Regression analysis Two variables

(Montgomery and Runger: ch 11 Brani Vidakovic: ch 14)

Reminder

Covariance Defined

Covariance is a number qunatifying average dependence between two random variables.

The covariance between the random variables X and Y, denoted as cov(X,Y) or σ_{XY} is

$$\sigma_{XY} = E[(X - \mu_X)(Y - \mu_Y)] = E(XY) - \mu_X \mu_Y$$
 (5-14)

The units of σ_{yy} are units of X times units of Y.

Unlike the range of variance, $-\infty < \sigma_{XY} < \infty$.

Correlation is "normalized covariance"

Also called:

Pearson correlation coefficient

 $\rho_{XY} = \sigma_{XY} / \sigma_X \sigma_Y$ is the covariance normalized to be $-1 \le \rho_{XY} \le 1$



Karl Pearson (1852–1936) English mathematician and biostatistician

Covariance and Scatter Patterns

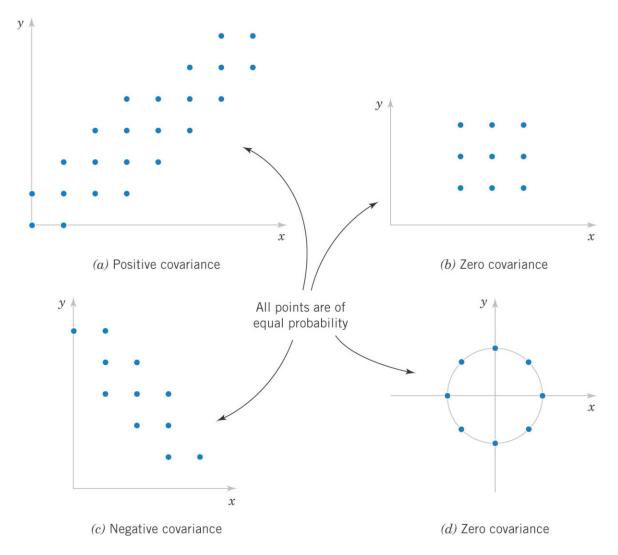
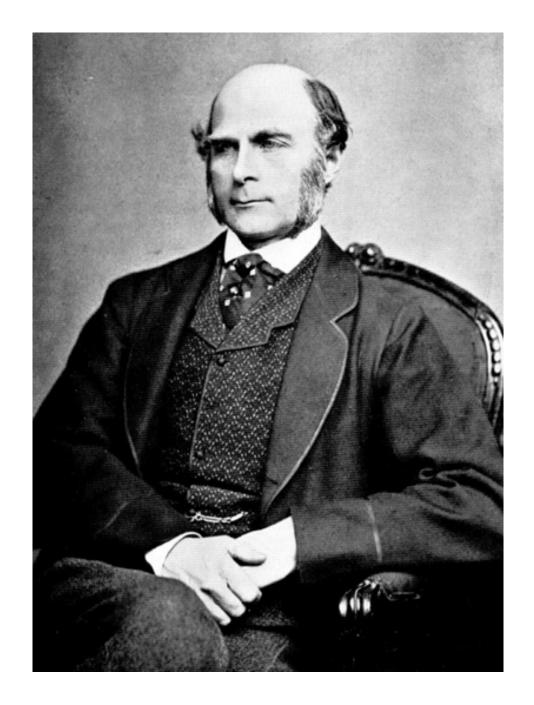


Figure 5-13 Joint probability distributions and the sign of cov(X, Y). Note that covariance is a measure of linear relationship. Variables with non-zero covariance are correlated.

Regression analysis

- Many problems in engineering and science involve sample in which two or more variables were measured. They may not be independent from each other and one (or several) of them can be used to predict another
- Everyday example: in most samples height and weight of people are related to each other
- Biological example: in a cell sorting experiment the copy number of a protein may be measured alongside its volume
- Regression analysis uses a sample to build a model to predict protein copy number given a cell volume

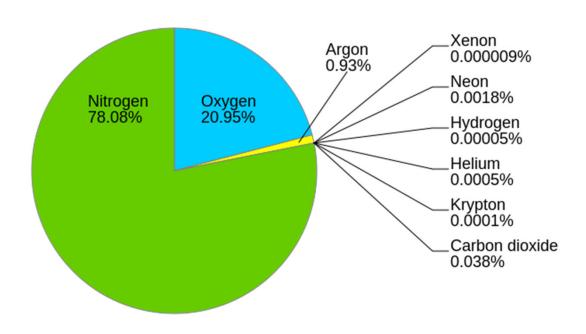


Sir Francis Galton, (1822 -1911) was an English statistician, anthropologist, proto-geneticist, psychometrician, eugenicist, ("Nature vs Nurture", inheritance of intelligence), tropical explorer, geographer, inventor (Galton Whistle to test hearing), meteorologist (weather map, anticyclone).

