Regression
Bios 662

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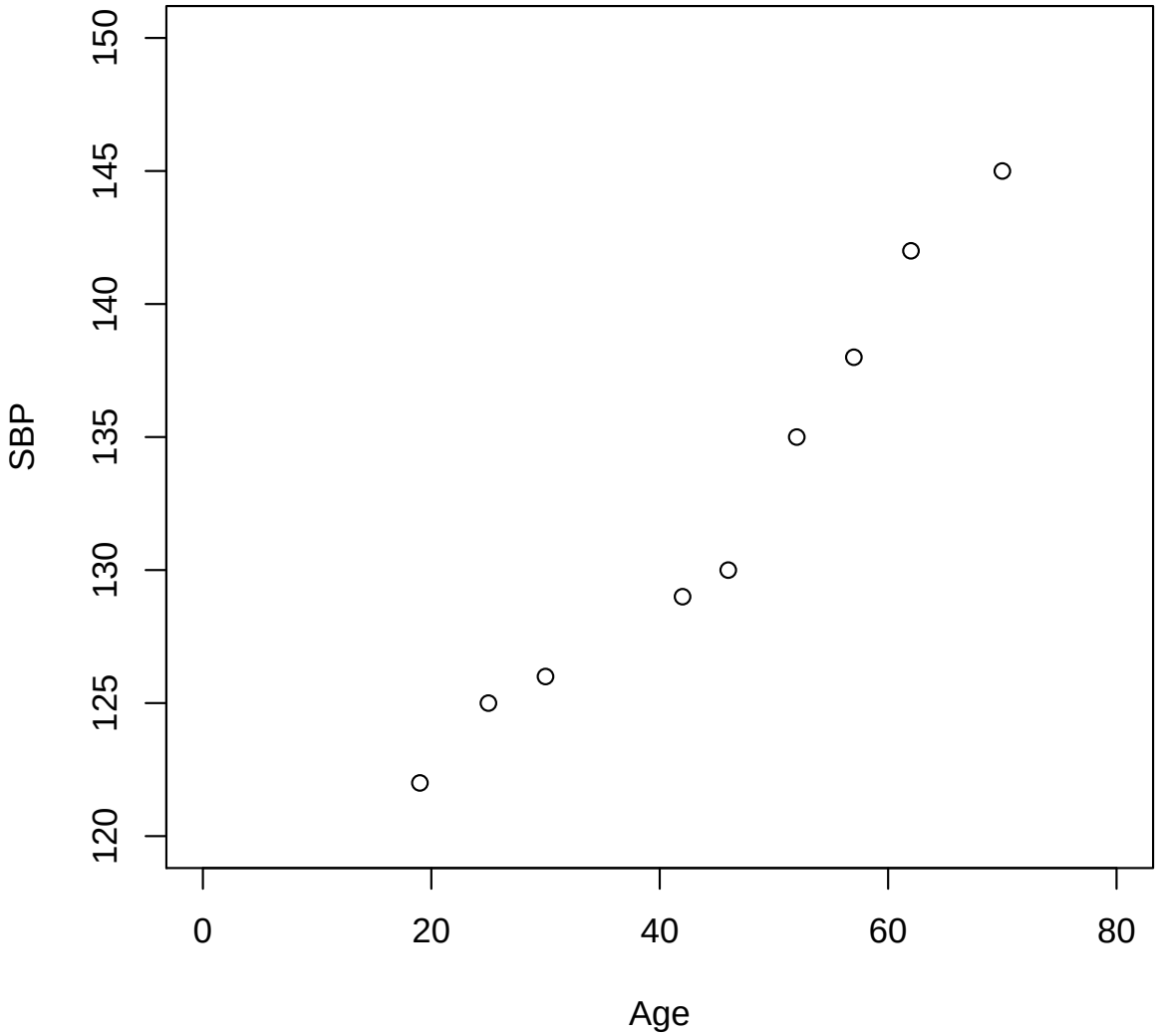
Outline

- Introduction: assumptions, least-squares estimation
- CI and hyp test for regression coefficients
- CI for mean
- Prediction intervals
- r^2

Example: SBP and Age

Obs	Age	SBP
1	19	122
2	25	125
3	30	126
4	42	129
5	46	130
6	52	135
7	57	138
8	62	142
9	70	145

Example: SBP and Age



Simple Linear Model

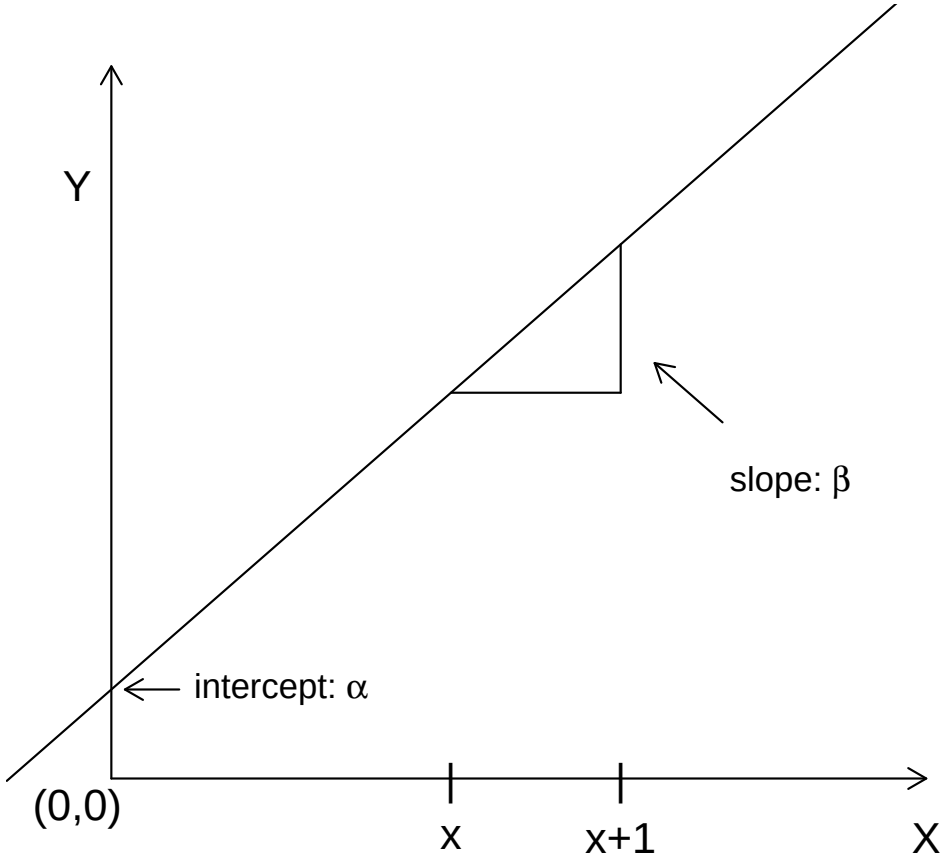
- Line

$$Y = \alpha + \beta X$$

- α = intercept; value of Y when $X = 0$
- β = slope; change in Y when X changes 1 unit

