Chapter 2

Simple Linear Regression

Motivation

- The Simplest model relating Response Y and Predictor X.
 - Simple Linear Regression
- Mean function:
 - $E(Y|X=x)=\beta_0 + \beta_1 x$
- Variance function
 - Var(Y|X=x)=σ²
- Parameters to estimates:
 - β_0 = intercept (Expectation of Y when X=0)
 - β_1 = slope (changes in E(Y) for 1 unit increase of X)
 - σ^2 = error variance



Simple Linear Regression

- Instead of expressing E(Y|X) and Var(Y|X) separately, we may say
 - $y_i = \beta_0 + \beta_1 x_i + e_i$
 - $E(e_i)=0$, $Var(e_i)=\sigma^2$, e_i 's are i.i.d.
- Compare with
 - Mean function: $E(Y|X=x) = \beta_0 + \beta_1 x$
 - Variance function: Var(Y|X=x)=σ²
- e_i : statistical error
 - Vertical distance between y and the "truth" E(Y|X=x_i)
 - $e_i = y_i \beta_0 \beta_1 x_i = Random error component$

We can assume x is known and e, y are random

How to find the estimators?

•
$$y_i = \beta_0 + \beta_1 x_i + e_i$$

• Vary β_0 , β_1 to find the best fit line



What's meant by the "best fit"?

How to find the estimators?

- Method of Least Square.
- Residual sum of squares

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



- Residual = vertical dist b/w y_i and its fitted value on the fitted regression line
- We find (β_0 , β_1) that minimize RSS

 $(\hat{\beta}_0, \hat{\beta}_1) = \operatorname{argmin}_{\beta_0, \beta_1} RSS(\beta_0, \beta_1)$

Least Squares estimators

Minimize Residual sum of squares

$$RSS(\beta_0, \beta_1) = \sum_{i=1}^n [y_i - (\beta_0 + \beta_1 x_i)]^2$$

- Step 1. Differentiate RSS w.r.t. $\beta_0 \& \beta_1$
- Step 2. Solving 2 equations 2 unknowns
- Answer:

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}, \quad \hat{\beta}_1 = \frac{\sum (x_i - \overline{x})(y_i - \overline{y})}{\sum (x_i - \overline{x})^2}$$

(see textbook P.273)

Example – Forbes Data Measure pressure from boiling point of water



Least Squares estimator



Least Squares estimator

• Hat is important!!!

$$y_i = \beta_0 + \beta_1 x_i + e_i$$
$$\hat{y}_i = \hat{E}(Y|X = x_i) = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

$$\hat{\mathbf{e}}_i = \mathbf{y}_i - \hat{\mathbf{y}}_i = \mathbf{y}_i - \hat{\beta}_0 - \hat{\beta}_1 \mathbf{x}_i$$

- Be familiar with the terms: observed data, parameter, parameter estimates, error, residual, fitted value...
- With hat = Known estimated value
 = Involve data only
 - No hat = Observed/Unknown true value

How to estimate σ^2 ?

• There are 3 parameters

•
$$y_i = \beta_0 + \beta_1 x_i + e_i$$

- $E(e_i)=0$, $Var(e_i)=\sigma^2$, e_i 's are i.i.d.
- Note that $\sigma^2 = Var(e_i) = E(e_i^2)$,
 - Looking at $\sum \hat{e}_i^2$ helps estimate σ^2
 - Fact: $E(\sum \hat{e}_{i}^{2}) = (n-2) \sigma^{2}$
 - We estimate σ^2 by

$$\widehat{\sigma}^2 = \frac{\sum \widehat{e}_i^2}{n-2}$$

How to estimate σ^2 ?

