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Most common linear model:

- > Repeat experiment n times
- > Have p predictor variables and 1 response/output variable
- > We label the data, predictors $(x_{i1}, x_{i2}, \dots, x_{ip}; y_i)$, $i = 1, \dots, n$
- > Model given by $y_i = \beta_0 + \sum_{j=1}^p \beta_j x_{ij} + \varepsilon_i$, linear in terms of x_{ij} , must determine $p+1$ coefficients $\beta_0, \beta_1, \dots, \beta_p$, ε_i takes into account randomness
 - Statistical assumption $\varepsilon_i \sim N(0, \sigma^2) \quad \forall i$
 - Assumption that all data fits linearly w/ normal random perturbations
- > So, goal is to predict β_j for $j=0, 1, \dots, p$ and σ^2
- > How? Ans 1: Maximum Likelihood Estimator, MLE

$$y_i \sim N(\beta_0 + \sum_{j=1}^p \beta_j x_{ij}, \sigma^2), \quad i = 1, \dots, n$$

y_i 's independent & identically distributed, i.i.d.

Convert to likelihood function

$$L = \prod_{i=1}^n \frac{e^{-z_i^2/(2\sigma^2)}}{(2\pi\sigma^2)^{1/2}}, \quad z_i = y_i - (\beta_0 + \sum_{j=1}^p \beta_j x_{ij})$$

where $L = L(\beta_0, \dots, \beta_p, \sigma^2)$. We compute the parameters

by setting $\frac{\partial L}{\partial(\beta_i)} = \frac{\partial L}{\partial(\sigma^2)} = 0, \quad i = 0, \dots, p$

> Matrix Formulation of model:

$$\underline{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n, \quad \underline{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} \in \mathbb{R}^{n \times p+1},$$

$$\underline{\beta} = \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_p \end{bmatrix} \in \mathbb{R}^{p+1}, \quad \underline{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{bmatrix} \in \mathbb{R}^n$$

And model is

$$\underline{y} = \underline{X} \underline{\beta} + \underline{\varepsilon}$$

with assumption $\underline{\varepsilon} \sim N_n(0, \sigma^2 \mathbb{I})$

$$\underline{y} \sim N_n(\underline{\beta}, \sigma^2 I)$$

Multivariate Normal Distribution:

→ $\underline{x} \sim N_n(\underline{\mu}, \Sigma)$, $\underline{x}, \underline{\mu} \in \mathbb{R}^n$, $\Sigma \in \mathbb{R}^{n \times n}$

with Σ symmetric and positive (semi-) definite.

→ Means that \underline{x} is a random vector with pdf

$$\rightarrow f(\underline{x}) = \frac{\exp\left(-\frac{1}{2}(\underline{x}-\underline{\mu})^T \Sigma^{-1} (\underline{x}-\underline{\mu})\right)}{(2\pi)^{n/2} |\det \Sigma|^{1/2}}$$

→ Use change of variables to show $\int f(\underline{x}) d\underline{x} = 1$

→ Properties:

- If $\underline{r} \in \mathbb{R}^n$, then $\underline{x} + \underline{r} \sim N_n(\underline{\mu} + \underline{r}, \Sigma)$

- If $\underline{A} \in \mathbb{R}^{m \times n}$, then $\underline{A}\underline{x} \sim N_m(\underline{A}\underline{\mu}, \underline{A}\Sigma\underline{A}^T)$

Necessary Linear Algebra:

→ Properties of definite matrices

→ Eigenvalue decomposition

→ Cholesky decomposition

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Let $\underline{A} \in \mathbb{R}^{m \times n}$

→ The row-rank of \underline{A} is the # of linearly independent rows

→ The column-rank —  columns

→ Define $C(\underline{A}) = \text{span}\{\text{cols of } \underline{A}\}$, $R(\underline{A}) = \text{span}\{\text{rows of } \underline{A}\}$

Theorem: row-rank = $\dim(R(\underline{A})) = \dim(C(\underline{A})) = \underline{\text{column-rank}}$

→ Nullspace $N(\underline{A}) = \{\underline{x} \mid \underline{A}\underline{x} = \underline{0}\}$

Theorem: Rank Nullity: $\text{rank}(\underline{A}) + \dim N(\underline{A}) = n$

Let $\underline{A} \in \mathbb{R}^{n \times n}$ with rank $1 \leq r \leq \min(n, m)$. Then $(\underline{P}, \underline{Q})$ is a rank factorization of \underline{A} if $\underline{P} \in \mathbb{R}^{m \times r}$, $\underline{Q} \in \mathbb{R}^{r \times n}$, and $\underline{A} = \underline{P} \underline{Q}$.

