Maximum Likelihood Estimation

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STA721 Linear Models

Duke University

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Outline

Topics

- Likelihood Function
- Projections
- Maximum Likelihood Estimates

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

Models

Take an random vector $\mathbf{Y} \in \mathbb{R}^n$ which is observable and decompose

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- $\boldsymbol{\epsilon}_i \overset{\text{iid}}{\sim} \mathsf{N}(0, \sigma^2)$ implies that $Y_i \overset{\text{ind}}{\sim} \mathsf{N}(\mu_i, \sigma^2)$

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

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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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- $\mathbf{P_X}$ is the orthogonal projection operator on the column space of $\mathbf{X}$; e.g.
- $\mathbf{P} = \mathbf{P}^2$ idempotent (projection)

$$\begin{aligned}
\mathbf{P}_X^2 = \mathbf{P_X}\mathbf{P_X} &= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T \\
&= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T \\
&= \mathbf{P_X}
\end{aligned}$$

- $\mathbf{P} = \mathbf{P}^T$ symmetry (orthogonal)

$$\begin{aligned}
\mathbf{P_X}^T &= (\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T)^T \\
&= (\mathbf{X}^T)^T((\mathbf{X}^T\mathbf{X})^{-1})^T(\mathbf{X})^T \\
&= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T \\
&= \mathbf{P_X}
\end{aligned}$$

- $\mathbf{P_X}\boldsymbol{\mu} = \mathbf{P_X}\mathbf{X}\boldsymbol{\beta} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} = \mathbf{X}\boldsymbol{\beta} = \boldsymbol{\mu}$

Projections

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

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

Projections

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

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

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

Projections

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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)

Projections

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- idempotent

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(\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)
- if $\mathbf{v} \in C(\mathbf{X})$, $(\mathbf{I} - \mathbf{P_X})\mathbf{v} = \mathbf{v} - \mathbf{v} = \mathbf{0}$

Log Likelihood

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

Log Likelihood

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Claim: Maximum Likelihood Estimator (MLE) of $\boldsymbol{\mu}$ is $\mathbf{P_X Y}$

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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 $\mathbf{Y} = \mathbf{P_X Y} + (\mathbf{I} - \mathbf{P_X})\mathbf{Y}$

Log Likelihood

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

Log Likelihood

$\mathbf{Y} \sim \mathrm{N}(\boldsymbol{\mu}, \sigma^2 \mathbf{I}_n)$ with $\boldsymbol{\mu} = \mathbf{X}\beta$ and $\mathbf{X}$ full column rank
Claim: Maximum Likelihood Estimator (MLE) of $\boldsymbol{\mu}$ is $\mathbf{P_X Y}$

- Log Likelihood:

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

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

Expand

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

Expand

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

Expand

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

Expand

$$
\begin{aligned}
\|\mathbf{Y} - \boldsymbol{\mu}\|^2 &= \|(\mathbf{I} - \mathbf{P_X})\mathbf{Y} + \mathbf{P}_x\mathbf{Y} - \boldsymbol{\mu}\|^2 \\
&= \|(\mathbf{I} - \mathbf{P_X})\mathbf{Y} + \mathbf{P}_x\mathbf{Y} - \mathbf{P_X}\boldsymbol{\mu}\|^2 \\
&= \|(\mathbf{I} - \mathbf{P_x})\mathbf{Y} + \mathbf{P_X}(\mathbf{Y} - \boldsymbol{\mu})\|^2 \\
&= \color{red}{\|(\mathbf{I} - \mathbf{P_x})\mathbf{Y}\|^2}
\end{aligned}
$$

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

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

Crossproduct term is zero

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

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

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

Crossproduct term is zero

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

Likelihood

Substitute decomposition into log likelihood

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

Likelihood

Substitute decomposition into log likelihood

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

Likelihood

Substitute decomposition into log likelihood

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

Likelihood

Substitute decomposition into log likelihood

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

Likelihood

Substitute decomposition into log likelihood

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

Likelihood

Substitute decomposition into log likelihood

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

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

Likelihood

Substitute decomposition into log likelihood

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

Maximize with respect to $\boldsymbol{\mu}$ for each σ^2
RHS is largest when $\boldsymbol{\mu} = \mathbf{P}_\mathbf{X}\mathbf{Y}$ for any choice of σ^2

Likelihood

Substitute decomposition into log likelihood

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\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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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

$$\therefore \quad \hat{\boldsymbol{\mu}} = \mathbf{P_X}\mathbf{Y}$$

is the MLE of μ

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

$$\therefore \quad \hat{\boldsymbol{\mu}} = \mathbf{P_X}\mathbf{Y}$$

is the MLE of μ (yields fitted values $\hat{\mathbf{Y}} = \mathbf{P_X}\mathbf{Y}$)

