11. Regression and Least Squares

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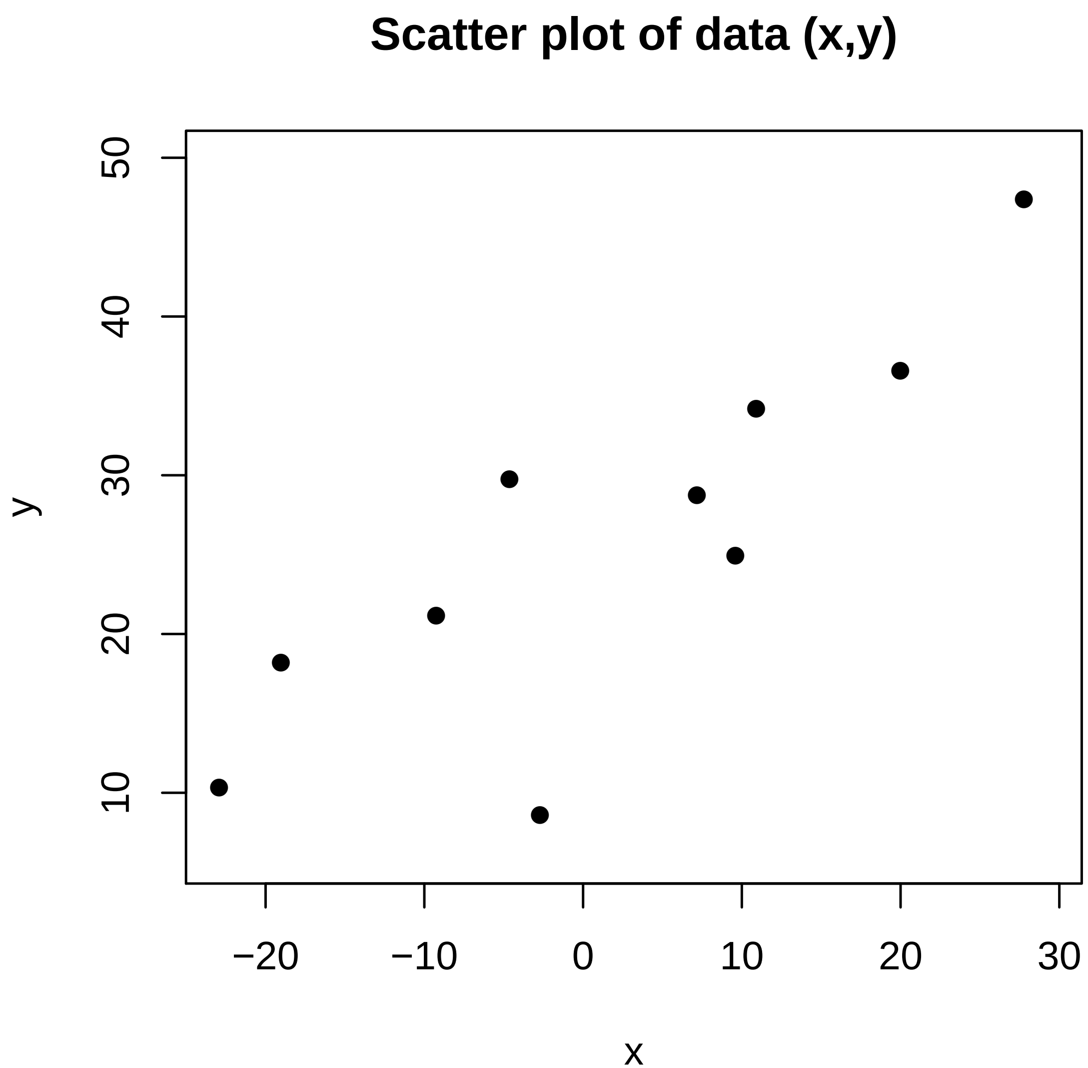
Math 186
Winter 2019

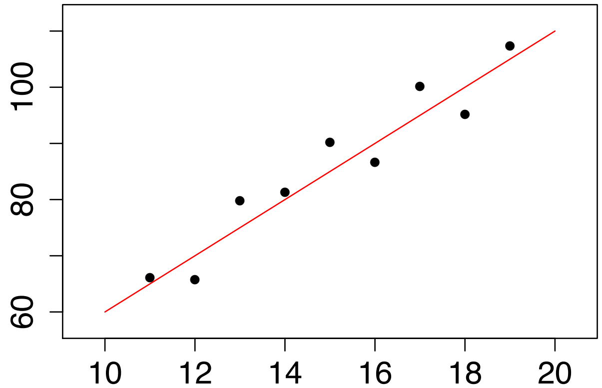
Regression

Given n points $(x_1, y_1), (x_2, y_2), \ldots,$ we want to determine a function $y = f(x)$ that is close to them.

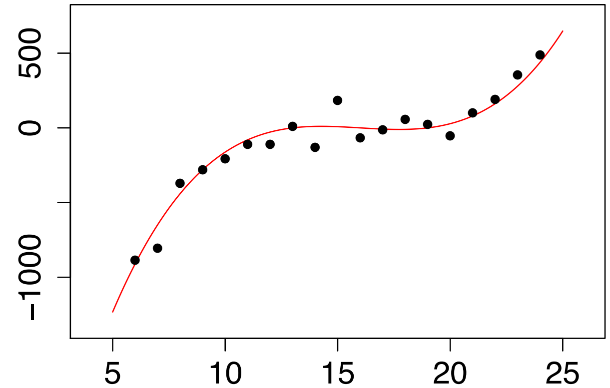


Based on knowledge of the underlying problem or on plotting the data, you have an idea of the general form of the function, such as:

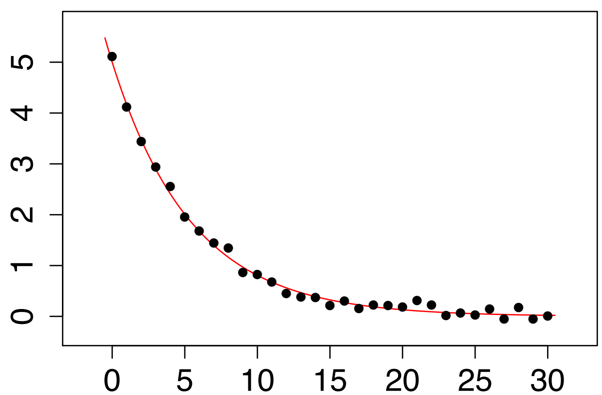
Line $y = \beta_0 + \beta_1 x$



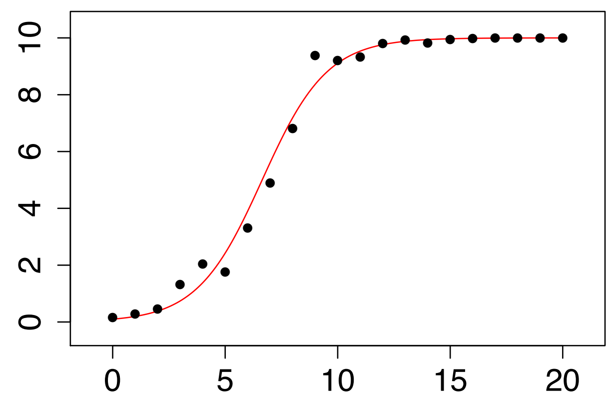
Polynomial $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$



Exponential Decay $y = Ae^{-Bx}$



Logistic Curve $y = A/(1 + B/C^x)$



Goal: Compute the parameters ($\beta_0, \beta_1, \ldots$ or $A, B, C, \ldots$) that give a "best fit" to the data.

Regression

- The methods we consider require the *parameters* to occur linearly. It is fine if (x, y) do not occur linearly.
  E.g., plugging $(x, y) = (2, 3)$ into $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$
  gives $3 = \beta_0 + 2\beta_1 + 4\beta_2 + 8\beta_3$.

- For exponential decay, $y = Ae^{-Bx}$, parameter B does not occur linearly. Transform the equation to:

$$\ln y = \ln(A) - Bx = A' - Bx$$

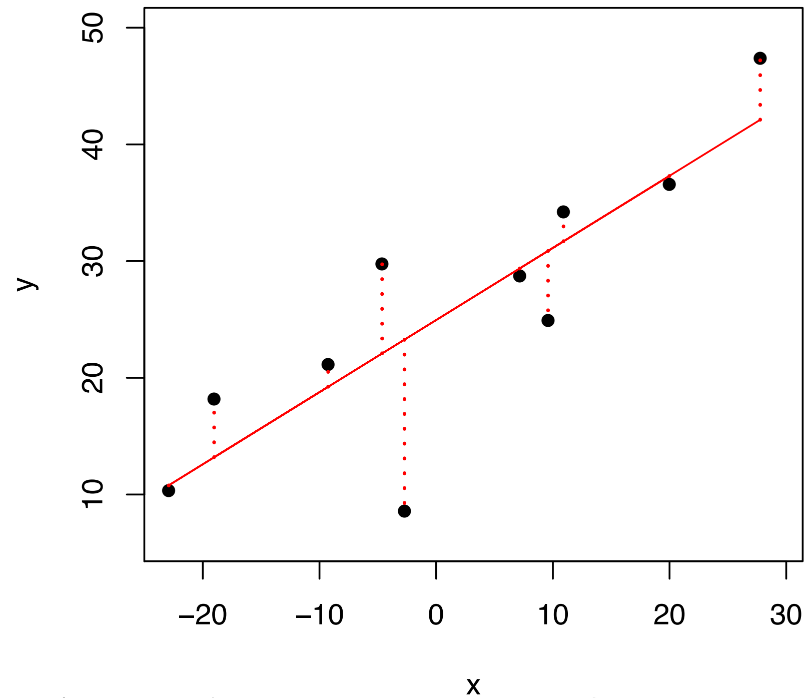
  When we plug in (x, y) values, the parameters A', B occur linearly.

- Transform the logistic curve $y = A/(1 + B/C^x)$ to:

$$\ln\left(\frac{A}{y} - 1\right) = \ln(B) - x\ln(C) = B' + C'x$$

  where A is determined from $A = \lim_{x\to\infty} y(x)$. Now B', C' occur linearly.

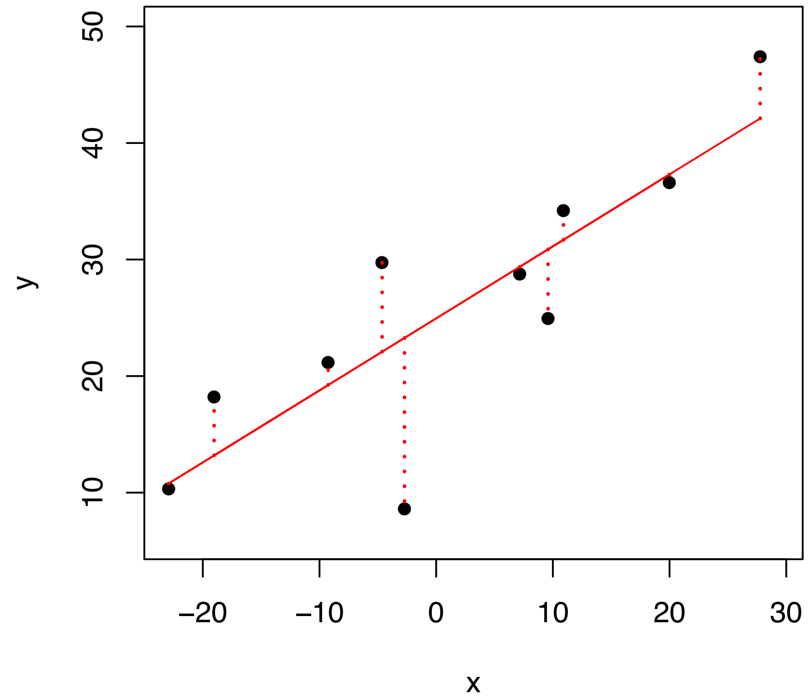
Least squares fit to a line



Given n points $(x_1, y_1), (x_2, y_2), \ldots,$ we will fit them to a line $\hat{y} = \beta_0 + \beta_1 x$:

- *Independent variable: x.* We assume the x's are known exactly or have negligible measurement errors.
- *Dependent variable: y.* We assume the y's depend on the x's but fluctuate due to a random process.
- We do not have $y = f(x)$, but instead, $y = f(x) + \text{error}$.

