

Maximum Likelihood Estimation

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STA721 Linear Models

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Topics

- Likelihood Function
- Projections
- Maximum Likelihood Estimates

Readings: Christensen Chapter 1-2, Appendix A, and Appendix B

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- $\epsilon_i \stackrel{\text{iid}}{\sim} N(0, \sigma^2)$ implies that $Y_i \stackrel{\text{ind}}{\sim} N(\mu_i, \sigma^2)$

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Last line is the density of $\mathbf{Y} \sim N_n(\mu, \sigma^2 \mathbf{I}_n)$

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or equivalently the log likelihood

Clearly, $\hat{\boldsymbol{\mu}} = \mathbf{Y}$ but $\hat{\sigma}^2 = 0$ is outside the parameter space

Need restrictions on $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$

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- $\mathbf{P}_X \mu = \mathbf{P}_X \mathbf{X}\beta = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{X}\beta = \mathbf{X}\beta = \mu$

Claim: $\mathbf{I} - \mathbf{P}_{\mathbf{X}}$ is an orthogonal projection onto $C(\mathbf{X})^\perp$

Projections

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Projections

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- idempotent

$$\begin{aligned}(\mathbf{I} - \mathbf{P}_X)^2 &= (\mathbf{I} - \mathbf{P}_X)(\mathbf{I} - \mathbf{P}_X) \\ &= \mathbf{I} - \mathbf{P}_X - \mathbf{P}_X + \mathbf{P}_X\mathbf{P}_X\end{aligned}$$

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Claim: $\mathbf{I} - \mathbf{P}_X$ is an orthogonal projection onto $C(\mathbf{X})^\perp$

- idempotent

$$\begin{aligned}(\mathbf{I} - \mathbf{P}_X)^2 &= (\mathbf{I} - \mathbf{P}_X)(\mathbf{I} - \mathbf{P}_X) \\&= \mathbf{I} - \mathbf{P}_X - \mathbf{P}_X + \mathbf{P}_X\mathbf{P}_X \\&= \mathbf{I} - \mathbf{P}_X - \mathbf{P}_X + \mathbf{P}_X\end{aligned}$$

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$$\begin{aligned}(\mathbf{I} - \mathbf{P}_X)^2 &= (\mathbf{I} - \mathbf{P}_X)(\mathbf{I} - \mathbf{P}_X) \\&= \mathbf{I} - \mathbf{P}_X - \mathbf{P}_X + \mathbf{P}_X \mathbf{P}_X \\&= \mathbf{I} - \mathbf{P}_X - \mathbf{P}_X + \mathbf{P}_X \\&= \mathbf{I} - \mathbf{P}_X\end{aligned}$$

- Symmetry $\mathbf{I} - \mathbf{P}_X = (\mathbf{I} - \mathbf{P}_X)^T$

Claim: $\mathbf{I} - \mathbf{P}_X$ is an orthogonal projection onto $C(\mathbf{X})^\perp$

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$$\begin{aligned}(\mathbf{I} - \mathbf{P}_X)^2 &= (\mathbf{I} - \mathbf{P}_X)(\mathbf{I} - \mathbf{P}_X) \\&= \mathbf{I} - \mathbf{P}_X - \mathbf{P}_X + \mathbf{P}_X \mathbf{P}_X \\&= \mathbf{I} - \mathbf{P}_X - \mathbf{P}_X + \mathbf{P}_X \\&= \mathbf{I} - \mathbf{P}_X\end{aligned}$$

- Symmetry $\mathbf{I} - \mathbf{P}_X = (\mathbf{I} - \mathbf{P}_X)^T$
- $\mathbf{u} \in C(\mathbf{X})^\perp \Rightarrow \mathbf{u} \perp C(\mathbf{X})$ that is $u \in C(\mathbf{X})^\perp$ and $v \in C(\mathbf{X})$
then $\mathbf{u}^T \mathbf{v} = 0$
- $(\mathbf{I} - \mathbf{P}_X)\mathbf{u} = \mathbf{u}$ (projection)

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- Symmetry $\mathbf{I} - \mathbf{P}_X = (\mathbf{I} - \mathbf{P}_X)^T$
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- $(\mathbf{I} - \mathbf{P}_X)\mathbf{u} = \mathbf{u}$ (projection)
- if $\mathbf{v} \in C(\mathbf{X})$, $(\mathbf{I} - \mathbf{P}_X)\mathbf{v} = \mathbf{v} - \mathbf{v} = \mathbf{0}$

