# Purdue-NCKU program 

# Lecture 7 <br> Simple Linear Regression 

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## Goals of Regression Analysis

Regression: use data $\left(Y_{i}, X_{i}\right)$ to find out a relationship

$$
E(Y)=f_{\beta}(X)
$$

or median, mode of $Y$ if possible.

- Serve three purposes
- Describes an association between $X$ and $Y$
* In some applications, the choice of which variable is $X$ and which is Y can be arbitrary
* Association generally does not imply causality
- In experimental settings, helps select $X$ to control $Y$ at the desired level
- Predict a future value of $Y$ at a specific value of $X$


## Straight Line Mean Equation

- Formula for a straight line

$$
E\left(Y_{i}\right)=\beta_{0}+\beta_{1} X_{i}, \text { or } E\left(Y_{i} \mid X_{i}\right)=\beta_{0}+\beta_{1} X_{i}
$$

$-\beta_{0}$ is the intercept
$-\beta_{1}$ is the slope

- Need to estimate $\beta_{0}$ and $\beta_{1}$
i.e. determine their plausible values from the data
- Will use method of least squares (OLS estimator).


## Simple Linear Regression Model

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

- $\beta_{0}$ is the intercept
- $\beta_{1}$ is the slope
- $\varepsilon_{i}$ is the $i^{\text {th }}$ random error term
- Mean 0, i.e. $E\left(\varepsilon_{i}\right)=0$
- Constant Variance $\sigma^{2}$, i.e. $\operatorname{Var}\left(\varepsilon_{i}\right)=\sigma^{2}$
- Uncorrelated, i.e. $\operatorname{Cov}\left(\varepsilon_{i}, \varepsilon_{j}\right)=0$
- Independent to $X_{i}$ if $X_{i}$ is random


## Estimation of Regression Function

- Consider the deviation of observed data $Y_{i}$ from a straight line with slope $a$ and intercept $b$,

$$
Y_{i}-\left(a X_{i}+b\right)
$$

it measures how good the line $a x+b$ fits the data $\left(X_{i}, Y_{i}\right)$ in terms of vertical distance

- Method of least squares (smallest sum of squared derivation)
- Find the value of $a$ and $b$ which minimize

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

- Motivated by $E(Y)=\arg \min _{b} E(Y-b)^{2} \approx \arg \min _{b} \sum\left(Y_{i}-\right.$ $b)^{2} / n$.


## Estimating $\beta^{\prime}$ 's

- $\beta_{1}$ is the true unknown slope
- Defines change in $E(Y)$ for change in $X$, i.e.,

$$
\beta_{1}=\frac{\Delta E(Y)}{\Delta X}
$$

- $b_{1}$ is the least squares estimate of $\beta_{1}$

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

- $\beta_{0}$ is the true unknown intercept
- $\beta_{0}$ is the expected value of $Y$ under $X=0$

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

- $b_{0}$ is the least squares estimate of $\beta_{0}$

$$
b_{0}=\bar{Y}-b_{1} \bar{X}
$$

that is, the fitted line goes through $(\bar{X}, \bar{Y})$.

## Properties of Estimates

- $b_{1}$ is a linear estimator, i.e., a linear combination of $Y_{i}$ 's.

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

where $k_{i}=\left(X_{i}-\bar{X}\right) / \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}$

- Note that $\sum k_{i}=0, \sum k_{i} X_{i}=1$, thus

$$
\begin{aligned}
E\left(b_{1}\right) & =\sum k_{i} E\left(Y_{i}\right)=\sum k_{i}\left(\beta_{0}+\beta_{1} X_{i}\right) \\
& =\beta_{0} \sum k_{i}+\beta_{1} \sum k_{i} X_{i} \\
& =0+\beta_{1},
\end{aligned}
$$

- $b_{0}$ is also a linear combination of $Y_{i}$ 's,

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

where

$$
\tilde{k}_{i}=\frac{1}{n}-\frac{\bar{X}\left(X_{i}-\bar{X}\right)}{\sum\left(X_{i}-\bar{X}\right)^{2}}
$$