Theorem: Every matrix has a rank factorization.

Pf: If $\text{rank}(\underline{A}) = n$, $\underline{A} = \underline{I} \underline{A}$, and if $\text{rank}(\underline{A}) = n$, then $\underline{A} = \underline{A} \underline{I}$. Otherwise, partial SVD is $\underline{A} = \underline{U} \underline{\Sigma} \underline{V}^T$, \underline{U} is $m \times r$, $\underline{\Sigma}$ is $r \times r$, \underline{V}^T is $r \times n$, so a factorization given by $(\underline{U} \underline{\Sigma}) \underline{V}^T$ or $\underline{U} (\underline{\Sigma} \underline{V}^T)$.

A matrix $\underline{A} \in \mathbb{R}^{n \times n}$ is idempotent if $\underline{A}^2 = \underline{A}$

ex: Projection matrices

Theorem: If \underline{A} is idempotent, then $\text{rank}(\underline{A}) = \text{trace}(\underline{A})$

Pf: Let $r = \text{rank}(\underline{A})$. By rank factorization, $\underline{A} = \underline{P} \underline{Q}$, \underline{P} is $n \times r$, \underline{Q} is $r \times n$. Then $\underline{P} \underline{Q} \underline{P} \underline{Q} = \underline{P} \underline{I}_{r \times r} \underline{Q}$. From this, $\underline{P} (\underline{Q} \underline{P} - \underline{I}_{r \times r}) \underline{Q} = \underline{0}$
 $\Rightarrow \underline{P}^T \underline{P} (\underline{Q} \underline{P} - \underline{I}_{r \times r}) \underline{Q} \underline{Q}^T = \underline{0}$ with $\underline{P}^T \underline{P}$ and $\underline{Q} \underline{Q}^T$ invertible since $r \times r$, hence,
 $\underline{Q} \underline{P} = \underline{I}_{r \times r}$. Thus, $\text{trace}(\underline{Q} \underline{P}) = \text{trace}(\underline{I}_{r \times r}) = r$. And by cyclic property of trace, $\text{trace}(\underline{A}) = \text{trace}(\underline{P} \underline{Q}) = \text{trace}(\underline{Q} \underline{P}) = r$.

Theorem: If $\underline{A}^2 = \underline{A} \in \mathbb{R}^{n \times n}$, then $\text{rank}(\underline{A}) + \text{rank}(\underline{I} - \underline{A}) = n$.

Proof: By last thm, $\text{rank}(\underline{A}) = \text{trace}(\underline{A})$. And, $(\underline{I} - \underline{A})^2 = (\underline{I} - \underline{A})$
so $\text{rank}(\underline{I} - \underline{A}) = \text{trace}(\underline{I} - \underline{A}) = n - \text{trace}(\underline{A}) = n - \text{rank}(\underline{A})$.

Let V be a vector space and $S \subseteq V$ a subspace. Then the complement of S is $S^\circ := \{y \in V : \langle y, s \rangle = 0 \ \forall s \in S\}$.

Fact: S° is also a subspace.

Theorem: Let $\{\underline{x}_i\}_{i=1}^k$ be an orthogonal basis for subspace $S \subseteq V$. This can be extended into an orthogonal basis $\{\underline{x}_i\}_{i=1}^n$ for V s.t. $\{\underline{x}_i\}_{i=k+1}^n$ is an orthogonal basis for S° .