Invented both correlation and regression analysis when studied heights of fathers and sons

Found that fathers with height above average tend to have sons with height also above average but closer to the average. Hence "regression" to the mean

Two variable samples



- Oxygen can be distilled from the air
- Hydrocarbons need to be filtered out or the whole thing would go kaboom!!!
- When more hydrocarbons were removed, the remaining oxygen stays cleaner
- Except we don't know how dirty was the air to begin with

Table 11-1 Oxygen and Hydrocarbon Levels

Observation Number	Hydrocarbon Level $x(\%)$	Purity y(%)
1	0.99	90.01
2	1.02	89.05
3	1.15	91.43
4	1.29	93.74
5	1.46	96.73
6	1.36	94.45
7	0.87	87.59
8	1.23	91.77
9	1.55	99.42
10	1.40	93.65
11	1.19	93.54
12	1.15	92.52
13	0.98	90.56
14	1.01	89.54
15	1.11	89.85
16	1.20	90.39
17	1.26	93.25
18	1.32	93.41
19	1.43	94.98
20	0.95	87.33

$$Y = \beta_0 + \beta_1 \times + \epsilon$$

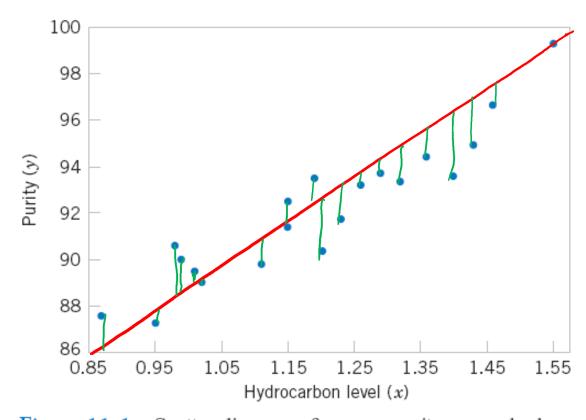


Figure 11-1 Scatter diagram of oxygen purity versus hydrocarbon level from Table 11-1.

Linear regression

The simple linear regression model is given by

$$Y = \beta_0 + \beta_1 X + E = \hat{Y} + E$$

E is the random error

slope β_1 and intercept β_0 of the line are called regression coefficients

Note: Y, \hat{Y} , X and E are random variables

Let's assume that
$$E(E|x)=0 \rightarrow E(Y|x) = \beta_0 + \beta_1 x + E(E|x) = \beta_0 + \beta_1 x$$

Y=
$$\beta_0 + \beta_1 \times + \epsilon$$
; $E(\epsilon|x) = 0$ $\forall x$
How does one find $\beta_0 + \beta_1 = 0$.
 $Cov(Y,X) = Cov((\beta_0 + \beta_1 \times + \epsilon), X) = 0$
 $E(x,X) = Cov(X,X) + Cov(X,X) + Cov(X,X)$
 $E(x,X) = 0$ Since $\beta_0 = 0$ Since $\beta_0 = 0$ Cov $(x,x) = E(x^2) - E(x)^2 = Var(X)$
 $E(x,X) = E(x^2) - E(x) = E(x) = 0$
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Method of least squares

• The method of least squares is used to estimate the parameters, β_0 and β_1 by minimizing the sum of the squares of the vertical deviations in Figure 11-3.

Figure 11-3 Deviations of the data from the estimated regression model.

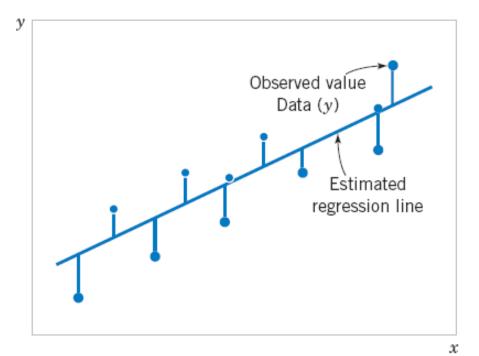


Figure 11-3 Deviations of the data from the estimated regression model.

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i, \qquad i = 1, 2, ..., n$$
 (11-3)

and the sum of the squares of the deviations of the observations from the true regression line is

$$L = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$
 (11-4)

The least squares estimators of β_0 and β_1 , say, $\hat{\beta}_0$ and $\hat{\beta}_1$, must satisfy

$$\frac{\partial L}{\partial \beta_{0}}\Big|_{\hat{\beta}_{0},\hat{\beta}_{1}} = -2\sum_{i=1}^{n} (y_{i} - \hat{\beta}_{0} - \hat{\beta}_{1}x_{i}) = 0$$

$$\frac{\partial L}{\partial \beta_{1}}\Big|_{\hat{\beta}_{0},\hat{\beta}_{1}} = -2\sum_{i=1}^{n} (y_{i} - \hat{\beta}_{0} - \hat{\beta}_{1}x_{i})x_{i} = 0$$

$$\hat{\beta}_{0} + \hat{\beta}_{1} \sum_{i=1}^{n} x_{i} = \sum_{i=1}^{n} y_{i}$$

$$\hat{\beta}_{0} \sum_{i=1}^{n} x_{i} + \hat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2} = \sum_{i=1}^{n} y_{i}x_{i}$$

$$(11-5)$$

$$\hat{\beta}_{0} \sum_{i=1}^{n} x_{i} + \hat{\beta}_{1} \sum_{i=1}^{n} x_{i}^{2} = \sum_{i=1}^{n} y_{i}x_{i}$$

$$(11-6) + \sum y_{i} \sum x_{i}^{2} = \sum x_{i}^{2} + \sum x_{i}^{2} + \sum x_{i}^{2} = \sum x_{i}^{2} + \sum x_{i}^{2} + \sum x_{i}^{2} = \sum x_{i}^{2} + \sum x_{i}^{$$

Traditional notation

Definition

The **least squares estimates** of the intercept and slope in the simple linear regression model are

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x} \tag{11-7}$$

$$\hat{\beta}_{1} = \frac{\sum_{i=1}^{n} y_{i} x_{i} - \frac{\left(\sum_{i=1}^{n} y_{i}\right) \left(\sum_{i=1}^{n} x_{i}\right)}{n}}{\sum_{i=1}^{n} x_{i}^{2} - \frac{\left(\sum_{i=1}^{n} x_{i}\right)^{2}}{n}} = \frac{\sum_{i=1}^{n} y_{i} x_{i}}{\sum_{i=1}^{n} x_{i}} = \frac{\sum_{i=1}^{n} y_{i}}{\sum_{i=1}^{n} x_{i}} = \frac{\sum_{i=1}^{n}$$

where $\overline{y} = (1/n) \sum_{i=1}^{n} y_i$ and $\overline{x} = (1/n) \sum_{i=1}^{n} x_i$.