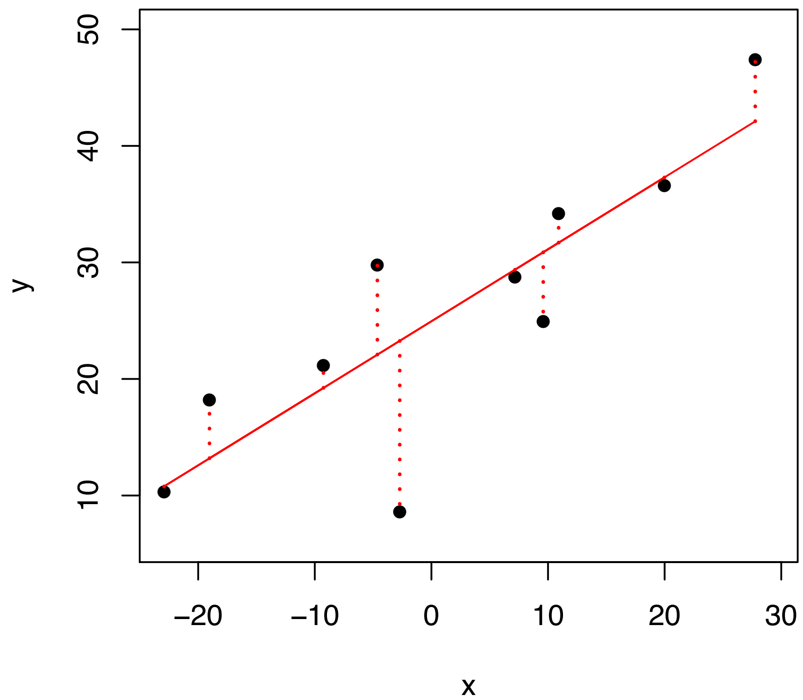
Least squares fit to a line



Given n points $(x_1, y_1), (x_2, y_2), \ldots,$ we will fit them to a line $\hat{y} = \beta_0 + \beta_1 x$:

Predicted y value (on the line):	$\hat{y}_i = \beta_0 + \beta_1 x_i$
Actual data (•):	$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$
Residual (actual y minus prediction):	$\epsilon_i = y_i - \hat{y}_i = y_i - (\beta_0 + \beta_1 x_i)$

Least squares fit to a line



We will use the *least squares method*: pick parameters β_0, β_1 that minimize the sum of squares of the residuals.

$$L = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2$$

Least squares fit to a line

$$L = \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i))^2$$

To find β_0, β_1 that minimize this, solve $\nabla L = \left(\frac{\partial L}{\partial \beta_0}, \frac{\partial L}{\partial \beta_1}\right) = (0,0)$:

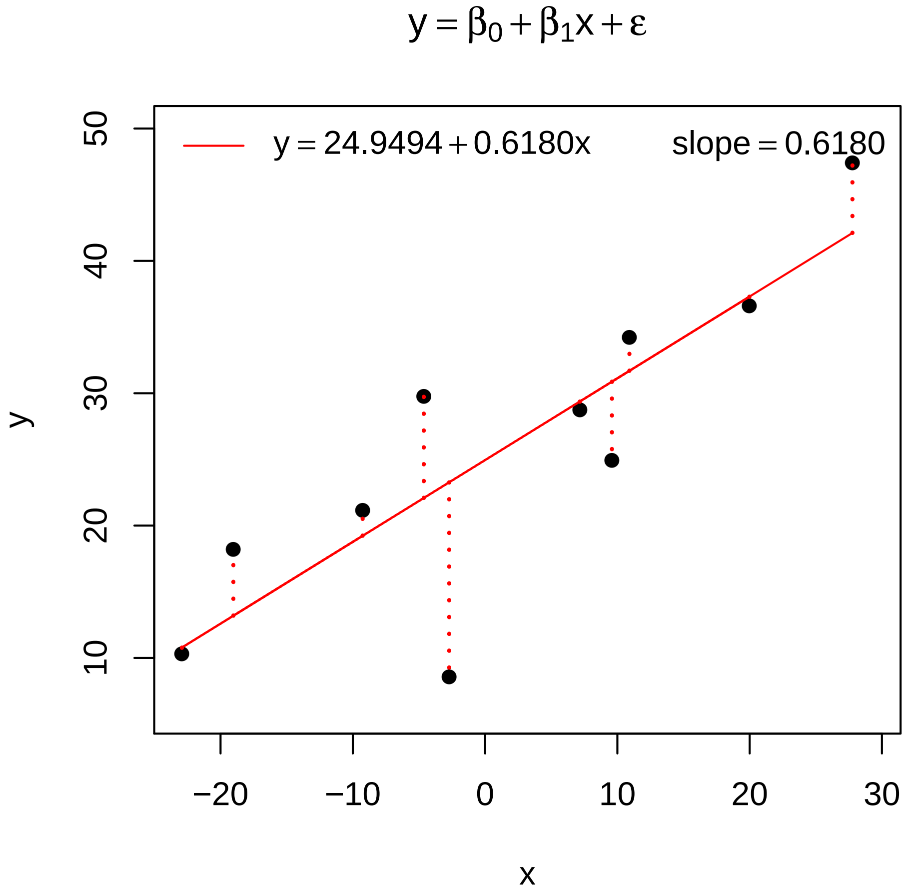
$$\frac{\partial L}{\partial \beta_0} = -2 \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i)) = 0 \quad \Rightarrow \quad n\beta_0 + \left(\sum_{i=1}^{n} x_i\right) \beta_1 = \sum_{i=1}^{n} y_i$$