- Note $\sum \tilde{k}_{i}=1, \sum \tilde{k}_{i} X_{i}=0$.

$$
\begin{aligned}
E\left(b_{0}\right) & =\sum \tilde{k}_{i} E\left(Y_{i}\right)=\sum \tilde{k}_{i}\left(\beta_{0}+\beta_{1} X_{i}\right) \\
& =\beta_{0} \sum \tilde{k}_{i}+\beta_{1} \sum \tilde{k}_{i} X_{i} \\
& =\beta_{0}+0
\end{aligned}
$$

## Estimated Regression Line

- Using the estimated parameters, the fitted regression line is

$$
\widehat{Y}_{i}=b_{0}+b_{1} X_{i}
$$

where $\widehat{Y}_{i}$ is the estimated value at $X_{i}$ (Fitted value).

- Fitted value $\hat{Y}_{i}$ is also an estimate of the mean response $E\left(Y_{i}\right)$
- $\widehat{Y}_{i}=\sum_{j=1}^{n}\left(\widetilde{k}_{j}+X_{i} k_{j}\right) Y_{j}=\sum_{j=1}^{n} \check{k}_{i j} Y_{j}$ is also a linear estimator
- $E\left(\widehat{Y}_{i}\right)=E\left(b_{0}+b_{1} X_{i}\right)=E\left(b_{0}\right)+E\left(b_{1}\right) X_{i}=\beta_{0}+\beta_{1} X_{i}=E\left(Y_{i}\right)$
- Gauss-Markov theorem: $b_{0}, b_{1}$ and $\widehat{Y}_{i}$ have minimum variance among all unbiased linear estimators.


## Residuals

- The residual is the difference between the observed and fitted values

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

- This is not the error term $\varepsilon_{i}=Y_{i}-E\left(Y_{i}\right)$
- The $e_{i}$ is observable while $\varepsilon_{i}$ is not
$-\sum e_{i}=0$
$-\sum Y_{i}=\sum \hat{Y}_{i}$
$-\sum X_{i} e_{i}=0$
$-\sum \hat{Y}_{i} e_{i}=0$


## Estimation of Error Variance

- In regression model

$$
s^{2}=\frac{\sum\left(Y_{i}-\widehat{Y}_{i}\right)^{2}}{n-2}
$$

- Also known as the mean square error (MSE)
- Two df lost by using ( $b_{0}, b_{1}$ ) in place of $\left(\beta_{0}, \beta_{1}\right)$
- unbiased estimation

$$
\begin{aligned}
\sum\left(Y_{i}-\widehat{Y}_{i}\right)^{2} & =\sum e_{i}\left(Y_{i}-\widehat{Y}_{i}\right)=\sum e_{i} Y_{i} \\
& =\sum e_{i}\left(\beta_{0}+\beta_{1} X_{i}+\varepsilon_{i}\right)=\sum e_{i} \varepsilon_{i} \\
& =\sum Y_{i} \varepsilon_{i}-\sum \widehat{Y}_{i} \varepsilon_{i} \\
E\left(Y_{i} \varepsilon_{i}\right) & =E\left(\beta_{0}+\beta_{1} X_{i}+\varepsilon_{i}\right) \varepsilon_{i}=E\left(\varepsilon^{2}\right)=\sigma^{2}, \\
E\left(\widehat{Y}_{i} \varepsilon_{i}\right) & =E\left(\sum_{j=1}^{n} \check{k}_{i j} Y_{j}\right) \varepsilon_{i}=E \check{k}_{i i} Y_{i} \varepsilon_{i}=\check{k}_{i i} \sigma^{2}
\end{aligned}
$$

Note that $\breve{k}_{i i}=\widetilde{k}_{i}+X_{i} k_{i}$ and the properties of $k_{i}$ and $\widetilde{k}_{i}$, we can show that $E\left(s^{2}\right)=\sigma^{2}$

## Normal Error Regression Model

$$
Y_{i}=\beta_{0}+\beta_{1} X_{i}+\varepsilon_{i}, \varepsilon_{i} \sim^{i i d} N\left(0, \sigma^{2}\right)
$$