11-2: Simple Linear Regression

Definition

The **least squares estimates** of the intercept and slope in the simple linear regression model are

$$\hat{\beta}_{0} = \overline{y} - \hat{\beta}_{1}\overline{x}$$

$$\hat{\beta}_{1} = \frac{\sum_{i=1}^{n} y_{i} x_{i}}{\sum_{i=1}^{n} y_{i}} - \frac{\left(\sum_{i=1}^{n} y_{i}\right) \left(\sum_{i=1}^{n} x_{i}\right)}{n^{2}} = \frac{Cov\left(X, Y\right)}{\sqrt{qv\left(X\right)}}$$

$$\sum_{i=1}^{n} x_{i}^{2} - \frac{\left(\sum_{i=1}^{n} x_{i}\right)^{2}}{n^{2}} = \frac{Vqv\left(X\right)}{\sqrt{qv\left(X\right)}}$$
(11-8)

where $\overline{y} = (1/n) \sum_{i=1}^{n} y_i$ and $\overline{x} = (1/n) \sum_{i=1}^{n} x_i$.

11-4.2 Analysis of Variance Approach to Test Significance of Regression

The analysis of variance identity is

$$\sum_{i=1}^{n} (y_i - \bar{y})^2 = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
 (11-24)

Symbolically,

$$SS_T = SS_R + SS_E \tag{11-25}$$

11-7: Adequacy of the Regression Model

11-7.2 Coefficient of Determination (R²) <u>VERY COMMONLY USED</u>

• The quantity

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T}$$

is called the **coefficient of determination** and is often used to judge the adequacy of a regression model.

- $0 \le R^2 \le 1$;
- We often refer (loosely) to R² as the amount of variability in the data explained or accounted for by the regression model.

Adjusted R-Squared

• Adjusted R-Squared uses unbiased estimates of σ_{ε}^2 and σ_{Y}^2 :

$$= 1 - \frac{\sigma_{\varepsilon}^{2}}{s_{Y}^{2}} = 1 - \frac{\frac{SS_{\varepsilon}}{n-2}}{\frac{SS_{\tau}}{n-1}}$$

• For small samples it is different from the regular R-Squared: $R^2 = 1 - \frac{SS_E}{SS_T}$

11-7: Adequacy of the Regression Model

11-7.2 Coefficient of Determination (R²)

• For the oxygen purity regression model,

$$R^2 = SS_R/SS_T$$

= 152.13/173.38
= 0.877

• Thus, the model accounts for 87.7% of the variability in the data.

11-2: Simple Linear Regression

Estimating $\sigma_{\underline{\epsilon}}^2$

An unbiased estimator of σ_{ϵ}^{2} is

$$\hat{\mathbf{g}}^2 = \frac{SS_E}{n-2} \tag{11-13}$$

where SS_E can be easily computed using

$$SS_E = SS_T - \hat{\beta}_1 S_{xy} \tag{11-14}$$

11-3: Properties of the Least Squares Estimators

Slope Properties

$$E(\hat{\beta}_1) = \beta_1$$

• Intercept Properties

$$V(\hat{\beta}_1) = \frac{\sigma_{\epsilon}^2}{S_{xx}} = \frac{\delta_{\epsilon}^2}{n \delta_{\epsilon}^2}$$

$$Large \quad n \rightarrow Small \quad Variance \quad of \quad R_1$$

$$E(\hat{\beta}_0) = \beta_0 \quad \text{and} \quad V(\hat{\beta}_0) = \hat{\sigma}_2^2 \left[\frac{1}{n} + \frac{\overline{x}^2}{S_{xx}} \right] =$$

$$= \hat{\delta}_2^2 \left[1 + \frac{\mu_{\lambda}^2}{\delta_x^2} \right]^{\lambda} \frac{1}{h}$$

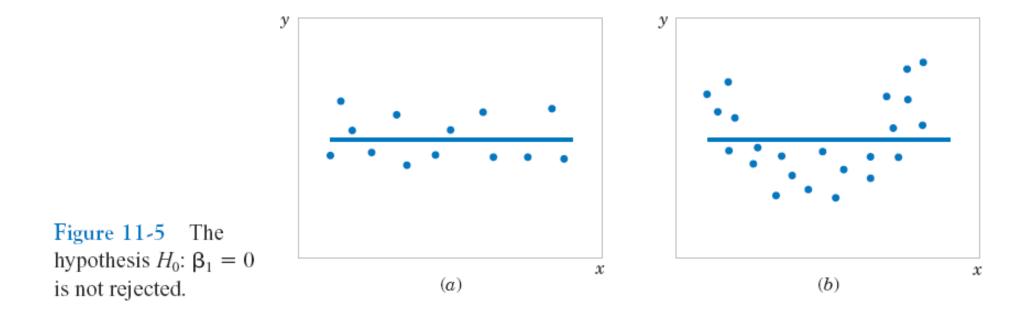


Figure 11-5 The null hypothesis H_0 : $\beta_1 = 0$ is accepted.

