

MSDS 596 Regression & Time Series

Lecture 02 Gauss Markov theorem and the R^2

Department of Statistics
Rutgers University

Sept 19, 2022

Do not reproduce or distribute lecture slides without permission

Welcome to MSDS 596: Regression & Time Series

- Meeting time: **Mondays 6-9pm**
- Instructor: **Koulik Khamaru** (kk1241@rutgers.edu)
Office hour: Monday 4-5pm, 479 Hill center
- Teaching Assistant: **Suvrojit Ghosh** (sg1565@scarletmail.rutgers.edu)
Office hour: Wednesdays 3:30-4:30pm, 260 Hill center.
- Course website (piazza):
<https://piazza.com/rutgers/fall2022/1695459602>
The course website is our main means of communication for all things class-related.

Gauss-Markov Theorem

Gauss-Markov Theorem

Suppose $\mathbb{E}(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$, where \mathbf{X} has full rank and $\text{Var}(\mathbf{y}) = \sigma^2\mathbf{I}$. The least squares estimator

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

is the **best linear unbiased estimator (BLUE)** of $\boldsymbol{\beta}$, in the sense that for any $\boldsymbol{\psi} = \mathbf{c}'\boldsymbol{\beta}$, of all unbiased estimators of $\boldsymbol{\psi}$ that are linear in \mathbf{y} , $\mathbf{c}'\hat{\boldsymbol{\beta}}$ has minimum variance.

Gauss Markov theorem proof

- Let

$$\tilde{\beta} = By = \left\{ (X^{\top}X)^{-1}X^{\top} + G \right\} y$$

- Show that $GX = 0$.
- Show $\text{var}(Gy) = \text{var}(\hat{\beta}_{OLS}) + \sigma^2 GG^{\top}$.

Variance estimate

- Recall the linear model is

$$y_i = \mathbf{x}_i' \boldsymbol{\beta} + \epsilon_i, \quad 1 \leq i \leq n,$$

assuming $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are independent and identically distributed (iid) with mean **zero** and variance σ^2 .

- The estimate of σ^2 is given by

$$\hat{\sigma}^2 = \frac{1}{n - (p + 1)} \sum_{i=1}^n (y_i - \hat{y}_i)^2.$$

– Unbiased estimate, i.e. $\mathbb{E}\hat{\sigma}^2 = \sigma^2$.

- The covariance matrix of $\hat{\boldsymbol{\beta}}$ is

$$\text{Cov}(\hat{\boldsymbol{\beta}}) = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1}.$$

– It is estimated by $\widehat{\text{Cov}}(\hat{\boldsymbol{\beta}}) = \hat{\sigma}^2 (\mathbf{X}'\mathbf{X})^{-1}$.

Variance estimate

- Recall the linear model is

$$y_i = \mathbf{x}_i' \boldsymbol{\beta} + \epsilon_i, \quad 1 \leq i \leq n,$$

assuming $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are independent and identically distributed (iid) with mean **zero** and variance σ^2 .

- The estimate of σ^2 is given by

$$\hat{\sigma}^2 = \frac{1}{n - (p + 1)} \sum_{i=1}^n (y_i - \hat{y}_i)^2.$$

- **Unbiased** estimate, i.e. $\mathbb{E}\hat{\sigma}^2 = \sigma^2$.

- The covariance matrix of $\hat{\boldsymbol{\beta}}$ is

$$\text{Cov}(\hat{\boldsymbol{\beta}}) = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1}.$$

- It is estimated by $\widehat{\text{Cov}}(\hat{\boldsymbol{\beta}}) = \hat{\sigma}^2 (\mathbf{X}'\mathbf{X})^{-1}$.

Variance estimate

- Recall the linear model is

$$y_i = \mathbf{x}_i' \boldsymbol{\beta} + \epsilon_i, \quad 1 \leq i \leq n,$$

assuming $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are independent and identically distributed (iid) with mean **zero** and variance σ^2 .

- The estimate of σ^2 is given by

$$\hat{\sigma}^2 = \frac{1}{n - (p + 1)} \sum_{i=1}^n (y_i - \hat{y}_i)^2.$$

– **Unbiased** estimate, i.e. $\mathbb{E}\hat{\sigma}^2 = \sigma^2$.

- The covariance matrix of $\hat{\boldsymbol{\beta}}$ is

$$\text{Cov}(\hat{\boldsymbol{\beta}}) = \sigma^2 (\mathbf{X}'\mathbf{X})^{-1}.$$

– It is estimated by $\widehat{\text{Cov}}(\hat{\boldsymbol{\beta}}) = \hat{\sigma}^2 (\mathbf{X}'\mathbf{X})^{-1}$.

Goodness of fit

We need to measure how well the model fits the data.

- Total sum of squares (Total SS): $\sum_{i=1}^n (y_i - \bar{y})^2$.
- Residual sum of squares (RSS): $\sum_{i=1}^n (y_i - \hat{y}_i)^2$.
- Coefficient of determination:

$$R^2 := 1 - \frac{\text{RSS}}{\text{Total SS}},$$

noting that $0 \leq R^2 \leq 1$.

- hint: Look at the definition of least square estimate.

Goodness of fit

We need to measure how well the model fits the data.

- Total sum of squares (Total SS): $\sum_{i=1}^n (y_i - \bar{y})^2$.
- Residual sum of squares (RSS): $\sum_{i=1}^n (y_i - \hat{y}_i)^2$.
- Coefficient of determination:

$$R^2 := 1 - \frac{\text{RSS}}{\text{Total SS}},$$

noting that $0 \leq R^2 \leq 1$.

- hint: Look at the definition of least square estimate.

Goodness of fit

We need to measure how well the model fits the data.