- the random error term is assumed to be independent normally distributed
- Defines distribution of random variable $Y_{i}$

$$
Y_{i} \sim N\left(\beta_{0}+\beta_{1} X_{i}, \sigma^{2}\right)
$$

- The normality assumption will greatly simplifies the theory of analysis beyond estimations, allows us to construct confidence intervals / perform hypothesis tests
- Most inferences are only sensitive to large departures from normality


## Sampling Distribution of $b_{i}$ 's

- Under the normality assumption, $b_{1}$ also follows a normal distribution since it is a linear combination of normal r.v.s.
- It is sufficient to figure the first two moments of $b_{1}$ :

$$
\begin{aligned}
E\left(b_{1}\right) & =\beta_{1} \\
\operatorname{Var}\left(b_{1}\right) & =\sum k_{i}^{2} \operatorname{Var}\left(Y_{i}\right)=\frac{\sigma^{2}}{\sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}
\end{aligned}
$$

- Therefore

$$
b_{1} \sim N\left(\beta_{1}, \sigma^{2} / \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}\right)
$$

- $b_{0}$ is also a linear combination of $Y_{i}{ }^{\prime}$ s, $b_{0}=\sum \tilde{k}_{i} Y_{i}$, thus by normal assumption, $b_{0} \sim N\left(E\left(b_{0}\right), \operatorname{Var}\left(b_{0}\right)\right)$, where

$$
\begin{aligned}
E\left(b_{0}\right) & =\beta_{0} \\
\operatorname{Var}\left(b_{0}\right) & =\sum \tilde{k}_{i}^{2} \operatorname{Var}\left(Y_{i}\right)=\sigma^{2}\left[\frac{1}{n}+\frac{\bar{X}^{2}}{\sum\left(X_{i}-\bar{X}\right)^{2}}\right]
\end{aligned}
$$

## $t$-test for $H_{0}: \beta_{1}=\beta_{1}^{0}$

- Consider statistics $\frac{b_{1}-\beta_{1}^{0}}{s e\left(b_{1}\right)}$, where standard error of $b_{1}$ means an estimation for the $\sqrt{\operatorname{Var}\left(b_{1}\right)}$.
- $s e\left(b_{1}\right)=\sqrt{s^{2} / \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}$, that is to replace the unknown $\sigma^{2}$ by its unbiased estimator $s^{2}=M S E=\sum\left(Y_{i}-\widehat{Y}_{i}\right)^{2} /(n-2)$,
- The test statistics is

$$
\frac{b_{1}-\beta_{1}^{0}}{s e\left(b_{1}\right)}=\frac{b_{1}-\beta_{1}^{0}}{\sqrt{s^{2} / \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}}}
$$

- $(n-2) s^{2} / \sigma^{2} \sim \chi_{n-2}^{2}$ and $s^{2}$ is independent to $b_{1}$ (will be proved later), then $\frac{b_{1}-\beta_{1}^{0}}{s e\left(b_{1}\right)} \sim t_{n-2}$


## $t$-test for $H_{0}: \beta_{1}=\beta_{1}^{0}$

$t$-test statistics $t^{*}=\frac{b_{1}-\beta_{1}^{0}}{s e\left(b_{1}\right)}$ under level $\alpha$

- Reject if $\left|t^{*}\right| \geq t(1-\alpha / 2, n-2)$ or p -value $P\left(\left|t_{n-2}\right| \geq\left|t^{*}\right|\right) \leq \alpha$


## C.I for $\beta_{1}$

$b_{1} \pm t(1-\alpha / 2, n-2) s e\left(b_{1}\right)$
Similar inference for $\beta_{0}$.