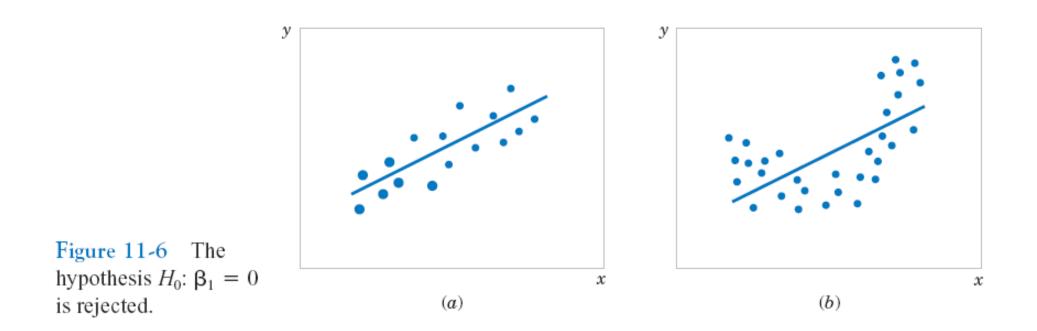


Figure 11-6 The null hypothesis H_0 : $\beta_1 = 0$ is rejected.

11-4.1 Use of Z-tests for large n

An important special case of the hypotheses of Equation 11-18 is

$$H_0: \beta_1 = 0$$

$$H_1: \beta_1 \neq 0$$

These hypotheses relate to the **significance of regression**. *Failure* to reject H_0 is equivalent to concluding that there is no linear relationship between X and Y.

$$H_0: \beta_1 = 0$$

$$H_1: \beta_1 \neq 0$$

$$\frac{1}{2} = \frac{\beta_1}{\beta_6}$$

$$\frac{3}{5} = \frac{1}{5}$$

Choose d (e.g. d=5%) for 95% confidence (n rejecting Ho)

$$Reject H_0 - \{ Z \} > Z_{2}^{=1.96}$$

11-4.1 Use of *t*-tests for smaller n.

The number of degrees of freedom in **n-2**

One can always fit a straight line through two points so one needs n>=3

$$H_0: \beta_1 = 0 \qquad \text{Choose d}$$

$$H_1: \beta_1 \neq 0 \qquad \text{(e.g. d=3\%)}$$

$$Confidence}$$

$$\text{(n rejecting)}$$

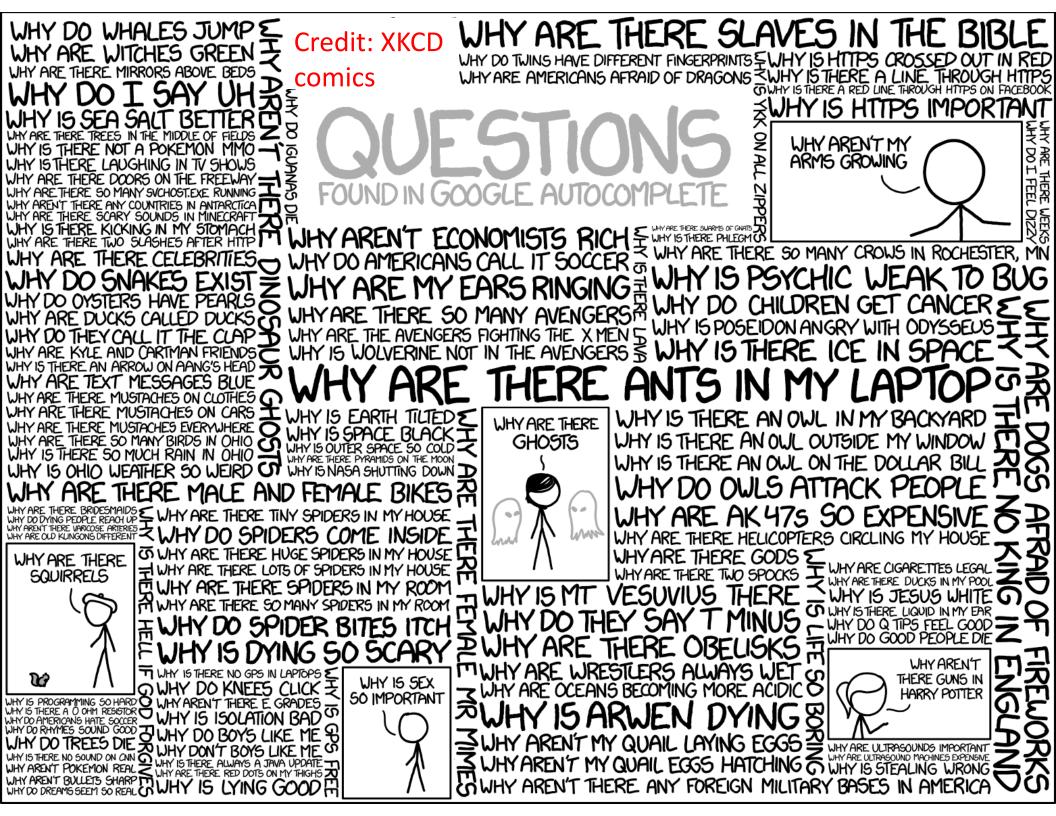
$$H_0) \hat{\beta}_{\delta} \qquad \text{(n rejecting)}$$

$$\frac{\beta_{\delta}}{\beta_{\delta}} \qquad \text{(n rejecting)}$$

$$\frac{\beta_{\delta}}{\beta_{\delta}} \qquad \text{(n rejecting)}$$

$$Reject H_0 - \mathcal{A} = t cdf(t_{\delta} \chi_1 + 2)^{\frac{1}{2}}$$

$$Reject H_0 - \mathcal{A} = t cdf(t_{\delta} \chi_1 + 2)^{\frac{1}{2}}$$



Multiple Linear Regression

(Chapters 12-13 in Montgomery, Runger)

12-1: Multiple Linear Regression Model

12-1.1 Introduction

- Many applications of regression analysis involve situations in which there are more than one regressor variable X_k used to predict Y.
- A regression model then is called a multiple regression model.