How to estimate σ^2 ?

$$\widehat{\sigma}^2 = \frac{\sum \widehat{e}_i^2}{n-2} = \frac{SYY - \frac{SXY^2}{SXX}}{n-2}$$

Forbe's data

$$RSS = 427.79402 - \frac{475.31224^2}{530.78235}$$
$$= 2.15493$$

square root of $\hat{\sigma}^2$, $\hat{\sigma} = \sqrt{0.14366} = 0.37903$ is also called the standard error of regression

Properties of least squares estimators

1. $\widehat{\beta}_0$ and $\widehat{\beta}_1$ can be written as a linear combination of y_i

•
$$\hat{\beta}_1 = \sum \left(\frac{x_i - \bar{x}}{SXX}\right) y_i \quad \hat{\beta}_0 = \sum \left[\frac{1}{n} - \bar{x} \left(\frac{x_i - \bar{x}}{SXX}\right)\right] y_i$$

- 2. The fitted line passes through (x,y)
 Check the derivative of RSS w.r.t. β₀
- 3. The sum of residuals=0 (not errors!)
 - Check the derivative of RSS w.r.t. β_0
- 4. The estimators are unbiased (Expectation=true value)

$$E(\widehat{\beta}_0|X) = \beta_0, \quad E(\widehat{\beta}_1|X) = \beta_1, \quad E(\widehat{\sigma}^2|X) = \sigma^2$$

Variance of least squares estimators

Unknown True Variance

Estimators of Variance

$$\operatorname{Var}(\widehat{\beta}_{1}|X) = \sigma^{2} \frac{1}{SXX}$$
$$\operatorname{Var}(\widehat{\beta}_{0}|X) = \sigma^{2} (\frac{1}{n} + \frac{\bar{x}^{2}}{SXX})$$
$$\operatorname{Cov}(\widehat{\beta}_{0}, \widehat{\beta}_{1}|X) = -\sigma^{2} \frac{\bar{x}}{SXX}$$
$$\rho(\widehat{\beta}_{0}, \widehat{\beta}_{1}) = \frac{-\bar{x}}{\sqrt{SXX/n + \bar{x}^{2}}}$$

$$\widehat{\operatorname{Var}}(\widehat{\beta}_{1}|X) = \widehat{\sigma}^{2} \frac{1}{SXX}$$
$$\widehat{\operatorname{Var}}(\widehat{\beta}_{0}|X) = \widehat{\sigma}^{2} (\frac{1}{n} + \frac{\bar{x}^{2}}{SXX})$$
$$\widehat{\operatorname{Cov}}(\widehat{\beta}_{0}, \widehat{\beta}_{1}|X) = -\widehat{\sigma}^{2} \frac{\bar{x}}{SXX}$$
$$\widehat{\rho}(\widehat{\beta}_{0}, \widehat{\beta}_{1}) = \frac{-\bar{x}}{\sqrt{SXX/n + \bar{x}^{2}}}$$

See textbook p.273-275

- Regression is the study of dependence of variables
 - $y_i = \beta_0 + \beta_1 x_i + e_i$
 - $\beta_1=0 \rightarrow x$ and y are independent
 - $\beta_1 \neq 0 \rightarrow x$ and y are dependent
- Question:
 - Are x and y dependent?

- Regression is the study of dependence of variables
 - $y_i = \beta_0 + \beta_1 x_i + e_i$
 - $\beta_1=0 \rightarrow x$ and y are dependent
 - $\beta_1 \neq 0 \rightarrow x$ and y are not dependent
- Question:
 - Are x and y dependent?
- Answer:
 - Method 1) test whether $\beta_1=0$
 - Method 2) Compare the two models
 - $E(y|x)=\beta_0$ i.e. $y_i=\beta_0 + e_i$
 - $E(y|x)=\beta_0 + \beta_1 x$ i.e. $y_i = \beta_0 + \beta_1 x_i + e_i$