$\mathbf{Y} \sim N(\boldsymbol{\mu}, \sigma^2 \mathbf{I}_n)$ with $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ and \mathbf{X} full column rank

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- Log Likelihood:

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- Log Likelihood:

$$\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) = -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}$$

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- Decompose $\mathbf{Y} = \mathbf{P}_\mathbf{X}\mathbf{Y} + (\mathbf{I} - \mathbf{P}_\mathbf{X})\mathbf{Y}$

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- Decompose $\mathbf{Y} = \mathbf{P}_\mathbf{X}\mathbf{Y} + (\mathbf{I} - \mathbf{P}_\mathbf{X})\mathbf{Y}$
- Use $\mathbf{P}_\mathbf{X}\boldsymbol{\mu} = \boldsymbol{\mu}$

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- Decompose $\mathbf{Y} = \mathbf{P}_X \mathbf{Y} + (\mathbf{I} - \mathbf{P}_X) \mathbf{Y}$
- Use $\mathbf{P}_X \boldsymbol{\mu} = \boldsymbol{\mu}$
- Simplify $\|\mathbf{Y} - \boldsymbol{\mu}\|^2$

$$\|\mathbf{Y} - \boldsymbol{\mu}\|^2 = \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\ &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\ &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\ &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 2(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X) \mathbf{Y}\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 2(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X) \mathbf{Y} \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 0\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 2(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X)\mathbf{Y} \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 0 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 2(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X)\mathbf{Y} \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 0 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2\end{aligned}$$

Crossproduct term is zero

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 2(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X)\mathbf{Y} \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 0 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2\end{aligned}$$

Crossproduct term is zero

$$\mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X) = \mathbf{P}_X (\mathbf{I} - \mathbf{P}_X)$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 2(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X)\mathbf{Y} \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 0 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2\end{aligned}$$

Crossproduct term is zero

$$\begin{aligned}\mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X) &= \mathbf{P}_X (\mathbf{I} - \mathbf{P}_X) \\&= \mathbf{P}_X - \mathbf{P}_X \mathbf{P}_X\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 2(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X)\mathbf{Y} \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 0 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2\end{aligned}$$

Crossproduct term is zero

$$\begin{aligned}\mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X) &= \mathbf{P}_X (\mathbf{I} - \mathbf{P}_X) \\&= \mathbf{P}_X - \mathbf{P}_X \mathbf{P}_X \\&= \mathbf{P}_X - \mathbf{P}_X\end{aligned}$$

Expand

$$\begin{aligned}\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X\mathbf{Y} - \mathbf{P}_X\boldsymbol{\mu}\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y} + \mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 2(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X) \mathbf{Y} \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X(\mathbf{Y} - \boldsymbol{\mu})\|^2 + 0 \\&= \|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2 + \|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2\end{aligned}$$

Crossproduct term is zero

$$\begin{aligned}\mathbf{P}_X^T (\mathbf{I} - \mathbf{P}_X) &= \mathbf{P}_X (\mathbf{I} - \mathbf{P}_X) \\&= \mathbf{P}_X - \mathbf{P}_X \mathbf{P}_X \\&= \mathbf{P}_X - \mathbf{P}_X \\&= 0\end{aligned}$$

Substitute decomposition into log likelihood

$$\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) = -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}$$

Substitute decomposition into log likelihood

$$\begin{aligned}\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \\ &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \right)\end{aligned}$$

Substitute decomposition into log likelihood

$$\begin{aligned}\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \\&= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \right) \\&= \underbrace{-\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2}} + \underbrace{-\frac{1}{2} \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}}\end{aligned}$$

Substitute decomposition into log likelihood

$$\begin{aligned}\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \\&= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \right) \\&= \underbrace{-\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2}}_{\text{constant with respect to } \boldsymbol{\mu}} + \underbrace{-\frac{1}{2} \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}}_{\text{constant with respect to } \boldsymbol{\mu}} \\&= \text{constant with respect to } \boldsymbol{\mu}\end{aligned}$$