Proposition: For any $x \in V$, there exists unique $y_s \in S$ & $y_{\circ} \in S^\circ$ s.t.

$$x = y_s + y_{\circ}$$

$$\rightarrow y_s = \text{Proj}_S(x), \quad y_{\circ} = \text{Proj}_{S^\circ}(x)$$

$\rightarrow \text{Proj}_S: V \rightarrow S$ is a linear mapping

Linearity means $\text{Proj}_S(\underline{x} + \underline{y}) = \text{Proj}_S(\underline{x}) + \text{Proj}_S(\underline{y})$ and $\exists \underline{P}_S \in \mathbb{R}^{n \times n}$

s.t. $\text{Proj}_S(\underline{x}) = \underline{P}_S \underline{x}$

Lemma: \underline{P}_S is idempotent

Lemma: $\underline{P}_S^T \underline{P}_S = \underline{P}_S$

Proof: Recall $(\underline{I} - \underline{P}_S)$ projects onto orthogonal space S^\perp , so we have

$$0 = \langle \underline{P}_S \underline{x}, (\underline{I} - \underline{P}_S) \underline{x} \rangle = \underline{x}^T (\underline{P}_S^T - \underline{P}_S^T \underline{P}_S) \underline{x} \quad \forall \underline{x}, \text{ hence}$$

$$\underline{P}_S^T = \underline{P}_S^T \underline{P}_S \Rightarrow \underline{P}_S = (\underline{P}_S^T \underline{P}_S)^T = \underline{P}_S^T \underline{P}_S.$$

$\underline{A} \in \mathbb{R}^{n \times n}$ is an orthogonal matrix if $\underline{A}^T \underline{A} = \underline{A} \underline{A}^T = \underline{I}$. I.e., the columns of \underline{A} are orthonormal (and hence the rows too)

Theorem: \underline{A} is orthogonal $\Leftrightarrow \langle \underline{A} \underline{x}, \underline{A} \underline{y} \rangle = \langle \underline{x}, \underline{y} \rangle \quad \forall \underline{x}, \underline{y}$

$$\Leftrightarrow \|\underline{A} \underline{x} - \underline{A} \underline{y}\| = \|\underline{x} - \underline{y}\| \quad \forall \underline{x}, \underline{y}$$

Proof: $\langle \underline{x}, \underline{y} \rangle = \langle \underline{A}^T \underline{A} \underline{x}, \underline{y} \rangle = \langle \underline{A} \underline{x}, \underline{A} \underline{y} \rangle \Leftrightarrow \underline{A}^T \underline{A} = \underline{I}$ so \underline{A} orthogonal.

And $\|\underline{A} \underline{x} - \underline{A} \underline{y}\|^2 = \langle \underline{A}(\underline{x} - \underline{y}), \underline{A}(\underline{x} - \underline{y}) \rangle = \langle \underline{x} - \underline{y}, \underline{x} - \underline{y} \rangle = \|\underline{x} - \underline{y}\|^2 \Leftrightarrow$ see above

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Let $\underline{A} \in \mathbb{R}^{n \times n}$. The determinant of \underline{A} can be defined recursively.

A cofactor of \underline{A} given by $\underline{A}_{ij}^{\circ}$ where it is an $n-1$ by $n-1$ matrix with row i and column j removed. Then

$$\begin{aligned} \det(\underline{A}) &= \sum_{k=1}^n (-1)^{i+k} a_{ik} \det(\underline{A}_{i,k}^{\circ}) \quad \text{for any } 1 \leq i \leq n \\ &= \sum_{k=1}^n (-1)^{k+j} a_{kj} \det(\underline{A}_{k,j}^{\circ}) \quad \text{for any } 1 \leq j \leq n. \end{aligned}$$

We can also define it as the unique map $\det: \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$ satisfying

1) Fixing $n-1$ cols, it is linear in the last column

2) Exchanging two cols flips the sign of the determinant

3) $I \mapsto 1$

Theorem: Letting S_n be the permutation group on $\{1, 2, \dots, n\}$, we have that

$$\det(\underline{A}) = \sum_{\pi \in S_n} \text{sgn}(\pi) \prod_{i=1}^n a_{i, \pi(i)}$$

where $\text{sgn}(\pi) = \begin{cases} 1 & \text{if } \pi \text{ an even permutation} \\ -1 & \text{if } \pi \text{ odd} \end{cases}$

→ Can prove by 3 properties above

Theorem: $\det(\underline{AB}) = \det(\underline{A}) \det(\underline{B})$.

