# Rank Deficient Models

STA 721: Lecture 3

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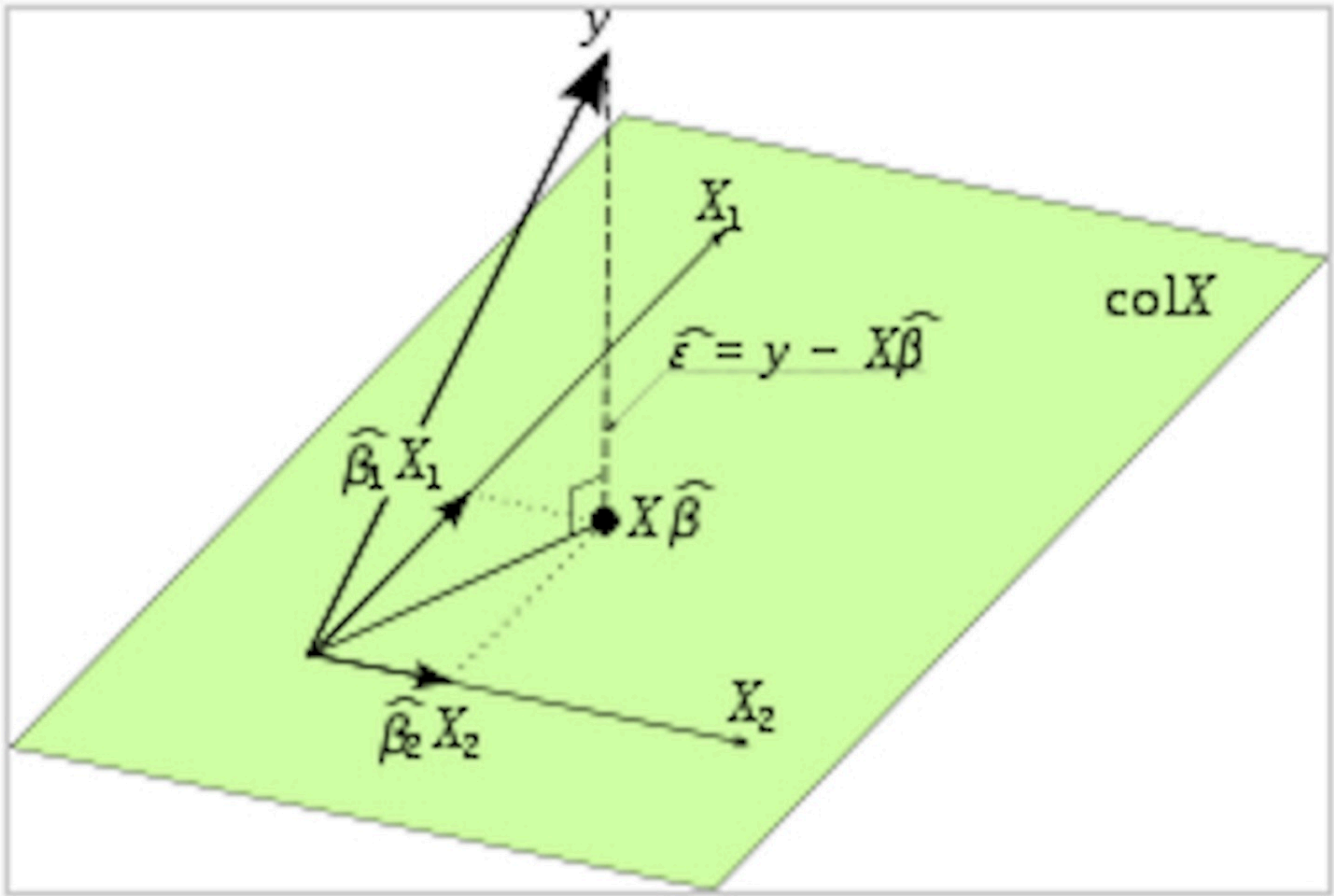
# Outline

- Rank Deficient Models
- Generalized Inverses, Projections and MLEs/OLS
- Class of Unbiased Estimators

