Identifiability, Gauss Markov & Predictive Distributions

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STA721 Linear Models

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Outline

Topics

- Gauss-Markov Theorem
- Estimability and Prediction

Readings: Christensen Chapter 2, Chapter 6.3, (Appendix A, and Appendix B as needed)

Non-Identifiable

Recall the One-way ANOVA model

$$\mu_{ij} = \mu + \tau_j \qquad \boldsymbol{\mu} = (\mu_{11}, \ldots, \mu_{n_1 1}, \mu_{12}, \ldots, \mu_{n_2,2}, \ldots, \mu_{1J}, \ldots, \mu_{n_J J})^T$$

- Let $\boldsymbol{\beta}_1 = (\mu, \tau_1, \ldots, \tau_J)^T$
- Let $\boldsymbol{\beta}_2 = (\mu - 42, \tau_1 + 42, \ldots, \tau_J + 42)^T$
- Then $\boldsymbol{\mu}_1 = \boldsymbol{\mu}_2$ even though $\boldsymbol{\beta}_1 \neq \boldsymbol{\beta}_2$
- $\boldsymbol{\beta}$ is not identifiable
- yet $\boldsymbol{\mu}$ is identifiable, where $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ (a linear combination of $\boldsymbol{\beta}$)

Identifiability and Estimability

Theorem

A function $g(\boldsymbol{\beta})$ *is identifiable if and only if* $g(\boldsymbol{\beta})$ *is a function of* $\mu(\boldsymbol{\beta})$

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Definition

A scalar function $\boldsymbol{\lambda}^T\boldsymbol{\beta}$ is *estimable* if $\boldsymbol{\lambda}^T\boldsymbol{\beta} = \mathbf{a}^T\mathbf{X}\boldsymbol{\beta}$ for some vector $\mathbf{a} \in \mathbb{R}^n$

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Equivalently

Definition

A function $\boldsymbol{\lambda}^T\boldsymbol{\beta}$ is *estimable* if it has an unbiased linear estimator, i.e. there exists an $\mathbf{a}$ such that $\mathsf{E}(\mathbf{a}^T\mathbf{Y}) = \boldsymbol{\lambda}^T\boldsymbol{\beta}$ for all $\boldsymbol{\beta}$

Estimability

Theorem

The function $\psi = \boldsymbol{\lambda}^T \beta$ *is estimable if and only if* $\boldsymbol{\lambda}^T$ *is a linear combination of the rows of* $\mathbf{X}$*. i.e. there exists* $\mathbf{a}^T$ *such that* $\boldsymbol{\lambda}^T = \mathbf{a}^T \mathbf{X}$

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Proof.

The function $\psi = \boldsymbol{\lambda}^T \boldsymbol{\beta}$ is estimable if there exists an $\mathbf{a}^T$ such that $\mathrm{E}[\mathbf{a}^T \mathbf{Y}] = \boldsymbol{\lambda}^T \boldsymbol{\beta}$

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$$\mathsf{E}[\mathbf{a}^T \mathbf{Y}] = \mathbf{a}^T \mathsf{E}[\mathbf{Y}]$$

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The function $\psi = \boldsymbol{\lambda}^T \beta$ *is estimable if and only if* $\boldsymbol{\lambda}^T$ *is a linear combination of the rows of* $\mathbf{X}$. *i.e. there exists* $\mathbf{a}^T$ *such that* $\boldsymbol{\lambda}^T = \mathbf{a}^T \mathbf{X}$

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if and only if $\boldsymbol{\lambda}^T = \mathbf{a}^T \mathbf{X}$ for all $\boldsymbol{\beta}$ $\square$

Estimability of Individual β_j

Proposition

For

$$\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta} = \sum_j \mathbf{X}_j \beta_j$$

β_j is not identifiable if and only if there exists α_j such that $\mathbf{X}_j = \sum_{i \neq j} \mathbf{X}_i \alpha_i$

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One-way Anova Model:

$$Y_{ij} = \mu + \tau_j + \epsilon_{ij}$$

$$\boldsymbol{\mu} = \begin{bmatrix} \mathbf{1}_{n_1} & \mathbf{1}_{n_1} & \mathbf{0}_{n_1} & \dots & \mathbf{0}_{n_1} \\ \mathbf{1}_{n_2} & \mathbf{0}_{n_2} & \mathbf{1}_{n_2} & \dots & \mathbf{0}_{n_2} \\ \vdots & \vdots & \ddots & \vdots & \\ \mathbf{1}_{n_J} & \mathbf{0}_{n_J} & \mathbf{0}_{n_J} & \dots & \mathbf{1}_{n_J} \end{bmatrix} \begin{pmatrix} \mu \\ \tau_1 \\ \tau_2 \\ \vdots \\ \tau_J \end{pmatrix}$$

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Are any parameters μ or τ_j identifiable?