Substitute decomposition into log likelihood

$$\begin{aligned}\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \\&= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \right) \\&= \underbrace{-\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2}}_{\text{constant with respect to } \boldsymbol{\mu}} + \underbrace{-\frac{1}{2} \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}}_{\leq 0} \\&= \text{constant with respect to } \boldsymbol{\mu} \leq 0\end{aligned}$$

Substitute decomposition into log likelihood

$$\begin{aligned}\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \\&= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \right) \\&= \underbrace{-\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2}}_{\text{constant with respect to } \boldsymbol{\mu}} + \underbrace{-\frac{1}{2} \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}}_{\leq 0} \\&= \text{constant with respect to } \boldsymbol{\mu} \leq 0\end{aligned}$$

Maximize with respect to $\boldsymbol{\mu}$ for each σ^2

Substitute decomposition into log likelihood

$$\begin{aligned}\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \\&= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \right) \\&= \underbrace{-\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2}}_{\text{constant with respect to } \boldsymbol{\mu}} + \underbrace{-\frac{1}{2} \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}}_{\leq 0} \\&= \text{constant with respect to } \boldsymbol{\mu} \leq 0\end{aligned}$$

Maximize with respect to $\boldsymbol{\mu}$ for each σ^2

RHS is largest when $\boldsymbol{\mu} = \mathbf{P}_X\mathbf{Y}$ for any choice of σ^2

Substitute decomposition into log likelihood

$$\begin{aligned}\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \\&= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \right) \\&= \underbrace{-\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2}}_{\text{constant with respect to } \boldsymbol{\mu}} + \underbrace{-\frac{1}{2} \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}}_{\leq 0} \\&= \text{constant with respect to } \boldsymbol{\mu} \leq 0\end{aligned}$$

Maximize with respect to $\boldsymbol{\mu}$ for each σ^2

RHS is largest when $\boldsymbol{\mu} = \mathbf{P}_X\mathbf{Y}$ for any choice of σ^2

$$\therefore \hat{\boldsymbol{\mu}} = \mathbf{P}_X\mathbf{Y}$$

is the MLE of $\boldsymbol{\mu}$

Substitute decomposition into log likelihood

$$\begin{aligned}\log \mathcal{L}(\boldsymbol{\mu}, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \\&= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2} \right) \\&= \underbrace{-\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2}}_{\text{constant with respect to } \boldsymbol{\mu}} + \underbrace{-\frac{1}{2} \frac{\|\mathbf{P}_X\mathbf{Y} - \boldsymbol{\mu}\|^2}{\sigma^2}}_{\leq 0} \\&= \text{constant with respect to } \boldsymbol{\mu} \leq 0\end{aligned}$$

Maximize with respect to $\boldsymbol{\mu}$ for each σ^2

RHS is largest when $\boldsymbol{\mu} = \mathbf{P}_X\mathbf{Y}$ for any choice of σ^2

$$\therefore \hat{\boldsymbol{\mu}} = \mathbf{P}_X\mathbf{Y}$$

is the MLE of $\boldsymbol{\mu}$ (yields fitted values $\hat{\mathbf{Y}} = \mathbf{P}_X\mathbf{Y}$)

$$\mathcal{L}(\mu, \sigma^2) = -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \mu\|^2}{\sigma^2} \right)$$

$$\begin{aligned}\mathcal{L}(\mu, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \mu\|^2}{\sigma^2} \right) \\ \mathcal{L}(\beta, \sigma^2) &= -\frac{n}{2} \log(\sigma^2) - \frac{1}{2} \left(\frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2} + \frac{\|\mathbf{P}_X\mathbf{Y} - \mathbf{X}\beta\|^2}{\sigma^2} \right)\end{aligned}$$

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Similar argument to show that RHS is maximized by minimizing

$$\|\mathbf{P}_X\mathbf{Y} - \mathbf{X}\beta\|^2$$

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Therefore $\hat{\beta}$ is a MLE of β if and only if satisfies

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$$\mathbf{P}_X\mathbf{Y} = \mathbf{X}\hat{\beta}$$

