Purdue-NCKU program

Lecture 7 Simple Linear Regression

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Goals of Regression Analysis

Regression: use data (Y_i, X_i) 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 \boldsymbol{X} to control \boldsymbol{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

 $E(Y_i) = \beta_0 + \beta_1 X_i$, or $E(Y_i|X_i) = \beta_0 + \beta_1 X_i$

- $-\beta_0$ is the intercept
- β_1 is the slope
- Need to **estimate** β_0 and β_1 i.e. determine their plausible values from the data
- Will use method of least squares (OLS estimator).

Simple Linear Regression Model

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

- β_0 is the intercept
- β_1 is the slope
- ε_i is the i^{th} random error term
 - Mean 0, i.e. $E(\varepsilon_i) = 0$
 - Constant Variance σ^2 , i.e. $Var(\varepsilon_i) = \sigma^2$
 - Uncorrelated, i.e. $Cov(\varepsilon_i, \varepsilon_j) = 0$
 - 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,

$$Y_i - (aX_i + b)$$

it measures how good the line ax + b fits the data (X_i, Y_i) in terms of vertical distance

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

$$Q = \sum_{i=1}^{n} [Y_i - (aX_i + b)]^2$$

- Motivated by $E(Y) = \arg \min_b E(Y-b)^2 \approx \arg \min_b \sum (Y_i - b)^2/n$.

Estimating β 's

- β_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 β_1

$$b_1 = \frac{\sum_{i=1}^n (X_i - \overline{X})(Y_i - \overline{Y})}{\sum_{i=1}^n (X_i - \overline{X})^2}$$

• β_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 β_0

$$b_0 = \overline{Y} - b_1 \overline{X}$$

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

Properties of Estimates

• b_1 is a linear estimator, i.e., a linear combination of Y_i 's.

$$b_1 = \sum_{i=1}^n \frac{(X_i - \overline{X})(Y_i - \overline{Y})}{\sum_{i=1}^n (X_i - \overline{X})^2} = \sum_{i=1}^n \frac{(X_i - \overline{X})Y_i}{\sum_{i=1}^n (X_i - \overline{X})^2}$$
$$= \sum_{i=1}^n \frac{(X_i - \overline{X})}{\sum_{i=1}^n (X_i - \overline{X})^2} Y_i$$
$$= \sum_{i=1}^n k_i Y_i$$

where $k_i = (X_i - \overline{X}) / \sum_{i=1}^n (X_i - \overline{X})^2$

• Note that $\sum k_i = 0$, $\sum k_i X_i = 1$, thus

$$E(b_1) = \sum k_i E(Y_i) = \sum k_i (\beta_0 + \beta_1 X_i)$$

= $\beta_0 \sum k_i + \beta_1 \sum k_i X_i$
= $0 + \beta_1$,

• b_0 is also a linear combination of Y_i 's,

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

where

$$\tilde{k}_i = \frac{1}{n} - \frac{\overline{X}(X_i - \overline{X})}{\sum (X_i - \overline{X})^2}$$

• Note $\sum \tilde{k}_i = 1$, $\sum \tilde{k}_i X_i = 0$.

$$E(b_0) = \sum \tilde{k}_i E(Y_i) = \sum \tilde{k}_i (\beta_0 + \beta_1 X_i)$$

= $\beta_0 \sum \tilde{k}_i + \beta_1 \sum \tilde{k}_i X_i$
= $\beta_0 + 0$,

Estimated Regression Line

• Using the estimated parameters, the fitted regression line is

$$\widehat{Y}_i = b_0 + b_1 X_i$$

where \hat{Y}_i is the estimated value at X_i (Fitted value).

- Fitted value \hat{Y}_i is also an estimate of the mean response $E(Y_i)$
- $\hat{Y}_i = \sum_{j=1}^n (\tilde{k}_j + X_i k_j) Y_j = \sum_{j=1}^n \check{k}_{ij} Y_j$ is also a linear estimator
- $E(\hat{Y}_i) = E(b_0 + b_1 X_i) = E(b_0) + E(b_1) X_i = \beta_0 + \beta_1 X_i = E(Y_i)$

• Gauss-Markov theorem: b_0 , b_1 and \hat{Y}_i have minimum variance among all unbiased linear estimators.