Readings: - Christensen Chapter 2 and Appendix B - Seber & Lee Chapter 3

# Geometric View



# Non-Full Rank Case

- Model: $\mathbf{Y} = \boldsymbol{\mu} + \boldsymbol{\epsilon}$
- Assumption: $\boldsymbol{\mu} \in C(\mathbf{X})$ for $\mathbf{X} \in \mathbb{R}^{n \times p}$
- What if the rank of $\mathbf{X}$, $r(\mathbf{X}) \equiv r \neq p$?
- Still have result that the OLS/MLE solution satisfies

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

- How can we characterize $\mathbf{P}$ and $\hat{\beta}$ in this case? 3 cases

1. $p \leq n, r(\mathbf{X}) \neq p \Rightarrow r(\mathbf{X}) < p$
2. $p > n, r(\mathbf{X}) \neq p$
3. $p > n, r(\mathbf{X}) = p$

Focus on the first case for OLS/MLE for now…

# Model Space

- $\boldsymbol{\mathcal{M}} = C(\mathbf{X})$ is an $r$-dimensional subspace of $\mathbb{R}^n$
- $\boldsymbol{\mathcal{M}}$ has an $(n-r)$-dimensional orthogonal complement $\boldsymbol{\mathcal{N}}$
- each $\mathbf{y} \in \mathbb{R}^n$ has a unique representation as

$$\mathbf{y} = \hat{\mathbf{y}} + \mathbf{e}$$

  for $\hat{\mathbf{y}} \in \boldsymbol{\mathcal{M}}$ and $\mathbf{e} \in \boldsymbol{\mathcal{N}}$

- $\hat{\mathbf{y}}$ is the orthogonal projection of $\mathbf{y}$ onto $\boldsymbol{\mathcal{M}}$ and is the OLS/MLE estimate of $\boldsymbol{\mu}$ that satisfies

$$\mathbf{P}_{\mathbf{X}}\mathbf{y} = \mathbf{X}\hat{\boldsymbol{\beta}}$$

- $\mathbf{X}^T\mathbf{X}$ is not invertible so need another way to represent $\mathbf{P}_{\mathbf{X}}$ and $\hat{\boldsymbol{\beta}}$

# Spectral Decomposition (SD)

Every symmetric $n \times n$ matrix, $\mathbf{S}$, has an eigen decomposition $\mathbf{S} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$

- $\boldsymbol{\lambda}$ is a diagonal matrix with eigenvalues $(\lambda_1, \ldots, \lambda_n)$ of $\mathbf{S}$
- $\mathbf{U}$ is a $n \times n$ *orthogonal* matrix $\mathbf{U}^T\mathbf{U} = \mathbf{U}\mathbf{U}^T = \mathbf{I}_n$ ( $\mathbf{U}^{-1} = \mathbf{U}^T$)
- the columns of $\mathbf{U}$ from an Orthonormal Basis (ONB) for $\mathbb{R}^n$
- the columns of $\mathbf{U}$ associated with non-zero eigenvalues form an ONB for $C(\mathbf{S})$
- the number of non-zero eigenvalues is the rank of $\mathbf{S}$
- the columns of $\mathbf{U}$ associated with zero eigenvalues form an ONB for $C(\mathbf{S})^\perp$
- $\mathbf{S}^d = \mathbf{U}\boldsymbol{\Lambda}^d\mathbf{U}^T$ (matrix powers)

# Positive Definite and Non-Negative Definite Matrices

▼ **Definition:** B.21 Positive Definite and Non-Negative Definite

A symmetric matrix $\mathbf{S}$ is *positive definite* ($\mathbf{S} > 0$) if and only if $\mathbf{x}^T\mathbf{S}\mathbf{x} > 0$ for $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{x} \neq \mathbf{0}_n$, and *positive semi-definite* or *non-negative definite* ($\mathbf{S} \geq 0$) if and only if $\mathbf{x}^T\mathbf{S}\mathbf{x} \geq 0$ for $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{x} \neq \mathbf{0}_n$

**Exercise**

Show that a symmetric matrix $\mathbf{S}$ is positive definite if and only if its eigenvalues are all strictly greater than zero, and positive semi-definite if all the eigenvalues are non-negative.

