

VE401 Probabilistic Methods in Eng.

Final Review Part 1

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Table of contents

Simple Linear Regression

- Simple Linear Regression Model

- Estimators and Predictors

- Model Analysis

- Calculations for Simple Linear Regression

Multiple Linear Regression

- Linear Algebra Basics

- Multiple Linear Regression Model

- Model Analysis

Simple Linear Regression

- Simple Linear Regression Model

- Estimators and Predictors

- Model Analysis

- Calculations for Simple Linear Regression

Multiple Linear Regression

- Linear Algebra Basics

- Multiple Linear Regression Model

- Model Analysis

Simple Linear Regression Model

Model. We assume that

$$Y|x = \beta_0 + \beta_1 x + E,$$

where $E[E] = 0$. We want to find estimators

$$B_0 := \widehat{\beta_0} = \text{estimator for } \beta_0, \quad b_0 = \text{estimate for } \beta_0,$$

$$B_1 := \widehat{\beta_1} = \text{estimator for } \beta_1, \quad b_1 = \text{estimate for } \beta_1.$$

Assumptions.

- ▶ For each value of x , the random variable follows a normal distribution with variance σ^2 and mean $\mu_{Y|x} = \beta_0 + \beta_1 x$.
- ▶ The random variables $Y|x_1$ and $Y|x_2$ are independent if $x_1 \neq x_2$.

Least Squares Estimation

Least squares estimation. We have the *error sum of squares*

$$SS_E := \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - (b_0 + b_1 x_i))^2.$$

To minimize it, we take

$$\begin{aligned}\frac{\partial SS_E}{\partial b_0} &= -2 \sum_{i=1}^n (y_i - b_0 - b_1 x_i) = 0, \\ \frac{\partial SS_E}{\partial b_1} &= -2 \sum_{i=1}^n (y_i - b_0 - b_1 x_i) x_i = 0.\end{aligned}$$

which gives

$$b_1 = \frac{S_{xy}}{S_{xx}}, \quad b_0 = \bar{y} - b_1 \bar{x},$$

Useful Properties

Properties.

$$S_{xx} = \sum_{i=1}^n (x_i - \bar{x})^2 = \sum_{i=1}^n (x_i - \bar{x})x_i = \sum_{i=1}^n x_i^2 - \frac{1}{n} \left(\sum_{i=1}^n x_i \right)^2 = \sum_{i=1}^n x_i^2 - n\bar{x}^2,$$

$$S_{yy} = \sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (y_i - \bar{y})y_i = \sum_{i=1}^n y_i^2 - \frac{1}{n} \left(\sum_{i=1}^n y_i \right)^2 = \sum_{i=1}^n y_i^2 - n\bar{y}^2,$$

$$\begin{aligned} S_{xy} &= \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) = \sum_{i=1}^n (x_i - \bar{x})y_i = \sum_{i=1}^n (y_i - \bar{y})x_i = \sum_{i=1}^n x_i y_i - n\bar{x} \cdot \bar{y} \\ &= \sum_{i=1}^n x_i y_i - \frac{1}{n} \left(\sum_{i=1}^n x_i \right) \left(\sum_{i=1}^n y_i \right). \end{aligned}$$

$$b_1 = \frac{S_{xy}}{S_{xx}}, \quad b_0 = \bar{y} - b_1 \bar{x}, \quad SS_E = S_{yy} - b_1 S_{xy}.$$

Useful Properties

Properties. The last property follows from

$$\begin{aligned}SS_E &= \sum_{i=1}^n (y_i - \bar{y} + \bar{y} - (b_0 + b_1 x_i))^2 \\&= \sum_{i=1}^n (y_i - \bar{y} + \bar{y} - (\bar{y} - b_1 \bar{x} + b_1 x_i))^2 \\&= \sum_{i=1}^n (y_i - \bar{y})^2 + \sum_{i=1}^n b_1^2 (\bar{x} - x_i)^2 - 2 \sum_{i=1}^n b_1 (y_i - \bar{y})(x_i - \bar{x}) \\&= S_{yy} + b_1 \cdot \frac{S_{xy}}{S_{xx}} \cdot S_{xx} - 2b_1 S_{xy} \\&= S_{yy} - b_1 S_{xy}.\end{aligned}$$