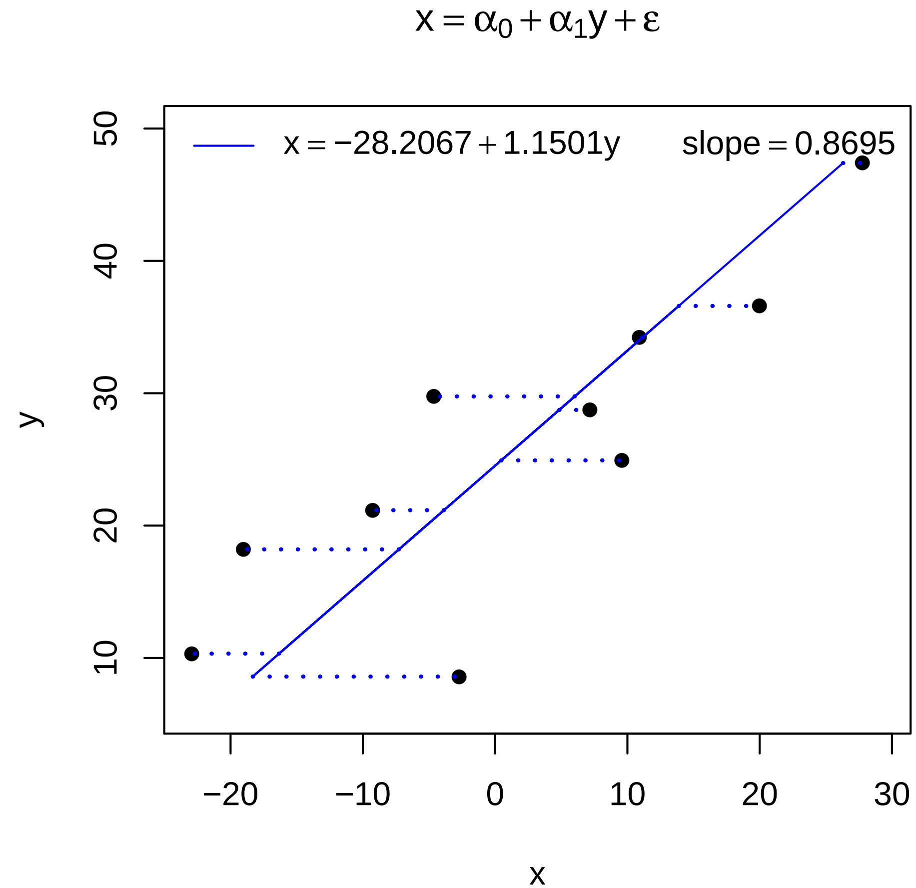
$$\frac{\partial L}{\partial \beta_1} = -2 \sum_{i=1}^{n} (y_i - (\beta_0 + \beta_1 x_i)) x_i = 0 \quad \Rightarrow \quad \left(\sum_{i=1}^{n} x_i\right) \beta_0 + \left(\sum_{i=1}^{n} {x_i}^2\right) \beta_1 = \sum_{i=1}^{n} x_i y_i$$

which has solution (all sums are $i = 1$ to n)

$$\beta_1 = \frac{n\left(\sum_i x_i\, y_i\right) - \left(\sum_i x_i\right)\left(\sum_i y_i\right)}{n\left(\sum_i {x_i}^2\right) - \left(\sum_i x_i\right)^2} = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2} \qquad \beta_0 = \bar{y} - \beta_1 \bar{x}$$

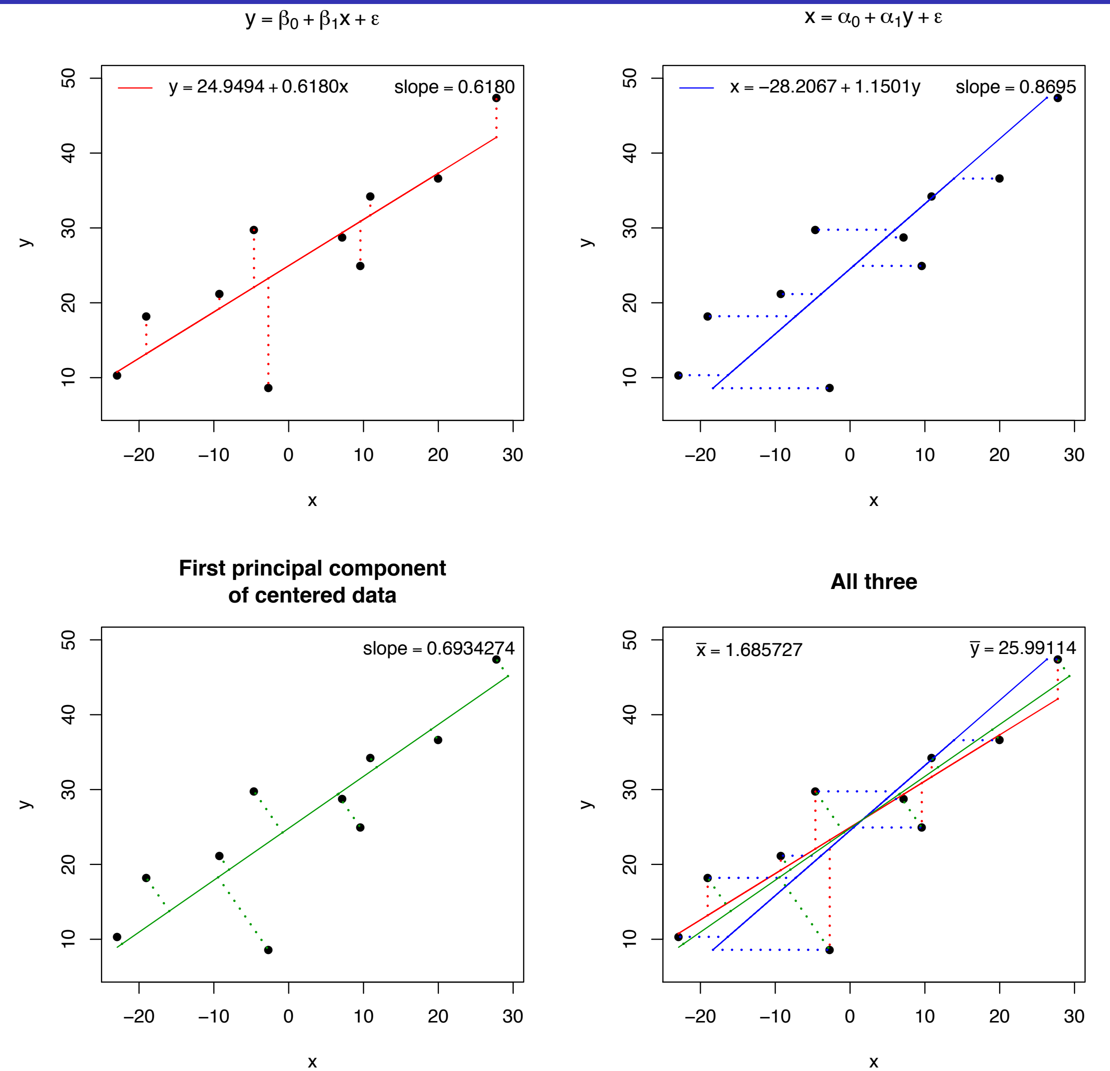
Not shown: use 2nd derivatives to confirm it's a minimum rather than a maximum or saddle point.