→ Can prove by above form

Corollary: If \underline{A} is invertible, then $\det(\underline{A}^{-1}) = 1 / \det(\underline{A})$.

Let $\underline{A} \in \mathbb{R}^{n \times n}$. The algebraic eigenvalues of \underline{A} are given by roots to the polynomial $\det(\lambda \underline{I} - \underline{A})$, $\lambda \in \mathbb{C}$. The geometric eigenvalues are defined to be any $\lambda \in \mathbb{C}$ for which there exists $\underline{x} \neq \underline{0}$ s.t. $\underline{Ax} = \lambda \underline{x}$. The geometric multiplicity of λ is k if \exists exactly k linearly independent, nonzero \underline{x}_i s.t. $\underline{Ax}_i = \lambda \underline{x}_i$ for each \underline{x}_i . (Algebraic is mult. of root)

Fact: Geometric multiplicity \leq Algebraic multiplicity (usually " $=$ " here).

Theorem: If $\underline{Ax} = \lambda \underline{x}$, $\underline{x} \neq \underline{0}$, then $\underline{A}^k \underline{x} = \lambda^k \underline{x}$.

Theorem: If f a polynomial, and λ an eigenvalue of \underline{A} , then $f(\lambda)$ an eigenvalue of $f(\underline{A})$.

Corollary: If $\underline{A}^2 = \underline{A}$ (idempotent), then the eigenvalues of \underline{A} are either 0 or 1.

Proof: $\underline{Ax} = \lambda \underline{x} \Rightarrow \underline{Ax} = \underline{A}^2 \underline{x} = \lambda^2 \underline{x} \Rightarrow \lambda = \lambda^2 \Rightarrow \lambda \in \{0, 1\}$

Theorem: If $\lambda_1, \dots, \lambda_k$ are distinct eigenvalues of \underline{A} with corresponding eigenvectors $\underline{x}_1, \dots, \underline{x}_k$, then the eigenvectors are linearly independent.

Proof: Suppose not, let j be the smallest integer s.t. $\underline{x}_j = \sum_{i=1}^{j-1} \beta_i \underline{x}_i$. Applying \underline{A} , $\lambda_j \underline{x}_j = \underline{A} \underline{x}_j = \sum_{i=1}^{j-1} \beta_i \underline{A} \underline{x}_i = \sum_{i=1}^{j-1} \lambda_i \beta_i \underline{x}_i$. Now, we cannot have

$\lambda_j = 0$ or else first $j-1$ eigenvectors linearly dependent. Dividing through by λ_j , so $\underline{x}_j = \sum_{i=1}^{j-1} \frac{\lambda_i}{\lambda_j} \beta_i \underline{x}_i$. But from $\underline{x}_j = \sum_{i=1}^{j-1} \beta_i \underline{x}_i$, must have

$\frac{\lambda_i}{\lambda_j} \beta_i = \beta_i$, $i = 1, \dots, j-1$, by linear independence. Since $\lambda_i \neq \lambda_j$ for

$i = 1, \dots, j-1$, must have $\beta_i = 0$ for $i = 1, \dots, j$. But then $\underline{x}_j = \underline{0}$, a contradiction.

Let $\underline{A} \in \mathbb{R}^{n \times n}$. The diagonalization of \underline{A} is a pair $(\underline{T}, \underline{\Delta})$ of non zero matrices s.t.

- 1) \underline{T} is invertible
- 2) $\underline{\Delta}$ is diagonal
- 3) $\underline{A} = \underline{T} \underline{\Delta} \underline{T}^{-1}$.

Theorem: Let $\underline{A} \in \mathbb{R}^{n \times n}$ be invertible with n distinct eigenvalues, then there exists a diagonalization $\underline{A} = \underline{T} \underline{\Delta} \underline{T}^{-1}$. Moreover, $\exists \underline{x} \neq \underline{0}$ s.t. $\underline{A}\underline{x} = \lambda \underline{x}$ for every λ on the diagonal of $\underline{\Delta}$.