# Projections

Let $\mathbf{P}$ be an orthogonal projection matrix onto $\boldsymbol{\mathcal{M}}$, then

1. the eigenvalues of $\mathbf{P}$, $\lambda_i$, are either zero or one
2. the trace of $\mathbf{P}$ is the rank of $\mathbf{P}$
3. the dimension of the subspace that $\mathbf{P}$ projects onto is the rank of $\mathbf{P}$
4. the columns of $\mathbf{U}_r = [u_1, u_2, \ldots u_r]$ form an ONB for the $C(\mathbf{P})$
5. the projection $\mathbf{P}$ has the representation $\mathbf{P} = \mathbf{U}_r \mathbf{U}_r^T = \sum_{i=1}^r u_i u_i^T$ (the sum of $r$ rank 1 projections)
6. the projection $\mathbf{I}_n - \mathbf{P} = \mathbf{I} - \mathbf{U}_r \mathbf{U}_r^T = \mathbf{U}_\perp \mathbf{U}_\perp^T$ where $\mathbf{U}_\perp = [u_{r+1}, \ldots u_n]$ is an orthogonal projection onto $\boldsymbol{\mathcal{N}}$

MLE/OLS:

- $\mathbf{P}_X \mathbf{y} = \mathbf{U}_r \mathbf{U}_r^T \mathbf{y} = \mathbf{U}_r \tilde{\boldsymbol{\beta}}$
- Claim $\tilde{\boldsymbol{\beta}}$ is a MLE/OLS estimate of $\boldsymbol{\beta}$ where $\tilde{\mathbf{X}} = \mathbf{U}_r$.

# Singular Value Decomposition & Connections to Spectral Decompositions

A matrix $\mathbf{X} \in \mathbb{R}^{n \times p}, p \leq n$ has a *singular value decomposition*

$$\mathbf{X} = \mathbf{U}_p \mathbf{D} \mathbf{V}^T$$

- $\mathbf{U}_p$ is a $n \times p$ matrix with the first $p$ eigenvectors in $\mathbf{U}$ associated with the $p$ largest eigenvectors of $\mathbf{X}\mathbf{X}^T = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$ with $\mathbf{U}_p^T \mathbf{U}_p = I_p$
- $\mathbf{V}$ is a $p \times p$ orthogonal matrix associated with the $p$ eigenvectors of $\mathbf{X}^T\mathbf{X} = \mathbf{V}\boldsymbol{\Lambda}_p\mathbf{V}^T$ where $\boldsymbol{\Lambda}_p$ is the diagonal matrix of eigenvalues associated with the $p$ largest eigenvalues of $\boldsymbol{\Lambda}$
- $\mathbf{D}$ = $\boldsymbol{\Lambda}_p^{1/2}$ are the singular values
- if $\mathbf{X}$ has rank $r < p$, then $C(\mathbf{X}) = C(\mathbf{U}_p) = C(\mathbf{U}_r)$, where $\mathbf{U}_r$ are the eigenvectors of $\mathbf{U}$ or $\mathbf{U}_p$ associated with the non-zero eigenvalues.

# MLE/OLS for non-full rank case

- if $\mathbf{X}^T\mathbf{X}$ is invertible, $\mathbf{P}_X = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ and $\hat{\boldsymbol{\beta}}$ is the unique estimator that satisfies $\mathbf{P}_{\mathbf{X}}\mathbf{y} = \mathbf{X}\hat{\boldsymbol{\beta}}$ or $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$
- if $\mathbf{X}^T\mathbf{X}$ is not invertible, replace $\mathbf{X}$ by $\tilde{\mathbf{X}}$ that is rank $r$
- or represent $\mathbf{P}_{\mathbf{X}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-}\mathbf{X}^T$ where $(\mathbf{X}^T\mathbf{X})^{-}$ is a generalized inverse of $\mathbf{X}^T\mathbf{X}$ and $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-}\mathbf{X}^T\mathbf{y}$

# Generalized Inverses

**Definition:** Generalized-Inverse (B.36)

A generalized inverse of any matrix $\mathbf{A}$: $\mathbf{A}^-$ satisfies $\mathbf{A}\mathbf{A}^-\mathbf{A} = \mathbf{A}$

- A generalized inverse of $\mathbf{A}$ symmetric always exists!

