Regression Estimation - Least Squares and Maximum Likelihood

Dr. Frank Wood

Least Squares Max(min)imization

1. Function to minimize w.r.t. β_0, β_1

$$Q = \sum_{i=1}^{n}(Y_i - (\beta_0 + \beta_1 X_i))^2$$

2. Minimize this by maximizing $-Q$
3. Find partials and set both equal to zero

$$\begin{aligned} \frac{dQ}{d\beta_0} &= 0 \\ \frac{dQ}{d\beta_1} &= 0 \end{aligned}$$

Normal Equations

1. The result of this maximization step are called the normal equations. b_0 and b_1 are called point estimators of β_0 and β_1 respectively.

$$\begin{aligned} \sum Y_i &= nb_0 + b_1 \sum X_i \\ \sum X_i Y_i &= b_0 \sum X_i + b_1 \sum X_i^2 \end{aligned}$$

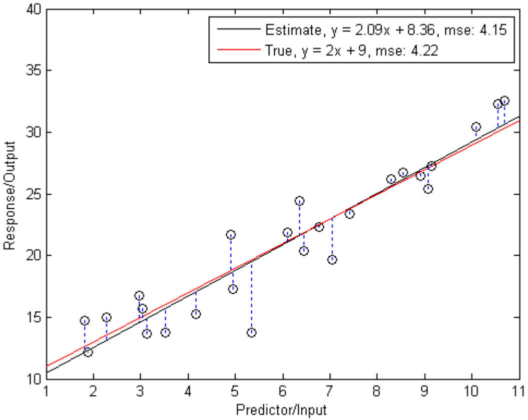
2. This is a system of two equations and two unknowns. The solution is given by ...

Solution to Normal Equations

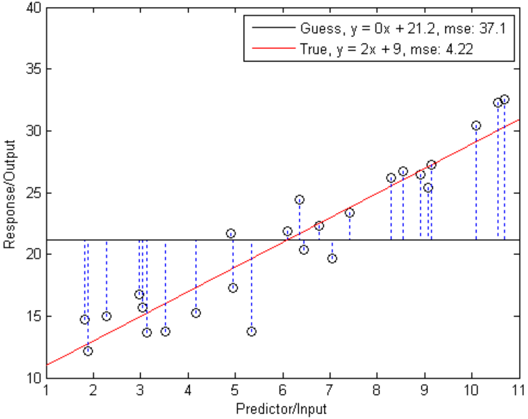
After a lot of algebra one arrives at

$$
\begin{aligned}
b_1 &= \frac{\sum (X_i - \bar{X})(Y_i - \bar{Y})}{\sum (X_i - \bar{X})^2} \\
b_0 &= \bar{Y} - b_1 \bar{X} \\
\bar{X} &= \frac{\sum X_i}{n} \\
\bar{Y} &= \frac{\sum Y_i}{n}
\end{aligned}
$$

Least Squares Fit



Guess #1



Guess, y = 0x + 21.2, mse: 37.1
True, y = 2x + 9, mse: 4.22
40
35
30
25
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10
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2
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6
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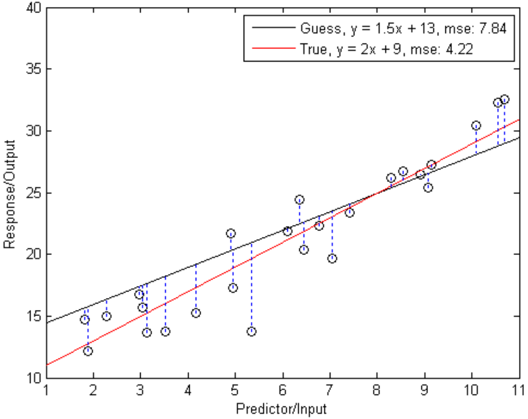
8
9
10
11
Response/Output
Predictor/Input

Guess #2



Guess, y = 1.5x + 13, mse: 7.84
True, y = 2x + 9, mse: 4.22
Response/Output
Predictor/Input
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11

Looking Ahead: Matrix Least Squares

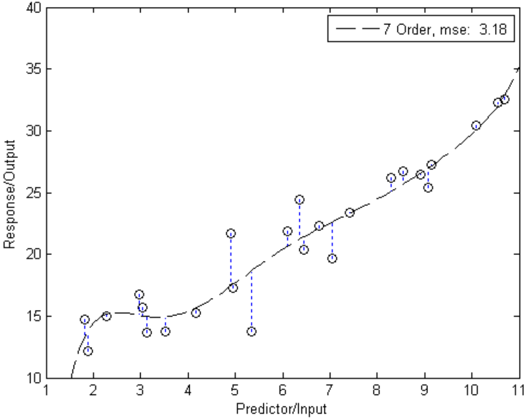
$$\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} X_1 & 1 \\ X_2 & 1 \\ \vdots & \\ X_n & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_0 \end{bmatrix}$$

Solution to this equation is solution to least squares linear regression (and maximum likelihood under normal error distribution assumption)

Questions to Ask

1. Is the relationship really linear?
2. What is the distribution of the of "errors"?
3. Is the fit good?
4. How much of the variability of the response is accounted for by including the predictor variable?
5. Is the chosen predictor variable the best one?