- Analysis of variance (ANOVA) is a method that compares two models of mean functions
 - E(y|x)=β₀
 - $E(y|x)=\beta_0+\beta_1x$
- For the first model: $E(y|x)=\beta_0$
 - β_0 can be estimated by minimizing $\sum (y_i \beta_0)^2$
 - differentiate w.r.t. β_0 gives $\hat{\beta_0} = \overline{y}$
 - Residual sum of square RSS is

$$\sum (y_i - \hat{\beta}_0)^2 = \sum (y_i - \overline{y})^2 = SYY$$

Compare

- E(y|x)=β₀
- $E(y|x)=\beta_0+\beta_1x$
- For the first model: $E(y|x)=\beta_0$
 - Residual sum of square, RSS₁, is

$$\sum (y_i - \hat{\beta}_0)^2 = \sum (y_i - \overline{y})^2 = SYY$$

• For the second model: $E(y|x)=\beta_0+\beta_1x$

• Residual sum of square, RSS₂, is $\sum_{i=1}^{n} [y_i - (\hat{\beta}_0 + \hat{\beta}_1 x_i)]^2 = SYY - \frac{(SXY)^2}{SXX}$ RSS₁>RSS₂... Is the 2nd model always better?

 $\begin{array}{ll} \text{RSS}_{1} \text{ for } E(y|x) = \beta_{0} & \rightarrow & \text{SYY} \\ \text{RSS}_{2} \text{ for } E(y|x) = \beta_{0} + \beta_{1}x & \rightarrow & syy - \frac{(SXY)^{2}}{syy} \end{array}$

The second model is useful only if RSS₁>>>RSS₂

- Difference sum of square due to regression (ssreg)
 - SSreg = RSS₁-RSS₂ = $\frac{(SXY)^2}{SXX}$
 - Large SSreg
 → 2nd model explains much more variation

How large is large?

Difference sum of square due to regression (ssreg)

- SSreg = RSS₁-RSS₂ = $\frac{(SXY)^2}{SYY}$

• How large is large?

Study the distribution of SSreg under model 1 (idea)

• After some algebra, SSreg = $\left[\sum_{\overline{SXX}} (\frac{x_i - \overline{x}}{SXX}) y_i\right]^2$

- By CLT, $\sum \left(\frac{x_i \bar{x}}{\int SXX}\right) y_i$ is approximately N(0, σ^2)
- SSreg ~ σ^2 (N(0,1))² = $\sigma^2 X_1^2$ (Chi-square with d.f. 1)
- $\hat{\sigma}^2 = \frac{\sum \hat{e}_i^2}{n-2} \sim \sigma^2 X_{n-2}^2/(n-2)$ (Chi-square with d.f. n-2)
- SSreg/ô² ~ X²₁ /(X²_{n-2}/(n-2))=F(1,n-2)

- Statistical facts we have used:
 - Degree of freedom = number of values in the final calculation of a statistic that are free to vary
 - $\sum_{i=1}^{n} y_i$: d.f.=n, each of the y_i is free to vary
 - $\sum_{i=1}^{j=1} (y_i \overline{y})^2$: d.f.=n-1, there is a constraint: $\sum_{i=1}^{n} y_i = n\overline{y}$
 - $RSS = \sum_{i=1}^{n} [y_i (\hat{\beta}_0 + \hat{\beta}_1 x_i)]^2$: d.f.=n-2, there are 2 constraints, $\hat{\beta}_0$, $\hat{\beta}_1$
 - About distributions
 - If $z \sim N(0,1)$, then $z^2 \sim X_1^2$ (Chi-square with d.f. 1)
 - If $z_i \sim N(0,1)$, then $z_1^2 + z_2^2 + ... + z_k^2 \sim X_k^2$ (Chi-square with d.f. k)
 - If $Y_1 \sim X_m^2$ and $Y_2 \sim X_n^2$, then $[Y_1/m]/[Y_2/n] \sim F(m,n)$

ANOVA table: a break-down of squares (variation)

Source	df	SS	MS	F	<i>p</i> -value
Regression	1	SSreg	SSreg/1	MS reg $/\hat{\sigma}^2$	
Residual	<i>n</i> – 2	RSS	$\hat{\sigma}^2 = RSS/(n-2)$		
Total	n - 1	SYY			

$$\sum_{i=1}^{n} [y_i - \overline{y}_i]^2 = \sum_{i=1}^{n} [y_i - \hat{y}_i]^2 + \sum_{i=1}^{n} [\hat{y}_i - \overline{y}_i]^2$$

$$TSS = SYY = RSS + SSreg$$
Variation of the variation not explained by regression variation explained by regression