- Y dependent variable, response variable
- X covariate, independent variable, predictor

Simple Linear Model



Simple Linear Model with Error

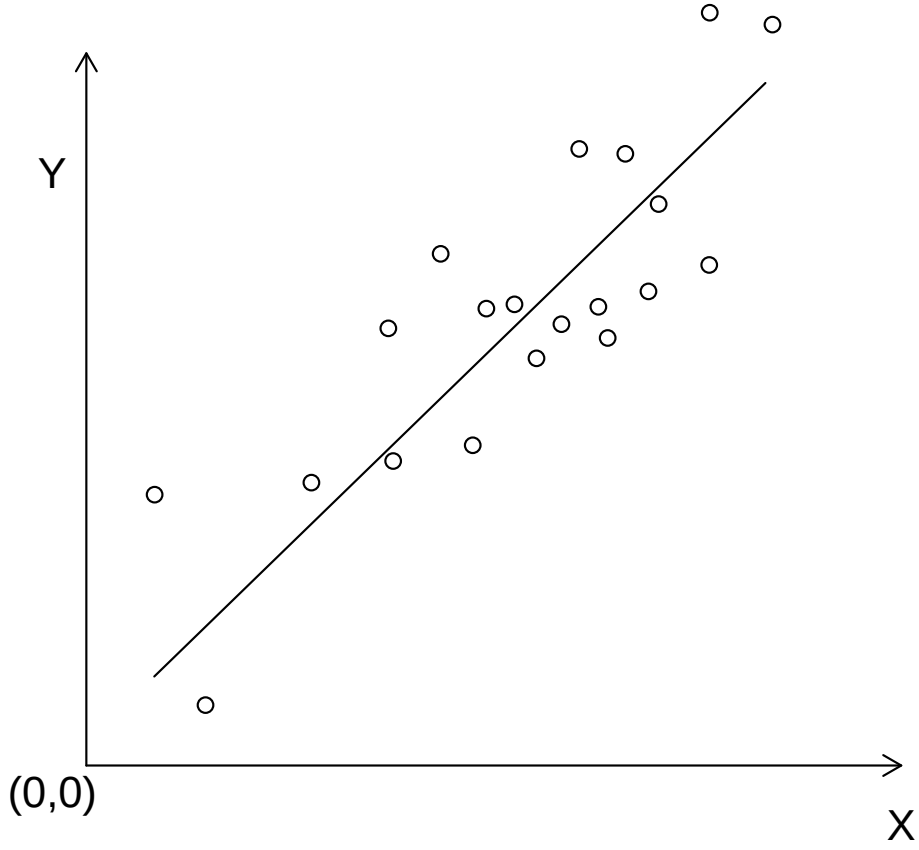
- Linear regression

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

$$\epsilon = Y - \alpha - \beta X$$

- ϵ equals vertical distance from Y to line defined by $\alpha + \beta X$

Simple Linear Model with Error



Model Assumptions

- Data are (Y_i, X_i); $i = 1, 2, \ldots, N$
- Assume:

  1. Linearity: $Y_i = \alpha + \beta X_i + \epsilon_i$
  2. X's are fixed constants
  3. ϵ_i iid $N(0, \sigma^2)$

Least Squares Estimation

- Least squares estimators are values of α and β that minimize

$$\sum_{i=1}^{N} \epsilon_i^2 = \sum_{i=1}^{N} (Y_i - \alpha - \beta X_i)^2$$

- Set partial derivatives equal to 0, solve for α and β
- Can also derive these estimators via maximum likelihood

Least Squares Estimation

- For α:

$$\frac{\partial \sum_i \epsilon_i^2}{\partial \alpha} = -2 \sum_i (Y_i - \alpha - \beta X_i)$$

$$= -2N\bar{Y} + 2N\alpha + 2N\beta\bar{X}$$

- For β:

$$\frac{\partial \sum_i \epsilon_i^2}{\partial \beta} = -2 \sum_i (Y_i - \alpha - \beta X_i) X_i$$

$$= -2 \sum_i X_i Y_i + 2\alpha \sum_i X_i + 2\beta \sum_i X_i^2$$

Least Squares Estimation

- Two equations with two unknowns

$$-2N\bar{Y} + 2N\alpha + 2N\beta\bar{X} = 0 \qquad (1)$$

$$-2\sum_i X_i Y_i + 2\alpha\sum_i X_i + 2\beta\sum_i X_i^2 = 0 \qquad (2)$$

- From (1)

$$\hat{\alpha} = \bar{Y} - \hat{\beta}\bar{X}$$

Least Squares Estimation

- Substituting into (2)

$$-\sum_i X_i Y_i + (\bar{Y} - \hat{\beta}\bar{X})\sum_i X_i + \hat{\beta}\sum_i X_i^2 = 0,$$

  implying

$$\hat{\beta}(\sum_i X_i^2 - N\bar{X}^2) = \sum_i X_i Y_i - N\bar{X}\bar{Y}.$$

- Therefore

$$\hat{\beta} = \frac{\sum_i X_i Y_i - N\bar{X}\bar{Y}}{\sum_i X_i^2 - N\bar{X}^2}$$

Least Squares Estimation

- Equivalent form:

$$\hat{\beta} = \frac{\sum_i X_i Y_i - N\bar{X}\bar{Y}}{\sum_i X_i^2 - N\bar{X}^2} = \frac{[XY]}{[X^2]}$$

  where

$$[XY] = \sum_i (X_i - \bar{X})(Y_i - \bar{Y})$$

$$[X^2] = \sum_i (X_i - \bar{X})^2$$

- Note if $X_i = Y_i$ for all i, then $\hat{\beta} = 1$ as expected
- Also if $Y_i = \bar{Y}$ for all i, then $\hat{\beta} = 0$

Least Squares Estimation

- Predicted response (aka *fitted values*)

$$\hat{Y}_i = \hat{\alpha} + \hat{\beta} X_i$$

- Estimate variance by mean square error (MSE)