Gauss-Markov Theorem

Theorem

Under the assumptions:

$$E[\mathbf{Y}] = \boldsymbol{\mu}$$

Gauss-Markov Theorem

Theorem

Under the assumptions:

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\begin{aligned}
E[\mathbf{Y}] &= \boldsymbol{\mu} \\
Cov(\mathbf{Y}) &= \sigma^2 \mathbf{I}_n
\end{aligned}
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every estimable function $\psi = \boldsymbol{\lambda}^T \boldsymbol{\beta}$ *has a unique unbiased linear estimator* $\hat{\psi}$ *which has minimum variance in the class of all unbiased linear estimators.*

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every estimable function $\psi = \boldsymbol{\lambda}^T \boldsymbol{\beta}$ *has a unique unbiased linear estimator* $\hat{\psi}$ *which has minimum variance in the class of all unbiased linear estimators.* $\hat{\psi} = \boldsymbol{\lambda}^T \hat{\boldsymbol{\beta}}$ *where* $\hat{\boldsymbol{\beta}}$ *is any set of ordinary least squares estimators.*

Unique Unbiased Estimator

Lemma

- If $\psi = \boldsymbol{\lambda}^T \boldsymbol{\beta}$ is estimable, there exists a unique linear unbiased estimator of $\psi = \mathbf{a}^{*T}\mathbf{Y}$ with $a^* \in C(\mathbf{X})$.

Unique Unbiased Estimator

Lemma

- If $\psi = \boldsymbol{\lambda}^T \boldsymbol{\beta}$ is estimable, there exists a unique linear unbiased estimator of $\psi = \mathbf{a}^{*T}\mathbf{Y}$ with $a^* \in C(\mathbf{X})$.
- If $\mathbf{a}^T\mathbf{Y}$ is any unbiased linear estimator of ψ then a^* is the projection of $\mathbf{a}$ onto $C(\mathbf{X})$, i.e. $\mathbf{a}^* = \mathbf{P_X a}$.

Unique Unbiased Estimator

Proof

- Since ψ is estimable, there exists an $\mathbf{a} \in \mathbb{R}^n$ for which $\mathsf{E}[\mathbf{a}^T\mathbf{Y}] = \boldsymbol{\lambda}^T\boldsymbol{\beta} = \psi$ with $\boldsymbol{\lambda}^T = \mathbf{a}^T\mathbf{X}$

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- Let $\mathbf{a} = \mathbf{a}^* + \mathbf{u}$ where $\mathbf{a}^* \in C(\mathbf{X})$ and $\mathbf{u} \in C(\mathbf{X})^\perp$

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Proof

- Since ψ is estimable, there exists an $\mathbf{a} \in \mathbb{R}^n$ for which $\mathsf{E}[\mathbf{a}^T\mathbf{Y}] = \boldsymbol{\lambda}^T\boldsymbol{\beta} = \psi$ with $\boldsymbol{\lambda}^T = \mathbf{a}^T\mathbf{X}$
- Let $\mathbf{a} = \mathbf{a}^* + \mathbf{u}$ where $\mathbf{a}^* \in C(\mathbf{X})$ and $\mathbf{u} \in C(\mathbf{X})^\perp$
- Then

$$\psi = \mathsf{E}[\mathbf{a}^T\mathbf{Y}] \quad = \quad \mathsf{E}[\mathbf{a}^{*T}\mathbf{Y}] + \mathsf{E}[\mathbf{u}^T\mathbf{Y}]$$

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Proof

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- Then

$$\begin{aligned} \psi = \textsf{E}[\mathbf{a}^T\mathbf{Y}] &= \textsf{E}[\mathbf{a}^{*T}\mathbf{Y}] + \textsf{E}[\mathbf{u}^T\mathbf{Y}] \\ &= \textsf{E}[\mathbf{a}^{*T}\mathbf{Y}] + 0 \end{aligned}$$

$$\textsf{E}[\mathbf{u}^T\mathbf{Y}] = \mathbf{u}^T\mathbf{X}\boldsymbol{\beta}$$

since $\mathbf{u} \perp C(\mathbf{X})$ (i.e. $\mathbf{u} \in C(\mathbf{X})^\perp$) $\textsf{E}[\mathbf{u}^T\mathbf{Y}] = 0$

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- Thus $\mathbf{a}^{*T}\mathbf{Y}$ is also an unbiased linear estimator of ψ with $\mathbf{a}^* \in C(\mathbf{X})$

Uniqueness

Proof.

