# Introduction to Simple Linear Regression 

Yang Feng

## Course Description

Theory and practice of regression analysis, Simple and multiple regression, including testing, estimation, and confidence procedures, modeling, regression diagnostics and plots, polynomial regression, colinearity and confounding, model selection, geometry of least squares. Extensive use of the computer to analyze data.

Course website: http://www.stat.columbia.edu/~yangfeng/W4315 Required Text: Applied Linear Regression Models (4th Ed.) Authors: Kutner, Nachtsheim, Neter

## Philosophy and Style

- Easy first half.
- Difficult second half.
- Some digressions from the required book.
- Understanding $=$ proof (derivation) + implementation.
- Practice makes perfect.


## Course Outline

First half of the course is single variable linear regression.

- Least squares
- Maximum likelihood, normal model
- Tests / inferences
- ANOVA
- Diagnostics
- Remedial Measures


## Course Outline (Continued)

Second half of the course is multiple linear regression and other related topics.

- Multiple linear Regression
- Linear algebra review
- Matrix approach to linear regression
- Multiple predictor variables
- Diagnostics
- Tests
- Model selection
- Other topics (If time permits)
- Principle Component Analysis
- Generalized Linear Models
- Introduction to Bayesian Inference


## Requirements

- Calculus
- Derivatives, gradients, convexity
- Linear algebra
- Matrix notation, inversion, eigenvectors, eigenvalues, rank
- Probability and Statistics
- Random variable
- Expectation, variance
- Estimation
- Bias/Variance
- Basic probability distributions
- Hypothesis Testing
- Confidence Interval


## Software

$\mathbf{R}$ will be used throughout the course and it is required in all homework. An $\mathbf{R}$ tutorial session will be given on Sep 5 (Bring your laptop!). Reasons for $\mathbf{R}$ :

- Completely free software. Can be downloaded from http://cran.r-project.org/
- Available on various systems, PC, MAC, Linux, and even


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- Completely free software. Can be downloaded from http://cran.r-project.org/
- Available on various systems, PC, MAC, Linux, and even Iphone and Ipad!
- Advanced yet easy to use.

An Introduction to R: http://cran.r-project.org/doc/manuals/R-intro.pdf

## Grading

- Weekly homework (20\%)
- DUE 6pm every Tuesday in W4315-Inbox at 904@SSW
- You can collect graded homework in W4315-Outbox at 904@SSW
- NO late homework accepted
- Lowest score will be dropped
- In Class Midterm exam (30\%)
- In Class Final exam (50\%).
- Exams are close book, close notes! One double-sided cheat sheet is allowed.


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## Office Hours / Website

- http://www.stat.columbia.edu/~yangfeng
- Course Materials and homework with the due dates will be posted on the course website.
- Office hours: Thursday 10am-noon subject to change
- Office Location : Room 1012, SSW Building (1255 Amsterdam Avenue, between 121st and 122nd street)


## Why regression?

- Want to model a functional relationship between an "predictor variable" (input, independent variable, etc.) and a "response variable" (output, dependent variable, etc.)
- Examples?
- But real world is noisy, no $f=m a$
- Observation noise
- Process noise
- Two distinct goals
- (Estimation) Understanding the relationship between predictor variables and response variables
- (Prediction) Predicting the future response given the new observed predictors.


## History

- Sir Francis Galton, $19^{\text {th }}$ century
- Studied the relation between heights of parents and children and noted that the children "regressed" to the population mean
- "Regression" stuck as the term to describe statistical relations between variables


## Example Applications

## Trend lines, eg. Google over 6 mo.



## Others

- Epidemiology
- Relating lifespan to obesity or smoking habits etc.
- Science and engineering
- Relating physical inputs to physical outputs in complex systems
- Brain



## Aims for the course

- Given something you would like to predict and some number of covariates
- What kind of model should you use?
- Which variables should you include?
- Which transformations of variables and interaction terms should you use?