Is This Better?



Goals for First Half of Course

1. How to do linear regression
    1.1 Self familiarization with software tools
2. How to interpret standard linear regression results
3. How to derive tests
4. How to assess and address deficiencies in regression models

Estimators for $\beta_0, \beta_1, \sigma^2$

1. We want to establish properties of estimators for β_0, β_1, and σ^2 so that we can construct hypothesis tests and so forth
2. We will start by establishing some properties of the regression solution.

Properties of Solution

1. The i^{th} residual is defined to be

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

2. The sum of the residuals is zero:

$$\begin{aligned}
\sum_i e_i &= \sum (Y_i - b_0 - b_1 X_i) \\
&= \sum Y_i - nb_0 - b_1 \sum X_i \\
&= 0
\end{aligned}$$

Properties of Solution

The sum of the observed values Y_i equals the sum of the fitted values $\widehat{Y}_i$

$$\begin{aligned}
\sum_i Y_i &= \sum_i \hat{Y}_i \\
&= \sum_i (b_1 X_i + b_0) \\
&= \sum_i (b_1 X_i + \bar{Y} - b_1 \bar{X}) \\
&= b_1 \sum_i X_i + n\bar{Y} - b_1 n\bar{X} \\
&= b_1 n\bar{X} + \sum_i Y_i - b_1 n\bar{X}
\end{aligned}$$

Properties of Solution

The sum of the weighted residuals is zero when the residual in the i^{th} trial is weighted by the level of the predictor variable in the i^{th} trial

$$\begin{aligned}\sum_i X_i e_i &= \sum (X_i(Y_i - b_0 - b_1 X_i)) \\ &= \sum_i X_i Y_i - b_0 \sum X_i - b_1 \sum (X_i^2) \\ &= 0\end{aligned}$$

Properties of Solution

The regression line always goes through the point

$$\bar{X}, \bar{Y}$$

Estimating Error Term Variance σ^2

1. Review estimation in non-regression setting.
2. Show estimation results for regression setting.

Estimation Review

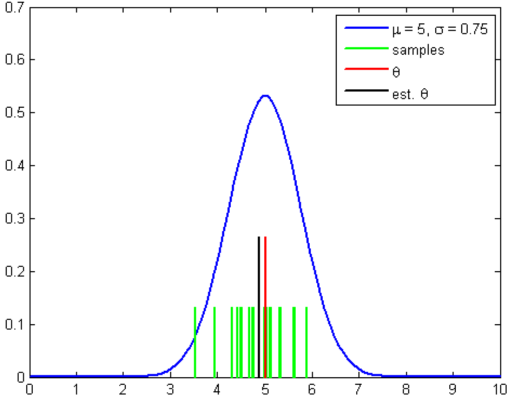
1. An estimator is a rule that tells how to calculate the value of an estimate based on the measurements contained in a sample
2. i.e. the sample mean

$$\bar{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i$$

Point Estimators and Bias

1. Point estimator
$$\hat{\theta} = f(\{Y_1, \ldots, Y_n\})$$
2. Unknown quantity / parameter
$$\theta$$
3. Definition: Bias of estimator
$$B(\hat{\theta}) = \mathbb{E}(\hat{\theta}) - \theta$$

One Sample Example



Distribution of Estimator

1. If the estimator is a function of the samples and the distribution of the samples is known then the distribution of the estimator can (often) be determined
   1.1 Methods
      1.1.1 Distribution (CDF) functions
      1.1.2 Transformations
      1.1.3 Moment generating functions
      1.1.4 Jacobians (change of variable)

Example

1. Samples from a *Normal*(μ, σ^2) distribution

$$Y_i \sim \mathrm{Normal}(\mu, \sigma^2)$$

2. Estimate the population mean

$$\theta = \mu, \quad \hat{\theta} = \bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i$$

Sampling Distribution of the Estimator

1. First moment

$$\begin{aligned} E(\hat{\theta}) &= E(\frac{1}{n}\sum_{i=1}^{n} Y_i) \\ &= \frac{1}{n}\sum_{i=1}^{n} E(Y_i) = \frac{n\mu}{n} = \theta \end{aligned}$$

