

STAT 571A — Advanced Statistical Regression Analysis

<u>Chapter 1 NOTES</u> Linear Regression with One Predictor Variable

© 2014 University of Arizona Statistics GIDP. All rights reserved, except where previous rights exist. No part of this material may be reproduced, stored in a retrieval system, or transmitted in any form or by any means — electronic, online, mechanical, photoreproduction, recording, or scanning — without the prior written consent of the course instructor.

Linear Regression

Linear regression is concerned with estimating relationships between a response variable, Y and an explanatory/predictor variable, X

The simple linear (straight-line) relationship is

 $Y = \beta_0 + \beta_1 X$ where β_1 is the slope ("rise-over-run") and β_0 is the Y-intercept.



Data model

In practice, we observe data pairs (X_i, Y_i) , i = 1,..., n, usually with observational/experimental error. Model this as

 $Y_{i} = (\beta_{0} + \beta_{1}X_{i}) + \varepsilon_{i}$ (1.1) i.e., observed Y = (simple linear model) + random error term

Can think of this as Y = (signal) + noise.

Historical Note

- As the text indicates, the originator of the term "regression" was Sir Francis Galton
- He plotted X = 'Mid-Parent' height (as the <u>vertical</u> axis), and Y = Adult child height (as the <u>horizontal</u> axis), and found that as adults, the offspring "regressed" to more central heights.
- Galton published the data in 1886 (in the J. Anthropol. Inst. Gr. Brit. & Ireland).

Galton's 1886 "Plate X"

Galton's original plot:



Model Assumptions

■ For our simple linear model, we assume

- X_i is a known constant
- β_0 and β_1 are unknown parameters
- $E[\epsilon_i] = 0$ for all i
- $\sigma^2[\epsilon_i] = \sigma^2$ (constant) for all i
- $\sigma[\epsilon_i, \epsilon_j] = 0$ (zero!) for all $i \neq j$
- Notice: ε_i is a random variable, thus so is Y_i.

Model Impact on Y_i

We find

- $\sigma[Y_i, Y_j] = \dots = 0$ for all $i \neq j$

Probability Model

Graphically, there is some probability function for Y_i resting at each X_i:



same variance!

Alternative Formulations

Alternative (but, essentially equivalent) formulations for the simple linear model include:

•
$$Y_i = \beta_0^* + \beta_1(X_i - \overline{X}) + \varepsilon_i$$

(so $\beta_0^* = \beta_0 + \beta_1\overline{X}$) for $\overline{X} = \frac{1}{n}\sum_{i=1}^n X_i$

•
$$Y_i = \beta_0 X_{0i} + \beta_1 X_{1i} + \varepsilon_i$$

where $X_{0i} = 1$ and $X_{1i} = X_i$ for all i.

These can be useful in select cases.

Data Generation Mechanisms

- Note that we can observe the data pairs in two fundamentally different ways:
 - Observational study: data are recorded without strict experimental controls ⇒ harder to relate cause & effect
 - <u>Experimental study</u>: data from controlled experiments

⇒ inference is truer but conduct is more expensive

We consider both forms in our data examples.

Least Squares (LS)

- Given data pairs (X_i,Y_i), i = 1,..., n, we estimate β₀ and β₁ using the method of least squares (LS) (from Appendix A.5).
- Denote these as b₀ and b₁, resp. (Equations will follow.)
- Then, the fitted value is $\hat{Y}_i = b_0 + b_1 X_i$. Find these by minimizing $Q = \sum (Y_i - \hat{Y}_i)^2$.
- The corresp. residual is $e_i = Y_i \hat{Y}_i$. We want \hat{Y}_i to be as close to Y_i as possible.

LS Line and Residuals

- Graphically, the idea is something
 like this →
- Points are data pairs; line is b₀ + b₁X



'Normal' Equations

To minimize Q with resp. to b₀ and b₁, via calculus (see pp.17-18), we find the LS estimators solve the system of equations

$$\sum \mathbf{Y}_i = \mathbf{nb}_0 + \mathbf{b}_1 \sum \mathbf{X}_i$$

$$\sum \mathbf{X}_{i} \mathbf{Y}_{i} = \mathbf{b}_{0} \sum \mathbf{X}_{i} + \mathbf{b}_{1} \sum \mathbf{X}_{i}^{2}$$

These are called the normal equations for the LS estimators.

Gauss-Markov Theorem

- A result known as the Gauss-Markov Theorem motivates use of the LS estimators: under model (1.1), the LS solutions for b₀ and b₁ are (a) unbiased and (b) have min. variance among all unbiased linear estimators.
- (a) says that E[b_j] = β_j for j=0,1

• (b) says $\sigma^2[b_0]$ and $\sigma^2[b_1]$ are minimized.

LS Solutions: Slope

The LS solution has, in fact, a closed form. First, the slope parameter is

$$\mathbf{b}_1 = \frac{\sum_{i=1}^n (\mathbf{X}_i - \overline{\mathbf{X}})(\mathbf{Y}_i - \overline{\mathbf{Y}})}{\sum_{i=1}^n (\mathbf{X}_i - \overline{\mathbf{X}})^2}$$

or also

$$b_{1} = \frac{\sum_{i=1}^{n} (X_{i} - \overline{X}) Y_{i}}{\sum_{m=1}^{n} (X_{m} - \overline{X})^{2}} = \sum_{i=1}^{n} k_{i} Y_{i}$$

for $k_{i} = \frac{(X_{i} - \overline{X})}{\sum_{m=1}^{n} (X_{m} - \overline{X})^{2}}$

LS Solutions: Intercept

Then, the intercept is expressed conveniently as

$$\mathbf{b}_0 = \overline{\mathbf{Y}} - \mathbf{b}_1 \overline{\mathbf{X}}$$

Indeed, b_0 can also be written in the form $b_0 = \sum_{i=1}^n k_i Y_i$ (...for a different set of k_i s)

Example CH01TA01 (p. 19)

X = lot size of refrig. parts productionY = hours worked (labor)at the Toluca Manufacturing Co.