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- Given something you would like to predict and some number of covariates
- What kind of model should you use?
- Which variables should you include?
- Which transformations of variables and interaction terms should you use?
- Given a model and some data
- How do you fit the model to the data?
- How do you express confidence in the values of the model parameters?
- How do you regularize the model to avoid over-fitting and other related issues?


## Data for Regression Analysis

- Observational Data Example: relation between age of employee $(X)$ and number of days of illness last year $(Y)$
Cannot be controlled!


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- Experimental Data

Example: an insurance company wishes to study the relation between productivity of its analysts in processing claims $(Y)$ and length of training $X$.

- Treatment: the length of training
- Experimental Units: the analysts included in the study.


## Data for Regression Analysis

- Observational Data

Example: relation between age of employee $(X)$ and number of days of illness last year ( $Y$ )
Cannot be controlled!

- Experimental Data

Example: an insurance company wishes to study the relation between productivity of its analysts in processing claims $(Y)$ and length of training $X$.

- Treatment: the length of training
- Experimental Units: the analysts included in the study.
- Completely Randomized Design: Most basic type of statistical design Example: same example, but every experimental unit has an equal chance to receive any one of the treatments.


## Questions?

## Good time to ask now.

## Simple Linear Regression

- Want to find parameters for a function of the form

$$
Y_{i}=\beta_{0}+\beta_{1} X_{i}+\epsilon_{i}
$$

- Distribution of error random variable not specified


## Quick Example - Scatter Plot



## Formal Statement of Model

$$
Y_{i}=\beta_{0}+\beta_{1} X_{i}+\epsilon_{i}
$$

- $Y_{i}$ value of the response variable in the $i^{\text {th }}$ trial
- $\beta_{0}$ and $\beta_{1}$ are parameters
- $X_{i}$ is a known constant, the value of the predictor variable in the $i^{t h}$ trial
- $\epsilon_{i}$ is a random error term with mean $\mathbb{E}\left(\epsilon_{i}\right)=0$ and variance $\operatorname{Var}\left(\epsilon_{i}\right)=\sigma^{2}$
- $\epsilon_{i}$ and $\epsilon_{j}$ are uncorrelated
- $i=1, \ldots, n$


## Properties

- The response $Y_{i}$ is the sum of two components
- Constant term $\beta_{0}+\beta_{1} X_{i}$
- Random term $\epsilon_{i}$
- The expected response is

$$
\begin{aligned}
\mathbb{E}\left(Y_{i}\right) & =\mathbb{E}\left(\beta_{0}+\beta_{1} X_{i}+\epsilon_{i}\right) \\
& =\beta_{0}+\beta_{1} X_{i}+\mathbb{E}\left(\epsilon_{i}\right) \\
& =\beta_{0}+\beta_{1} X_{i}
\end{aligned}
$$

## Expectation Review

- Suppose $X$ has probability density function $f(x)$.
- Definition

$$
\mathbb{E}(X)=\int x f(x) d x
$$

- Linearity property

$$
\begin{aligned}
\mathbb{E}(a X) & =a \mathbb{E}(X) \\
\mathbb{E}(a X+b Y) & =a \mathbb{E}(X)+b \mathbb{E}(Y)
\end{aligned}
$$

- Obvious from definition


## Example Expectation Derivation

Suppose p.d.f of $X$ is

$$
f(x)=2 x, 0 \leq x \leq 1
$$

Expectation

$$
\begin{aligned}
\mathbb{E}(X) & =\int_{0}^{1} x f(x) d x \\
& =\int_{0}^{1} 2 x^{2} d x \\
& =\left.\frac{2 x^{3}}{3}\right|_{0} ^{1} \\
& =\frac{2}{3}
\end{aligned}
$$