Proof: Let $\lambda_1, \dots, \lambda_n$ be such that $\underline{A}\underline{x}_i = \lambda_i \underline{x}_i$ for $i=1, \dots, n$ with $\underline{x}_1, \dots, \underline{x}_n$ linearly independent. Let $\underline{T} = [\underline{x}_1 \dots \underline{x}_n]$. By linear independence, \underline{T} invertible. Also, $\underline{A}\underline{T} = [\underline{A}\underline{x}_1 \dots \underline{A}\underline{x}_n] = [\lambda_1 \underline{x}_1 \dots \lambda_n \underline{x}_n]$. And this equals $\underline{T}\underline{\Delta} = [\underline{x}_1 \dots \underline{x}_n][\lambda_1 \dots \lambda_n]$. Hence, we have $\underline{A}\underline{T} = \underline{T}\underline{\Delta} \Rightarrow \underline{A} = \underline{T}\underline{\Delta}\underline{T}^{-1}$.

Spectral Theorem: Let \underline{A} be a symmetric $n \times n$ matrix. Then \exists an orthogonal matrix \underline{T} s.t. $\underline{A} = \underline{T}\underline{\Delta}\underline{T}^T$ where $\underline{\Delta}$ is diagonal with real entries.

Theorem: If $\underline{A} \in \mathbb{C}^{n \times n}$, hermitian, then all its eigenvalues are real, consequently, all eigenvalues can be chosen to have real entries. (or $A \in \mathbb{R}^{n \times n}$ symmetric)

Proof: If $\underline{A}\underline{x} = \lambda \underline{x}$, then $\underline{x}^* \underline{A} \underline{x} = \lambda \underline{x}^* \underline{x}$. And taking conjugate, $\underline{x}^* \underline{A}^* \underline{x} = \bar{\lambda} \underline{x}^* \underline{x}$. With \underline{A} real & hermitian, $\underline{A} = \underline{A}^*$, so $\lambda = \bar{\lambda} \Rightarrow \lambda \in \mathbb{R}$. In addition, suppose $\underline{x} = (\underline{a} + i\underline{b})$ an eigenvector. Then $\underline{A}(\underline{a} + i\underline{b}) = \underline{A}\underline{x} = \lambda \underline{x} = \lambda(\underline{a} + i\underline{b})$. Hence, $\underline{a}, \underline{b} \in \mathbb{R}^n$ are real eigenvectors for λ .

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Theorem: Let \underline{A} be real, symmetric. Then eigenvectors corresponding to distinct eigenvalues are orthogonal.

Proof: Let $\underline{A}\underline{x}_1 = \lambda_1 \underline{x}_1$ and $\underline{A}\underline{x}_2 = \lambda_2 \underline{x}_2$ for distinct λ_1, λ_2 .

$$\text{Then } \lambda_1 \underline{x}_1^T \underline{x}_2 = \underline{x}_1^T (\underline{A}\underline{x}_2) = (\underline{x}_1^T \underline{A}\underline{x}_2)^T = \underline{x}_2^T \underline{A}\underline{x}_1 = \lambda_2 \underline{x}_2^T \underline{x}_1 = \lambda_2 \underline{x}_2^T \underline{x}_2.$$

By $\lambda_1 \neq \lambda_2$, must have $\underline{x}_2^T \underline{x}_1 = 0 \Rightarrow \underline{x}_1 \perp \underline{x}_2$.

Corollary: Let \underline{A} be real symmetric & λ be an eigenvalue of multiplicity d . Then we can choose d orthonormal eigenvectors for λ that is also orthogonal to all other eigenvectors of \underline{A} .

The above theorems prove the Spectral Theorem.

Theorem: Let $\underline{A} \in \mathbb{R}^{n \times n}$, and suppose \exists a diagonalization exists $\underline{A} = \underline{T} \underline{\Lambda} \underline{T}^{-1}$. Then $\text{rank}(\underline{A}) = \text{rank}(\underline{\Lambda})$, number of nonzero diagonals.