Multiple Linear Regression Model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + ... \beta_k x_k + \varepsilon$$

One can also use powers and products of other variables or even non-linear functions like $exp(x_i)$ or $log(x_i)$ instead of x_3, \ldots, x_k .

Example: the general two-variable quadratic regression has 6 constants:

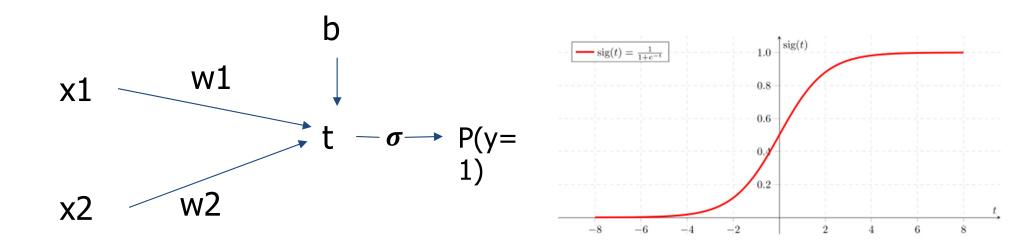
$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 (x_1)^2 + \beta_4 (x_2)^2 + \beta_5 (x_1 x_2) + \varepsilon$$

Nonlinear Regression Example: Logistic Regression

$$P(Y=1) = \sigma(x1*w1 + x2*w2 + b)$$

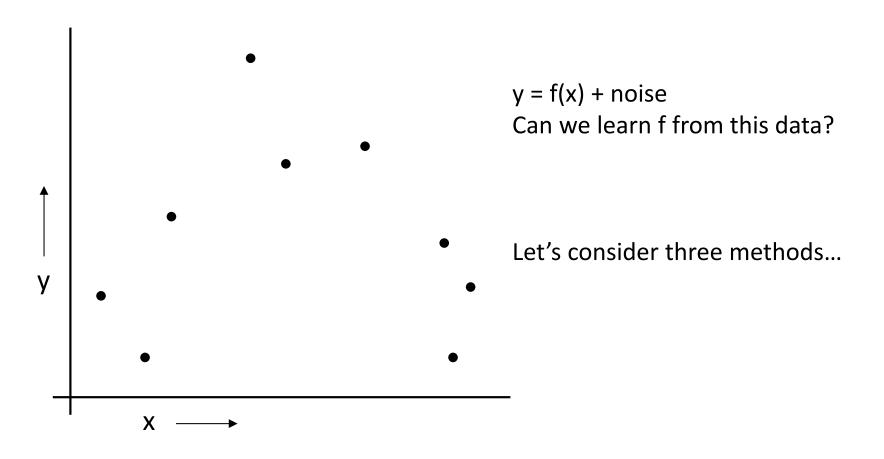
Linear regression analog

$$Y = X1*b1 + X2*b2 + b0$$

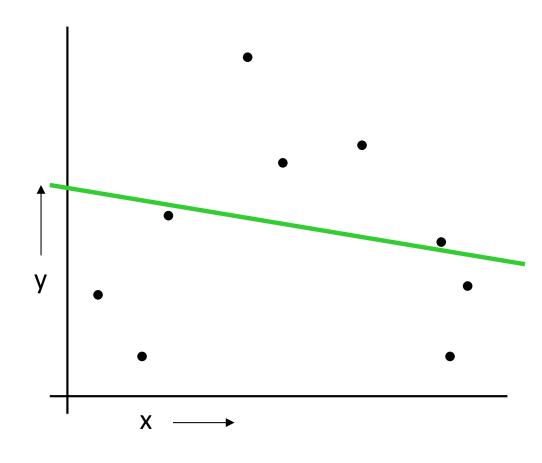


How to know where to stop adding new variables or powers of old variables?