## Expectation of a Product of Random Variables

If $X, Y$ are random variables with joint density function $f(x, y)$ then the expectation of the product is given by

$$
\mathbb{E}(X Y)=\int_{X Y} x y f(x, y) d x d y
$$

## Expectation of a product of random variables

What if $X$ and $Y$ are independent? If $X$ and $Y$ are independent with density functions $f_{1}$ and $f_{2}$ respectively then

$$
\begin{aligned}
\mathbb{E}(X Y)= & \int_{X Y} x y f_{1}(x) f_{2}(y) d x d y \\
& =\int_{X} \int_{Y} x y f_{1}(x) f_{2}(Y) d x d y \\
& =\int_{X} x f_{1}(x)\left[\int_{Y} y f_{2}(y) d y\right] d x \\
& =\int_{X} x f_{1}(x) \mathbb{E}(Y) d X \\
& =\mathbb{E}(X) \mathbb{E}(Y)
\end{aligned}
$$

## Regression Function

- The response $Y_{i}$ comes from a probability distribution with mean

$$
\mathbb{E}\left(Y_{i}\right)=\beta_{0}+\beta_{1} X_{i}
$$

- This means the regression function is

$$
\mathbb{E}(Y)=\beta_{0}+\beta_{1} X
$$

Since the regression function relates the means of the probability distributions of $Y$ for a given $X$ to the level of $X$

## Error Terms

- The response $Y_{i}$ in the $i^{\text {th }}$ trial exceeds or falls short of the value of the regression function by the error term amount $\epsilon_{i}$
- The error terms $\epsilon_{i}$ are assumed to have constant variance $\sigma^{2}$


## Response Variance

Responses $Y_{i}$ have the same constant variance

$$
\begin{aligned}
\operatorname{Var}\left(Y_{i}\right) & =\operatorname{Var}\left(\beta_{0}+\beta_{1} X_{i}+\epsilon_{i}\right) \\
& =\operatorname{Var}\left(\epsilon_{i}\right) \\
& =\sigma^{2}
\end{aligned}
$$

## Variance (2 $2^{\text {nd }}$ central moment) Review

- Continuous distribution

$$
\operatorname{Var}(X)=\mathbb{E}\left[(X-\mathbb{E}(X))^{2}\right]=\int(x-\mathbb{E}(X))^{2} f(x) d x
$$

- Discrete distribution

$$
\operatorname{Var}(X)=\mathbb{E}\left[(X-\mathbb{E}(X))^{2}\right]=\sum_{i}\left(X_{i}-\mathbb{E}(X)\right)^{2} P\left(X=X_{i}\right)
$$

- Alternative Form for Variance:

$$
\operatorname{Var}(X)=\mathbb{E}\left(X^{2}\right)-\mathbb{E}(X)^{2}
$$

## Example Variance Derivation

$$
\begin{aligned}
f(x) & =2 x, 0 \leq x \leq 1 \\
\operatorname{Var}(X) & =\mathbb{E}\left(X^{2}\right)-\mathbb{E}(X)^{2} \\
& =\int_{0}^{1} 2 x x^{2} d x-\left(\frac{2}{3}\right)^{2} \\
& =\left.\frac{2 x^{4}}{4}\right|_{0} ^{1}-\frac{4}{9} \\
& =\frac{1}{2}-\frac{4}{9} \\
& =\frac{1}{18}
\end{aligned}
$$

## Variance Properties

$$
\begin{aligned}
\operatorname{Var}(a X) & =a^{2} \operatorname{Var}(X) \\
\operatorname{Var}(a X+b Y) & =a^{2} \operatorname{Var}(X)+b^{2} \operatorname{Var}(Y) \text { if } X \perp Y \\
\operatorname{Var}(a+c X) & =c^{2} \operatorname{Var}(X) \text { if } a \text { and } c \text { are both constants }
\end{aligned}
$$

More generally

$$
\operatorname{Var}\left(\sum a_{i} X_{i}\right)=\sum_{i} \sum_{j} a_{i} a_{j} \operatorname{Cov}\left(X_{i}, X_{j}\right)
$$