Corollary: Let $\underline{A} \in \mathbb{R}^{n \times n}$ with diagonalization $\underline{A} = \underline{T} \underline{\Lambda} \underline{T}^{-1}$ and $\text{rank}(\underline{A}) = n$. Then, $\underline{A}^{-1} = (\underline{T} \underline{\Lambda} \underline{T}^{-1})^{-1} = (\underline{T}^{-1})^{-1} \underline{\Lambda}^{-1} \underline{T}^{-1} = \underline{T} \underline{\Lambda}^{-1} \underline{T}^{-1}$.

Let $\underline{A} \in \mathbb{R}^{n \times n}$ be symmetric. \underline{A} is non-negative definite if $\underline{x}^T \underline{A} \underline{x} \geq 0 \quad \forall \underline{x} \in \mathbb{R}^n$. \underline{A} is strictly positive definite if $\underline{x}^T \underline{A} \underline{x} > 0 \quad \forall \underline{x} \in \mathbb{R}^n \setminus \{0\}$.

Note: $\underline{x}^T \underline{A} \underline{x} = \sum_{i=1}^n \sum_{j=1}^n a_{ij} x_i x_j$, a quadratic polynomial in \underline{x} .

We call $\underline{x}^T \underline{A} \underline{x}$ a quadratic form.

Theorem: If $\underline{A} \in \mathbb{R}^{n \times n}$ is symmetric, \underline{A} is nonnegative definite iff its eigenvalues are nonnegative. Same for positive definite.

Proof: $\underline{x}^T \underline{A} \underline{x} = \underline{x}^T \underline{T}^T \underline{\Lambda} \underline{T} \underline{x} = (\underline{T} \underline{x})^T \underline{\Lambda} (\underline{T} \underline{x})$, and since $\underline{\Lambda}$ diagonal, \underline{T} full rank, $\underline{x}^T \underline{A} \underline{x} \geq 0 \Leftrightarrow \lambda_{ii} \geq 0$. Similarly, $\underline{x}^T \underline{A} \underline{x} > 0 \Leftrightarrow \lambda_{ii} > 0$ and $\underline{x} \neq 0$.

Theorem: Let \underline{A} be nonnegative definite. $\det(\underline{A}) = 0$ iff the smallest eigenvalue of \underline{A} is zero.

Proof: $\det(\underline{A}) = \det(\underline{T} \underline{\Lambda} \underline{T}^T) = \det(\underline{\Lambda}) = \prod_{i=1}^n \lambda_i$.

Theorem: Let $\underline{A} \in \mathbb{R}^{n \times n}$ be symmetric with all eigenvalues either 0 or 1. Then $\underline{A}^2 = \underline{A}$.

Proof: $\underline{A} = \underline{T} \underline{\Lambda} \underline{T}^T$. By $\lambda_i \in \{0, 1\}$, $\underline{\Lambda}^2 = \underline{\Lambda}$. Hence,
 $\underline{A}^2 = \underline{T} \underline{\Lambda} \underline{T}^T \underline{T} \underline{\Lambda} \underline{T}^T = \underline{T} \underline{\Lambda}^2 \underline{T}^T = \underline{T} \underline{\Lambda} \underline{T}^T = \underline{A}$.

Theorem: Let \underline{A} be nonnegative definite and $\lambda_1, \dots, \lambda_n$ be the eigenvalues of \underline{A} in nonincreasing order: $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$. Then, the largest eigenvalue is $\lambda_1 = \max_{\|\underline{x}\|=1} \underline{x}^T \underline{A} \underline{x}$.

Proof: By \underline{A} nonnegative definite, $\max_{\|x\|=1} x^T \underline{A} x = \max_{\|y\|=1} y^T \underline{A} y$. This is easier as $y^T \underline{A} y = \sum_{i=1}^n \lambda_i y_i^2$. To maximize this, set $y = (1, 0, \dots, 0)^T$, giving us $y^T \underline{A} y = \lambda_1$.

Theorem: Let \underline{A} be positive definite. Then $\lambda_n \|x\|^2 \leq x^T \underline{A} x \leq \lambda_1 \|x\|^2$

where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ are the eigenvalues of \underline{A} .