## Comments

- When errors not normal, procedures are generally reasonable approximations
- Procedures can be modified for one-sided test / confidence intervals
- To obtain an accurate interval estimation, at design stage, choose $X_{i}$ such that
$-\sum\left(X_{i}-\bar{X}\right)^{2}$ is large $\rightarrow$ smaller margin of error for $\beta_{1}$
$-\sum\left(X_{i}-\bar{X}\right)^{2}$ is large and $|\bar{X}|$ is small $\rightarrow$ smaller margin of error for $\beta_{0}$


## Interval Estimation of $E\left(Y_{h}\right)$

- Often interested in estimating the mean response for particular $X_{h}$, i.e., the parameter of interests is $E\left(Y_{h}\right)=\beta_{0}+\beta_{1} X_{h}$.
- Unbiased estimation is $\hat{Y}_{h}=b_{0}+b_{1} X_{h}$.
- Derive the sampling distribution of $b_{0}+b_{1} X_{h}$ in order to make test and CI.

$$
\begin{aligned}
& -\widehat{Y}_{h}=\sum \breve{k}_{i} Y_{i} \text { where } k_{i}=\frac{1}{n}+\frac{\left(X_{h}-\bar{X}\right)\left(X_{i}-\bar{X}\right)}{\sum\left(X_{i}-\bar{X}\right)^{2}} \\
& -E\left(\hat{Y}_{h}\right)=\beta_{0}+\beta_{1} X_{h} \\
& -\operatorname{Var}\left(\widehat{Y}_{h}\right)=\sigma^{2}\left[\frac{1}{n}+\frac{\left(X_{h}-\bar{X}\right)^{2}}{\sum\left(X_{i}-\bar{X}\right)^{2}}\right], s e^{2}\left(\widehat{Y}_{h}\right)=s^{2}\left[\frac{1}{n}+\frac{\left(X_{h}-\bar{X}\right)^{2}}{\sum\left(X_{i}-\bar{X}\right)^{2}}\right] . \\
& \text { - Test: }\left(\widehat{Y}_{h}-\text { null value }\right) / s e\left(\widehat{Y}_{h}\right) ; \text { CI: } \hat{Y}_{h} \pm t(1-\alpha / 2, n-2) \operatorname{se}\left(\widehat{Y}_{h}\right)
\end{aligned}
$$

## Interval Prediction of $Y_{h(n e w)}$

- Predicting future observation $Y_{h(n e w)}=E\left[Y_{h}\right]+\varepsilon_{h(n e w)}$
- The prediction interval for a unknown r.v., i.e., $P\left(L<Y_{h(n e w)}<\right.$ $U)=1-\alpha$
- Comparing with CI of $E\left[Y_{h}\right]$, one need to take account of future error $\varepsilon_{h(n e w)}$.
$-E\left(b_{0}+b_{1} X_{h}\right)=E\left(Y_{h(n e w)}\right)$
$-\operatorname{Var}\left(Y_{h(n e w)}-b_{0}+b_{1} X_{h}\right)=\sigma^{2}\left[1+\frac{1}{n}+\frac{\left(X_{h}-\bar{X}\right)^{2}}{\sum\left(X_{i}-\bar{X}\right)^{2}}\right]$
$-s e^{2}\left(Y_{h(n e w)}-b_{0}+b_{1} X_{h}\right)=s^{2}\left[1+\frac{1}{n}+\frac{\left(X_{h}-\bar{X}\right)^{2}}{\sum\left(X_{i}-\bar{X}\right)^{2}}\right]$
- PI: $b_{0}+b_{1} X_{h} \pm t(1-\alpha / 2, n-2) \sqrt{s^{2}\left[1+\frac{1}{n}+\frac{\left(X_{h}-\bar{X}\right)^{2}}{\sum\left(X_{i}-\bar{X}\right)^{2}}\right]}$


## Confidence Band for Response Means

- Consider the entire regression line
- Want to define a likely region within which this unknown real line lies
- Rigorously, $P\left(L(x)<\beta_{0}+\beta_{1} x<U(x)\right.$ for all $\left.x\right) \geq 1-\alpha$
- One can show

$$
\max _{x}\left[\frac{b_{0}+b_{1} x-\left(\beta_{0}+\beta_{1} x\right)}{\operatorname{se}\left(\hat{Y}_{h}\right)(x)}\right]^{2} \sim 2 F_{2, n-2}
$$