ANOVA table: a break-down of squares (variation)

Source	df	SS	MS	F	<i>p</i> -value
Regression	1	SSreg	SSreg/1	MS reg $/\hat{\sigma}^2$	
Residual	<i>n</i> – 2	RSS	$\hat{\sigma}^2 = RSS/(n-2)$		
Total	n - 1	SYY			

Forbe's data

	Source	df	SS	MS	F	<i>p</i> -value
-	Regression on Temp	1	425.639			
	Residual	15	2.155			

conclusion?

Forbe's data

Source	df	SS	MS	F	<i>p</i> -value
Regression on Temp	1	425.639	425.639	2962.79	≈ 0
Residual	15	2.155	0.144		

2.7 Coefficient of Determination, R²

Definition

$$R^2 = \frac{SSreg}{SYY}$$

- Proportion of variability explained by regression
- Scale-free one number summary of strength of relationship between x and y.
- Connections to sample correlation r²_{xy}

$$R^{2} = \frac{SSreg}{SYY} = \frac{(SXY)^{2}}{SXX \ SYY} = r_{xy}^{2}$$

- R² is always between 0 and 1.
 - Close to 1→ good fit
 - Close to 0→ bad fit

• Regression model:

• E(Y|X=x)= $\beta_0 + \beta_1 x$

Quantities of interests

- Intercept: β₀
- Slope: β₁

• Prediction: If we observe x*, what is the y?

• Fitted value: E(Y|X=x) for different values of x

 Confidence intervals give estimates for the above quantities of interests

Statistics facts:

 If z_i are independent, then z₁+ z₂+...+ z_k ~ Normal (Central limit theorem)

• If $z_i \sim iid N(0,1)$, then $z_1^2 + z_2^2 + ... + \underline{z_k^2} \sim X_k^2$

• If Z~N(0,1) and Y~ X_m^2 , then $Z/\sqrt{(Y/m)}$ ~ t(m)

Recall what we have shown

• $\hat{\beta}_0 = \sum \left[\frac{1}{n} - \overline{x} \left(\frac{x_i - \overline{x}}{SXX}\right)\right] y_i$ $\widehat{\operatorname{Var}}(\hat{\beta}_0 | X) = \hat{\sigma}^2 \left(\frac{1}{n} + \frac{\overline{x}^2}{SXX}\right)$ • $\hat{\beta}_1 = \sum \left(\frac{x_i - \overline{x}}{SXX}\right) y_i$ $\widehat{\operatorname{Var}}(\hat{\beta}_1 | X) = \hat{\sigma}^2 \frac{1}{SXX}$ • $\hat{\sigma}^2 = \frac{\sum \hat{e}_i^2}{n-2} \sim \sigma^2 X_{n-2}^2 / (n-2)$ (Chi-square with d.f. n-2)

Intercept: β₀

Testing: NH:
$$\beta_0 = \beta_0^*$$
, β_1 arbitrary
AH: $\beta_0 \neq \beta_0^*$, β_1 arbitrary
 $t = \frac{\hat{\beta}_0 - \beta_0^*}{\operatorname{se}(\hat{\beta}_0)}$ t-distribution with $n - 2$ df
where $\operatorname{se}(\hat{\beta}_0) = \hat{\sigma}(\frac{1}{n} + \frac{\bar{x}^2}{SXX})^{\frac{1}{2}}$

(1-α)x100% confidence interval:

$$\hat{\beta}_0 - t(\alpha/2, n-2)\operatorname{se}(\hat{\beta}_0) \le \beta_0 \le \hat{\beta}_0 + t(\alpha/2, n-2)\operatorname{se}(\hat{\beta}_0)$$