Theorem: Let \underline{A} be nonnegative definite. Then, we have that

$\underline{A} = \underline{I} \underline{\Lambda} \underline{I}^T \Rightarrow \underline{A} = (\underline{I} \underline{\Lambda}^{1/2} \underline{I}^T)^2$, so we can find the square root of \underline{A} to be $\underline{I} \underline{\Lambda}^{1/2} \underline{I}^T$ ($\underline{\Lambda}^{1/2} = [\lambda_1^{1/2} \dots \lambda_n^{1/2}]$).
(in general, $\underline{A}^{1/2} = \underline{B}$ if $\underline{B} \underline{B}^T = \underline{A}$)

9/6/23:

The standard normal is characterized by the density function

$$\varphi(t) = \frac{1}{\sqrt{2\pi}} e^{-t^2/2}, \quad N(0, 1).$$

How to show integrates to 1? Square it:

$$\left[\int_{-\infty}^{\infty} \varphi(t) dt \right]^2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(t^2+s^2)/2} ds dt \xrightarrow{\text{Polar coords}} = 1.$$

The cumulative density function is given by

$$\Phi(t) = \int_{-\infty}^t \varphi(x) dx.$$

Let $N \sim N(0, 1)$.

$$1) E[N] = \int_{-\infty}^{\infty} t \varphi(t) dt = 0 \quad (\text{anti-symmetric})$$

$$2) E[N^2] = \int_{-\infty}^{\infty} t^2 \cdot \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt \quad u=t \quad du=t e^{-t^2/2}$$

$$= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt \quad \text{int. pdf} = 1$$

$$3) E[N^k] = 0 \quad \text{for } k=1, 3, 5, \dots \quad \text{by anti-symmetric}$$

4) Now let k be even

$$\begin{aligned}
 E[N^k] &= \int_{-\infty}^{\infty} t^k \cdot \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt \\
 &= \int_{-\infty}^{\infty} t^{k-1} \cdot \frac{1}{2\pi} \cdot t e^{-t^2/2} dt \\
 &\stackrel{IBP}{=} \int_{-\infty}^{\infty} (k-1) t^{k-2} \cdot \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt \\
 &= (k-1) E[N^{k-2}] \\
 &= \prod_{i=0}^{k/2+1} (k-1-2i)
 \end{aligned}$$

The Gamma Distribution with shape parameter $R > 0$ is

$$\Gamma(R) = \int_0^{\infty} x^{R-1} e^{-x} dx.$$

The corresponding density function is

$$f(x) = \begin{cases} \frac{1}{\Gamma(R)} x^{R-1} e^{-x}, & x > 0 \\ 0, & x \leq 0 \end{cases}$$

Note: The density function is not unique. Can change countable # of points and the cdf $F(x) = \int_{-\infty}^x f(t) dt$ doesn't change.

Feller's Inequality: $\frac{x}{x^2+1} \varphi(x) \leq 1 - \Phi(x) \leq \frac{1}{x} \varphi(x), x > 0$

> Will be proved in HW.

The moment generating function of the standard normal is

$$\begin{aligned}
 m_N(t) &= E[e^{Nt}] = \int_{-\infty}^{\infty} e^{tx} \varphi(x) dx \\
 &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{tx-x^2/2} dx = \frac{1}{\sqrt{2\pi}} e^{\frac{t^2}{2}} \int_{-\infty}^{\infty} e^{-(t-x)^2/2} dx = e^{t^2/2}.
 \end{aligned}$$

The characteristic function is

$$C_N(t) = E[e^{itX}].$$

Can show the complex part disappears,

$$C_N(t) = e^{-t^2/2}.$$

If X_1, \dots, X_n are independent, then the properties hold

$$m_{X_1 + X_2 + \dots + X_n}(t) = \prod_{i=1}^n m_{X_i}(t)$$

$$\text{and } C_{X_1 + X_2 + \dots + X_n}(t) = \prod_{i=1}^n C_{X_i}(t).$$

Suppose X_1, \dots, X_n iid $\exp(1)$, $f_{X_i}(x) = e^{-x} \cdot I\{x \geq 0\}$. We can show that $\sum_{i=1}^n X_i \sim \text{Gamma}(n)$. This will be homework.