- Replace $t(1-\alpha / 2, n-2)$ with Working-Hotelling value in each confidence interval

$$
W=\sqrt{2 F(1-\alpha ; 2, n-2)} \Rightarrow \widehat{Y}_{h} \pm W \times \operatorname{se}\left(\hat{Y}_{h}\right)
$$

- Boundary values define a hyperbola


## Confidence Band vs C.I. vs P.I.



- Blue - 95\% confidence band; widest when $X_{h}-X$ is large
- Red - 95\% confidence interval for the mean; always narrowest
- Green - 95\% confidence interval for the individual prediction; widest when $X_{h}-\bar{X}$ is small


## ANOVA approach

- Organizes results arithmetically
- The total sum of squares in $Y$ is defined

$$
\mathrm{SSTO}=\sum\left(Y_{i}-\bar{Y}\right)^{2}
$$

- Can partition the total sum of squares into
- Model (explained by regression)
- Error (unexplained / residual)

$$
\begin{aligned}
\sum\left(Y_{i}-\bar{Y}\right)^{2} & =\sum\left(Y_{i}-\hat{Y}_{i}+\widehat{Y}_{i}-\bar{Y}\right)^{2} \\
& =\sum\left(Y_{i}-\widehat{Y}_{i}\right)^{2}+\sum_{\text {SSTO }}\left(\widehat{Y}_{i}-\bar{Y}\right)^{2} \\
& =\mathrm{SSE}+\mathrm{SSR}
\end{aligned}
$$

## Sum of Squares

- Can also express

$$
\begin{aligned}
\mathrm{SSR} & =\sum\left(\hat{Y}_{i}-\bar{Y}\right)^{2} \\
& =\sum\left(b_{0}+b_{1} X_{i}-b_{0}-b_{1} \bar{X}\right)^{2} \\
& =b_{1}^{2} \sum\left(X_{i}-\bar{X}\right)^{2}
\end{aligned}
$$

- Degrees of freedom is 1 due to normality of $b_{1}$ for some $\delta$.
- SSR large when $\hat{Y}_{i}$ 's are different from $\bar{Y}$
- Error sum of squares is equal to the sum of squared residuals

$$
\text { SSE }=\sum\left(Y_{i}-\widehat{Y}_{i}\right)^{2}=\sum e_{i}^{2}
$$

- Degrees of freedom is $n-2$ due to using $\left(b_{0}, b_{1}\right)$ in place of ( $\beta_{0}, \beta_{1}$ ), and SSE $\sim \sigma^{2} \chi_{n-2}^{2}$
- The MSE $=$ SSE/ $(n-2)$ and represents an unbiased estimate of $\sigma^{2}$ when taking $X$ into account


## F Test

- Can use this structure to test $H_{0}: \beta_{1}=0$
- Consider

$$
F^{*}=\frac{\mathrm{MSR}}{\mathrm{MSE}}
$$

- If $\beta_{1}=0$, then $F^{*}$ should be near one, since both denominator and numerator are of mean
sigma ${ }^{2}$.
- Need sampling distribution of $F^{*}$ under $H_{0}$ to obtain p-value.

$$
F^{*} \operatorname{sim} \quad F_{1, n-2}
$$

- When $H_{0}$ is false, $F^{*}$ tends to be large
- p -value $=\operatorname{Pr}\left(F(1, n-2)>F^{*}\right)$
- Reject when $F^{*}>F_{1, n-2,1-\alpha}$, or p-value $<\alpha$


## General Linear Test

- A third way to test for linear association
- Consider two models
- Full model: $Y_{i}=\beta_{0}+\beta_{1} X_{i}+\varepsilon_{i}$
- Reduced model: $Y_{i}=\beta_{0}+\varepsilon_{i}$
- Will compare models using SSE's
- Error sum of squares of the full model will be labeled SSE(F)
- Error sum of squares of the reduced model will be labeled SSE(R)
- Note: SSTO is the same under each model
- Reduced model corresponds to $H_{0}: \beta_{1}=0$
- Can be shown that $\operatorname{SSE}(F) \leq \operatorname{SSE}(R)$
- Idea: more parameters provide better fit
- If SSE (F) is not much smaller than SSE(R), full model doesn't better explain $Y$.