Simple Linear Regression

Simple Linear Regression Model

Estimators and Predictors

Model Analysis

Calculations for Simple Linear Regression

Multiple Linear Regression

Linear Algebra Basics

Multiple Linear Regression Model

Model Analysis

Distribution of Estimator for Variance

LSE for variance. An unbiased estimator for variance σ^2 is given by

$$S^2 = \frac{SS_E}{n-2} = \frac{1}{n-2} \sum_{i=1}^n (Y_i - \hat{\mu}_{Y|x_i})^2.$$

Distribution of estimator for variance. The statistic

$$\chi_{n-2}^2 = \frac{(n-2)S^2}{\sigma^2} = \frac{SS_E}{\sigma^2}$$

follows a chi-squared distribution with $n - 2$ degrees of freedom.

Distribution of B_1

Theorem. The least squares estimator B_1 for β_1 follows a normal distribution with

$$E[B_1] = \beta_1, \quad \text{Var}[B_1] = \frac{\sigma^2}{\sum (x_i - \bar{x})^2} = \frac{\sigma^2}{S_{xx}}.$$

Proof.

$$\begin{aligned} B_1 &= \frac{1}{S_{xx}} \sum_{i=1}^n (x_i - \bar{x})(Y_i - \bar{Y}) = \frac{1}{S_{xx}} \sum (x_i - \bar{x}) Y_i \\ &= \frac{1}{S_{xx}} \sum (x_i - \bar{x})(\beta_0 + \beta_1 x_i + E_i) \\ &= \frac{1}{S_{xx}} \cdot \beta_1 S_{xx} + \frac{1}{S_{xx}} \sum (x_i - \bar{x}) E_i \\ &= \beta_1 + \frac{\sum (x_i - \bar{x}) E_i}{S_{xx}}. \end{aligned}$$

Distribution of B_1 with Estimated Variance

Distribution. The statistics

$$T_{n-2} = \frac{B_1 - \beta_1}{S/\sqrt{S_{xx}}}$$

follows T -distributions with $n - 2$ degrees of freedom.

Confidence interval. The $100(1 - \alpha)\%$ confidence interval of β_1 is given by

$$B_1 \pm t_{\alpha/2, n-2} \frac{S}{\sqrt{S_{xx}}}.$$

Test for Significance

Test for significance of regression. Let $(x_i, Y|x_i), i = 1, \dots, n$ be a random sample from $Y|x$. We reject

$$H_0 : \beta_1 = 0$$

at significance level α if the test statistic

$$T_{n-2} = \frac{B_1}{S/\sqrt{S_{xx}}}$$

satisfies $|T_{n-2}| > t_{\alpha/2, n-2}$.

Distribution of B_0

Theorem. The least squares estimator B_0 for β_0 follows a normal distribution with

$$E[B_0] = \beta_0, \quad \text{Var}[B_0] = \frac{\sigma^2 \sum x_i^2}{n \sum (x_i - \bar{x})^2}.$$

Proof. Since

$$\begin{aligned} B_0 &= \bar{Y} - B_1 \bar{x} = \beta_0 + \beta_1 \bar{x} + \bar{E} - \left(\beta_1 + \frac{\sum (x_i - \bar{x}) E_i}{S_{xx}} \right) \bar{x} \\ &= \beta_0 + \bar{E} - \frac{\bar{x} \sum (x_i - \bar{x}) E_i}{S_{xx}}, \end{aligned}$$

we can see that

$$\begin{aligned} E[B_0] &= \beta_0, \quad \text{Var}[B_0] = \frac{\sigma^2}{n} + \bar{x}^2 \frac{\sigma^2}{S_{xx}} - 2 \sum \text{Cov} \left[\frac{E_i}{n}, \frac{\bar{x} \sum (x_i - \bar{x}) E_i}{S_{xx}} \right] \\ &= \sigma^2 \cdot \frac{S_{xx} + n \bar{x}^2}{n S_{xx}} = \frac{\sigma^2 \sum x_i^2}{n S_{xx}}. \end{aligned}$$

Distribution of B_0 with Estimated Variance

Distribution. The statistics

$$T_{n-2} = \frac{B_0 - \beta_0}{S \sqrt{\sum x_i^2 / \sqrt{n S_{xx}}}}$$

follows T -distributions with $n - 2$ degrees of freedom.