Suppose that there is another $\mathbf{v} \in C(\mathbf{X})$ such that $\mathrm{E}[\mathbf{v}^T\mathbf{Y}] = \psi$. Then for all $\boldsymbol{\beta}$

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$$0 = \mathsf{E}[\mathbf{a}^{*T}\mathbf{Y}] - \mathsf{E}[\mathbf{v}^T\mathbf{Y}]$$

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- Implies $(\mathbf{a}^* - \mathbf{v}) \in C(\mathbf{X})^\perp$

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- but by assumption $(\mathbf{a}^* - \mathbf{v}) \in C(\mathbf{X})$ ($C(\mathbf{X})$ is a vector space)

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- the only vector in BOTH is $\mathbf{0}$, so $\mathbf{a}^* = \mathbf{v}$

Uniqueness

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Suppose that there is another $\mathbf{v} \in C(\mathbf{X})$ such that $\mathsf{E}[\mathbf{v}^T\mathbf{Y}] = \psi$. Then for all $\boldsymbol{\beta}$

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- the only vector in BOTH is $\mathbf{0}$, so $\mathbf{a}^* = \mathbf{v}$

Therefore $\mathbf{a}^{*T}\mathbf{Y}$ is the unique linear unbiased estimator of ψ with $\mathbf{a}^* \in C(\mathbf{X})$. $\square$

Proof of Minimum Variance (G-M)

- Let $\mathbf{a}^{*T}\mathbf{Y}$ be the unique unbiased linear estimator of ψ with $\mathbf{a}^* \in C(\mathbf{X})$.

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- Let $\mathbf{a}^{*T}\mathbf{Y}$ be the unique unbiased linear estimator of ψ with $\mathbf{a}^* \in C(\mathbf{X})$.
- Let $\mathbf{a}^T\mathbf{Y}$ be any unbiased estimate of ψ; $\mathbf{a} = \mathbf{a}^* + \mathbf{u}$ with $\mathbf{a}^* \in C(\mathbf{X})$ and $\mathbf{u} \in C(\mathbf{X})^\perp$

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$$\mathrm{Var}(\mathbf{a}^T\mathbf{Y}) = \mathbf{a}^T\mathrm{Cov}(\mathbf{Y})\mathbf{a}$$

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$$\begin{aligned} \mathrm{Var}(\mathbf{a}^T\mathbf{Y}) &= \mathbf{a}^T\mathrm{Cov}(\mathbf{Y})\mathbf{a} \\ &= \sigma^2\|\mathbf{a}\|^2 \end{aligned}$$

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$$
\begin{aligned}
\mathrm{Var}(\mathbf{a}^T\mathbf{Y}) &= \mathbf{a}^T\mathrm{Cov}(\mathbf{Y})\mathbf{a} \\
&= \sigma^2\|\mathbf{a}\|^2 \\
&= \sigma^2(\|\mathbf{a}^*\|^2 + \|\mathbf{u}\|^2 + 2\mathbf{a}^{*T}\mathbf{u})
\end{aligned}
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\end{aligned}$$

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&= \sigma^2(\|\mathbf{a}^*\|^2 + \|\mathbf{u}\|^2) + 0 \\
&= \mathrm{Var}(\mathbf{a}^{*T}\mathbf{Y}) + \sigma^2\|\mathbf{u}\|^2 \\
&\geq \mathrm{Var}(\mathbf{a}^{*T}\mathbf{Y})
\end{aligned}
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with equality if and only if $\mathbf{a} = \mathbf{a}^*$

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&= \sigma^2\|\mathbf{a}\|^2 \\
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&= \sigma^2(\|\mathbf{a}^*\|^2 + \|\mathbf{u}\|^2) + 0 \\
&= \mathrm{Var}(\mathbf{a}^{*T}\mathbf{Y}) + \sigma^2\|\mathbf{u}\|^2 \\
&\geq \mathrm{Var}(\mathbf{a}^{*T}\mathbf{Y})
\end{aligned}
$$

with equality if and only if $\mathbf{a} = \mathbf{a}^*$

Hence $\mathbf{a}^{*T}\mathbf{Y}$ is the unique linear unbiased estimator of ψ with minimum variance

Proof of Minimum Variance (G-M)

- Let $\mathbf{a}^{*T}\mathbf{Y}$ be the unique unbiased linear estimator of ψ with $\mathbf{a}^* \in C(\mathbf{X})$.
- Let $\mathbf{a}^T\mathbf{Y}$ be any unbiased estimate of ψ; $\mathbf{a} = \mathbf{a}^* + \mathbf{u}$ with $\mathbf{a}^* \in C(\mathbf{X})$ and $\mathbf{u} \in C(\mathbf{X})^\perp$

$$
\begin{aligned}
\mathrm{Var}(\mathbf{a}^T\mathbf{Y}) &= \mathbf{a}^T\mathrm{Cov}(\mathbf{Y})\mathbf{a} \\
&= \sigma^2\|\mathbf{a}\|^2 \\
&= \sigma^2(\|\mathbf{a}^*\|^2 + \|\mathbf{u}\|^2 + 2\mathbf{a}^{*T}\mathbf{u}) \\
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Hence $\mathbf{a}^{*T}\mathbf{Y}$ is the unique linear unbiased estimator of ψ with minimum variance "BLUE" = Best Linear Unbiased Estimator

Continued

Proof.