$$\hat{\sigma}^2 = s^2_{y.x} = \frac{1}{N-2} \sum_i (Y_i - \hat{Y}_i)^2$$

- Residual

$$r_i = Y_i - \hat{Y}_i$$

Example: SBP and Age

$$\bar{Y} = 132.4; \bar{X} = 44.8$$

$$\sum_i X_i Y_i = 54461; \sum_i X_i^2 = 20463$$

$$\hat{\beta} = \frac{54461 - 9(132.4)(44.8)}{20463 - 9(44.8)^2} = 0.45$$

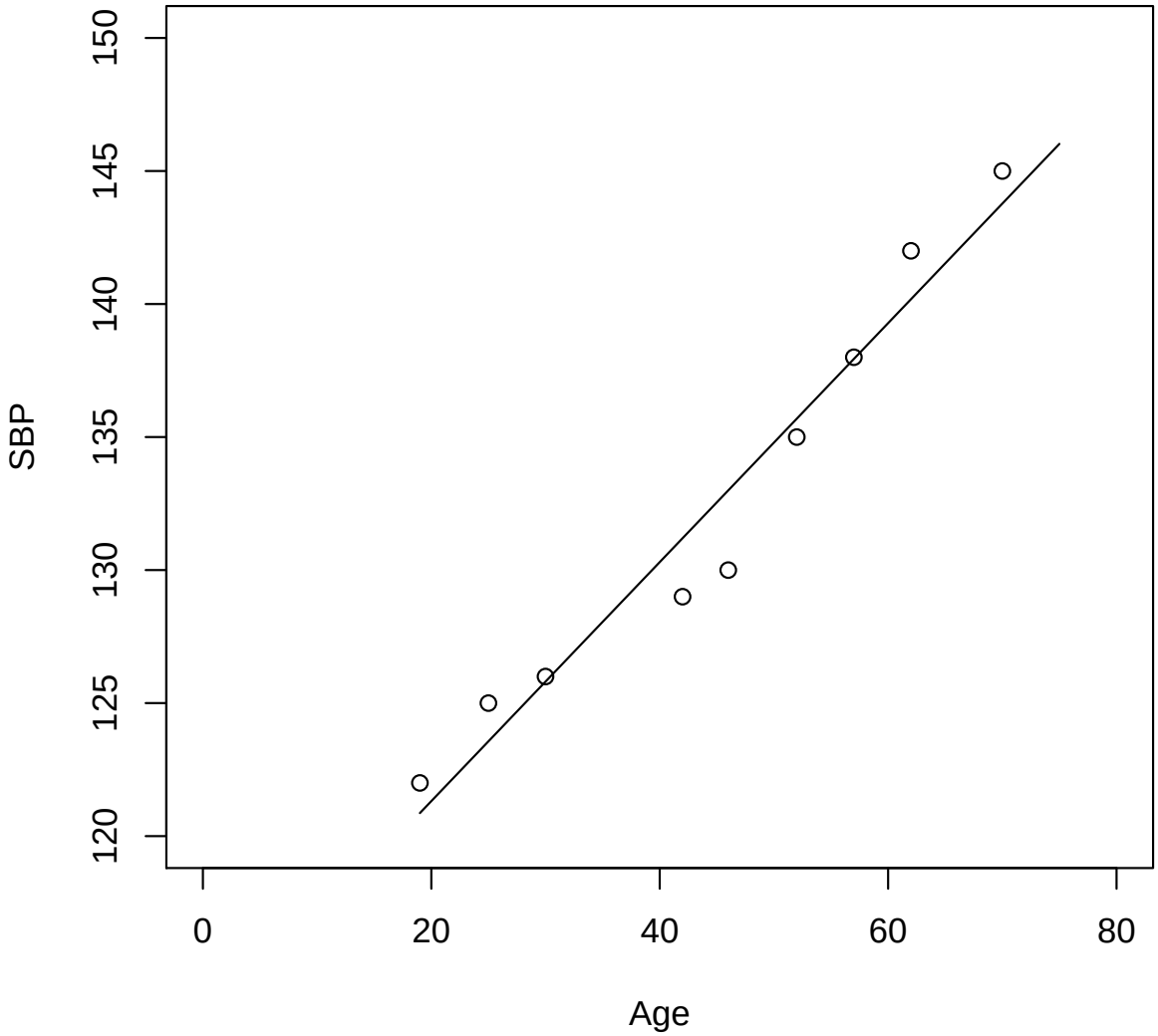
$$\hat{\alpha} = 132.4 - .45(44.8) = 112.3$$

$$\hat{Y}_i = 112.3 + .45X_i$$

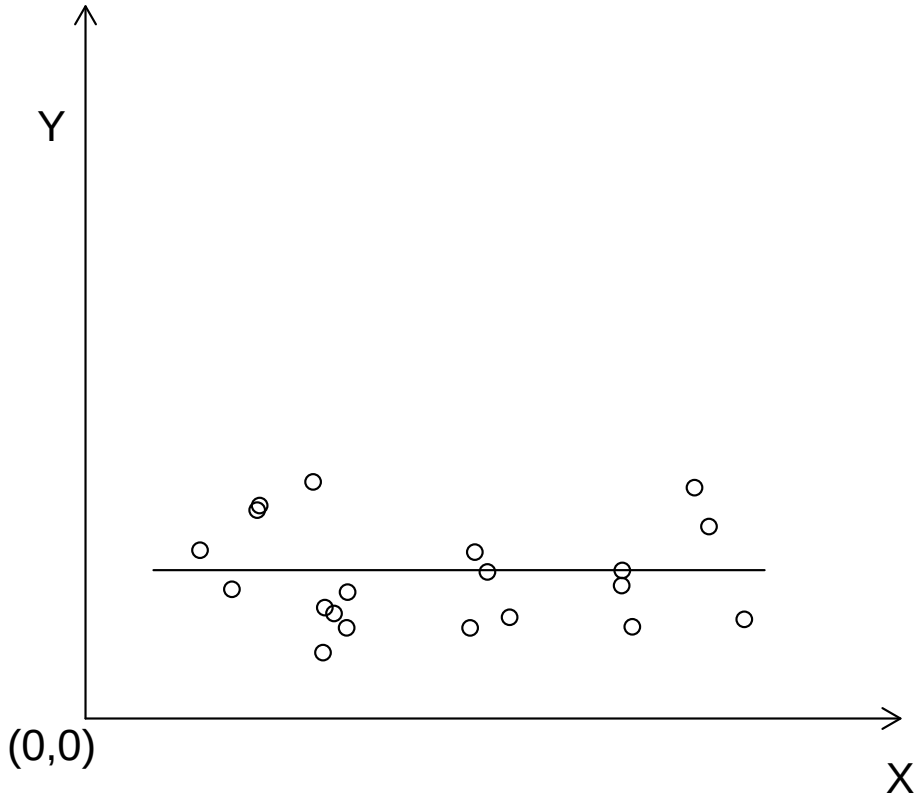
Example: Interpretation

- $\hat{\beta} = 0.45 \rightarrow$ expected SBP increases 0.45 (mmHg) for each one year increase in age
- $\hat{\alpha} = 112.3 \rightarrow$? Beware extrapolation (see section 9.4.3)

