Regression Estimation - Least Squares and Maximum Likelihood

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Least Squares Max(min)imization

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

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

- Minimize this by maximizing $-Q$
- 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

- 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.

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

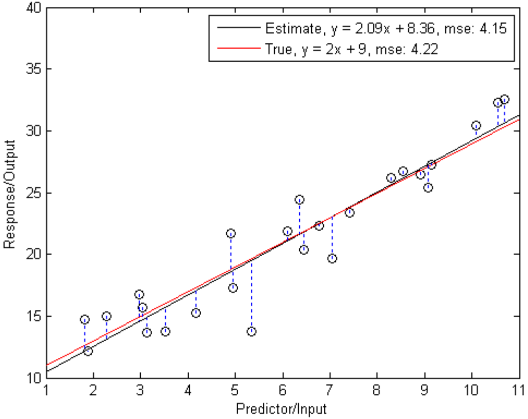
- This is a system of two equations and two unknowns. The solution is given by ...

Solution to Normal Equations

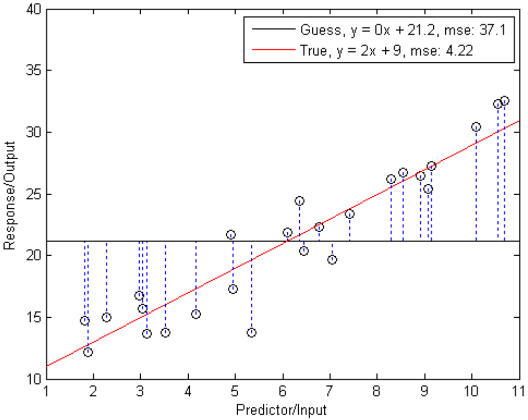
After a lot of algebra one arrives at

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

Least Squares Fit

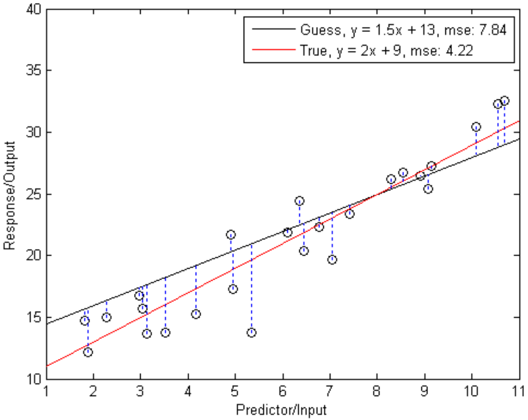


Guess #1



Guess, y = 0x + 21.2, mse: 37.1
True, y = 2x + 9, mse: 4.22
Response/Output
Predictor/Input
40
35
30
25
20
15
10
1
2
3
4
5
6
7
8
9
10
11

Guess #2



Guess, y = 1.5x + 13, mse: 7.84
True, y = 2x + 9, mse: 4.22
Response/Output
Predictor/Input
40
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Looking Ahead: Matrix Least Squares

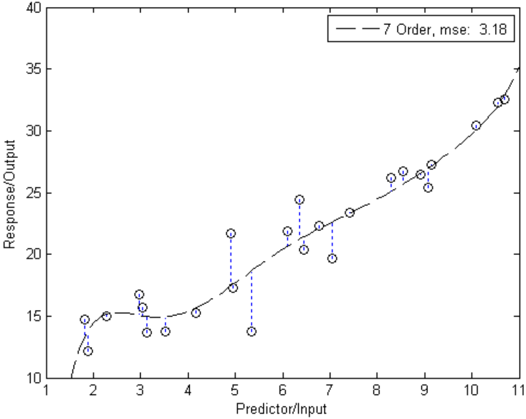
$$
\begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} X_1 & 1 \\ X_2 & 1 \\ \vdots & \\ X_n & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_0 \end{bmatrix}
$$

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

Questions to Ask

- Is the relationship really linear?
- What is the distribution of the of "errors"?
- Is the fit good?
- How much of the variability of the response is accounted for by including the predictor variable?
- Is the chosen predictor variable the best one?

Is This Better?



Goals for First Half of Course

- How to do linear regression
  - Self familiarization with software tools
- How to interpret standard linear regression results
- How to derive tests
- How to assess and address deficiencies in regression models

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

- 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
- We will start by establishing some properties of the regression solution.

Properties of Solution

- The i^{th} residual is defined to be

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

- 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

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

Estimation Review

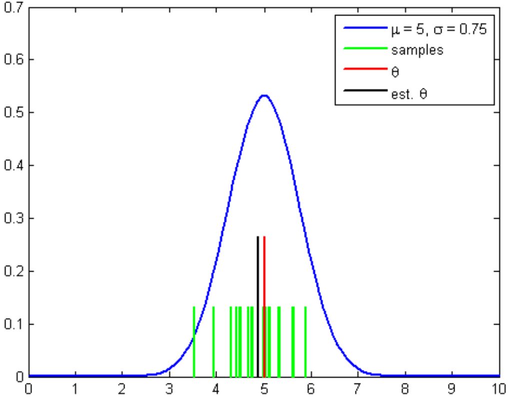
- An estimator is a rule that tells how to calculate the value of an estimate based on the measurements contained in a sample
- i.e. the sample mean

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

Point Estimators and Bias

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

One Sample Example



Distribution of Estimator

- 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
  - Methods
    - Distribution (CDF) functions
    - Transformations
    - Moment generating functions
    - Jacobians (change of variable)

Example

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

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

- 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

- First moment

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

- This is an example of an unbiased estimator

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

Variance of Estimator

- Definition: Variance of estimator

$$\mathsf{Var}(\hat{\theta}) = \mathbb{E}([\hat{\theta} - \mathbb{E}(\hat{\theta})]^2)$$

- Remember:

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

Only if the Y_i are independent with finite variance

Example Estimator Variance

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

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

- Note assumptions

Central Limit Theorem Review

Central Limit Theorem

Let $Y_1, Y_2, \ldots, Y_n$ be iid random variables with $\mathbb{E}(Y_i) = \mu$ and $\mathrm{Var}(Y_i) - \sigma^2 < \infty$. Define.