- Total sum of squares (Total SS): $\sum_{i=1}^n (y_i - \bar{y})^2$.
- Residual sum of squares (RSS): $\sum_{i=1}^n (y_i - \hat{y}_i)^2$.
- Coefficient of determination:

$$R^2 := 1 - \frac{\text{RSS}}{\text{Total SS}},$$

noting that $0 \leq R^2 \leq 1$.

- hint: Look at the definition of least square estimate.

Goodness of fit

We need to measure how well the model fits the data.

- Total sum of squares (Total SS): $\sum_{i=1}^n (y_i - \bar{y})^2$.
- Residual sum of squares (RSS): $\sum_{i=1}^n (y_i - \hat{y}_i)^2$.
- Coefficient of determination:

$$R^2 := 1 - \frac{\text{RSS}}{\text{Total SS}},$$

noting that $0 \leq R^2 \leq 1$.

- hint: Look at the definition of least square estimate.

Goodness of fit

We need to measure how well the model fits the data.

- Total sum of squares (Total SS): $\sum_{i=1}^n (y_i - \bar{y})^2$.
- Residual sum of squares (RSS): $\sum_{i=1}^n (y_i - \hat{y}_i)^2$.
- Coefficient of determination:

$$R^2 := 1 - \frac{\text{RSS}}{\text{Total SS}},$$

noting that $0 \leq R^2 \leq 1$.

- hint: Look at the definition of least square estimate.

Goodness of fit

- Coefficient of determination:

$$R^2 := 1 - \frac{\text{RSS}}{\text{Total SS}}.$$

- Large value of R^2 indicates better fit.
 - In biological and social sciences, and finances, the variables are usually weakly correlated, with a lot of noise, we would expect low values of R^2 .
 - In physics and engineering, most data come from controlled experiments, typically get higher R^2 .
 - Background knowledge may be required to judge the R^2 value.
- Do **NOT** rely on R^2 as the only measure of fit! (Chapters 6,7,8,10)

Maximum Likelihood Estimation (Next class)

- Linear model $y_i = \mathbf{x}_i' \boldsymbol{\beta} + \epsilon_i$, $1 \leq i \leq n$.
- If the assumption is stronger: $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are iid $N(0, \sigma^2)$, then...
- In the simple regression case, likelihood and log likelihood:

$$L(\boldsymbol{\beta}) = \prod_{i=1}^n \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2} \right] \right\},$$

$$\log L(\boldsymbol{\beta}) = -\frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2.$$

Solve for the MLEs: $\frac{\partial \log L}{\partial \beta_0} \big|_{\hat{\beta}_0, \hat{\beta}_1} = 0$ and $\frac{\partial \log L}{\partial \beta_1} \big|_{\hat{\beta}_0, \hat{\beta}_1} = 0$.

- $\hat{\boldsymbol{\beta}}$ is also the **maximum likelihood estimate (MLE)** of $\boldsymbol{\beta}$.

1

¹Read chap 1 and 3 of the book Statistical Inference 2nd ed. by Casella and Berger

Maximum Likelihood Estimation (Next class)

- Linear model $y_i = \mathbf{x}_i' \boldsymbol{\beta} + \epsilon_i$, $1 \leq i \leq n$.
- If the assumption is stronger: $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are iid $N(0, \sigma^2)$, then...
- In the simple regression case, likelihood and log likelihood:

$$L(\boldsymbol{\beta}) = \prod_{i=1}^n \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2} \right] \right\},$$
$$\log L(\boldsymbol{\beta}) = -\frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2.$$

Solve for the MLEs: $\frac{\partial \log L}{\partial \beta_0} \big|_{\hat{\beta}_0, \hat{\beta}_1} = 0$ and $\frac{\partial \log L}{\partial \beta_1} \big|_{\hat{\beta}_0, \hat{\beta}_1} = 0$.

- $\hat{\boldsymbol{\beta}}$ is also the maximum likelihood estimate (MLE) of $\boldsymbol{\beta}$.

1

¹Read chap 1 and 3 of the book Statistical Inference 2nd ed. by Casella and Berger

Maximum Likelihood Estimation (Next class)

- Linear model $y_i = \mathbf{x}_i' \boldsymbol{\beta} + \epsilon_i$, $1 \leq i \leq n$.
- If the assumption is stronger: $\epsilon_1, \epsilon_2, \dots, \epsilon_n$ are iid $N(0, \sigma^2)$, then...
- In the simple regression case, likelihood and log likelihood:

$$L(\boldsymbol{\beta}) = \prod_{i=1}^n \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[-\frac{(y_i - \beta_0 - \beta_1 x_i)^2}{2\sigma^2} \right] \right\},$$

$$\log L(\boldsymbol{\beta}) = -\frac{n}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2.$$

Solve for the MLEs: $\frac{\partial \log L}{\partial \beta_0} \big|_{\hat{\beta}_0, \hat{\beta}_1} = 0$ and $\frac{\partial \log L}{\partial \beta_1} \big|_{\hat{\beta}_0, \hat{\beta}_1} = 0$.

- $\hat{\boldsymbol{\beta}}$ is also the **maximum likelihood estimate (MLE)** of $\boldsymbol{\beta}$.

1

¹Read chap 1 and 3 of the book Statistical Inference 2nd ed. by Casella and Berger

Distribution of $\hat{\beta}$ (Next class)

- σ known
 - Distribution of $\hat{\beta}$.
 - Distribution of $a^T \hat{\beta}$.
 - What happens when σ^2 is unknown?
- σ^2 is unknown
 - What is the MLE for $\hat{\beta}$?
 - What is the MLE for $\hat{\sigma}^2$?