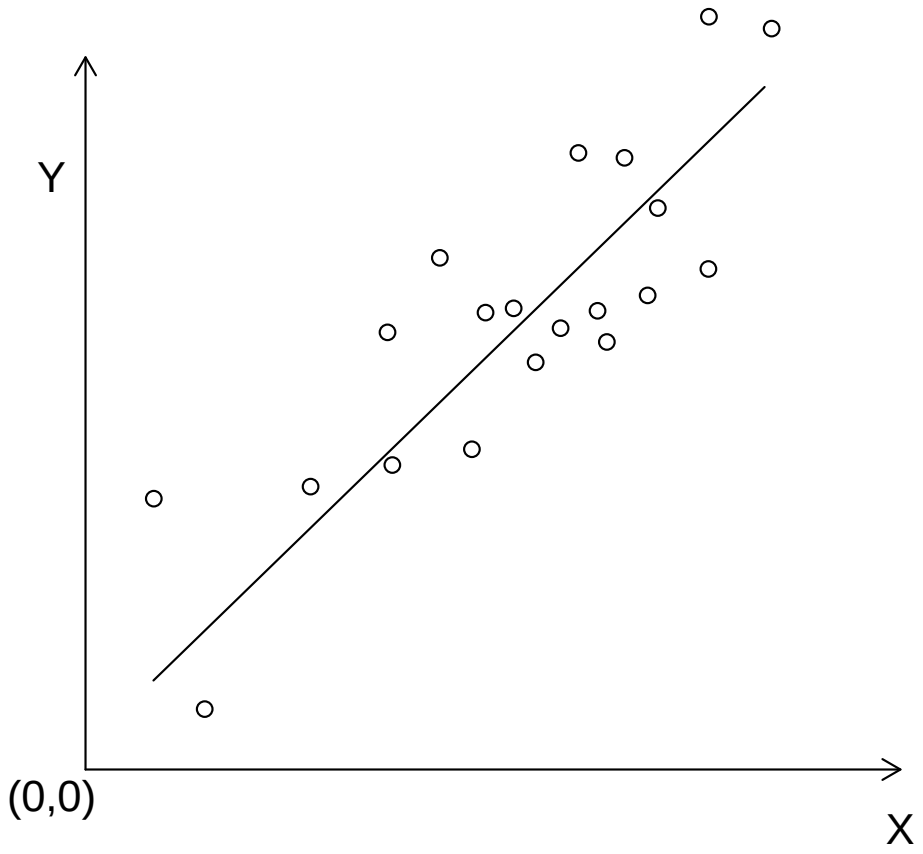
Example: SBP and Age



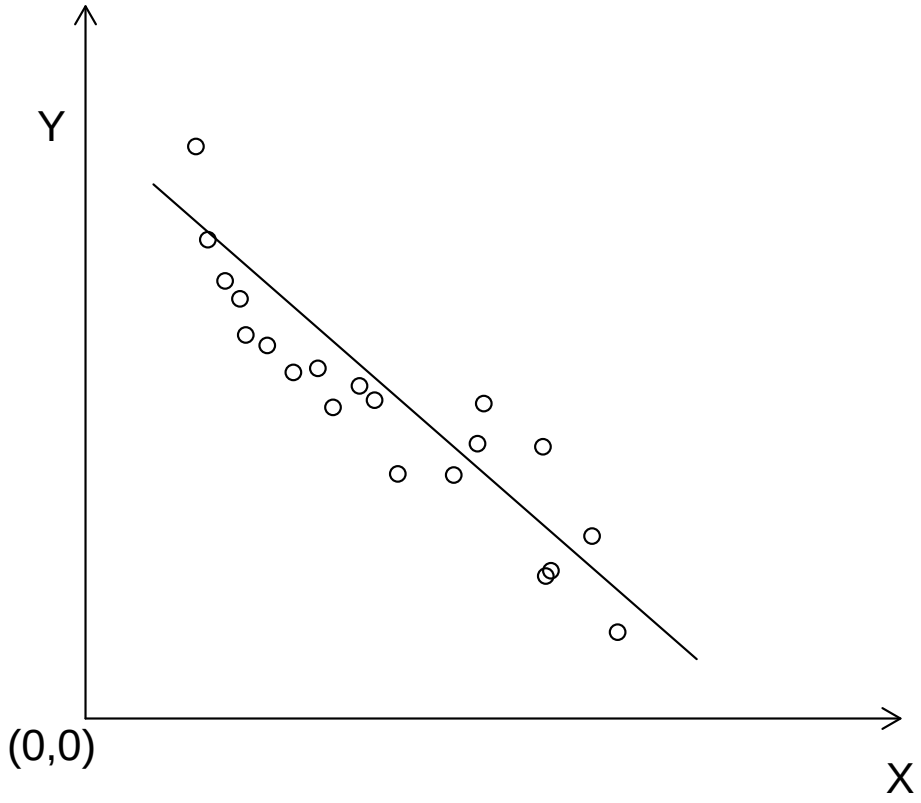
$$\hat{\beta} = 0$$



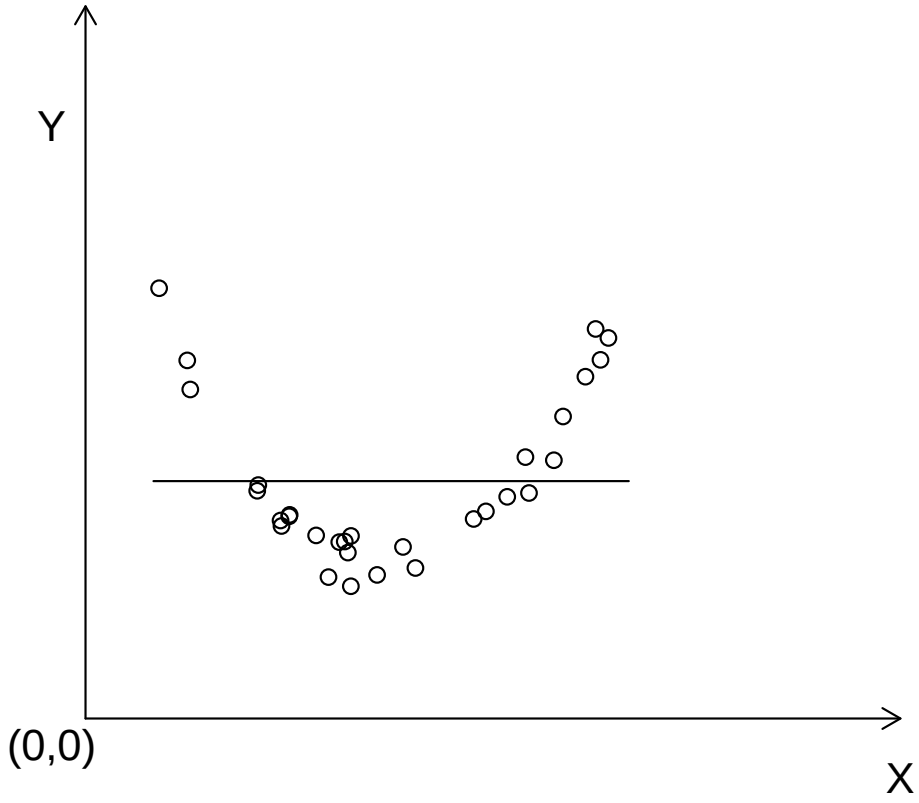
$$\hat{\beta} > 0$$



$$\hat{\beta} < 0$$



$$\hat{\beta} = 0$$



CI and Hypotheses Tests

- Can write

$$\hat{\beta} = \sum c_i Y_i$$

  where

$$c_i = \frac{X_i - \bar{X}}{\sum_j (X_j - \bar{X})^2}$$

- Under model,

$$Y_i \sim N(\alpha + \beta X_i, \sigma^2)$$

- Thus

$$\hat{\beta} \sim N\left(\sum_i c_i(\alpha + \beta X_i), \sigma^2 \sum_i c_i^2\right)$$