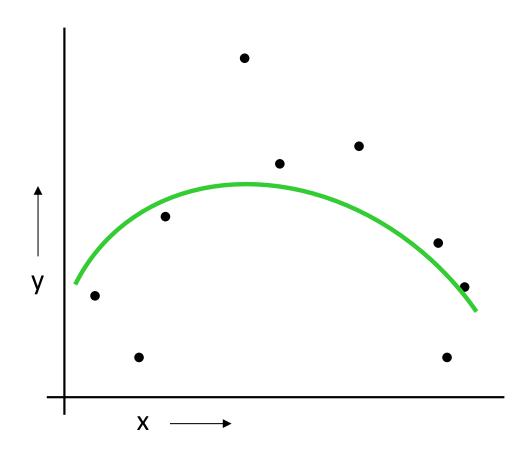
A Regression Problem



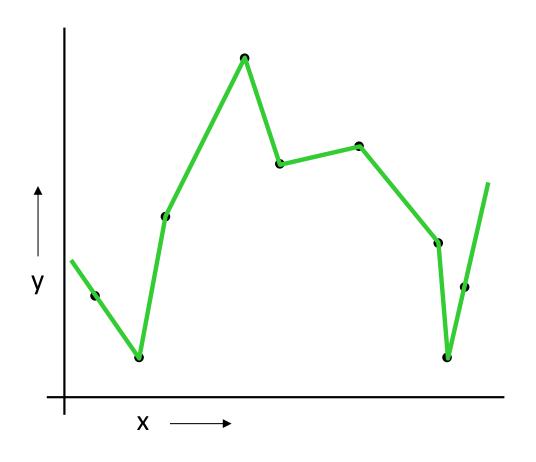
Linear Regression



Quadratic Regression

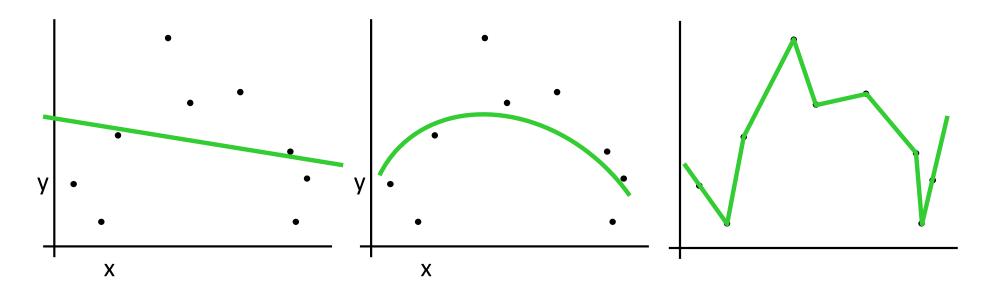


Join-the-dots



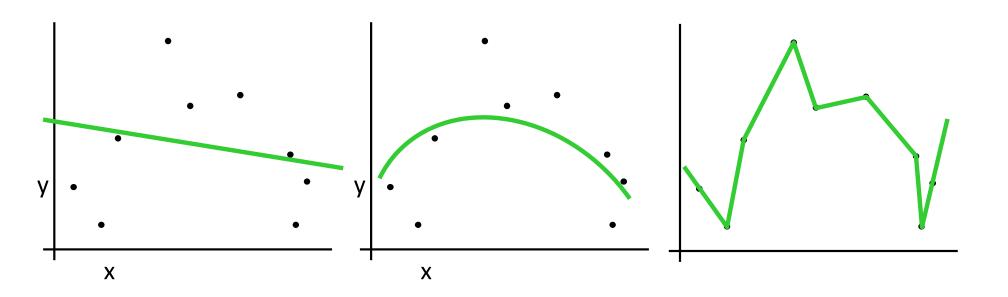
Also known as piecewise linear nonparametric regression if that makes you feel better

Which is best?



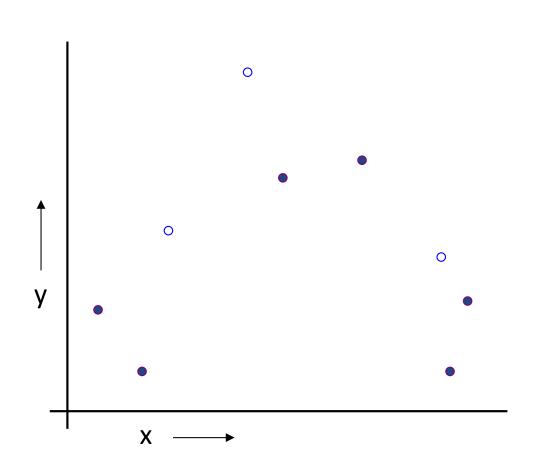
Why not choose the method with the best fit to the data?

What do we really want?

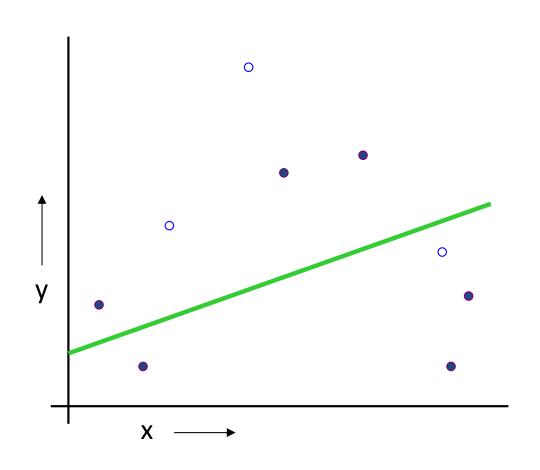


Why not choose the method with the best fit to the data?

"How well are you going to predict future data drawn from the same distribution?"

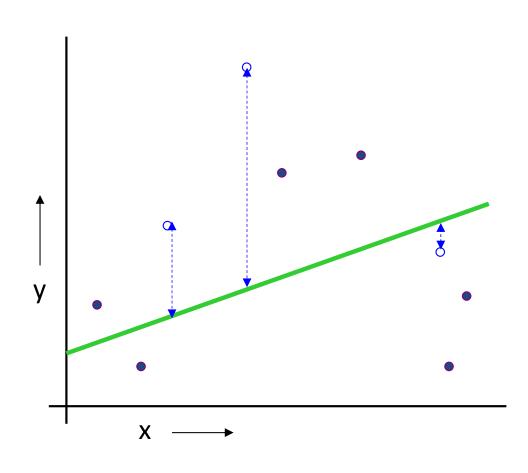


Randomly choose
 of the data to
 in a test set
 The remainder is a training set



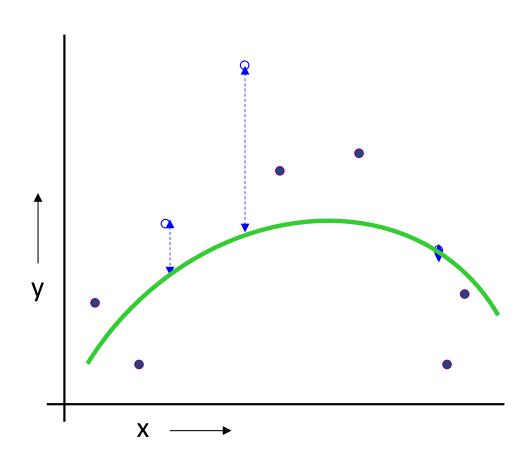
(Linear regression example)