Residuals

• The *residual* is the difference between the observed and fitted values

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

- This is not the error term $\varepsilon_i = Y_i E(Y_i)$
- The e_i is observable while ε_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

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

- Also known as the mean square error (MSE)
- Two df lost by using (b_0, b_1) in place of (β_0, β_1)
- unbiased estimation

$$\sum (Y_i - \hat{Y}_i)^2 = \sum e_i (Y_i - \hat{Y}_i) = \sum e_i Y_i$$

=
$$\sum e_i (\beta_0 + \beta_1 X_i + \varepsilon_i) = \sum e_i \varepsilon_i$$

=
$$\sum Y_i \varepsilon_i - \sum \hat{Y}_i \varepsilon_i,$$

$$E(Y_i \varepsilon_i) = E(\beta_0 + \beta_1 X_i + \varepsilon_i) \varepsilon_i = E(\varepsilon^2) = \sigma^2,$$

$$E(\hat{Y}_i \varepsilon_i) = E(\sum_{j=1}^n \check{k}_{ij} Y_j) \varepsilon_i = E\check{k}_{ii} Y_i \varepsilon_i = \check{k}_{ii} \sigma^2$$

Note that $\check{k}_{ii} = \tilde{k}_i + X_i k_i$ and the properties of k_i and \tilde{k}_i , we can show that $E(s^2) = \sigma^2$

Normal Error Regression Model

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \varepsilon_i \sim^{iid} N(0, \sigma^2)$$

- the random error term is assumed to be **independent nor**mally distributed
- Defines distribution of random variable Y_i

$$Y_i \sim N(\beta_0 + \beta_1 X_i, \sigma^2)$$

- 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 :

$$E(b_1) = \beta_1,$$

$$Var(b_1) = \sum k_i^2 Var(Y_i) = \frac{\sigma^2}{\sum_{i=1}^n (X_i - \overline{X})^2}.$$

• Therefore

$$b_1 \sim N(\beta_1, \sigma^2 / \sum_{i=1}^n (X_i - \overline{X})^2)$$

• b_0 is also a linear combination of Y_i 's, $b_0 = \sum \tilde{k}_i Y_i$, thus by normal assumption, $b_0 \sim N(E(b_0), Var(b_0))$, where

$$E(b_0) = \beta_0,$$

$$Var(b_0) = \sum \tilde{k}_i^2 Var(Y_i) = \sigma^2 \left[\frac{1}{n} + \frac{\overline{X}^2}{\sum (X_i - \overline{X})^2} \right].$$
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t-test for H_0 : $\beta_1 = \beta_1^0$

- Consider statistics $\frac{b_1 \beta_1^0}{se(b_1)}$, where standard error of b_1 means an estimation for the $\sqrt{Var(b_1)}$.
- $se(b_1) = \sqrt{s^2 / \sum_{i=1}^n (X_i \overline{X})^2}$, that is to replace the unknown σ^2 by its unbiased estimator $s^2 = MSE = \sum (Y_i \hat{Y}_i)^2 / (n-2)$,
- The test statistics is

$$\frac{b_1 - \beta_1^0}{se(b_1)} = \frac{b_1 - \beta_1^0}{\sqrt{s^2 / \sum_{i=1}^n (X_i - \overline{X})^2}}$$

• $(n-2)s^2/\sigma^2 \sim \chi^2_{n-2}$ and s^2 is independent to b_1 (will be proved later), then $\frac{b_1-\beta_1^0}{se(b_1)}\sim t_{n-2}$

t-test for
$$H_0$$
 : $\beta_1 = \beta_1^0$

t-test statistics
$$t^* = rac{b_1 - eta_1^0}{se(b_1)}$$
 under level $lpha$

• Reject if $|t^*| \ge t(1 - \alpha/2, n - 2)$ or p-value $P(|t_{n-2}| \ge |t^*|) \le \alpha$

C.I for β_1

 $b_1 \pm t(1 - \alpha/2, n - 2)se(b_1)$

Similar inference for β_0 .

<u>Comments</u>

- 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
 - $-\sum (X_i \overline{X})^2$ is large \rightarrow smaller margin of error for β_1
 - $-\sum (X_i \overline{X})^2$ is large and $|\overline{X}|$ is small \rightarrow smaller margin of error for β_0

Interval Estimation of $E(Y_h)$

- Often interested in estimating the mean response for particular X_h , i.e., the parameter of interests is $E(Y_h) = \beta_0 + \beta_1 X_h$.
- 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.