Confidence interval. The $100(1 - \alpha)\%$ confidence interval of β_0 is given by

$$B_0 \pm t_{\alpha/2, n-2} \frac{S \sqrt{\sum x_i^2}}{\sqrt{n S_{xx}}}.$$

Distribution of Estimated Mean

Distribution. The estimated mean $\hat{\mu}_{Y|x}$ follows a normal distribution with mean and variance

$$E[\hat{\mu}_{Y|x}] = \mu_{Y|x}, \quad \text{Var}[\hat{\mu}_{Y|x}] = \left(\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}} \right) \sigma^2.$$

Therefore, the statistic

$$T_{n-2} = \frac{\hat{\mu}_{Y|x} - \mu_{Y|x}}{S \sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}}$$

follows a T -distribution with $n - 2$ degrees of freedom. A $100(1 - \alpha)\%$ confidence interval for $\mu_{Y|x}$ is given by

$$\hat{\mu}_{Y|x} \pm t_{\alpha/2, n-2} S \sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}.$$

Distribution and CI for Predictor

Predictor. The statistic $Y|x - \widehat{Y}|x$ follows a normal distribution with mean and variance

$$E[Y|x - \widehat{Y}|x] = 0, \quad \text{Var}[Y|x - \widehat{Y}|x] = \left(1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}\right) \sigma^2.$$

Therefore, the statistic

$$T_{n-2} = \frac{Y|x - \widehat{Y}|x}{S \sqrt{1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}}$$

follows a T -distribution with $n - 2$ degrees of freedom. A $100(1 - \alpha)\%$ confidence interval for $Y|x$ is given by

$$\widehat{Y}|x \pm t_{\alpha/2, n-2} S \sqrt{1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}}.$$

Simple Linear Regression

Simple Linear Regression Model

Estimators and Predictors

Model Analysis

Calculations for Simple Linear Regression

Multiple Linear Regression

Linear Algebra Basics

Multiple Linear Regression Model

Model Analysis

Model Analysis

Crucial quantities.

- **Total sum of squares:**

$$SS_T = S_{yy} = \sum_{i=1}^n (Y_i - \bar{Y})^2.$$

- **Error sum of squared:**

$$SS_E = \sum_{i=1}^n (Y_i - (B_0 + B_1 x_i))^2 = S_{yy} - B_1 S_{xy} = S_{yy} - \frac{S_{xy}^2}{S_{xx}}.$$

- **Coefficient of determination:** the proportion of the total variation in Y that is explained by the linear model.

$$R^2 = \frac{SS_T - SS_E}{SS_T} = \frac{S_{xy}^2}{S_{xx} S_{yy}}.$$

Test for Significance with R^2

Test for significance of regression. Let $(x_i, Y|x_i), i = 1, \dots, n$ be a random sample from $Y|x$. We reject

$$H_0 : \beta_1 = 0$$

at significance level α if the test statistic

$$T_{n-2} = \frac{B_1}{S/\sqrt{S_{xx}}} = \frac{R\sqrt{n-2}}{\sqrt{1-R^2}}$$

satisfies $|T_{n-2}| > t_{\alpha/2, n-2}$.

Test for Correlation with R^2

Test for correlation. Let (X, Y) follow a bivariate normal distribution with correlation coefficient $\rho \in (-1, 1)$. Let R be the estimator for ρ . Then we reject

$$H_0 : \rho = 0$$

at significance level α if the test statistic

$$T_{n-2} = \frac{R\sqrt{n-2}}{\sqrt{1-R^2}}$$

satisfies $|T_{n-2}| > t_{\alpha/2, n-2}$.

Lack-of-Fit and Pure Error

Source of SS_E . SS_E is the variance of Y explained by the model.

► **Error sum of squares due to pure error:**

$$SS_{E,pe} := \sum_{i=1}^k \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_i)^2 = \sum_{i=1}^k \sum_{j=1}^{n_i} Y_{ij}^2 - \sum_{i=1}^k \frac{1}{n_i} \left(\sum_{j=1}^{n_i} Y_{ij} \right)^2.$$

The statistic $SS_{E,pe}/\sigma^2$ follows a chi-squared distribution with $\sum_{i=1}^k (n_i - 1) = n - k$ degrees of freedom. (Recall that with sample variance S^2 of some sample X_1, \dots, X_n , the statistic $(n-1)S^2/\sigma^2$ follows chi-squared distribution with $n-1$ d.o.f.)