**Theorem:** Christensen B.39

If $\mathbf{G}_1$ and $\mathbf{G}_2$ are generalized inverses of $\mathbf{A}$ then $\mathbf{G}_1\mathbf{A}\mathbf{G}_2$ is also a generalized inverse of $\mathbf{A}$

- if $\mathbf{A}$ is symmetric, then $\mathbf{A}^-$ need not be!

# Orthogonal Projections in General

**Lemma B.43**

If $\mathbf{G}$ and $\mathbf{H}$ are generalized inverses of $\mathbf{X}^T\mathbf{X}$ then

$$\mathbf{X}\mathbf{G}\mathbf{X}^T\mathbf{X} = \mathbf{X}\mathbf{H}\mathbf{X}^T\mathbf{X} = \mathbf{X}$$
$$\mathbf{X}\mathbf{G}\mathbf{X}^T = \mathbf{X}\mathbf{H}\mathbf{X}^T$$

**Theorem:** B.44

$\mathbf{X}(\mathbf{X}^T\mathbf{X})^-\mathbf{X}^T$ is an orthogonal projection onto $C(\mathbf{X})$.

We need to show that (i) $\mathbf{P}\mathbf{m} = \mathbf{m}$ for $\mathbf{m} \in C(\mathbf{X})$ and (ii) $\mathbf{P}\mathbf{n} = 0$ for $\mathbf{n} \in C(\mathbf{X})^\perp$.

i. For $\mathbf{m} \in C(\mathbf{X})$, write $\mathbf{m} = \mathbf{X}\mathbf{b}$. Then $\mathbf{P}\mathbf{m} = \mathbf{P}\mathbf{X}\mathbf{b} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^-\mathbf{X}^T\mathbf{X}\mathbf{b}$ and by Lemma B43, we have that $\mathbf{X}(\mathbf{X}^T\mathbf{X})^-\mathbf{X}^T\mathbf{X}\mathbf{b} = \mathbf{X}\mathbf{b} = \mathbf{m}$

ii. For $\mathbf{n} \perp C(\mathbf{X})$, $\mathbf{P}\mathbf{n} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^-\mathbf{X}^T\mathbf{n} = \mathbf{0}_n$ as $C(\mathbf{X})^\perp = N(\mathbf{X}^T)$.

# MLEs & OLS

MLE/OLS satisfies

- $\mathbf{P}\mathbf{y} = \mathbf{X}\hat{\boldsymbol{\beta}}$
- $\mathbf{P}\mathbf{y} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-}\mathbf{X}^T\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}\hat{\boldsymbol{\beta}}$ (does not depend on choice of generalized inverse)
- $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-}\mathbf{X}^T\mathbf{y}$
- $\hat{\boldsymbol{\beta}}$ is not unique - does depend on choice of generalized inverse unless $\mathbf{X}$ is full rank

# Moore-Penrose Generalized Inverse:

- Decompose symmetric $\mathbf{A} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T$ (i.e $\mathbf{X}^T\mathbf{X}$)
- $\mathbf{A}^-_{MP} = \mathbf{U}\boldsymbol{\Lambda}^-\mathbf{U}^T$
- $\boldsymbol{\Lambda}^-$ is diagonal with

$$\lambda_i^- = \begin{cases} 1/\lambda_i \text{ if } \lambda_i \neq 0 \\ 0 \qquad \text{if } \lambda_i = 0 \end{cases}$$

- Symmetric $\mathbf{A}^-_{MP} = (\mathbf{A}^-_{MP})^T$
- Reflexive $\mathbf{A}^-_{MP}\mathbf{A}\mathbf{A}^-_{MP} = \mathbf{A}^-_{MP}$
- Can you construct another generalized inverse of $\mathbf{X}^T\mathbf{X}$ ?
- Can you find the Moore-Penrose generalized inverse of $\mathbf{X} \in \mathbb{R}^{n \times p}$?