$$- \hat{Y}_{h} = \sum \check{k}_{i}Y_{i} \text{ where } k_{i} = \frac{1}{n} + \frac{(X_{h} - \overline{X})(X_{i} - \overline{X})}{\sum(X_{i} - \overline{X})^{2}}$$

$$- E(\hat{Y}_{h}) = \beta_{0} + \beta_{1}X_{h}$$

$$- Var(\hat{Y}_{h}) = \sigma^{2} \left[\frac{1}{n} + \frac{(X_{h} - \overline{X})^{2}}{\sum(X_{i} - \overline{X})^{2}} \right], se^{2}(\hat{Y}_{h}) = s^{2} \left[\frac{1}{n} + \frac{(X_{h} - \overline{X})^{2}}{\sum(X_{i} - \overline{X})^{2}} \right]$$

$$- \text{Test: } (\hat{Y}_{h} - \text{null value})/se(\hat{Y}_{h}); \text{ CI: } \hat{Y}_{h} \pm t(1 - \alpha/2, n - 2)se(\hat{Y}_{h})$$

Interval Prediction of $Y_{h(new)}$

- Predicting future observation $Y_{h(new)} = E[Y_h] + \varepsilon_{h(new)}$
- The prediction interval for a unknown r.v., i.e., $P(L < Y_{h(new)} < U) = 1 \alpha$
- Comparing with CI of $E[Y_h]$, one need to take account of future error $\varepsilon_{h(new)}$.

$$- E(b_0 + b_1 X_h) = E(Y_{h(new)})$$

$$- Var(Y_{h(new)} - b_0 + b_1 X_h) = \sigma^2 \left[1 + \frac{1}{n} + \frac{(X_h - \overline{X})^2}{\sum (X_i - \overline{X})^2} \right]$$

$$- se^2(Y_{h(new)} - b_0 + b_1 X_h) = s^2 \left[1 + \frac{1}{n} + \frac{(X_h - \overline{X})^2}{\sum (X_i - \overline{X})^2} \right]$$

$$- \text{PI: } b_0 + b_1 X_h \pm t(1 - \alpha/2, n - 2) \sqrt{s^2 \left[1 + \frac{1}{n} + \frac{(X_h - \overline{X})^2}{\sum (X_i - \overline{X})^2} \right]}$$

Confidence Band for Response Means

- Consider the *entire regression line*
- Want to define a likely region within which this unknown real line lies
- Rigorously, $P(L(x) < \beta_0 + \beta_1 x < U(x) \text{ for all } x) \ge 1 \alpha$
- One can show

$$\max_{x} \left[\frac{b_0 + b_1 x - (\beta_0 + \beta_1 x)}{se(\hat{Y}_h)(x)} \right]^2 \sim 2F_{2,n-2}$$

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

$$W = \sqrt{2F(1-\alpha; 2, n-2)} \Rightarrow \hat{Y}_h \pm W \times se(\hat{Y}_h)$$

• Boundary values define a hyperbola

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



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

ANOVA approach

- Organizes results arithmetically
- The total sum of squares in Y is defined $\mathsf{SSTO} = \sum (Y_i \overline{Y})^2$
- Can partition the total sum of squares into
 - Model (explained by regression)
 - Error (unexplained / residual)

$$\sum (Y_i - \overline{Y})^2 = \sum (Y_i - \hat{Y}_i + \hat{Y}_i - \overline{Y})^2$$

=
$$\sum (Y_i - \hat{Y}_i)^2 + \sum (\hat{Y}_i - \overline{Y})^2$$

SSTO = SSE + SSR

• Can also express

SSR =
$$\sum (\hat{Y}_i - \overline{Y})^2$$

= $\sum (b_0 + b_1 X_i - b_0 - b_1 \overline{X})^2$
= $b_1^2 \sum (X_i - \overline{X})^2$

- Degrees of freedom is 1 due to normality of b_1 for some δ .
- SSR large when \hat{Y}_i 's are different from \overline{Y}
- Error sum of squares is equal to the sum of squared residuals

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

- Degrees of freedom is n-2 due to using (b_0,b_1) in place of (β_0,β_1) , and SSE $\sim \sigma^2 \chi^2_{n-2}$
- The MSE = SSE/(n-2) and represents an unbiased estimate of σ^2 when taking X into account

F Test

- Can use this structure to test $H_0: \beta_1 = 0$
- Consider

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

- 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.
- ullet

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

- When H_0 is false, F^* tends to be large
- p-value = $Pr(F(1, n-2) > F^*)$
- 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 $SSE(F) \leq SSE(R)$
- Idea: more parameters provide better fit
- If SSE(F) is not much smaller than SSE(R), full model doesn't better explain Y.

$$F^* = \frac{(SSE(R) - SSE(F))/(df_R - df_F)}{SSE(F)/df_F}$$
$$= \frac{(SSTO - SSE)/1}{SSE(F)/(n-2)}$$