2. This is an example of an unbiased estimator

$$B(\hat{\theta}) = E(\hat{\theta}) - \theta = 0$$

Variance of Estimator

1. Definition: Variance of estimator

$$V(\hat{\theta}) = E([\hat{\theta} - E(\hat{\theta})]^2)$$

2. Remember:

$$\begin{aligned} V(cY) &= c^2 V(Y) \\ V(\sum_{i=1}^{n} Y_i) &= \sum_{i=1}^{n} V(Y_i) \end{aligned}$$

Only if the Y_i are independent with finite variance

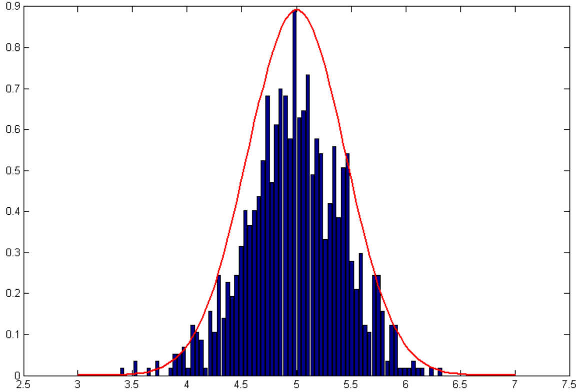
Example Estimator Variance

1. For $N(0,1)$ mean estimator

$$\begin{aligned} V(\hat{\theta}) &= V(\frac{1}{n}\sum_{i=1}^{n} Y_i) \\ &= \frac{1}{n^2}\sum_{i=1}^{n} V(Y_i) = \frac{n\sigma^2}{n^2} = \frac{\sigma^2}{n} \end{aligned}$$

2. Note assumptions

Distribution of sample mean estimator



Bias Variance Trade-off

1. The mean squared error of an estimator

$$MSE(\hat{\theta}) = E([\hat{\theta} - \theta]^2)$$

2. Can be re-expressed

$$MSE(\hat{\theta}) = V(\hat{\theta}) + (B(\hat{\theta})^2)$$

MSE = VAR + $BIAS^2$

Proof

$$
\begin{aligned}
MSE(\hat{\theta}) &= E((\hat{\theta}-\theta)^2) \\
&= E(([\hat{\theta}-E(\hat{\theta})]+[E(\hat{\theta})-\theta])^2) \\
&= E([\hat{\theta}-E(\hat{\theta})]^2)+2E([E(\hat{\theta})-\theta][\hat{\theta}-E(\hat{\theta})])+E([E(\hat{\theta})-\theta] \\
&= V(\hat{\theta})+2E([E(\hat{\theta})[\hat{\theta}-E(\hat{\theta})]-\theta[\hat{\theta}-E(\hat{\theta})]])+(B(\hat{\theta}))^2 \\
&= V(\hat{\theta})+2(0+0)+(B(\hat{\theta}))^2 \\
&= V(\hat{\theta})+(B(\hat{\theta}))^2
\end{aligned}
$$

Trade-off

1. Think of variance as confidence and bias as correctness.
   1.1 Intuitions (largely) apply
2. Sometimes a biased estimator can produce lower MSE if it lowers the variance.

Estimating Error Term Variance σ^2

1. Regression model
2. Variance of each observation Y_i is σ^2 (the same as for the error term ϵ_i)
3. Each Y_i comes from a different probability distribution with different means that depend on the level X_i
4. The deviation of an observation Y_i must be calculated around its own estimated mean.

s^2 estimator for σ^2

$$s^2 = MSE = \frac{SSE}{n-2} = \frac{\sum(Y_i - \hat{Y}_i)^2}{n-2} = \frac{\sum e_i^2}{n-2}$$

1. MSE is an unbiased estimator of σ^2

$$E(MSE) = \sigma^2$$

2. The sum of squares SSE has n-2 degrees of freedom associated with it.

Normal Error Regression Model

1. No matter how the error terms ϵ_i are distributed, the least squares method provides unbiased point estimators of β_0 and β_1
   1.1 that also have minimum variance among all unbiased linear estimators
2. To set up interval estimates and make tests we need to specify the distribution of the ϵ_i
3. We will assume that the ϵ_i are normally distributed.

Normal Error Regression Model

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

1. Y_i value of the response variable in the i^{th} trial
2. β_0 and β_1 are parameters
3. X_i is a known constant, the value of the predictor variable in the i^{th} trial
4. $\epsilon_i \sim_{iid} N(0, \sigma^2)$
5. $i = 1, \ldots, n$

Notational Convention

1. When you see $\epsilon_i \sim_{iid} N(0, \sigma^2)$
2. It is read as ϵ_i is distributed identically and independently according to a normal distribution with mean 0 and variance σ^2
3. Examples
   3.1 $\theta \sim Poisson(\lambda)$
   3.2 $z \sim G(\theta)$

Maximum Likelihood Principle

The method of maximum likelihood chooses as estimates those values of the parameters that are most consistent with the sample data.