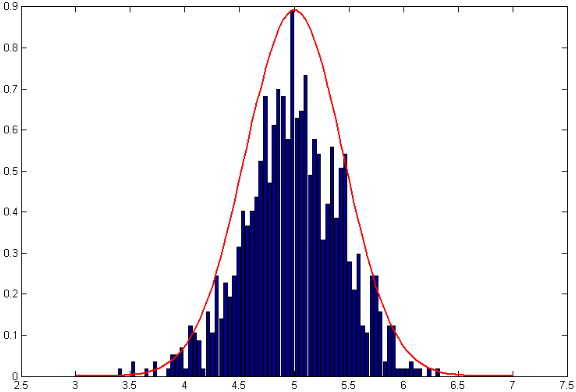
$$U_n = \sqrt{n}\left(\frac{\bar{Y} - \mu}{\sigma}\right) \quad \text{where} \quad \bar{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i \tag{1}$$

Then the distribution function of U_n converges to a standard normal distribution function as $n \to \infty$.

Alternately

$$P(a \leq U_n \leq b) \to \int_a^b \left(\frac{1}{\sqrt{2\pi}}\right) e^{\frac{-u^2}{2}}\, du \tag{2}$$

Distribution of sample mean estimator



Bias Variance Trade-off

- The mean squared error of an estimator

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

- Can be re-expressed

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

MSE = VAR + $BIAS^2$

Proof

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

Trade-off

- Think of variance as confidence and bias as correctness.
  - Intuitions (largely) apply
- Sometimes choosing a biased estimator can result in an overall lower MSE if it exhibits lower variance.
- Bayesian methods (later in the course) specifically introduce bias.

Estimating Error Term Variance σ^2

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

s^2 estimator for σ^2

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

- MSE is an unbiased estimator of σ^2

$$\mathbb{E}(MSE) = \sigma^2$$

- The sum of squares SSE has n-2 “degrees of freedom” associated with it.
- Cochran’s theorem (later in the course) tells us where degree’s of freedom come from and how to calculate them.

Normal Error Regression Model

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

Normal Error Regression Model

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

- Y_i value of the response variable in the i^{th} trial
- β_0 and β_1 are parameters
- X_i is a known constant, the value of the predictor variable in the i^{th} trial
- $\epsilon_i \sim_{iid} N(0, \sigma^2)$
  note this is different, now we know the distribution
- $i = 1, \ldots, n$

Notational Convention

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

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

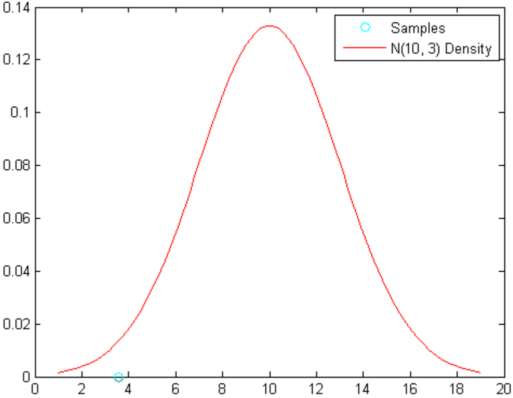
If

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

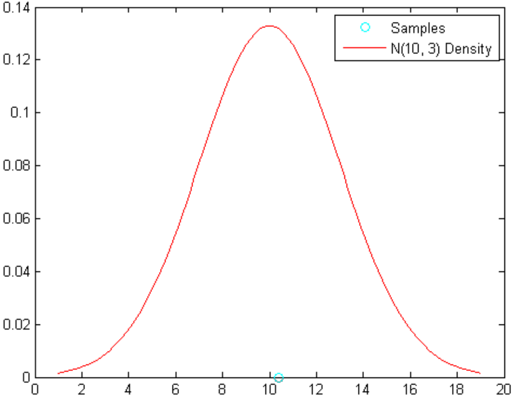
then the likelihood function is

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

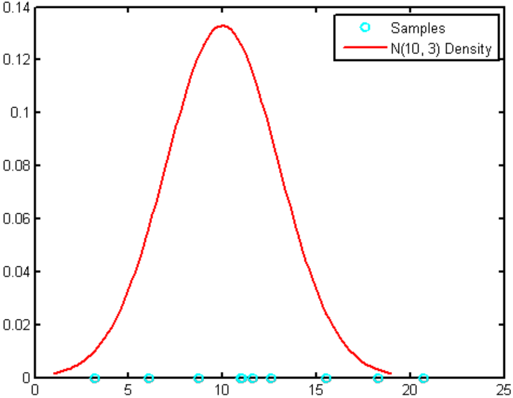
Example, $N(10, 3)$ Density, Single Obs.



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



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



Maximum Likelihood Estimation

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

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

- 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)

- β_0
  b_0 same as in least squares case
- β_1
  b_1 same as in least squares case
- σ_2

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

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

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

Comments

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