- slope: β_1
- **Testing:** NH: $\beta_1 = \beta_1^*$, β_0 arbitrary AH: $\beta_1 \neq \beta_1^*$, β_0 arbitrary $t = \frac{\hat{\beta}_1 - \beta_1^*}{\operatorname{se}(\hat{\beta}_1)}$ t-distribution with n - 2 df where $\operatorname{se}(\hat{\beta}_1) = \frac{\hat{\sigma}}{\sqrt{SXX}}$
- (1-α)x100% confidence interval:

$$\hat{\beta}_1 - t(\alpha/2, n-2)\operatorname{se}(\hat{\beta}_1) \le \beta_1 \le \hat{\beta}_1 + t(\alpha/2, n-2)\operatorname{se}(\hat{\beta}_1)$$

2.8 T-test = F-test in testing β_1 =0!

- A common test of slope
 - NH: β₁=0
 - AH: β₁≠0
- It is equivalent to comparing the models
 - y_i= β₀ +e_i
 - $y_i = \beta_0 + \beta_1 x_i + e_i$
- F-stat=(t-stat)² *t*-statistic: $t = \frac{\hat{\beta}_1 - 0}{se(\hat{\beta}_1)} = \frac{\hat{\beta}_1}{\hat{\sigma}/\sqrt{SXX}}$ $t^2 = \frac{\hat{\beta}_1^2}{\hat{\sigma}^2/SXX} = \frac{\hat{\beta}_1^2 SXX}{\hat{\sigma}^2} = \frac{(SXY)^2}{\hat{\sigma}^2 SXX} = \frac{SSreg}{\hat{\sigma}^2} = F$ -statistic

 $F(1,m) = X_1^2/[X_m^2/m] = N(0,1)^2/[X_m^2/m] = t(m)^2$

- Prediction: If we observe x_{*}, what is the y_{*}?
 - New observation (x*,?):
 - Prediction > $\tilde{y}_* = \hat{\beta}_0 + \hat{\beta}_1 x_*$
 - Prediction uncertainty

This is the notation used in the textbook. It should be understood as $V_{all}(v_* - \tilde{v}_* | x_*)$

•
$$Var(y_* - \tilde{y}_* | x_*) = Var((\beta_o - \hat{\beta}_o) + (\beta_1 - \hat{\beta}_1)x_* + e)$$

• (predicting a particular observation incorporate the error, giving σ^2)

$\Rightarrow \operatorname{Var}(\tilde{y}_* x_*) = \sigma^2 + \sigma^2(\frac{1}{n} + \frac{(x_* - \bar{x})^2}{SXX})$	9
sepred $(\tilde{y}_* x_*) = \hat{\sigma}(1 + \frac{1}{n} + \frac{(x_* - \bar{x})^2}{SXX})^{\frac{1}{2}}$	

Prediction interval for y_{*} (pointwise)

 $\tilde{y}_* \pm t_{(\frac{\alpha}{2}, n-2)} \operatorname{sepred}(\tilde{y}_* | x_*)$

- Fitted value: E(Y|X=x) for different values of x
 - What is the mean daughter height if mothers height=x?
 - Fitted value: $E(Y|X=x)=\beta_0+\beta_1x$
 - Estimation:

$$\hat{\gamma} = \hat{\beta}_0 + \hat{\beta}_1 x$$

• Estimation uncertainty: $Var(E(Y | x) - \hat{y} | x) = Var((\beta_o - \hat{\beta}_o) + (\beta_1 - \hat{\beta}_1)x))$

• It is not a prediction, no error term, so no σ^2

sefit
$$(\hat{y}|x) = \hat{\sigma}(\frac{1}{n} + \frac{(x-\bar{x})^2}{SXX})^{\frac{1}{2}}$$

Confidence interval for E(Y|X=x): (pointwise)

 $\hat{y} \pm t_{(\frac{\alpha}{2},n-2)} \operatorname{sefit}(\hat{y} | x)$

Confidence band for E(Y|X=x): (for entire line)