The data are in Table 1.1. We could just 'do the math':

 $\sum_{i=1}^{n} (X_i - \overline{X}) Y_i = 70690 \quad \& \quad \sum_{i=1}^{n} (X_i - \overline{X})^2 = 19800$ so $b_1 = \frac{\sum_{i=1}^{n} (X_i - \overline{X}) Y_i}{\sum_{i=1}^{n} (X_i - \overline{X})^2} = \frac{70690}{19800} = 3.5702$

Example CH01TA01 (cont'd)

Also,
$$\overline{Y} = 312.28$$
 and $\overline{X} = 70$, so
 $b_0 = \overline{Y} - b_1 \overline{X} = 312.28 - (3.5702)(70)$
= 62.37.

The prediction equation for $\hat{Y}_i = b_0 + b_1 X_i$ is then $\hat{Y}_i = 62.37 + 3.5702 X_i$.

But, it's so much easier in R \rightarrow

Example CH01TA01 (cont'd)

Toluca Co. example: LS fit for simple linear model via R:

- > X = c(80, 30, ..., 70)
- > Y = c(399, 121, ..., 323)
- > CH01TA01.lm = lm($Y \sim X$)

> summary(CH01TA01.lm)

summary() output for Toluca example

```
Call:
lm(formula = Y \sim X)
Residuals:
   Min 1Q Median 3Q
                                  Max
-83.876 -34.088 -5.982 38.826 103.528
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 62.366 26.177 2.382 0.0259 *
             3.570 0.347 10.290 4.45e-10 ***
X
LS estimates of the regr. parameters highlighted in red here.
```

Example CH01TA01 (cont'd)

ALWAYS PLOT THE DATA! Toluca example. <u>Scatterplot</u> plot in R:

- > plot(Y ~ X)
- > abline(CH01TA01.lm)

abline() command overlays line from LS fit



Example CH01TA01 (p.22)

What about predicting the fitted value at a given X_i?

For instance, at X₁ = 80 we see $\hat{Y}_1 = b_0 + b_1(80) = 62.37 + (3.5702)(80) = 347.98$

The corresp. residual is $e_1 = Y_1 - \hat{Y}_1 = 399 - 347.98 = 51.02.$ (See Table 1.2.)

Consequences of the LS Fit

The LS estimators produce the following, interesting, mathematical consequences:

- $\sum e_i = 0$ (always!)
- $\sum e_i^2$ is a minimum (since it's LS)
- $\sum \mathbf{Y}_i = \sum \hat{\mathbf{Y}}_i$
- $\sum e_i X_i = 0$ (weighted sum of e_i 's is zero)
- $\sum \mathbf{e}_i \hat{\mathbf{Y}}_i = \mathbf{0}$
- $\hat{\mathbf{Y}}(\overline{\mathbf{X}}) = \mathbf{b}_0 + \mathbf{b}_1 \overline{\mathbf{X}} = \overline{\mathbf{Y}}$

Estimating σ^2

- How to estimate a variance?
- Think of the single-sample case. For Y₁,...,Y_n, we use the sample variance:

$$S^{2} = \frac{\sum_{i=1}^{n} (Y_{i} - \overline{Y})^{2}}{n-1} \longleftrightarrow \qquad \frac{a \text{ "sum of squares"}}{\text{degrees of freedom}}$$

■ Now do the same thing with the simple linear model, but replace \overline{Y} with $\hat{Y}_i \rightarrow$

SSE

The resulting sum of squares is called the **Sum of Squared Errors**, or SSE:

SSE =
$$\sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} e_i^2$$

(Notice that it's just the sum of squared residuals, so it's also called the **Residual Sum of Squares**.)

This has d.f. = n – 2. (Why? Think of it as "# observations" – "# fitted components")

MSE

Now, divide SSE by its d.f.: $MSE = \frac{SSE}{d.f.} = \frac{\sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2}{n-2}$

We call this the Mean Squared Error, or MSE.

Under (1.1), can show that E[MSE] = σ^2 (unbiased!).

To estimate σ , use the root mean squared error: $\sqrt{\text{MSE}}$

Normal Error Model

- Let's add one last model component: impose a formal distribution on the error terms in ε_i.
- **Recall:** $Y_i = (\beta_0 + \beta_1 X_i) + \varepsilon_i$.
- Now, let ε_i ~ i.i.d. N(E[ε_i], σ²[ε_i]). Since we already specified E[ε_i] = 0 and σ²[ε_i] = σ², this yields

 $ε_i ~ i.i.d. N(0, σ^2).$

Maximum Likelihood

- The combination of the simple linear model in (1.1) with normal errors is called a Simple Linear Regression (SLR) model.
- By imposing a formal probability distribution into the model, a form of estimation known as Maximum Likelihood is available.
- We use ML occasionally. For now, know that ML estimators and LS estimators for the SLR model actually coincide (i.e., they're identical).