CI and Hypotheses Tests

- Equivalently

$$\hat{\beta} \sim N\left(\beta, \frac{\sigma^2}{\sum_i (X_i - \bar{X})^2}\right)$$

- $(1-\alpha) * 100\%$ CI for β

$$\hat{\beta} \pm z_{1-\alpha/2}\sqrt{\frac{\sigma^2}{\sum_i (X_i - \bar{X})^2}}$$

- Test for $H_0 : \beta = \beta_0$

$$z = \frac{\hat{\beta} - \beta_0}{\sqrt{\sigma^2 / \sum_i (X_i - \bar{X})^2}}$$

CI and Hypotheses Tests

- If σ^2 is unknown, use $s^2_{y.x}$ and t_{N-2}
- $(1-\alpha) * 100\%$ CI for β

$$\hat{\beta} \pm t_{N-2,1-\alpha/2} \sqrt{s^2_{y.x} / \sum_i (X_i - \bar{X})^2}$$

- Test for $H_0 : \beta = \beta_0$

$$t = \frac{\hat{\beta} - \beta_0}{\sqrt{s^2_{y.x} / \sum_i (X_i - \bar{X})^2}}$$

CI and Hypotheses Tests: SBP

- For SBP example, $H_0 : \beta = 0$ versus $H_A : \beta \neq 0$

$$C_{.05} = \{t : |t| > t_{7,.975} = 2.365\}$$

- Observed test statistic implies reject H_0

$$t = \frac{0.449 - 0}{\sqrt{3.21/2417.56}} = 12.32$$

- 95% CI

$$0.449 \pm 2.365\sqrt{3.21/2417.56} = (0.363, 0.535)$$

CI and Hypotheses Tests

- It can be shown that $\bar{Y}$ and $\hat{\beta}$ are independent
- Therefore

$$\hat{\alpha} \sim N\left(\alpha, \sigma^2\left\{\frac{1}{N} + \frac{\bar{X}^2}{\sum_i (X_i - \bar{X})^2}\right\}\right)$$

- $H_0 : \alpha = \alpha_0$

$$t = \frac{\hat{\alpha} - \alpha_0}{s_{y.x}\sqrt{\frac{1}{N} + \frac{\bar{X}^2}{\sum_i (X_i - \bar{X})^2}}} \sim t_{N-2}$$

SBP Example in R

```
> fit <- lm(sbp~age)
> summary(fit)

Call:
lm(formula = sbp ~ age)

Residuals:
    Min      1Q  Median      3Q     Max
-2.9934 -0.6884  0.1933  1.2265  1.8199

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 112.33169    1.73773   64.64 5.57e-11 ***
age           0.44917    0.03644   12.32 5.31e-06 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.792 on 7 degrees of freedom
Multiple R-Squared: 0.9559,     Adjusted R-squared: 0.9497
F-statistic: 151.9 on 1 and 7 DF,  p-value: 5.313e-06
```

SBP Example in SAS

```
proc reg; model sbp=age; run;
```

The REG Procedure
Model: MODEL1
Dependent Variable: sbp

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	487.74667	487.74667	151.91	<.0001
Error	7	22.47555	3.21079		
Corrected Total	8	510.22222			

Root MSE	1.79187	R-Square	0.9559
Dependent Mean	132.44444	Adj R-Sq	0.9497
Coeff Var	1.35292		

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	112.33169	1.73773	64.64	<.0001
age	1	0.44917	0.03644	12.33	<.0001

CI for $E(Y|X = x)$

- Goal: CI for the mean of Y given $X = x$
- Let $\mu_x = E(Y|X = x)$
- Estimator for μ_x:

$$\begin{aligned}\hat{\mu}_x &= \hat{\alpha} + \hat{\beta}x \\ &= \bar{Y} - \hat{\beta}\bar{X} + \hat{\beta}x \\ &= \bar{Y} + \hat{\beta}(x - \bar{X})\end{aligned}$$

- $E(\hat{\mu}_x) = \mu_x$

CI for $E(Y|X = x)$

- Recall $\bar{Y}$ and $\hat{\beta}$ are independent Normal RVs
- Thus $\hat{\mu}_x$ is Normal and

$$Var(\hat{\mu}_x) = Var(\bar{Y}) + (x - \bar{X})^2 Var(\hat{\beta})$$

$$= \frac{\sigma^2}{N} + \frac{\sigma^2 (x - \bar{X})^2}{\sum_i (X_i - \bar{X})^2}$$

$$= \sigma^2 \left[\frac{1}{N} + \frac{(x - \bar{X})^2}{\sum_i (X_i - \bar{X})^2} \right]$$

CI for $E(Y|X = x)$

- Therefore, a $(1-\alpha)100\%$ CI for μ_x is

$$\hat{\mu}_x \pm t_{N-2,1-\alpha/2}\sqrt{s^2_{y.x}\left\{\frac{1}{N} + \frac{(x-\bar{X})^2}{\sum_i (X_i - \bar{X})^2}\right\}}$$

- Note that $Var(\hat{\mu}_x)$ is a function of $x - \bar{X}$
- So, the farther x is from $\bar{X}$, the larger the CI will be
- Design considerations: note 9.3 in text