$$
\begin{aligned}
F^{*} & =\frac{(\operatorname{SSE}(\mathrm{R})-\operatorname{SSE}(F)) /\left(d f_{R}-d f_{F}\right)}{\operatorname{SSE}(F) / d f_{F}} \\
& =\frac{(\operatorname{SSTO}-\operatorname{SSE}) / 1}{\operatorname{SSE}(F) /(n-2)}
\end{aligned}
$$

- Same test as before, but will have a more general use in multiple regression


## Diagnose

- use a residual plots ( $e_{i}$ vs $\widehat{Y}_{i}$ ) to check
- linearity
- constant variance
- never plot $e_{i}$ vs $Y_{i}$
- normality
- Boxcox transformation


## Matrix Approach

- Consider example with $n=4$
- Consider expressing observations:

$$
\begin{aligned}
Y_{1} & = \\
Y_{2} & =\begin{array}{ll}
\beta_{0}+\beta_{1} X_{1} \\
\beta_{0}+\beta_{1} X_{2} & +\varepsilon_{1} \\
Y_{3} & =\begin{array}{l}
2 \\
\beta_{0}+\beta_{1} X_{3} \\
+\varepsilon_{3} \\
Y_{4}
\end{array}
\end{array} \begin{array}{ll}
\beta_{0}+\beta_{1} X_{4} & +\varepsilon_{4}
\end{array} \\
{\left[\begin{array}{l}
Y_{1} \\
Y_{2} \\
Y_{3} \\
Y_{4}
\end{array}\right] } & =\left[\begin{array}{ll}
\beta_{0}+\beta_{1} X_{1} \\
\beta_{0}+\beta_{1} X_{2} \\
\beta_{0}+\beta_{1} X_{3} \\
\beta_{0}+\beta_{1} X_{4}
\end{array}\right]
\end{aligned}+\left[\begin{array}{l}
\varepsilon_{1} \\
\varepsilon_{2} \\
\varepsilon_{3} \\
\varepsilon_{4}
\end{array}\right] .
$$

- $\mathbf{X}$ is called the design matrix


## Regression Matrices

- Can express observations

$$
\mathbf{Y}=\mathbf{X} \boldsymbol{\beta}+\varepsilon
$$

- Both Y and $\varepsilon$ are random vectors

$$
\begin{aligned}
E(\mathrm{Y}) & =\mathbf{X} \boldsymbol{\beta}+E(\varepsilon) \\
& =\mathbf{X} \boldsymbol{\beta} \\
\boldsymbol{\sigma}^{2}(\mathbf{Y}) & =0 \quad{ }^{+\boldsymbol{\sigma}^{2}(\varepsilon)} \\
& =\sigma^{2} \mathbf{I}
\end{aligned}
$$

## Least Squares

- Express quantity $Q$

$$
\begin{aligned}
Q & =(\mathbf{Y}-\mathbf{X} \boldsymbol{\beta})^{\prime}(\mathbf{Y}-\mathbf{X} \boldsymbol{\beta}) \\
& =\mathbf{Y}^{\prime} \mathbf{Y}-\boldsymbol{\beta}^{\prime} \mathbf{X}^{\prime} \mathbf{Y}-\mathbf{Y}^{\prime} \mathbf{X} \boldsymbol{\beta}+\boldsymbol{\beta}^{\prime} \mathbf{X}^{\prime} \mathbf{X} \boldsymbol{\beta} \\
& =\mathbf{Y}^{\prime} \mathbf{Y}-2 \boldsymbol{\beta}^{\prime} \mathbf{X}^{\prime} \mathbf{Y}+\boldsymbol{\beta}^{\prime} \mathbf{X}^{\prime} \mathbf{X} \boldsymbol{\beta}
\end{aligned}
$$

$$
-(\mathbf{X} \boldsymbol{\beta})^{\prime}=\boldsymbol{\beta}^{\prime} \mathbf{X}^{\prime}
$$