Likelihood Function

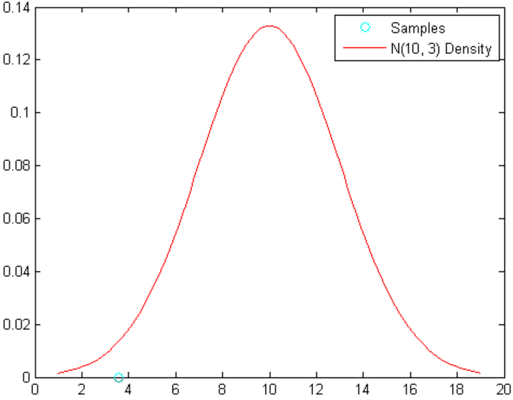
If

$$X_i \sim F(\Theta), i = 1 \dots n$$

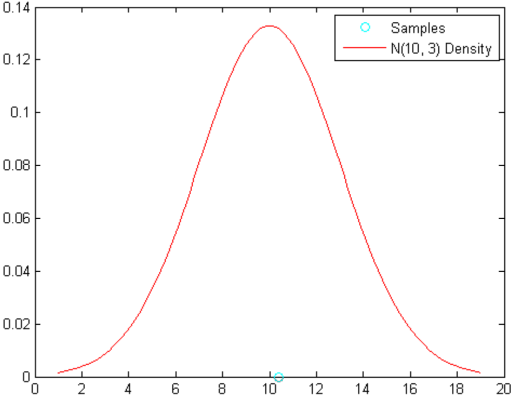
then the likelihood function is

$$\mathcal{L}(\{X_i\}_{i=1}^n, \Theta) = \prod_{i=1}^n F(X_i; \Theta)$$

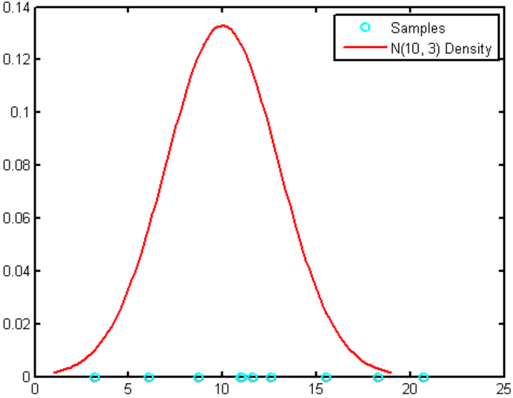
Example, $N(10, 3)$ Density, Single Obs.



Example, $N(10, 3)$ Density, Single Obs. Again



Example, $N(10, 3)$ Density, Multiple Obs.



Maximum Likelihood Estimation

1. The likelihood function can be maximized w.r.t. the parameter(s) Θ, doing this one can arrive at estimators for parameters as well.

$$\mathcal{L}(\{X_i\}_{i=1}^{n}, \Theta) = \prod_{i=1}^{n} F(X_i; \Theta)$$

2. To do this, find solutions to (analytically or by following gradient)

$$\frac{d\mathcal{L}(\{X_i\}_{i=1}^{n}, \Theta)}{d\Theta} = 0$$

Important Trick

Never (almost) maximize the likelihood function, maximize the log likelihood function instead.

$$\begin{aligned} log(\mathcal{L}(\{X_i\}_{i=1}^n, \Theta)) &= log(\prod_{i=1}^n F(X_i; \Theta)) \\ &= \sum_{i=1}^n log(F(X_i; \Theta)) \end{aligned}$$

Quite often the log of the density is easier to work with mathematically.

ML Normal Regression

Likelihood function

$$\begin{aligned}\mathcal{L}(\beta_0, \beta_1, \sigma^2) &= \prod_{i=1}^{n} \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-\frac{1}{2\sigma^2}(Y_i - \beta_0 - \beta_1 X_i)^2} \\ &= \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 X_i)^2}\end{aligned}$$

which if you maximize (how?) w.r.t. to the parameters you get...

Maximum Likelihood Estimator(s)

1. β_0
   b_0 same as in least squares case
2. β_1
   b_1 same as in least squares case
3. σ_2

$$\hat{\sigma}^2 = \frac{\sum_i (Y_i - \hat{Y}_i)^2}{n}$$

4. Note that ML estimator is biased as s^2 is unbiased and

$$s^2 = MSE = \frac{n}{n-2}\hat{\sigma}^2$$

Comments

1. Least squares minimizes the squared error between the prediction and the true output
2. The normal distribution is fully characterized by its first two central moments (mean and variance)
3. Food for thought:
   3.1 What does the bias in the ML estimator of the error variance mean? And where does it come from?