Example: SBP and Age

- Suppose we want a 95% CI of the mean SBP if age = 40

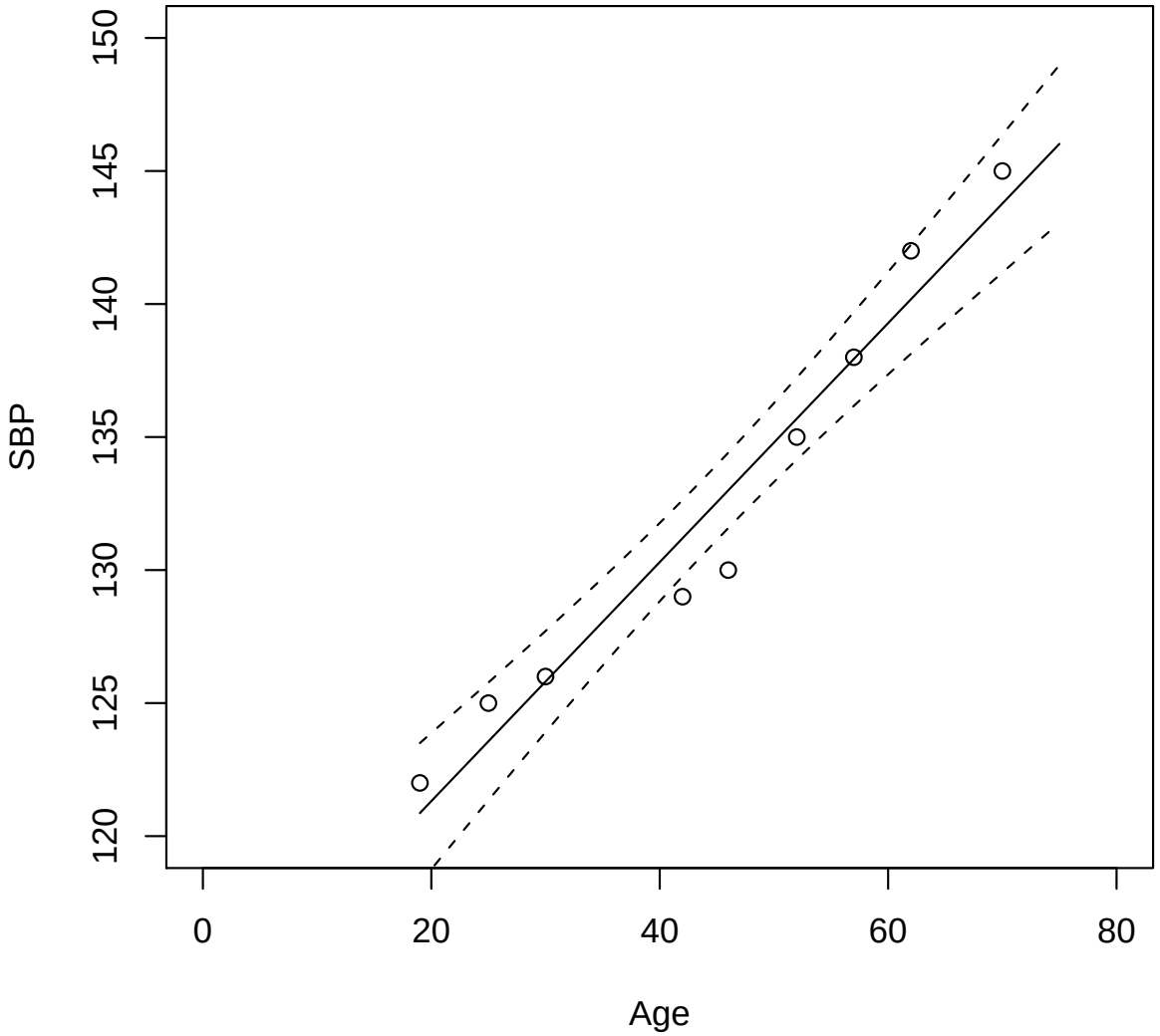
$$\hat{\mu}_{40} = 112.3 + .45(40) = 130.3$$

- CI

$$130.3 \pm 2.365(1.79)\sqrt{\frac{1}{9} + \frac{(40 - 44.8)^2}{2417.59}}$$

$$(128.8, 131.8)$$

Example: SBP and Age



CI for $E(Y|X = x)$

- These "bands" should be interpreted in a pointwise fashion only
- Books usage of term "bands" is nonstandard (p. 303-4)
- Usual interpretation of *confidence band*: covers the entire regression line with $(1 - \alpha)\%$ confidence
- Cf Section 2.6 of *Applied Linear Statistical Models*, Neter et al. 4th edition, 1996

Prediction

- Want prediction interval (PI) for future observation given $X = x$

$$\hat{Y}_x = \hat{\alpha} + \hat{\beta}x$$

- Note: Y_x is a RV, so we consider the RV $Y_x - \hat{Y}_x$

$$E(Y_x - \hat{Y}_x) = \alpha + \beta x - (\alpha + \beta x) = 0$$

$$V(Y_x - \hat{Y}_x) = V(Y_x) + V(\hat{Y}_x) - 2Cov(Y_x, \hat{Y}_x)$$

Prediction

- Since Y_x is not part of the sample, Y_x and $\hat{Y}_x$ are independent
- Therefore

$$V(Y_x - \hat{Y}_x) = \sigma^2 + \sigma^2 \left\{ \frac{1}{N} + \frac{(x-\bar{X})^2}{\sum_i (X_i - \bar{X})^2} \right\}$$

$$= \sigma^2 \left\{ 1 + \frac{1}{N} + \frac{(x-\bar{X})^2}{\sum_i (X_i - \bar{X})^2} \right\}$$

Prediction

- Since the ϵ's are normally distributed, it follows

$$Y_x - \hat{Y}_x \sim N\left(0, \sigma^2\left\{1 + \frac{1}{N} + \frac{(x-\bar{X})^2}{\sum(X_i - \bar{X})^2}\right\}\right)$$

- If σ^2 is not known,

$$\frac{Y_x - \hat{Y}_x}{s_{y.x}\sqrt{1 + \frac{1}{N} + \frac{(x-\bar{X})^2}{\sum(X_i-\bar{X})^2}}} \sim t_{N-2}$$

Prediction

- $(1-\alpha)100\%$ PI for future observation at $X = x$

$$\hat{Y}_x \pm t_{N-2,1-\alpha/2} s_{y.x} \sqrt{1 + \frac{1}{N} + \frac{(x-\bar{X})^2}{\sum (X_i - \bar{X})^2}}$$

- Aka *prediction interval* (PI). Cf Section 5-10 of *Applied Regression Analysis and Multvariable Methods*, Kleinbaum et al 3rd edtion, 1998