- Taking derivative $\longrightarrow-2 \mathbf{X}^{\prime} \mathbf{Y}+2 \mathbf{X}^{\prime} \mathbf{X} \boldsymbol{\beta}=0$

$$
\begin{aligned}
& -\frac{\partial}{\partial \beta} \boldsymbol{\beta}^{\prime} \mathbf{X}^{\prime} \mathbf{Y}=\mathbf{X}^{\prime} \mathbf{Y} \\
& -\frac{\partial}{\partial \beta} \boldsymbol{\beta}^{\prime} \mathbf{X}^{\prime} \mathbf{X} \boldsymbol{\beta}=2 \mathbf{X}^{\prime} \mathbf{X} \boldsymbol{\beta}
\end{aligned}
$$

- This means $\mathbf{b}=\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{Y}$


## Fitted Values

- The fitted values $\hat{\mathbf{Y}}=\mathbf{X} b=\mathbf{X}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{Y}$
- Matrix $\mathbf{H}=\mathbf{X}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime}$ is called the hat matrix
-H is symmetric, i.e., $\mathrm{H}^{\prime}=\mathrm{H}$
-H is idempotent, i.e., $\mathrm{HH}=\mathrm{H}$
- Equivalently write $\hat{\mathbf{Y}}=\mathbf{H Y}$
- Matrix H used in diagnostics (Chapter 9)


## Residuals

- Residual matrix

$$
\begin{aligned}
\mathbf{e} & =\mathbf{Y}-\hat{\mathbf{Y}} \\
& =\mathbf{Y}-\mathbf{H Y} \\
& =(\mathbf{I}-\mathbf{H}) \mathbf{Y}
\end{aligned}
$$

- $\mathbf{e}$ is a random vector

$$
\begin{aligned}
E(\mathrm{e}) & =(\mathbf{I}-\mathbf{H}) \times E(\mathbf{Y}) \\
& =(\mathbf{I}-\mathbf{H}) \mathbf{X} \boldsymbol{\beta} \\
& =\mathbf{X} \boldsymbol{\beta}-\mathbf{X} \boldsymbol{\beta} \\
& =0 \\
\sigma^{2}(\mathbf{e}) & =(\mathbf{I}-\mathbf{H}) \times \boldsymbol{\sigma}^{2}(\mathbf{Y}) \times(\mathbf{I}-\mathbf{H})^{\prime} \\
& =(\mathbf{I}-\mathbf{H}) \sigma^{2} \mathbf{I}(\mathbf{I}-\mathbf{H})^{\prime} \\
& =(\mathbf{I}-\mathbf{H}) \sigma^{2}
\end{aligned}
$$

## Inference

- Vector $\mathbf{b}=\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{Y}=\mathbf{A Y}$
- The mean and variance are

$$
\begin{aligned}
E(\mathbf{b}) & =\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} E(\mathbf{Y}) \\
& =\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1} \mathbf{X}^{\prime} \mathbf{X} \boldsymbol{\beta} \\
& =\boldsymbol{\beta} \\
\sigma^{2}(\mathbf{b}) & =\mathbf{A} \times \sigma^{2}(\mathbf{Y}) \times \mathbf{A}^{\prime} \\
& =\mathbf{A} \times \sigma^{2} \mathbf{I} \times \mathbf{A}^{\prime} \\
& =\sigma^{2} \mathbf{A A ^ { \prime }} \\
& =\sigma^{2}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1}
\end{aligned}
$$

- Thus, $\mathbf{b}$ is multivariate $\operatorname{Normal}\left(\boldsymbol{\beta}, \sigma^{2}\left(\mathbf{X}^{\prime} \mathbf{X}\right)^{-1}\right)$
- $S S E=(\mathbf{e})^{\prime}(\mathbf{e})=\mathbf{Y}^{\prime}(\mathbf{I}-\mathbf{H}) \mathbf{Y} \sim \sigma^{2} \chi_{n-2}^{2}$
- Since b and (e) are indep, SSE and b are independent


## Chapter Review

- Simple linear regression
- OLS estimation and prediction
- Inference and confidence band