► **Error sum of squares due to lack of fit:**

$$SS_{E,lf} := SS_E - SS_{E,pe}.$$

The statistic $SS_{E,lf}/\sigma^2$ follows a chi-squared distribution with $k - 2$ degrees of freedom.

Testing for Lack of Fit

Test for lack of fit. Let x_1, \dots, x_k be regressors and Y_{i1}, \dots, Y_{in_i} , $i = 1, \dots, k$ the measured responses at each of the regressors. Let $SS_{E,pe}$ and $SS_{E,lf}$ be the pure error and lack-of-fit sums of squares for a linear regression model. Then we reject at significance level α

H_0 : the linear regression model is appropriate

if the test statistic

$$F_{k-2, n-k} = \frac{SS_{E,lf}/(k-2)}{SS_{E,pe}/(n-k)}$$

satisfies $F_{k-2, n-k} > f_{\alpha, k-2, n-k}$.

Simple Linear Regression

Simple Linear Regression Model

Estimators and Predictors

Model Analysis

Calculations for Simple Linear Regression

Multiple Linear Regression

Linear Algebra Basics

Multiple Linear Regression Model

Model Analysis

Calculations for Simple Linear Regression

1. Find $\sum x_i$, $\sum y_i$, $\sum x_i^2$, $\sum y_i^2$, $\sum x_i y_i$ and calculate

$$S_{xx} = \sum x_i^2 - \frac{1}{n} \left(\sum x_i \right)^2, \quad S_{yy} = \sum y_i^2 - \frac{1}{n} \left(\sum y_i \right)^2,$$

$$S_{xy} = \sum x_i y_i - \frac{1}{n} \left(\sum x_i \right) \left(\sum y_i \right).$$

2. Obtain b_1 and b_0 by

$$b_1 = \frac{S_{xy}}{S_{xx}}, \quad b_0 = \bar{y} - b_1 \bar{x}.$$

3. Calculate other quantities as required, e.g.,

$$SS_E = S_{yy} - \frac{S_{xy}^2}{S_{xx}}, \quad R^2 = \frac{S_{xy}^2}{S_{xx} S_{yy}}.$$

Simple Linear Regression

Simple Linear Regression Model

Estimators and Predictors

Model Analysis

Calculations for Simple Linear Regression

Multiple Linear Regression

Linear Algebra Basics

Multiple Linear Regression Model

Model Analysis

Gradient of Matrix

Gradient. Suppose $a, x \in \mathbb{R}^n$, $A \in \text{Mat}(n \times n; \mathbb{R})$, then we have the following properties.

► $\nabla_x(a^T x) = a$, since

$$a^T x = \sum_{i=1}^n a_i x_i \quad \Rightarrow \quad \nabla_x(x^T x) = \begin{pmatrix} \frac{\partial a^T x}{\partial x_1} \\ \vdots \\ \frac{\partial a^T x}{\partial x_n} \end{pmatrix} = a.$$

► $\nabla_x(x^T A x) = 2Ax$ if $A^T = A$, since

$$\begin{aligned} x^T A x &= \sum_{i=1}^n \sum_{j=1}^n x_i a_{ij} x_j = \sum_{i=1}^n a_{ii} x_i^2 + 2 \sum_{i < j} x_i a_{ij} x_j \\ \Rightarrow \quad \frac{\partial x^T A x}{\partial x_i} &= 2 \sum_{j=1}^n a_{ij} x_j \quad \Rightarrow \quad \nabla_x(x^T x) = 2Ax. \end{aligned}$$

Idempotent Matrix

Idempotent matrix. A $n \times n$ matrix P satisfying the property that $P^2 = P$ is called idempotent. Then

$$(\mathbb{1}_n - P)^2 = \mathbb{1}_n - P - P + P^2 = \mathbb{1}_n - P$$

is also idempotent. Furthermore, its eigenvalues may only be 0 or 1, since

$$\lambda v = Pv = P^2 v = P(\lambda v) = \lambda^2 v,$$

where v is an eigenvector. This gives $\lambda^2 = \lambda$. In lecture slides, P is an *orthogonal projection* if

$$P^2 = P, \quad P^T = P.$$

The Spectral Theorem of Linear Algebra

Spectral theorem. Let $A \in \text{Mat}(n \times n; \mathbb{R})$ be a self-adjoint matrix, which means $A = A^* = A^T$. Then there exists an orthonormal basis of \mathbb{R}^n consisting of eigenvectors of A .