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$$\begin{aligned} \mathbf{a}^{*T}\mathbf{Y} &= \mathbf{a}^{*T}\mathbf{P}_X^T\mathbf{Y} \\ &= \mathbf{a}^{*T}\mathbf{P}_x\mathbf{Y} \end{aligned}$$

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for $\boldsymbol{\lambda}^T = \mathbf{a}^{*T}\mathbf{X}$ or $\boldsymbol{\lambda} = \mathbf{X}^T\mathbf{a}$ $\square$

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- For predicting at new $\mathbf{x}_*$ is there always a unique unbiased estimator of $E[\mathbf{Y} \mid \mathbf{x}_*]$?
- If one does exist, how do we know that if we are given $\boldsymbol{\lambda}$?

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- What about out of sample prediction?

Example

```
x1 = -4:4
x2 = c(-2, 1, -1, 2, 0, 2, -1, 1, -2)
x3 = 3*x1  -2*x2
x4 = x2 - x1 + 4
Y = 1+x1+x2+x3+x4 + c(-.5,.5,.5,-.5,0,.5,-.5,-.5,.5)
dev.set = data.frame(Y, x1, x2, x3, x4)
lm1234 = lm(Y ~ x1 + x2 + x3 + x4, data=dev.set)
round(coefficients(lm1234), 4)

## (Intercept)          x1          x2          x3          x4
##           5           3           0          NA          NA

lm3412 = lm(Y ~ x3 + x4 + x1 + x2, data = dev.set)
round(coefficients(lm3412), 4)

## (Intercept)          x3          x4          x1          x2
##         -19           3           6          NA          NA
```

In Sample Predictions

```r
cbind(dev.set, predict(lm1234), predict(lm3412))
```

```
##      Y x1 x2  x3 x4 predict(lm1234) predict(lm3412)
## 1 -7.5 -4 -2  -8  6              -7              -7
## 2 -3.5 -3  1 -11  8              -4              -4
## 3 -0.5 -2 -1  -4  5              -1              -1
## 4  1.5 -1  2  -7  7               2               2
## 5  5.0  0  0   0  4               5               5
## 6  8.5  1  2  -1  5               8               8
## 7 10.5  2 -1   8  1              11              11
## 8 13.5  3  1   7  2              14              14
## 9 17.5  4 -2  16 -2              17              17
```

Both models agree for estimating the mean at the observed $\mathbf{X}$ points!

Out of Sample

```
out = data.frame(test.set,
      Y1234=predict(lm1234, new=test.set),
      Y3412=predict(lm3412, new=test.set))
out

##   x1 x2 x3 x4 Y1234 Y3412
## 1  3  1  7  2    14    14
## 2  6  2 14  4    23    47
## 3  6  2 14  0    23    23
## 4  0  0  0  4     5     5
## 5  0  0  0  0     5   -19
## 6  1  2  3  4     8    14
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```

Agreement for cases 1, 3, and 4 only! Can we determine that without finding the predictions and comparing?

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Take $\mathbf{P}_{\mathbf{X}^T} = (\mathbf{X}^T\mathbf{X})(\mathbf{X}^T\mathbf{X})^-$ as a projection onto $C(\mathbf{X}^T)$ and show $(\mathbf{I} - \mathbf{P}_{\mathbf{X}^T})\boldsymbol{\lambda} = \mathbf{0}_p$

Example

```
library("estimability" )
cbind(epredict(lm1234, test.set), epredict(lm3412, test.set
```

```
##   [,1] [,2]
## 1   14   14
## 2   NA   NA
## 3   23   23
## 4    5    5
## 5   NA   NA
## 6   NA   NA
```

Rows 2, 5, and 6 are not estimable! No linear unbiased estimator

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- may occur with redundancies for modest $p < n$ and of course $p > n$
- Eliminate redundancies by removing variables (variable selection)
- Consider alternative estimators (Bayes and related)

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  where $\mathsf{Bias} = \mathsf{E}[g(\mathbf{Y})] - \boldsymbol{\lambda}^T\beta$
- Bias vs Variance tradeoff
- Can have smaller MSE if we allow some Bias!

Bayes

- Next Class Bayes Theorem & Conjugate Normal-Gamma Prior/Posterior distributions
- Read Chapter 2 in Christensen or Wakefield 5.7
- Review Multivariate Normal and Gamma distributions