## Covariance

The covariance between two real-valued random variables X and Y , with expected values $\mathbb{E}(X)=\mu$ and $\mathbb{E}(Y)=\nu$ is defined as

$$
\begin{aligned}
\operatorname{Cov}(X, Y) & =\mathbb{E}((X-\mu)(Y-\nu)) \\
& =\mathbb{E}(X Y)-\mu \nu
\end{aligned}
$$

If $X \perp Y$,

$$
\mathbb{E}(X Y)=\mathbb{E}(X) \mathbb{E}(Y)=\mu \nu
$$

Then

$$
\operatorname{Cov}(X, Y)=0
$$

## Formal Statement of Model

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- $i=1, \ldots, n$


## Example

An experimenter gave three subjects a very difficult task. Data on the age of the subject $(X)$ and on the number of attempts to accomplish the task before giving up $(Y)$ follow:

Table:

| Subject $i$ | 1 | 2 | 3 |
| ---: | ---: | ---: | ---: |
| Age $X_{i}$ | 20 | 55 | 30 |
| Number of Attempts $Y_{i}$ | 5 | 12 | 10 |

## Least Squares Linear Regression

- Goal: make $Y_{i}$ and $b_{0}+b_{1} X_{i}$ close for all $i$.


## Least Squares Linear Regression

- Goal: make $Y_{i}$ and $b_{0}+b_{1} X_{i}$ close for all $i$.
- Proposal 1: minimize $\sum_{i=1}^{n}\left[Y_{i}-\left(b_{0}+b_{1} X_{i}\right)\right]$.
- Proposal 2: minimize $\sum_{i=1}^{n}\left|Y_{i}-\left(b_{0}+b_{1} X_{i}\right)\right|$.


## Least Squares Linear Regression

- Goal: make $Y_{i}$ and $b_{0}+b_{1} X_{i}$ close for all $i$.
- Proposal 1: minimize $\sum_{i=1}^{n}\left[Y_{i}-\left(b_{0}+b_{1} X_{i}\right)\right]$.
- Proposal 2: minimize $\sum_{i=1}^{n}\left|Y_{i}-\left(b_{0}+b_{1} X_{i}\right)\right|$.
- Final Proposal: minimize

$$
Q\left(b_{0}, b_{1}\right)=\sum_{i=1}^{n}\left[Y_{i}-\left(b_{0}+b_{1} X_{i}\right)\right]^{2}
$$

- Choose $b_{0}$ and $b_{1}$ as estimators for $\beta_{0}$ and $\beta_{1}$.
- $b_{0}$ and $b_{1}$ will minimize the criterion $Q$ for the given sample observations $\left(X_{1}, Y_{1}\right),\left(X_{2}, Y_{2}\right), \cdots,\left(X_{n}, Y_{n}\right)$.


## Guess \#1



## Guess \#2



## Function maximization

- Important technique to remember!
- Take derivative
- Set result equal to zero and solve
- Test second derivative at that point
- Question: does this always give you the maximum?
- Going further: multiple variables, convex optimization


## Function Maximization

Find the value of $x$ that maximize the function

$$
f(x)=-x^{2}+\log (x), x>0
$$

## Function Maximization

Find the value of $x$ that maximize the function

$$
f(x)=-x^{2}+\log (x), x>0
$$

1. Take derivative

$$
\begin{align*}
\frac{d}{d x}\left(-x^{2}+\log (x)\right) & =0  \tag{1}\\
-2 x+\frac{1}{x} & =0  \tag{2}\\
2 x^{2} & =1  \tag{3}\\
x^{2} & =\frac{1}{2}  \tag{4}\\
x & =\frac{\sqrt{2}}{2} \tag{5}
\end{align*}
$$

2. Check second order derivative

$$
\begin{align*}
\frac{d^{2}}{d x^{2}}\left(-x^{2}+\log (x)\right) & =\frac{d}{d x}\left(-2 x+\frac{1}{x}\right)  \tag{6}\\
& =-2-\frac{1}{x^{2}}  \tag{7}\\
& <0 \tag{8}
\end{align*}
$$

Then we have found the maximum. $x^{*}=\frac{\sqrt{2}}{2}, f\left(x^{*}\right)=-\frac{1}{2}[1+\log (2)]$.