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

Diagnose

- use a residual plots (e_i vs \hat{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:

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

$$Y_{2} = \beta_{0} + \beta_{1}X_{2} + \varepsilon_{2}$$

$$Y_{3} = \beta_{0} + \beta_{1}X_{3} + \varepsilon_{3}$$

$$Y_{4} = \beta_{0} + \beta_{1}X_{4} + \varepsilon_{4}$$

$$\begin{bmatrix}Y_{1}\\Y_{2}\\Y_{3}\\Y_{4}\end{bmatrix} = \begin{bmatrix}\beta_{0} + \beta_{1}X_{1}\\\beta_{0} + \beta_{1}X_{2}\\\beta_{0} + \beta_{1}X_{3}\\\beta_{0} + \beta_{1}X_{4}\end{bmatrix} + \begin{bmatrix}\varepsilon_{1}\\\varepsilon_{2}\\\varepsilon_{3}\\\varepsilon_{4}\end{bmatrix}$$

$$\begin{bmatrix}Y_{1}\\Y_{2}\\Y_{3}\\Y_{4}\end{bmatrix} = \begin{bmatrix}1 & X_{1}\\1 & X_{2}\\1 & X_{3}\\1 & X_{4}\end{bmatrix} \begin{bmatrix}\beta_{0}\\\beta_{1}\end{bmatrix} + \begin{bmatrix}\varepsilon_{1}\\\varepsilon_{2}\\\varepsilon_{3}\\\varepsilon_{4}\end{bmatrix}$$

$$Y = X\beta + \varepsilon$$

 $\bullet~{\bf X}$ is called the design matrix

Regression Matrices

• Can express observations

$$Y = X\beta + \varepsilon$$

 \bullet Both Y and ε are random vectors

$$E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta} + E(\boldsymbol{\varepsilon})$$
$$= \mathbf{X}\boldsymbol{\beta}$$
$$\sigma^{2}(\mathbf{Y}) = \mathbf{0} + \sigma^{2}(\boldsymbol{\varepsilon})$$
$$= \sigma^{2}\mathbf{I}$$

Least Squares

• Express quantity \boldsymbol{Q}

$$Q = (Y - X\beta)'(Y - X\beta)$$

= Y'Y - \beta'X'Y - Y'X\beta + \beta'X'X\beta
= Y'Y - 2\beta'X'Y + \beta'X'X\beta

$$- (X\beta)' = \beta' X'$$

• Taking derivative $\rightarrow -2X'Y + 2X'X\beta = 0$

$$- \frac{\partial}{\partial \beta} \beta' \mathbf{X}' \mathbf{Y} = \mathbf{X}' \mathbf{Y}$$
$$- \frac{\partial}{\partial \beta} \beta' \mathbf{X}' \mathbf{X} \beta = 2\mathbf{X}' \mathbf{X} \beta$$

• This means
$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

Fitted Values

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

Residuals

• Residual matrix

$$e = Y - \hat{Y}$$
$$= Y - HY$$
$$= (I - H)Y$$

• e is a random vector

$$E(\mathbf{e}) = (\mathbf{I} - \mathbf{H}) \times E(\mathbf{Y})$$

= $(\mathbf{I} - \mathbf{H})\mathbf{X}\boldsymbol{\beta}$
= $\mathbf{X}\boldsymbol{\beta} - \mathbf{X}\boldsymbol{\beta}$
= 0

$$\sigma^{2}(e) = (I - H) \times \sigma^{2}(Y) \times (I - H)'$$

= (I - H)\sigma^{2}I(I - H)'
= (I - H)\sigma^{2}

Inference

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

$$E(\mathbf{b}) = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'E(\mathbf{Y})$$
$$= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\beta$$
$$= \beta$$

$$\sigma^{2}(\mathbf{b}) = \mathbf{A} \times \sigma^{2}(\mathbf{Y}) \times \mathbf{A}'$$
$$= \mathbf{A} \times \sigma^{2} \mathbf{I} \times \mathbf{A}'$$
$$= \sigma^{2} \mathbf{A} \mathbf{A}'$$
$$= \sigma^{2} (\mathbf{X}' \mathbf{X})^{-1}$$

• Thus, b is multivariate Normal(β , $\sigma^2(X'X)^{-1}$)

•
$$SSE = (e)'(e) = Y'(I - H)Y \sim \sigma^2 \chi^2_{n-2}$$

 \bullet Since b and (e) are indep, SSE and b are independent

Chapter Review

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