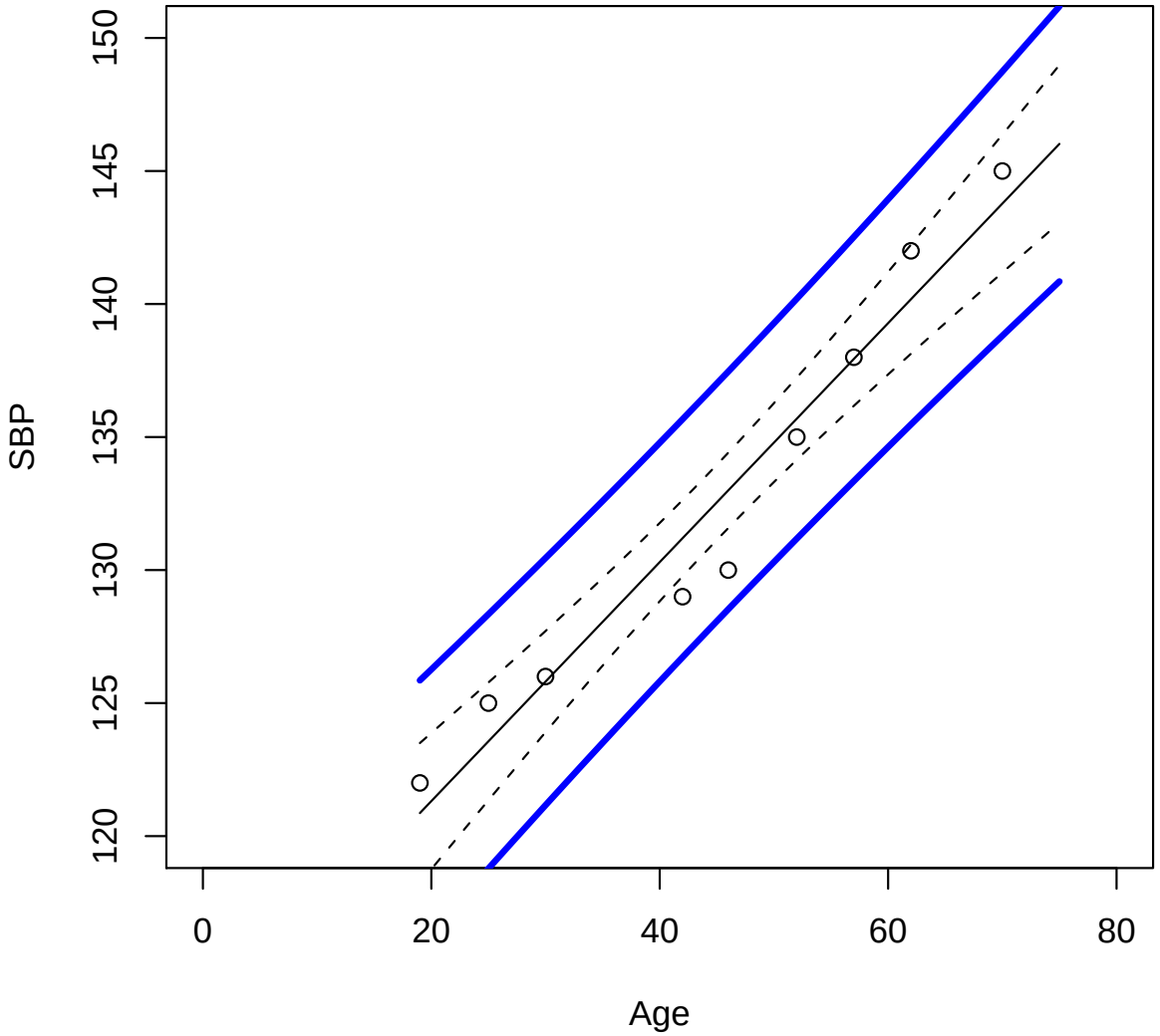
Prediction

- Suppose we want a 95% PI for an individual who is 40 years old:
- Point estimate: $\hat{Y}_{40} = 130.3$
- PI:

$$130.3 \pm 2.365(1.79)\sqrt{1 + \frac{1}{9} + \frac{(40 - 44.8)^2}{2417.59}}$$

$$(125.8, 134.8)$$

Example: SBP vs Age



SBP Example in R

```
> fit <- lm(sbp~age)

> predict(fit,data.frame(age=40),interval="confidence")
          fit      lwr      upr
[1,] 130.2984 128.8273 131.7696

> predict(fit,data.frame(age=40),interval="prediction")
          fit      lwr      upr
[1,] 130.2984 125.8132 134.7836
```

SBP Example in SAS

```
proc reg;
model sbp=age;
        output out=foo lcl=LCL lclm=LCLM p=P uclm=UCLM ucl=UCL;

proc print data=foo; run;
```

Obs	id	age	sbp	P	LCLM	UCLM	LCL	UCL
1	1	19	122	120.866	118.234	123.498	115.878	125.854
2	2	25	125	123.561	121.347	125.774	118.780	128.341
3	3	30	126	125.807	123.905	127.708	121.162	130.451
4	4	42	129	131.197	129.764	132.629	126.724	135.669
5	5	46	130	132.993	131.577	134.410	128.526	137.461
6	6	52	135	135.688	134.145	137.232	131.179	140.198
7	7	57	138	137.934	136.172	139.696	133.345	142.523
8	8	62	142	140.180	138.131	142.229	135.474	144.887
9	9	70	145	143.773	141.181	146.366	138.806	148.741
10	10	40	.	130.298	128.827	131.770	125.813	134.784

Sum of Squares Decomposition

- Can decompose total sum of squares

$$\sum_i (Y_i - \bar{Y})^2 = \sum_i (\hat{Y}_i - \bar{Y})^2 + \sum_i (Y_i - \hat{Y}_i)^2$$

$$SST = SSR + SSE$$

- Total sample variance of the Y's:

$$s_y^2 = \frac{SST}{N-1} = \frac{\sum_i (Y_i - \bar{Y})^2}{N-1}$$

(Unadjusted) r^2

- The unadjusted r^2 is given by

$$r^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

- *Coefficient of determination*
- Proportion of total variation attributable to regression
- Example

$$r^2 = \frac{487.75}{510.22} = 0.9559$$

Adjusted r^2

- Note that the sample variance of the Y's is $s_y^2 = 63.78$ while $s_{y.x}^2 = 3.21$
- Thus X "explains"

$$\frac{63.78 - 3.21}{63.78} = 0.9497$$

  proportion of the variance in Y.
- This quantity is called the *adjusted* r^2

$$r_a^2 = \frac{s_y^2 - s_{y.x}^2}{s_y^2} = 1 - \frac{s_{y.x}^2}{s_y^2} = 1 - \frac{SSE/(N-2)}{SST/(N-1)}$$