## Least Squares Minimization

- Function to minimize w.r.t. $b_{0}$ and $b_{1}$
- $b_{0}$ and $b_{1}$ are called point estimators of $\beta_{0}$ and $\beta_{1}$ respectively

$$
Q\left(b_{0}, b_{1}\right)=\sum_{i=1}^{n}\left[Y_{i}-\left(b_{0}+b_{1} X_{i}\right)\right]^{2}
$$

- Find partial derivatives and set both equal to zero

$$
\begin{aligned}
& \frac{\partial Q}{\partial b_{0}}=0 \\
& \frac{\partial Q}{\partial b_{1}}=0
\end{aligned}
$$

## Normal Equations

- The result of this maximization step are called the normal equations. $b_{0}$ and $b_{1}$ are called point estimators of $\beta_{0}$ and $\beta_{1}$ respectively.

$$
\begin{align*}
\sum Y_{i} & =n b_{0}+b_{1} \sum X_{i}  \tag{9}\\
\sum X_{i} Y_{i} & =b_{0} \sum X_{i}+b_{1} \sum X_{i}^{2} \tag{10}
\end{align*}
$$

- This is a system of two equations and two unknowns.


## Solution to Normal Equations

After a lot of algebra one arrives at

$$
\begin{aligned}
b_{1} & =\frac{\sum\left(X_{i}-\bar{X}\right)\left(Y_{i}-\bar{Y}\right)}{\sum\left(X_{i}-\bar{X}\right)^{2}} \\
b_{0} & =\bar{Y}-b_{1} \bar{X} \\
\bar{X} & =\frac{\sum X_{i}}{n} \\
\bar{Y} & =\frac{\sum Y_{i}}{n}
\end{aligned}
$$

## Least Square Fit



## Properties of Solution

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

$$
e_{i}=Y_{i}-\hat{Y}_{i}
$$

- The sum of the residuals is zero from (9).

$$
\begin{aligned}
\sum_{i} e_{i} & =\sum\left(Y_{i}-b_{0}-b_{1} X_{i}\right) \\
& =\sum Y_{i}-n b_{0}-b_{1} \sum X_{i} \\
& =0
\end{aligned}
$$

- The sum of the observed values $Y_{i}$ equals the sum of the fitted values $\widehat{Y}_{i}$

$$
\sum_{i} \hat{Y}_{i}=\sum_{i} Y_{i}
$$

## Properties of Solution

The sum of the weighted residuals is zero when the residual in the $i^{t h}$ trial is weighted by the level of the predictor variable in the $i^{t h}$ trial from (10).

$$
\begin{aligned}
\sum_{i} X_{i} e_{i} & =\sum\left(X_{i}\left(Y_{i}-b_{0}-b_{1} X_{i}\right)\right) \\
& =\sum_{i} X_{i} Y_{i}-b_{0} \sum X_{i}-b_{1} \sum X_{i}^{2} \\
& =0
\end{aligned}
$$

## Properties of Solution

The sum of the weighted residuals is zero when the residual in the $i^{\text {th }}$ trial is weighted by the fitted value of the response variable in the $i^{t h}$ trial

$$
\begin{aligned}
\sum_{i} \hat{Y}_{i} e_{i} & =\sum_{i}\left(b_{0}+b_{1} X_{i}\right) e_{i} \\
& =b_{0} \sum_{i} e_{i}+b_{1} \sum_{i} X_{i} e_{i} \\
& =0
\end{aligned}
$$