 $(\hat{\beta}_0 + \hat{\beta}_1 x) \pm [2F(\alpha; 2, n-2)]^{1/2} \operatorname{sefit}(\hat{y}|x)$

2.9 Residuals

2.9 Residuals

 Summary Statistics for Forbes' Data with All Data and with Case 12 deleted

Quantity	All Data	Delete Case 12	
$\hat{\beta}_0$	-42.138	-41.308	
$\hat{\beta}_1$	0.895	0.891	
$se(\hat{eta}_0)$	3.340	1.001	
$se(\hat{eta}_1)$	0.016	0.005	
$\hat{\sigma}$	0.379	0.113	
R^2	0.995	1.000	

2.9 Residuals

• Null plot:

- Mean function = 0
- Variance function = constant
- No separated points
- A null plot is a good residual plot

Chapter 2 summary

•	Estimators $\hat{\beta}_0 =$	$= \overline{y} - \hat{\beta}_1 \overline{x},$	$\hat{\beta}_1 = \sum_{i=1}^{n}$	$\sum_{i=1}^{n} (x_i - \overline{x}_i)$	$\frac{\overline{x}(y_i - \overline{y})}{\overline{x}^2} = \frac{SXY}{SXX}$	$\widehat{\sigma}^2 = \frac{\sum \widehat{e}_i^2}{2} =$	$= \frac{SYY - \frac{SXY^2}{SXX}}{SXX}$
•	Variances $\widehat{\operatorname{Var}}(\widehat{\beta}_1 X) = \widehat{\sigma}^2 \frac{1}{SXX}$	$\widehat{\operatorname{Var}}(\widehat{\beta_0} X)$	$= \widehat{\sigma}^2 (\frac{1}{n} +$	$\frac{\bar{x}^2}{SXX}$	$\widehat{\mathrm{Cov}}(\widehat{\beta}_0, \widehat{\beta}_1 X) = -\widehat{\sigma}$	$n-2$ $^{2}\frac{\bar{X}}{5XX} \widehat{\rho}(\widehat{\beta}_{0},\widehat{\beta}$	$n-2$ $\overline{F_1} = \frac{-\overline{x}}{\sqrt{SXY/n + \overline{x}^2}}$
	ANOVA table	Source	df	SS	MS	F	$\sqrt{3}$ / $n + x^2$
		Regression	1	SSreg	SSreg/1	$MSreg/\hat{\sigma}^2$	
		Residual	<u>n – 2</u>	RSS	$\hat{\sigma}^2 = RSS/(n-2)$		
•	Tests for dependence • F-test: $F = \frac{1}{2}$ • T-test $t = \frac{1}{2}$	$\frac{SSreg/1}{RSS/(n-2)}$ $\frac{\hat{\beta}_1 - \beta_1^*}{\operatorname{se}(\hat{\beta}_1)} \sim t(r)$	f x and ~ F(1,n-2)	у			
•	$R^2 = \frac{SSreg}{SYY}$			^	<u>^</u>		()2 1
	Confidence bai	nd for E(`	Ƴ X=x):	(β ₀	$+\beta_1 x$) $\pm [2F(\alpha; 2, n +$	$(-2)]^{1/2}\hat{\sigma}(\frac{1}{p}+$	$\left(\frac{(x-x)^{-}}{SXX}\right)^{\frac{1}{2}}$
k	Confidence inte	erval for E	Ξ(Y X=)	κ): ^{(β}₀ -	$(\hat{\beta}_1 x) \pm t_{(\frac{\alpha}{2}, n-2)} \hat{\sigma}(\frac{1}{n})$	$(\frac{1}{n} + \frac{(x-\bar{x})^2}{SXX})^{\frac{1}{2}}$	
	Prediction inter	val for ne	ew obs:	$(\hat{eta}_0$	$+\hat{\beta}_1 x) \pm t_{(\frac{\alpha}{2},n-2)} \hat{\sigma}($	$1 + \frac{1}{n} + \frac{(x_* - \bar{x})}{SXX}$	$(\frac{1}{2})^{\frac{1}{2}}$