Adjusted and Unadjusted 'r^2

- Note

$$r_a^2 = 1 - \frac{SSE/(N-2)}{SST/(N-1)}$$

and

$$r^2 = 1 - \frac{SSE}{SST}$$

- Implying

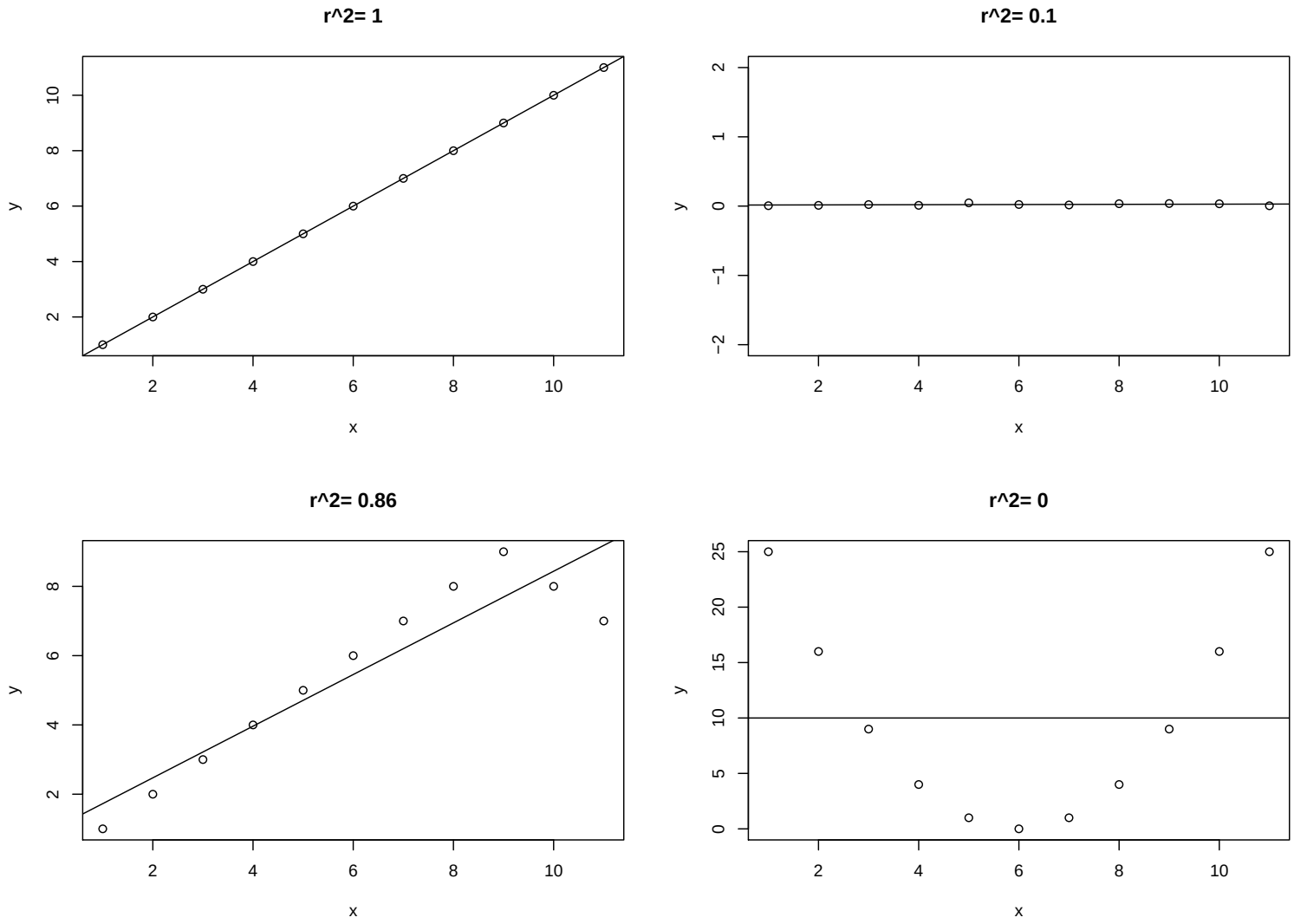
$$r_a^2 = 1 - \frac{N-1}{N-2}(1 - r^2)$$

- Thus $r^2 \approx r_a^2$ for large N

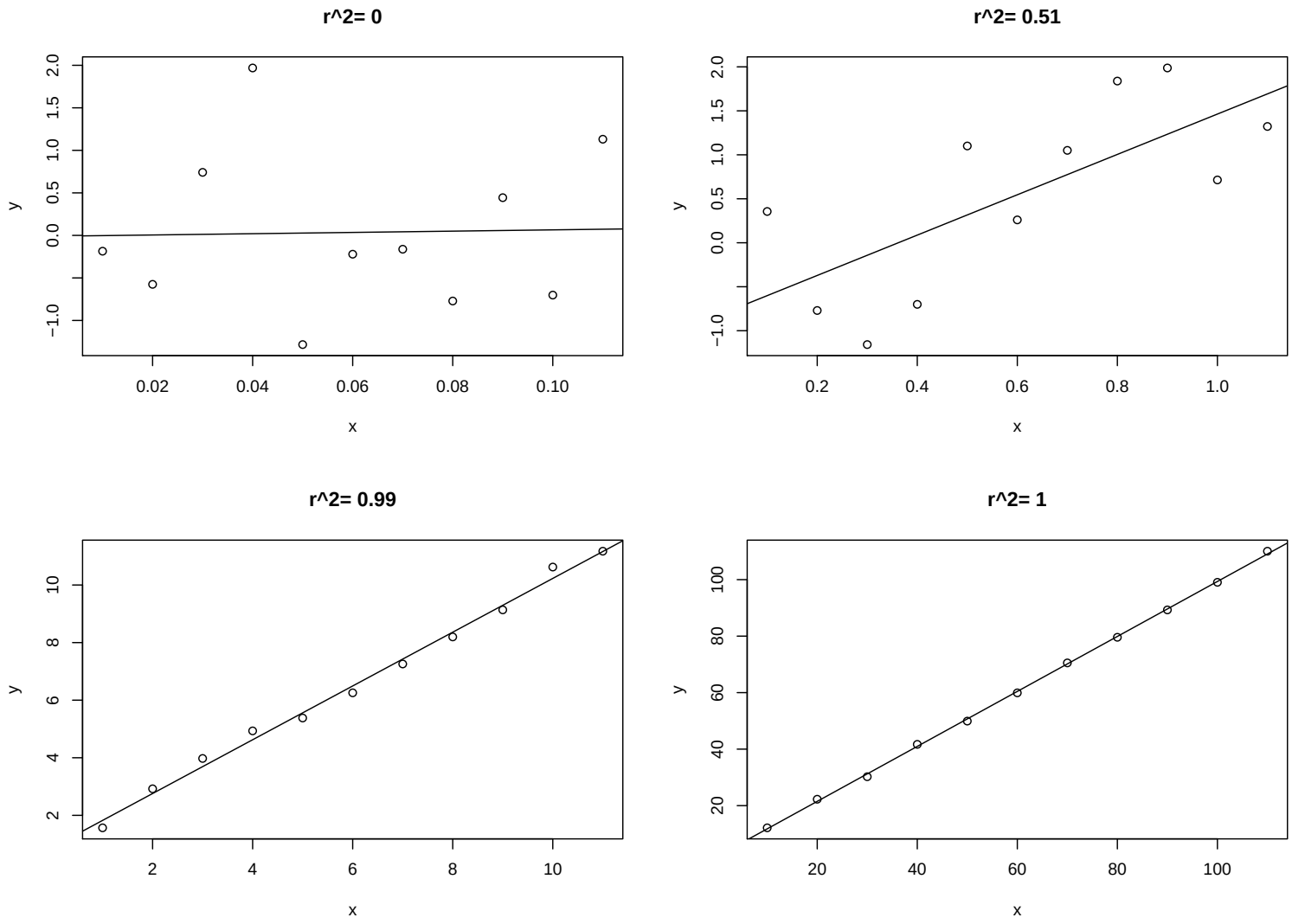
Unadjusted r^2

- Proportion of total variation attributable to regression
- Degree of linear association
- Ranges between 0 and 1
- $r^2 = 0 \rightarrow$ no linear association between X and Y; However, a non-linear association may still exist!
- $r^2 = 1 \rightarrow$ indicates perfect fit; assessment of fit also by diagnostics
- $r^2 = 1 - SSE/SST$ typically increases w/ range/spacing of X

Examples of r^2



Examples of r^2: $Y = 0 + 1 \cdot X + \epsilon$, $\epsilon \sim N(0, 1)$



Examples of r^2: $Y = 0 + 1 \cdot X + \epsilon$, $\epsilon \sim N(0, 4)$