If $\mathbf{X}^T\mathbf{X}$ is full rank, the MLE of β is

$$(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} = \hat{\beta}$$

- Plug-in MLE of $\hat{\mu}$ for μ and differentiate with respect to σ^2

- Plug-in MLE of $\hat{\boldsymbol{\mu}}$ for $\boldsymbol{\mu}$ and differentiate with respect to σ^2

$$\log \mathcal{L}(\hat{\boldsymbol{\mu}}, \sigma^2) = -\frac{n}{2} \log \sigma^2 - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{\sigma^2}$$

- Plug-in MLE of $\hat{\boldsymbol{\mu}}$ for $\boldsymbol{\mu}$ and differentiate with respect to σ^2

$$\begin{aligned}\log \mathcal{L}(\hat{\boldsymbol{\mu}}, \sigma^2) &= -\frac{n}{2} \log \sigma^2 - \frac{1}{2} \frac{\|(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{Y}\|^2}{\sigma^2} \\ \frac{\partial \log \mathcal{L}(\hat{\boldsymbol{\mu}}, \sigma^2)}{\partial \sigma^2} &= -\frac{n}{2} \frac{1}{\sigma^2} + \frac{1}{2} \|(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{Y}\|^2 \left(\frac{1}{\sigma^2}\right)^2\end{aligned}$$

- Plug-in MLE of $\hat{\boldsymbol{\mu}}$ for $\boldsymbol{\mu}$ and differentiate with respect to σ^2

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- Set derivative to zero and solve for MLE

$$0 = -\frac{n}{2} \frac{1}{\hat{\sigma}^2} + \frac{1}{2} \|(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{Y}\|^2 \left(\frac{1}{\hat{\sigma}^2} \right)^2$$

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- Plug-in MLE of $\hat{\boldsymbol{\mu}}$ for $\boldsymbol{\mu}$ and differentiate with respect to σ^2

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Maximum Likelihood Estimate of σ^2

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$$\begin{aligned}\hat{\sigma}^2 &= \frac{\|(\mathbf{I} - \mathbf{P}_X)\mathbf{Y}\|^2}{n} \\ &= \frac{\mathbf{Y}^T (\mathbf{I} - \mathbf{P}_X)^T (\mathbf{I} - \mathbf{P}_X) \mathbf{Y}}{n}\end{aligned}$$

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where $\mathbf{e} = (\mathbf{I} - \mathbf{P}_X)\mathbf{Y}$ **residuals** from the regression of \mathbf{Y} on \mathbf{X}

- Fitted Values $\hat{\mathbf{Y}} = \mathbf{P}_X \mathbf{Y} = \mathbf{X} \hat{\boldsymbol{\beta}}$

Geometric View

- Fitted Values $\hat{\mathbf{Y}} = \mathbf{P}_X \mathbf{Y} = \mathbf{X} \hat{\boldsymbol{\beta}}$
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Geometric View

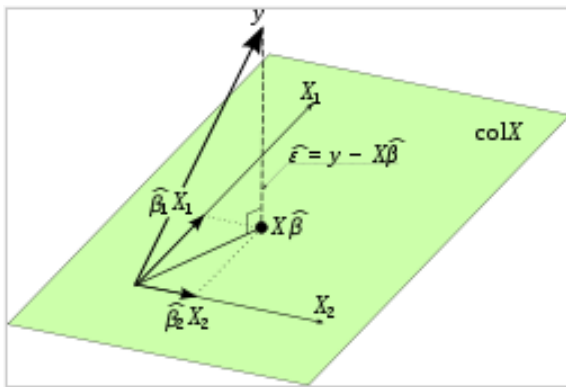
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Will not be $\mathbf{0}$ if $\boldsymbol{\mu} \notin C(\mathbf{X})$ (useful for model checking)

Estimate of σ^2

MLE of σ^2 :

$$\hat{\sigma}^2 = \frac{\mathbf{e}^T \mathbf{e}}{n} = \frac{\mathbf{Y}^T (\mathbf{I} - \mathbf{P}_X) \mathbf{Y}}{n}$$

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Is this an unbiased estimate of σ^2 ?

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Is this an unbiased estimate of σ^2 ?