Corollary of spectral theorem. Let $A \in \text{Mat}(n \times n; \mathbb{R})$ be a self-adjoint matrix. Then if (v_1, \dots, v_n) is an orthonormal basis of eigenvectors of A and $U = (v_1, \dots, v_n)$, then $U^{-1} = U^T$, and

$$D = U^{-1}AU = U^T AU$$

is a diagonal matrix containing eigenvalues of A . This can be seen from

$$De_k = U^{-1}AUe_k = U^{-1}Av_k = U^{-1}\lambda_k v_k = \lambda_k e_k.$$

Important Results from Linear Algebra for Regression

Results used multiple linear regression.

- ▶ If $A \in \text{Mat}(n \times n; \mathbb{R})$ is idempotent, then $\mathbb{1}_n - A$ is idempotent, and A has eigenvalues only 0 or 1.
- ▶ If $A \in \text{Mat}(n \times n; \mathbb{R})$ is symmetric, then there exists a matrix $U = (v_1, \dots, v_n)$ of eigenvectors of A and $U^{-1} = U^T$ such that

$$D = U^T A U \quad \Rightarrow \quad A = U D U^T.$$

- ▶ In discussions of multiple linear regression, the two properties above hold for matrices

$$P = \frac{1}{n} \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix} \quad \text{and} \quad H = X(X^T X)^{-1} X^T,$$

and thus $\mathbb{1}_n - P$ and $\mathbb{1}_n - H$.

Simple Linear Regression

Simple Linear Regression Model

Estimators and Predictors

Model Analysis

Calculations for Simple Linear Regression

Multiple Linear Regression

Linear Algebra Basics

Multiple Linear Regression Model

Model Analysis

Polynomial Regression Model

Model. For a polynomial model, we assume that

$$Y|x = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_p x^p + E \quad \Leftrightarrow \quad Y = X\beta + E,$$

where

$$Y = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix}, \quad X = \begin{pmatrix} 1 & x_1 & \cdots & x_1^p \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & \cdots & x_n^p \end{pmatrix}, \quad \beta = \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_p \end{pmatrix}, \quad E = \begin{pmatrix} E_1 \\ \vdots \\ E_n \end{pmatrix}.$$

Assumptions.

- ▶ For each value of x , the random variable follows a normal distribution with variance σ^2 and mean $\mu_{Y|x} = \beta_0 + \beta_1 x + \cdots + \beta_p x^p$.
- ▶ The random variables $Y|x_1$ and $Y|x_2$ are independent if $x_1 \neq x_2$.

The Multilinear Model

Model. For a multilinear model, we assume that Y depends on several factors,

$$Y|x = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p + E \quad \Leftrightarrow \quad Y = X\beta + E,$$

where

$$Y = \begin{pmatrix} Y_1 \\ \vdots \\ Y_n \end{pmatrix}, \quad X = \begin{pmatrix} 1 & x_{11} & \cdots & x_{p1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{1n} & \cdots & x_{pn} \end{pmatrix}, \quad \beta = \begin{pmatrix} \beta_0 \\ \vdots \\ \beta_p \end{pmatrix}, \quad E = \begin{pmatrix} E_1 \\ \vdots \\ E_n \end{pmatrix}.$$

Assumptions.

- ▶ For each value of x , the random variable follows a normal distribution with variance σ^2 and mean $\mu_{Y|x} = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$.
- ▶ The random variables $Y|x_1$ and $Y|x_2$ are independent if $x_1 \neq x_2$.

Least Squares Estimation

Least squares estimation. For both cases, we have the error sum of squares

$$SS_E = \langle Y - Xb, Y - Xb \rangle = (Y - Xb)^T (Y - Xb).$$

To minimize it, we take

$$\begin{aligned}\nabla_b SS_E &= \nabla_b (Y - Xb)^T (Y - Xb) \\ &= \nabla_b (Y^T Y - Y^T Xb - b^T X^T Y + b^T X^T Xb) \\ &= -2X^T Y + 2X^T Xb = 0 \quad \Rightarrow \quad b = (X^T X)^{-1} X^T Y,\end{aligned}$$

where we have used since both $Y^T Xb$ and $b^T X^T Y$ are scalars,

$$b^T X^T Y = (b^T X^T Y)^T = Y^T Xb.$$

Simple Linear Regression

Simple Linear Regression Model

Estimators and Predictors

Model Analysis

Calculations for Simple Linear Regression

Multiple Linear Regression

Linear Algebra Basics

Multiple Linear Regression Model

Model Analysis

Error Analysis

Crucial quantities.