## Properties of Solution

The regression line always goes through the point

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

Using the alternative format of linear regression model:

$$
Y_{i}=\beta_{0}^{*}+\beta_{1}\left(X_{i}-\bar{X}\right)+\epsilon_{i}
$$

The least squares estimator $b_{1}$ for $\beta_{1}$ remains the same as before. The least squares estimator for $\beta_{0}^{*}=\beta_{0}+\beta_{1} \bar{X}$ becomes

$$
b_{0}^{*}=b_{0}+b_{1} \bar{X}=\left(\bar{Y}-b_{1} \bar{X}\right)+b_{1} \bar{X}=\bar{Y}
$$

Hence the estimated regression function is

$$
\hat{Y}=\bar{Y}+b_{1}(X-\bar{X})
$$

Apparently, the regression line always goes through the point $(\bar{X}, \bar{Y})$.

## Estimating Error Term Variance $\sigma^{2}$

- 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

$$
\hat{\theta}=f\left(\left\{Y_{1}, \ldots, Y_{n}\right\}\right)
$$

- Unknown quantity / parameter
- Definition: Bias of estimator

$$
\operatorname{Bias}(\hat{\theta})=\mathbb{E}(\hat{\theta})-\theta
$$

## Example

- Samples

$$
Y_{i} \sim N\left(\mu, \sigma^{2}\right)
$$

- 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

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

- This is an example of an unbiased estimator

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

## Variance of Estimator

- Definition: Variance of estimator

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

- Remember:

$$
\begin{aligned}
\operatorname{Var}(c Y) & =c^{2} \operatorname{Var}(Y) \\
\operatorname{Var}\left(\sum_{i=1}^{n} Y_{i}\right) & =\sum_{i=1}^{n} \operatorname{Var}\left(Y_{i}\right)
\end{aligned}
$$

Only if the $Y_{i}$ are independent with finite variance

## Example Estimator Variance

$$
\begin{aligned}
\operatorname{Var}(\hat{\theta}) & =\operatorname{Var}\left(\frac{1}{n} \sum_{i=1}^{n} Y_{i}\right) \\
& =\frac{1}{n^{2}} \sum_{i=1}^{n} \operatorname{Var}\left(Y_{i}\right) \\
& =\frac{n \sigma^{2}}{n^{2}} \\
& =\frac{\sigma^{2}}{n}
\end{aligned}
$$

## Bias Variance Trade-off

- The mean squared error of an estimator

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

- Can be re-expressed

$$
\operatorname{MSE}(\hat{\theta})=\operatorname{Var}(\hat{\theta})+[\operatorname{Bias}(\hat{\theta})]^{2}
$$

## $\mathrm{MSE}=\mathrm{VAR}+B I A S^{2}$

## Proof

$$
\begin{aligned}
& \operatorname{MSE}(\hat{\theta}) \\
= & \mathbb{E}\left((\hat{\theta}-\theta)^{2}\right) \\
= & \mathbb{E}\left(([\hat{\theta}-\mathbb{E}(\hat{\theta})]+[\mathbb{E}(\hat{\theta})-\theta])^{2}\right) \\
= & \mathbb{E}\left([\hat{\theta}-\mathbb{E}(\hat{\theta})]^{2}\right)+2 \mathbb{E}([\mathbb{E}(\hat{\theta})-\theta][\hat{\theta}-\mathbb{E}(\hat{\theta})])+\mathbb{E}\left([\mathbb{E}(\hat{\theta})-\theta]^{2}\right) \\
= & \operatorname{Var}(\hat{\theta})+2 \mathbb{E}([\mathbb{E}(\hat{\theta})[\hat{\theta}-\mathbb{E}(\hat{\theta})]-\theta[\hat{\theta}-\mathbb{E}(\hat{\theta})]))+(\operatorname{Bias}(\hat{\theta}))^{2} \\
= & \operatorname{Var}(\hat{\theta})+2(0+0)+(\operatorname{Bias}(\hat{\theta}))^{2} \\
= & \operatorname{Var}(\hat{\theta})+(\operatorname{Bias}(\hat{\theta}))^{2}
\end{aligned}
$$