Need expectations of quadratic forms $\mathbf{Y}^T \mathbf{A} \mathbf{Y}$ for \mathbf{A} an $n \times n$ matrix
 \mathbf{Y} a random vector in \mathbb{R}^n

Without loss of generality we can assume that $\mathbf{A} = \mathbf{A}^T$

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- may take $\mathbf{A} = \mathbf{A}^T$

Expectations of Quadratic Forms

Theorem

Let \mathbf{Y} be a random vector in \mathbb{R}^n with $E[\mathbf{Y}] = \boldsymbol{\mu}$ and $\text{Cov}(\mathbf{Y}) = \boldsymbol{\Sigma}$.

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Let \mathbf{Y} be a random vector in \mathbb{R}^n with $E[\mathbf{Y}] = \boldsymbol{\mu}$ and $\text{Cov}(\mathbf{Y}) = \boldsymbol{\Sigma}$.
Then $E[\mathbf{Y}^T \mathbf{A} \mathbf{Y}] = \text{tr} \mathbf{A} \boldsymbol{\Sigma} + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu}$.

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Let \mathbf{Y} be a random vector in \mathbb{R}^n with $E[\mathbf{Y}] = \boldsymbol{\mu}$ and $\text{Cov}(\mathbf{Y}) = \boldsymbol{\Sigma}$.
Then $E[\mathbf{Y}^T \mathbf{A} \mathbf{Y}] = \text{tr} \mathbf{A} \boldsymbol{\Sigma} + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu}$.

Result useful for finding expected values of Mean Squares; no normality required!

Start with $(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A}(\mathbf{Y} - \boldsymbol{\mu})$, expand and take expectations

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$$E[(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A}(\mathbf{Y} - \boldsymbol{\mu})] = E[\mathbf{Y}^T \mathbf{A} \mathbf{Y} + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} - \boldsymbol{\mu}^T \mathbf{A} \mathbf{Y} - \mathbf{Y}^T \mathbf{A} \boldsymbol{\mu}]$$

Start with $(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A}(\mathbf{Y} - \boldsymbol{\mu})$, expand and take expectations

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Proof

Start with $(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A}(\mathbf{Y} - \boldsymbol{\mu})$, expand and take expectations

$$\begin{aligned} E[(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A}(\mathbf{Y} - \boldsymbol{\mu})] &= E[\mathbf{Y}^T \mathbf{A} \mathbf{Y} + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} - \boldsymbol{\mu}^T \mathbf{A} \mathbf{Y} - \mathbf{Y}^T \mathbf{A} \boldsymbol{\mu}] \\ &= E[\mathbf{Y}^T \mathbf{A} \mathbf{Y}] + \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} - \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} - \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \\ &= E[\mathbf{Y}^T \mathbf{A} \mathbf{Y}] - \boldsymbol{\mu}^T \mathbf{A} \boldsymbol{\mu} \end{aligned}$$

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Rearrange

Start with $(\mathbf{Y} - \boldsymbol{\mu})^T \mathbf{A}(\mathbf{Y} - \boldsymbol{\mu})$, expand and take expectations

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Expectation of $\hat{\sigma}^2$

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If \mathbf{X} is full rank ($r(\mathbf{X}) = p$) and $\mathbf{P}_X = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$ then the

$$\begin{aligned}\text{tr}(\mathbf{P}_X) &= \text{tr}(\mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T) \\&= \text{tr}(\mathbf{X}^T \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1}) \\&= \text{tr}(\mathbf{I}_p) = p\end{aligned}$$

Spectral Theorem

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If \mathbf{A} ($n \times n$) is a symmetric real matrix then there exists a \mathbf{U} ($n \times n$) such that $\mathbf{U}^T \mathbf{U} = \mathbf{U} \mathbf{U}^T = \mathbf{I}_n$ and a diagonal matrix $\mathbf{\Lambda}$ with elements λ_i such that $\mathbf{A} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^T$

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$$\mathbf{P} = [\mathbf{U}_P \mathbf{U}_{P^\perp}] \begin{bmatrix} \mathbf{I}_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0}_{n-r} \end{bmatrix} \begin{bmatrix} \mathbf{U}_P^T \\ \mathbf{U}_{P^\perp}^T \end{bmatrix} = \mathbf{U}_P \mathbf{U}_P^T$$

$$\mathbf{P} = \sum_{i=1}^r \mathbf{u}_i \mathbf{u}_i^T$$

sum of r rank 1 projections.

Next Class

distribution theory

Continue Reading Chapter 1-2 and Appendices A & B in
Christensen