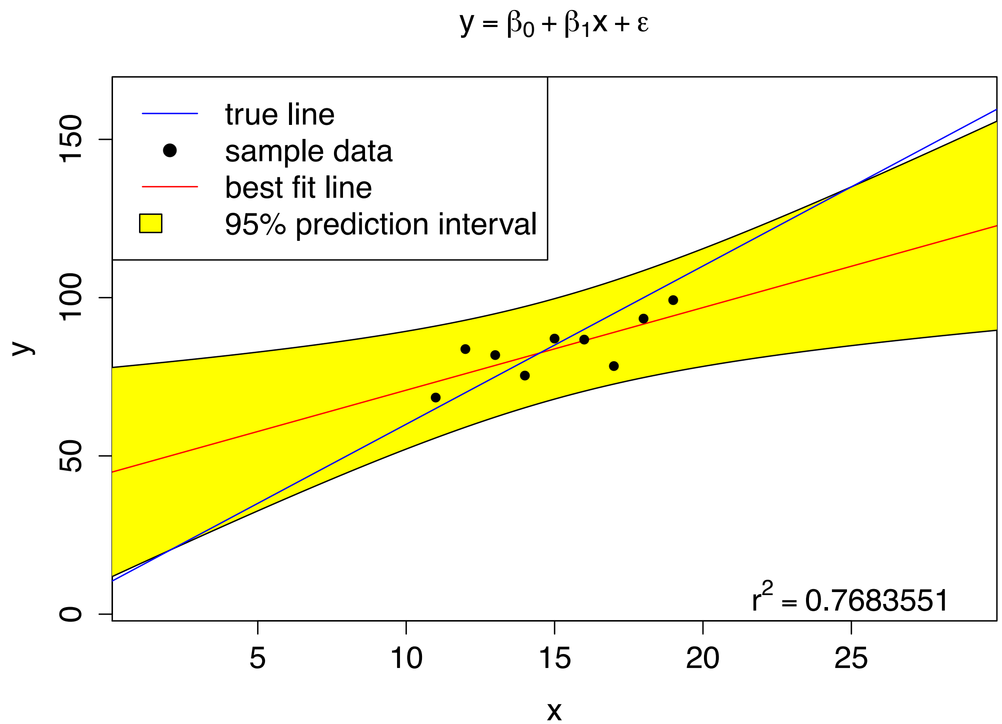
- The best fit for $y = \beta_0 + \beta_1 x +$ error or $x = \alpha_0 + \alpha_1 y +$ error give different lines!
- $y = \beta_0 + \beta_1 x +$ error assumes the x's are known exactly with no errors, while the y's have errors.
- $x = \alpha_0 + \alpha_1 y +$ error is the other way around.

Total Least Squares / Principal Components Analysis



- In many experiments, both x and y have measurement errors.
- Use *Total Least Squares* or *Principal Components Analysis*, in which the residuals are measured perpendicular to the line.
- Details require advanced linear algebra, beyond Math 18.

Confidence intervals



- The best fit line — is different than the true line —.
- We found point estimates of β_0 and β_1.
- Assuming errors are independent of x and normally distributed gives
  - Confidence intervals for β_0, β_1.
  - A *prediction interval* to extrapolate $y = f(x)$ at other x's.
    Warning: it may diverge from the true line when we go out too far.
  - **Not shown:** one can also do hypothesis tests on the values of β_0 and β_1, and on whether two samples give the same line.

Confidence intervals

- The method of least squares gave point estimates of β_0 and β_1:

$$\hat{\beta}_1 = \frac{n\sum_i x_i y_i - \left(\sum_i x_i\right)\left(\sum_i y_i\right)}{n\left(\sum_i {x_i}^2\right) - \left(\sum_i x_i\right)^2} = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2} \qquad \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

- The sample variance of the residuals is

$$s^2 = \frac{1}{n-2}\sum_{i=1}^{n}\left(y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i)\right)^2 \quad \text{(with } df = n-2\text{).}$$

- $100(1-\alpha)\%$ confidence intervals:

$$\beta_0 : \quad \left(\hat{\beta}_0 - t_{\alpha/2,n-2}\frac{s\sqrt{\sum_i {x_i}^2}}{\sqrt{n\sum_i (x_i - \bar{x})}},\ \hat{\beta}_0 + t_{\alpha/2,n-2}\frac{s\sqrt{\sum_i {x_i}^2}}{\sqrt{n\sum_i (x_i - \bar{x})}}\right)$$

$$\beta_1 : \quad \left(\hat{\beta}_1 - t_{\alpha/2,n-2}\frac{s}{\sqrt{\sum_i (x_i - \bar{x})}},\ \hat{\beta}_1 + t_{\alpha/2,n-2}\frac{s}{\sqrt{\sum_i (x_i - \bar{x})}}\right)$$

$$y \text{ at new } x : \quad (\hat{y} - w, \hat{y} + w) \ \text{ with } \ \hat{y} = \beta_0 + \beta_1 x$$

$$\text{and } \ w = t_{\alpha/2,n-2} \cdot s \cdot \sqrt{1 + \frac{1}{n} + \frac{(x-\bar{x})^2}{\sum_i (x_i - \bar{x})^2}}$$

Covariance

- Let X and Y be random variables, possibly dependent.
- Let $\mu_X = E(X)$, $\mu_Y = E(Y)$
- $$\begin{aligned} \mathrm{Var}(X+Y) &= E((X+Y-\mu_X-\mu_Y)^2) = E\left(\left((X-\mu_X)+(Y-\mu_Y)\right)^2\right) \\ &= E\left((X-\mu_X)^2\right) + E\left((Y-\mu_Y)^2\right) + 2E\left((X-\mu_X)(Y-\mu_Y)\right) \\ &= \mathrm{Var}(X) + \mathrm{Var}(Y) + 2\,\mathrm{Cov}(X,Y) \end{aligned}$$
  where the *covariance* of X and Y is defined as
  $$\mathrm{Cov}(X,Y) = E\left((X-\mu_X)(Y-\mu_Y)\right) = E(XY) - E(X)E(Y)$$
- Independent variables have $E(XY) = E(X)E(Y)$, so $\mathrm{Cov}(X,Y) = 0$. But $\mathrm{Cov}(X,Y) = 0$ does not guarantee X and Y are independent.