## 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 has much lower variance than the unbiased one.


## $s^{2}$ estimator for $\sigma^{2}$ for Single population

Sum of Squares:

$$
\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}\right)^{2}
$$

Sample Variance Estimator:

$$
s^{2}=\frac{\sum_{i=1}^{n}\left(Y_{i}-\bar{Y}\right)^{2}}{n-1}
$$

- $s^{2}$ is an unbiased estimator of $\sigma^{2}$.
- The sum of squares SSE has $n-1$ "degrees of freedom" associated with it, one degree of freedom is lost by using $\bar{Y}$ as an estimate of the unknown population mean $\mu$.


## Estimating Error Term Variance $\sigma^{2}$ for Regression Model

- Regression model
- Variance of each observation $Y_{i}$ is $\sigma^{2}$ (the same as for the error term $\epsilon_{i}$ )
- 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 $\sigma^{2}$

$$
s^{2}=M S E=\frac{S S E}{n-2}=\frac{\sum\left(Y_{i}-\hat{Y}_{i}\right)^{2}}{n-2}=\frac{\sum e_{i}^{2}}{n-2}
$$

- MSE is an unbiased estimator of $\sigma^{2}$

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

- 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 $\epsilon_{i}$ are distributed, the least squares method provides unbiased point estimators of $\beta_{0}$ and $\beta_{1}$
- 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 $\epsilon_{i}$
- We will assume that the $\epsilon_{i}$ 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 $i^{\text {th }}$ trial
- $\beta_{0}$ and $\beta_{1}$ are parameters
- $X_{i}$ is a known constant, the value of the predictor variable in the $i^{\text {th }}$ trial
- $\epsilon_{i} \sim_{i i d} N\left(0, \sigma^{2}\right)$ note this is different, now we know the distribution
- $i=1, \ldots, n$


## Notational Convention

- When you see $\epsilon_{i} \sim_{i i d} N\left(0, \sigma^{2}\right)$
- It is read as $\epsilon_{i}$ is identically and independently distributed according to a normal distribution with mean 0 and variance $\sigma^{2}$


## 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

$$
X_{i} \sim F(\Theta), i=1 \ldots n
$$

then the likelihood function is

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

## Maximum Likelihood Estimation

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

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

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

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

## Important Trick

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

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

Usually the log of the likelihood is easier to work with mathematically.

## ML Normal Regression

Likelihood function

$$
\begin{aligned}
\mathcal{L}\left(\beta_{0}, \beta_{1}, \sigma^{2}\right) & =\prod_{i=1}^{n} \frac{1}{\left(2 \pi \sigma^{2}\right)^{1 / 2}} e^{-\frac{1}{2 \sigma^{2}}\left(Y_{i}-\beta_{0}-\beta_{1} X_{i}\right)^{2}} \\
& =\frac{1}{\left(2 \pi \sigma^{2}\right)^{n / 2}} e^{-\frac{1}{2 \sigma^{2}} \sum_{i=1}^{n}\left(Y_{i}-\beta_{0}-\beta_{1} X_{i}\right)^{2}}
\end{aligned}
$$

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

## Maximum Likelihood Estimator(s)

- $\beta_{0}$
$b_{0}$ same as in least squares case
- $\beta_{1}$
$b_{1}$ same as in least squares case
- $\sigma^{2}$

$$
\hat{\sigma}^{2}=\frac{\sum_{i}\left(Y_{i}-\hat{Y}_{i}\right)^{2}}{n}
$$

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

$$
s^{2}=M S E=\frac{n}{n-2} \hat{\sigma}^{2}
$$

## 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)