- 1. Randomly choose 30% of the data to be in a test set
- 2. The remainder is a training set
- 3. Perform your regression on the training set



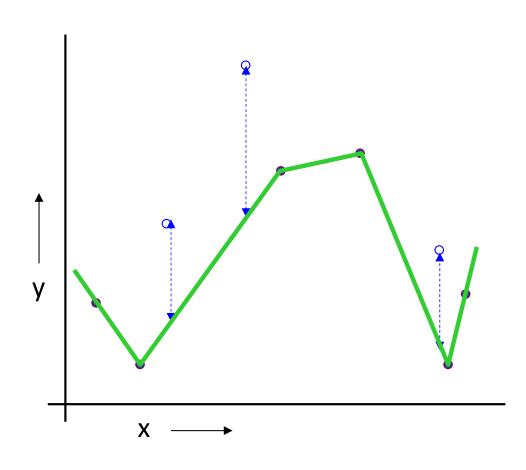
(Linear regression example) Mean Squared Error = 2.4

- 1. Randomly choose 30% of the data to be in a test set
- 2. The remainder is a training set
- 3. Perform your regression on the training set
- 4. Estimate your future performance with the test set



(Quadratic regression example) Mean Squared Error = 0.9

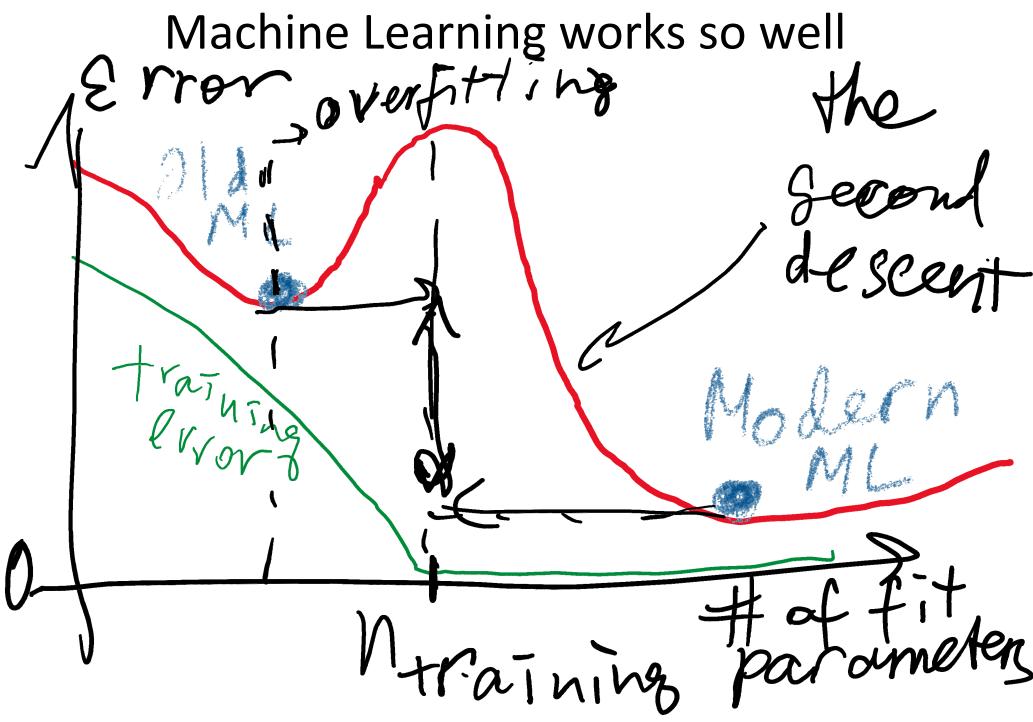
- 1. Randomly choose 30% of the data to be in a test set
- 2. The remainder is a training set
- 3. Perform your regression on the training set
- 4. Estimate your future performance with the test set