Covariance and independence

- Independent variables have $E(XY) = E(X)E(Y)$, so $\text{Cov}(X, Y) = 0$. But $\text{Cov}(X, Y) = 0$ does not guarantee X and Y are independent.
- Consider the standard normal distribution, Z.
- Z and Z^2 are dependent.
- $\text{Cov}(Z, Z^2) = E(Z^3) - E(Z)E(Z^2)$.
- The standard normal distribution has mean 0: $E(Z) = 0$.
- $E(Z^3) = 0$ since Z^3 is an odd function and the pdf of Z is symmetric around $Z = 0$.
- So $\text{Cov}(Z, Z^2) = 0$.

Covariance properties

We have

$$\mathrm{Var}(X+Y) = \mathrm{Var}(X) + \mathrm{Var}(Y) + 2\,\mathrm{Cov}(X,Y)$$

where the *covariance* of X and Y is defined as

$$\mathrm{Cov}(X,Y) = E\left((X-\mu_X)(Y-\mu_Y)\right) = E(XY) - E(X)E(Y)$$

Additional properties of covariance

- $\mathrm{Cov}(X,X) = \mathrm{Var}(X)$
- $\mathrm{Cov}(X,Y) = \mathrm{Cov}(Y,X)$
- $\mathrm{Cov}(aX+b, cY+d) = ac\,\mathrm{Cov}(X,Y)$

Sign of covariance

$$\mathrm{Cov}(X,Y) = E((X-\mu_X)(Y-\mu_Y))$$

- ***When*** $\mathbf{Cov}(X,Y)$ ***is positive:***
  There is a tendency to have $X > \mu_X$ when $Y > \mu_Y$ and vice-versa, and $X < \mu_X$ when $Y < \mu_Y$ and vice-versa.
- ***When*** $\mathbf{Cov}(X,Y)$ ***is negative:***
  There is a tendency to have $X > \mu_X$ when $Y < \mu_Y$ and vice-versa, and $X < \mu_X$ when $Y > \mu_Y$ and vice-versa.
- ***When*** $\mathbf{Cov}(X,Y) = \mathbf{0}$***:***
  a) X and Y **might** be independent, but it's not guaranteed.
  b) $\mathrm{Var}(X+Y) = \mathrm{Var}(X) + \mathrm{Var}(Y)$

Sample variance and covariance

Variance of a random variable:

$$\sigma^2 = \mathrm{Var}(X) = E((X-\mu_X)^2) = E(X^2) - (E(X))^2$$

Sample variance from data $x_1, \ldots, x_n$ to estimate σ^2:

$$s^2 = \mathrm{var}(x) = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{1}{n-1}\left(\sum_{i=1}^{n} {x_i}^2\right) - \frac{n}{n-1}\bar{x}^2$$

Covariance between random variables X, Y:

$$\sigma_{XY} = \mathrm{Cov}(X,Y) = E((X-\mu_X)(Y-\mu_Y)) = E(XY) - E(X)E(Y)$$

Sample covariance from data $(x_1,y_1), \ldots, (x_n,y_n)$ to estimate σ_{XY}:

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

Correlation coefficient

Let X and Y be two random variables.
Their *correlation coefficient* is

$$\rho(X,Y) = \frac{\operatorname{Cov}(X,Y)}{\sqrt{\operatorname{Var}(X)\operatorname{Var}(Y)}}$$

- This is a normalized version of covariance, and is between ± 1.
- For a line $Y = aX + b$ with a, b constants ($a \neq 0$),

$$\rho(X,Y) = \frac{a\operatorname{Var}(X)}{\sqrt{\operatorname{Var}(X)}\sqrt{\operatorname{Var}(aX)}} = \frac{a\sigma^2}{\sigma\cdot|a|\sigma} = \frac{a}{|a|} = \pm 1 \text{ (sign of } a\text{)}$$

- $\rho(X,Y) = \pm 1$ iff $Y = aX + b$ with a, b constants ($a \neq 0$).
- Closer to ± 1: more linear. Closer to 0: less linear.
- If X and Y are independent then $\rho(X,Y)=0$.
  The converse is not valid: dependent variables can have $\rho(X,Y)=0$.