# Properties of OLS (full rank case)

How good is $\hat{\boldsymbol{\beta}}$ as an estimator of $\beta$

- $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{\epsilon}$
- don't know $\boldsymbol{\epsilon}$, but can talk about behavior on average over
  - different runs of an experiment
  - different samples from a population
  - different values of $\boldsymbol{\epsilon}$
- with minimal assumption $\textsf{E}[\boldsymbol{\epsilon}] = \mathbf{0}_n$,

$$\begin{aligned}\textsf{E}[\hat{\boldsymbol{\beta}}] &= \textsf{E}[(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{\epsilon}] \\ &= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\textsf{E}[\boldsymbol{\epsilon}] \\ &= \boldsymbol{\beta}\end{aligned}$$

- *Bias* of $\hat{\boldsymbol{\beta}}$, $\text{Bias}[\hat{\boldsymbol{\beta}}] = \textsf{E}[\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}] = \mathbf{0}_p$ - $\hat{\boldsymbol{\beta}}$ is an unbiased estimator of $\boldsymbol{\beta}$ if $\boldsymbol{\mu} \in C(\mathbf{X})$

# Class of Unbiased Estimators

Class of linear statistical models:

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$
$$\boldsymbol{\epsilon} \sim P$$
$$P \in \mathcal{P}$$

An estimator $\tilde{\boldsymbol{\beta}}$ is unbiased for $\boldsymbol{\beta}$ if $\mathsf{E}_P[\tilde{\boldsymbol{\beta}}] = \boldsymbol{\beta} \quad \forall \boldsymbol{\beta} \in \mathbb{R}^p$ and $P \in \mathcal{P}$

Examples:

$\mathcal{P}_1 = \{\mathcal{P} = \mathsf{N}(\mathbf{0}_n, \mathbf{I}_n)\}$

$\mathcal{P}_2 = \{\mathcal{P} = \mathsf{N}(\mathbf{0}_n, \sigma^2\mathbf{I}_n), \sigma^2 > 0\}$

$\mathcal{P}_3 = \{\mathcal{P} = \mathsf{N}(\mathbf{0}_n, \boldsymbol{\Sigma}), \boldsymbol{\Sigma} \in \mathcal{S}^+\}$

$\mathcal{P}_4$ is the set of distributions with $\mathsf{E}_P[\boldsymbol{\epsilon}] = \mathbf{0}_n$ and $\mathsf{E}_P[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T] > 0$

$\mathcal{P}_5$ is the set of distributions with $\mathsf{E}_P[\boldsymbol{\epsilon}] = \mathbf{0}_n$ and $\mathsf{E}_P[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T] \geq 0$

# Linear Unbiased Estimation

**Exercise**

1. Explain why an estimator that is unbiased for the model with parameter space $\boldsymbol{\beta} \in \mathbb{R}^p$ and $P \in \mathcal{P}_{k+1}$ is unbiased for the model with parameter space $\boldsymbol{\beta} \in \mathbb{R}^p$ and $P \in \mathcal{P}_k$ .
2. Find an estimator that is unbiased for $\boldsymbol{\beta} \in \mathbb{R}^p$ and $P \in \mathcal{P}_1$ that but is biased for $\boldsymbol{\beta} \in \mathbb{R}^p$ and $P \in \mathcal{P}_2$.

Restrict attention to **linear** unbiased estimators

▼ **Definition:** Linear Unbiased Estimators (LUEs)

An estimator $\tilde{\boldsymbol{\beta}}$ is a **Linear Unbiased Estimator** (LUE) of $\boldsymbol{\beta}$ if

1. linearity: $\tilde{\boldsymbol{\beta}} = \mathbf{AY}$ for $\mathbf{A} \in \mathbb{R}^{p \times n}$
2. unbiasedness: $\mathsf{E}[\tilde{\boldsymbol{\beta}}] = \boldsymbol{\beta}$ for all $\boldsymbol{\beta} \in \mathbb{R}^p$

- Are there other LUEs besides the OLS/MLE estimator?
- Which is "best"? (and in what sense?)