $y = L/(1 + e^{a+bx})$, then $\ln\left(\dfrac{L-y}{y}\right)$ is linear with x.

d. If $y = \dfrac{1}{a+bx}$, then $\dfrac{1}{y}$ is linear with x.

e. If $y = \dfrac{x}{a+bx}$, then $\dfrac{1}{y}$ is linear with $\dfrac{1}{x}$.

f. If $y = 1 - e^{-x^b/a}$, then $\ln\ln\left(\dfrac{1}{1-y}\right)$ is linear with $\ln x$.