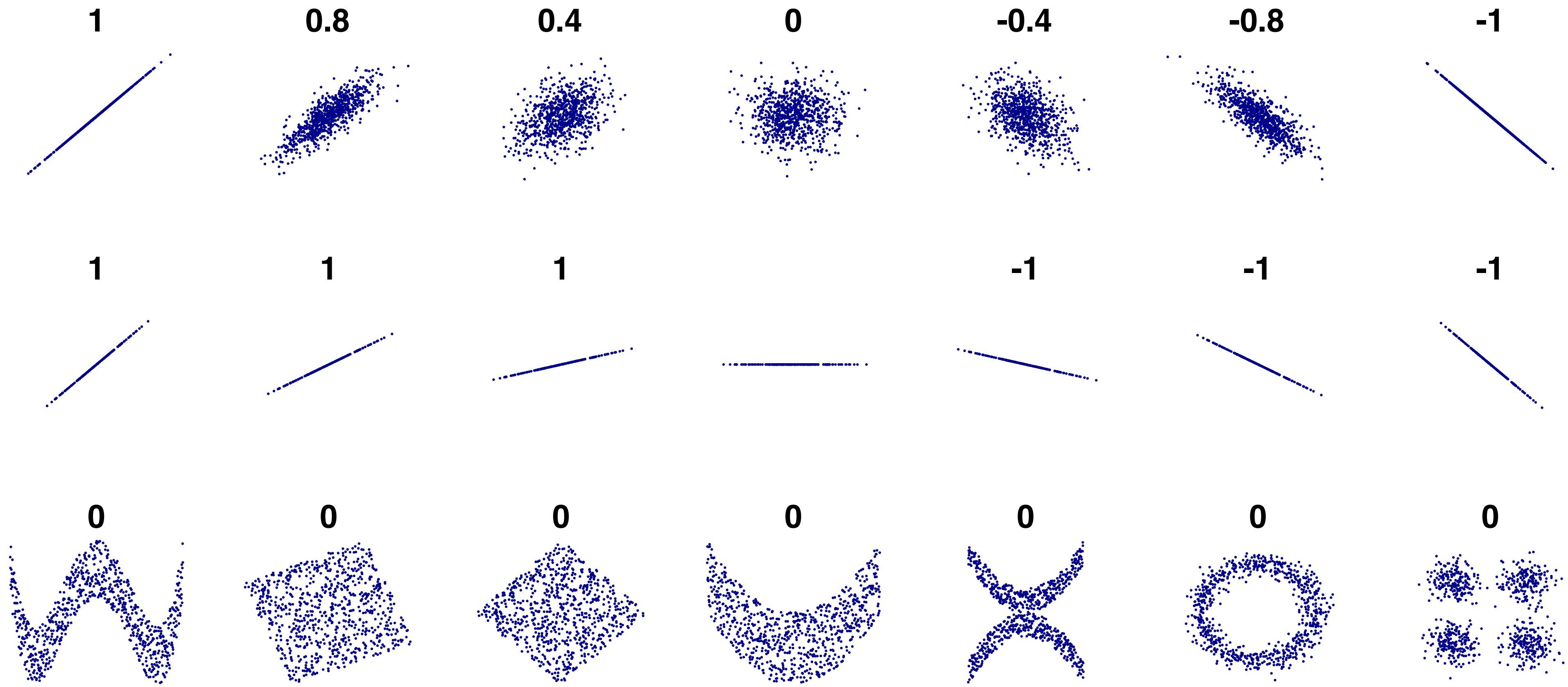
Correlation coefficient

- $\rho(X,Y)$ is estimated from data by the *sample correlation coefficient* (a.k.a. *Pearson product-moment correlation coefficient*):

$$r(x,y) = \frac{\operatorname{cov}(x,y)}{\sqrt{\operatorname{var}(x)\operatorname{var}(y)}} = \frac{\sum_i (x_i-\bar{x})(y_i-\bar{y})}{\sqrt{\sum_i (x_i-\bar{x})^2}\sqrt{\sum_i (y_i-\bar{y})^2}}$$
$$= \frac{n\sum_i x_i y_i - (\sum_i x_i)(\sum_i y_i)}{\sqrt{n\sum_i {x_i}^2 - (\sum_i x_i)^2}\sqrt{n\sum_i {y_i}^2 - (\sum_i y_i)^2}}$$

- People often report r^2 (between 0 and 1) instead of r.

Sample correlation coefficient r



http://en.wikipedia.org/wiki/File:Correlation_examples2.svg
http://en.wikipedia.org/wiki/Pearson_product-moment_correlation_coefficient

- **Middle row:** Perfect linear relation $Y = aX + b$ gives

$r = 1$	for lines with positive slope $(a > 0)$
$r = -1$	for lines with negative slope $(a < 0)$
r undefined	for horizontal line $(Y = b)$

- **Other rows:** coming up!

Interpretation of r^2

- Let $\hat{y}_i = \hat{\beta}_1 x_i + \hat{\beta}_0$
  be the predicted y-value for x_i based on the least squares line.
- Write the deviation of y_i from $\bar{y}$ as

$$\underbrace{y_i - \bar{y}}_{\text{Total deviation}} = \underbrace{(y_i - \hat{y}_i)}_{\text{Unexplained by line}} + \underbrace{(\hat{y}_i - \bar{y})}_{\text{Explained by line}}$$

- It can be shown that the sum of squared deviations for all y's is

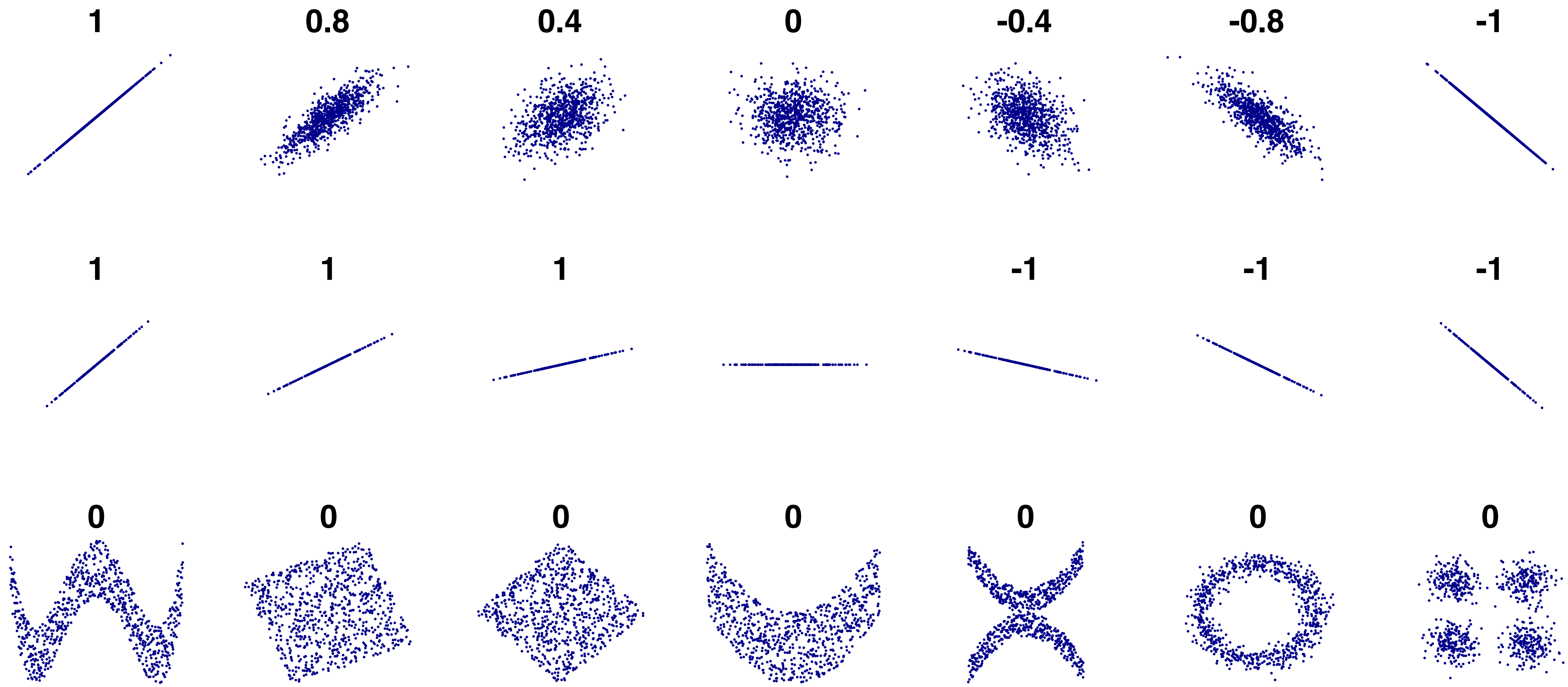
$$\underbrace{\textstyle\sum_i (y_i - \bar{y})^2}_{\text{Total variation}} = \underbrace{\textstyle\sum_i (y_i - \hat{y}_i)^2}_{\text{Unexplained variation}} + \underbrace{\textstyle\sum_i (\hat{y}_i - \bar{y})^2}_{\text{Explained variation}} + \underbrace{2 \textstyle\sum_i (y_i - \hat{y}_i)(\hat{y}_i - \bar{y})}_{\substack{= 0 \text{ by a miracle!} \\ \text{(Tedious algebra not shown)}}}$$