- **Total variation:** given orthogonal projection P ,

$$P := \frac{1}{n} \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix} \quad \Rightarrow \quad (\mathbb{1}_n - P)^2 = \mathbb{1}_n - P,$$

giving

$$SS_T = \langle (\mathbb{1}_n - P)Y, (\mathbb{1}_n - P)Y \rangle = \langle Y, (\mathbb{1}_n - P)Y \rangle.$$

- **Sum of squares error:** given orthogonal projection H ,

$$\begin{aligned} H &:= X(X^T X)^{-1} X^T \quad \Rightarrow \quad SS_E = \langle Y - Xb, Y - Xb \rangle \\ &= \langle (\mathbb{1}_n - H)Y, (\mathbb{1}_n - H)Y \rangle \\ &= \langle Y, (\mathbb{1}_n - H)Y \rangle = \langle E, (\mathbb{1}_n - H)E \rangle. \end{aligned}$$

- **Coefficient of multiple determination:**

$$R^2 = \frac{SS_R}{SS_T}, \quad SS_R = SS_T - SS_E = \langle Y, (H - P)Y \rangle = \langle (H - P)Y, (H - P)Y \rangle.$$

Distribution of SS_E

Distribution of sum of squares error. The statistic given by the SS_E and variance σ^2

$$\begin{aligned}\frac{SS_E}{\sigma^2} &= \left\langle \frac{E}{\sigma}, (\mathbb{1}_n - H) \frac{E}{\sigma} \right\rangle = \langle Z, (\mathbb{1}_n - H)Z \rangle \\ &= \langle Z, UD_{n-p-1}U^T Z \rangle = \langle U^T Z, D_{n-p-1}U^T Z \rangle \\ &= \sum_{i=1}^{n-p-1} (U^T Z)_i^2, \quad \left(U^T Z \sim N(0, \sigma^2 U U^T) = N(0, \sigma^2 \mathbb{1}_n) \right)\end{aligned}$$

follows a chi-squared distribution with $n - p - 1$ degrees of freedom, where the matrix U contains columns of eigenvectors of $(\mathbb{1}_n - H)$ such that

$$U^T(\mathbb{1}_n - H)U = D_{n-p-1} \quad \Rightarrow \quad \mathbb{1}_n - H = UD_{n-p-1}U^T.$$

Distribution of SS_E

- ▶ SS_E/σ^2 follows a chi-squared distribution with $n-p-1$ degrees of freedom.
- ▶ If $\beta = (\beta_0, 0, \dots, 0)$, then SS_R/σ^2 follows a chi-squared distribution with p degrees of freedom.
- ▶ SS_R and SS_E are independent random variables. (Fisher-Cochran theorem.)
- ▶ An unbiased estimator for σ^2 is given by

$$\hat{\sigma}^2 = S^2 = \frac{SS_E}{n-p-1}.$$

- ▶ The regression sum of squares can be expressed as

$$\begin{aligned} SS_R &= \langle Xb, Y \rangle - \frac{1}{n} \left(\sum_{i=1}^n Y_i \right)^2 \\ &= b_0 \sum_{i=1}^n Y_i + \sum_{j=1}^p b_j \sum_{i=1}^n x_{ji} Y_i - \frac{1}{2} \left(\sum_{i=1}^n Y_i \right)^2, \end{aligned}$$

for multilinear model, and substitute x_{ji} with x_i^j for polynomial model.

F-Test for Significance of Regression

F-test for significance of regression. Let x_1, \dots, x_p be the predictor variables in a multilinear model for Y . Then we reject at significance level α

$$H_0 : \beta_1 = \beta_2 = \dots = \beta_p = 0$$

if the test statistic

$$F_{p, n-p-1} = \frac{SS_R/p}{SS_E/(n-p-1)} = \frac{SS_R/p}{S^2} = \frac{n-p-1}{p} \frac{R^2}{1-R^2}$$

satisfies $F_{p, n-p-1} > f_{\alpha, p, n-p-1}$.

Thanks for your attention!
Good luck for Final exam!