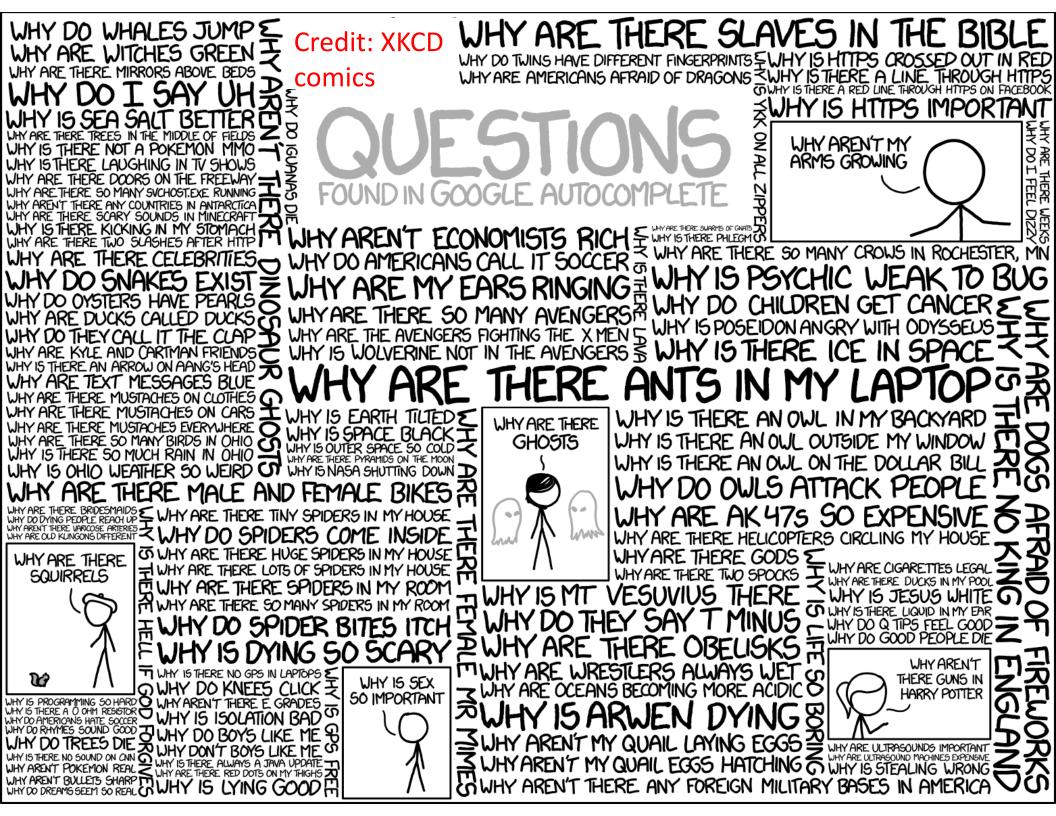


(Join the dots example)
Mean Squared Error = 2.2

- 1. Randomly choose 30% of the data to be in a test set
- 2. The remainder is a training set
- 3. Perform your regression on the training set
- 4. Estimate your future performance with the test set

Double descend- the main reason modern





12-1: Multiple Linear Regression Model

12-1.3 Matrix Approach to Multiple Linear Regression

Suppose the model relating the regressors to the response is

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik} + \varepsilon_i$$
 $i = 1, 2, \dots, n$

In matrix notation this model can be written as

$$y = X\beta + \varepsilon \tag{12-6}$$

12-1: Multiple Linear Regression Model

12-1.3 Matrix Approach to Multiple Linear Regression

where

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \boldsymbol{\beta}_0 \\ \boldsymbol{\beta}_1 \\ \vdots \\ \boldsymbol{\beta}_k \end{bmatrix} \text{ and } \boldsymbol{\varepsilon} = \begin{bmatrix} \boldsymbol{\varepsilon}_1 \\ \boldsymbol{\varepsilon}_2 \\ \vdots \\ \boldsymbol{\varepsilon}_n \end{bmatrix}$$

12-1.3 Matrix Approach to Multiple Linear Regression

We wish to find the vector $\hat{\beta}$ that minimizes the sum of squares of error terms:

$$L = \sum_{i=1}^{n} \epsilon_i^2 = \epsilon' \epsilon = (y - X\beta)' (y - X\beta)$$

$$0 = \frac{\partial L}{2\partial \beta} = -X' (\mathbf{y} - \mathbf{X}\beta) = -X' \mathbf{y} + (X'X)\boldsymbol{\beta}$$

The resulting least squares estimate is

$$\widehat{\beta} = (X'X)^{-1} X'y$$
(12-7)

Analog of \widehat{V} ov (X,Y)

Sec 12-1 Multiple Linear Regression Model

Multiple Linear Regression Model

$$\hat{\beta} = (X'X)^{-1} X'y$$

$$\hat{y} = X \hat{\beta} = X(X'X)^{-1} X'y,$$

$$\hat{y} = Hy, \text{ and } e = (I - H)y.$$

$$H = H^{1} \cdot H^{2} = X(X'X)^{-1} X'X(X'X)^{-1} X^{1} = X(X'X)^{-1} X^{1} + X(X'X)^{-1} X^{1} = X(X'X)^{-1} X^{$$

12-1: Multiple Linear Regression Models

12-1.4 Properties of the Least Squares Estimators

Unbiased estimators:

$$E(\hat{\boldsymbol{\beta}}) = E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}]$$

$$= E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'(\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon})]$$

$$= E[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\epsilon}]$$

$$= \boldsymbol{\beta}$$

Covariance Matrix of Estimators:

$$\mathbf{C} = (\mathbf{X}'\mathbf{X})^{-1} = \begin{bmatrix} C_{00} & C_{01} & C_{02} \\ C_{10} & C_{11} & C_{12} \\ C_{20} & C_{21} & C_{22} \end{bmatrix}$$

12-1: Multiple Linear Regression Models

12-1.4 Properties of the Least Squares Estimators

Individual variances and covariances:

$$V(\hat{\beta}_j) = \sigma^2 C_{jj}, \qquad j = 0, 1, 2$$
$$cov(\hat{\beta}_i, \hat{\beta}_j) = \sigma^2 C_{ij}, \qquad i \neq j$$

In general,

$$\operatorname{cov}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1} = \sigma^2\mathbf{C}$$

12-1: Multiple Linear Regression Models

Estimating error variance σ_{ϵ}^{2}

An unbiased estimator of error variance σ_{ϵ}^{2} is

$$\hat{g}^2 = \frac{\sum_{i=1}^n e_i^2}{n-p} = \frac{SS_E}{n-p}$$
 (12-16)

Here p=k+1 for k-variable multiple linear regression

R² and Adjusted R²

The coefficient of multiple determination R²

$$R^2 = \frac{SS_R}{SS_T} = 1 - \frac{SS_E}{SS_T}$$

The adjusted R^2 is

$$R_{\text{adj}}^2 = 1 - \frac{SS_E/(n-p)}{SS_T/(n-1)}$$

- The adjusted R² statistic penalizes adding terms to the MLR model.
- It can help guard against overfitting (including regressors that are not really useful)

How to know where to stop adding variables?

 Adding new variables x_i to MLR watch the adjusted R²

Once the adjusted R²
 no longer increases = stop.
 Now you did the best you can.