  and that

$$r^2 = \frac{\sum_i (\hat{y}_i - \bar{y})^2}{\sum_i (y_i - \bar{y})^2} = \frac{\text{Explained variation}}{\text{Total variation}}$$

- $r = 1$: 100% of the variation is explained by the line and 0% is due to other factors, and the slope is positive.
- $r = -.8$: 64% of the variation is explained by the line and 36% is due to other factors, and the slope is negative.

Sample correlation coefficient r



http://en.wikipedia.org/wiki/File:Correlation_examples2.svg
http://en.wikipedia.org/wiki/Pearson_product-moment_correlation_coefficient

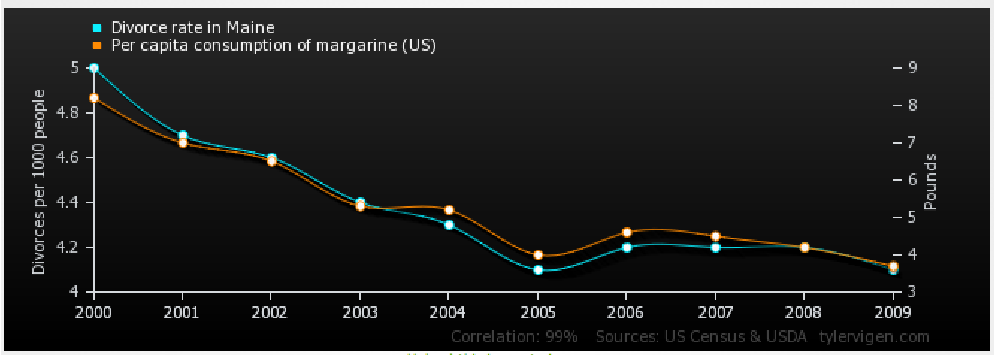
- **Top row:** Linear relations with varying r.
- **Bottom:** $r = 0$, yet X and Y are dependent in all of these (except possibly the last); it's just that the relationship is not a line.

Correlation does not imply causation

- High correlation between X and Y doesn't mean X causes Y or vice-versa. It could be a coincidence. Or they could both be caused by a third variable.
- Website tylervigen.com plots many data sets (various quantities by year) against each other to find spurious correlations:

spurious correlations

Divorce rate in Maine
correlates with
Per capita consumption of margarine (US)



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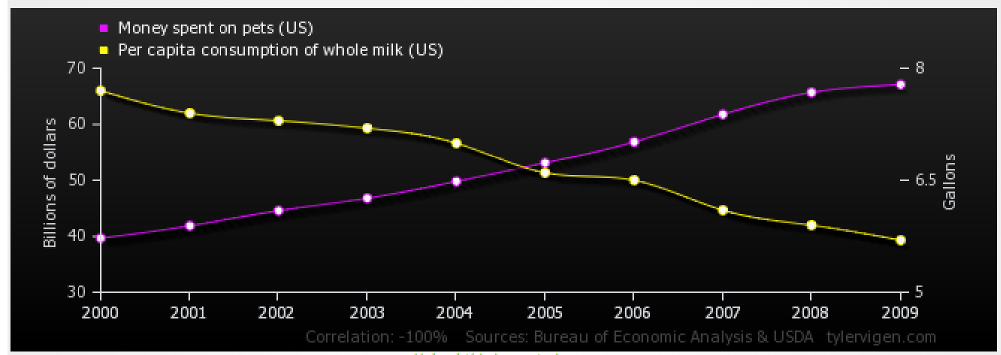
	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009
Divorce rate in Maine *Divorces per 1000 people (US Census)*	5	4.7	4.6	4.4	4.3	4.1	4.2	4.2	4.2	4.1
Per capita consumption of margarine (US) *Pounds (USDA)*	8.2	7	6.5	5.3	5.2	4	4.6	4.5	4.2	3.7

Correlation: 0.992558

http://www.tylervigen.com/view_correlation?id=1703

spurious correlations

Money spent on pets (US)
inversely correlates with
Per capita consumption of whole milk (US)



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	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009
Money spent on pets (US) *Billions of dollars (Bureau of Economic Analysis)*	39.7	41.9	44.6	46.8	49.8	53.1	56.9	61.8	65.7	67.1
Per capita consumption of whole milk (US) *Gallons (USDA)*	7.7	7.4	7.3	7.2	7	6.6	6.5	6.1	5.9	5.7

Correlation: -0.995478

http://tylervigen.com/view_correlation?id=1759

More about interpretation of correlation

- Low r^2 does NOT guarantee independence; it just means that a line $y = \beta_0 + \beta_1 x$ is not a good fit to the data.

- r is an estimate of ρ. The estimate improves with higher n. With additional assumptions on the underlying joint distribution of X, Y, we can use r to test

  H_0: $\rho = 0$ vs. H_1: $\rho \neq 0$ (or other values).

- Best fits and correlation generalize to other models, including

Polynomial regression	$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_p x^p$
Multiple linear regression	$y = \beta_0 + \beta_1 t + \beta_2 u + \cdots + \beta_p w$ $t, u, \ldots, w$: multiple independent variables y: dependent variable
Weighted versions	When the variance is different at each value of the independent variables