MLE of β

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

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\mathcal{L}(\boldsymbol{\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}$$

MLE of β

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

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Similar argument to show that RHS is maximized by minimizing

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

MLE of β

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\mathcal{L}(\boldsymbol{\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}-\boldsymbol{\mu}\|^2}{\sigma^2}\right) \\
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Therefore $\hat{\beta}$ is a MLE of β if and only if satisfies

$$\mathbf{P_X}\mathbf{Y} = \mathbf{X}\hat{\beta}$$

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\mathcal{L}(\boldsymbol{\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 Y} - \mathbf{X}\beta\|^2}{\sigma^2}\right)
\end{aligned}$$

Similar argument to show that RHS is maximized by minimizing

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

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

$$\mathbf{P_X Y} = \mathbf{X}\hat{\beta}$$

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

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

MLE of σ^2

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\end{aligned}$$

- Set derivative to zero and solve for MLE

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

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0 &= -\frac{n}{2}\frac{1}{\hat{\sigma}^2} + \frac{1}{2}\|(\mathbf{I}-\mathbf{P_X})\mathbf{Y}\|^2\left(\frac{1}{\hat{\sigma}^2}\right)^2 \\
\frac{n}{2}\hat{\sigma}^2 &= \frac{1}{2}\|(\mathbf{I}-\mathbf{P_X})\mathbf{Y}\|^2 \\
\hat{\sigma}^2 &= \frac{\|(\mathbf{I}-\mathbf{P_X})\mathbf{Y}\|^2}{n}
\end{aligned}
$$

Estimate of σ^2

Maximum Likelihood Estimate of σ^2

$$\hat{\sigma}^2 = \frac{\|(\mathbf{I} - \mathbf{P_X})\mathbf{Y}\|^2}{n}$$

Maximum Likelihood Estimate of σ^2

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

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&= \frac{\mathbf{e}^T\mathbf{e}}{n}
\end{aligned}$$

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

Geometric View

- Fitted Values $\hat{\mathbf{Y}} = \mathbf{P_X Y} = \mathbf{X}\hat{\beta}$

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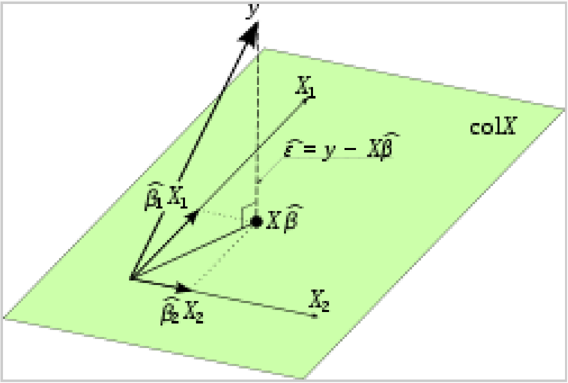

Properties

$\hat{\mathbf{Y}} = \hat{\boldsymbol{\mu}}$ is an unbiased estimate of $\boldsymbol{\mu} = \mathbf{X}\beta$

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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 $\mathbb{R}^n$

Quadratic Forms

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

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Quadratic Forms

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

Theorem

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

Expectations of Quadratic Forms

Theorem

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

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Theorem

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

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

Proof

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

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

Proof

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

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

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

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

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

$\mathrm{tr}\mathbf{A} \equiv \sum_{i=1}^{n} a_{ii}$

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

Use the theorem:

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$$E[\mathbf{Y}^T(\mathbf{I} - \mathbf{P_X})\mathbf{Y}] \quad = \quad \operatorname{tr}(\mathbf{I} - \mathbf{P_X})\sigma^2\mathbf{I} + \boldsymbol{\mu}^T(\mathbf{I} - \mathbf{P_X})\boldsymbol{\mu}$$

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&= \sigma^2\mathrm{tr}(\mathbf{I}-\mathbf{P_X}) \\
&= \sigma^2 r(\mathbf{I}-\mathbf{P_X})
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Therefore an unbiased estimate of σ^2 is

$$\frac{\mathbf{e}^T\mathbf{e}}{n - r(\mathbf{X})}$$

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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

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

Spectral Theorem

Theorem

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 $\boldsymbol{\Lambda}$ with elements λ_i such that $\mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$

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If $\mathbf{P}$ is an orthogonal projection matrix, then its eigenvalues λ_i are either zero or one with $\text{tr}(\mathbf{P}) = \sum_i(\lambda_i) = r(\mathbf{P})$

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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