> Recall timeless property of exponential distribution.

$$\Pr[X_i > a+h \mid X_i > a] = \Pr[X_i > h]$$

Let N_1, \dots, N_r be iid standard normal random variables. Can show that $\sum_{n=1}^r (N_n)^2 \sim \chi^2(r)$. Will also be on HW, use mgf. And from this, $E[\chi^2] = \sum_{n=1}^r E[N_n^2] = r$.

Lemma: X_1, \dots, X_n iid. Then $\text{var}(X_1 + \dots + X_n) = \text{var}(X_1) + \dots + \text{var}(X_n)$.

$$\begin{aligned} \text{So } \text{var}(\chi^2) &= r \cdot \text{var}(N_1^2) = r(E[N_1^4] - E[N_1^2]^2) \\ &= r \cdot (3 - 1) = 2r. \end{aligned}$$

We also have the property

$$\frac{\chi^2(r) - r}{\sqrt{2r}} \xrightarrow[r \rightarrow \infty]{\text{distribution}} N \quad \text{i.e. in cdf.}$$

9/11/23:

Recall the chi-squared distribution $\chi^2(r) = N_1^2 + \dots + N_r^2$ where each N_i is iid, $N(0, 1)$. And the T-distribution is given by

$$t(r) = \frac{N(0, 1)}{\sqrt{\chi^2(r)/r}}$$

with $N(0, 1)$, $\chi^2(r)$ independent. And the F-distribution is given by

$$F(r_1, r_2) = \frac{\chi^2(r_1)/r_1}{\chi^2(r_2)/r_2}$$

with each χ^2_i independent.

And, we can define

$$N(\mu, \sigma^2) := \mu + \sigma N(0, 1).$$

Note also that

$$\mu - \sigma N(0, 1) = N(\mu, \sigma^2).$$

Let $\underline{X} = (X_1, \dots, X_d)^T$ be a d -dimensional random vector.

The joint distribution is $P\{X_1 < t_1, X_2 < t_2, \dots, X_d < t_d\} = F_{\underline{X}}(\underline{t})$.

If we can write $F_{\underline{X}}(\underline{t}) = \int_{-\infty}^{t_1} \int_{-\infty}^{t_2} \dots \int_{-\infty}^{t_d} f_{\underline{X}}(u_1, \dots, u_d) du_1 du_2 \dots du_d$,

then $f_{\underline{X}}$ is the joint density function. (which implies $f_{\underline{X}}(\underline{t}) = \prod_{i=1}^d f_{X_i}(t_i)$)

We say X_1, \dots, X_d are independent iff $F_{\underline{X}}(\underline{t}) = \prod_{i=1}^d P(X_i < t_i)$.

The multinomial (p, n) , with $\sum p_i = 1$, simulates number of outcomes, $1, \dots, d$, with corresponding probabilities, p_1, \dots, p_d , over n samples.

We can define the covariance

$$\text{cov}(X_i, X_j) = E[(X_i - E[X_i])(X_j - E[X_j])].$$

$$=: \Sigma_{ij}$$

We then define the correlation

$$\text{correlation}(X_i, X_j) = \frac{\text{cov}(X_i, X_j)}{\sqrt{\text{var}(X_i) \text{var}(X_j)}}.$$

Suppose we're given random $\underline{X} \in \mathbb{R}^d$, $\underline{Y} \in \mathbb{R}^m$. Then,

$$\text{cov}(\underline{X}, \underline{Y}) = E[(\underline{X} - E[\underline{X}])(\underline{Y} - E[\underline{Y}])^T] \in \mathbb{R}^{d \times m}$$

This will satisfy $\text{cov}(\underline{X}, \underline{Y}) = \text{cov}(\underline{Y}, \underline{X})^T$.

The covariance matrix of \underline{X} is given by

$$\underline{\Sigma} = \text{cov}(\underline{X}, \underline{X}) \in \mathbb{R}^{d \times d}$$

We know $\underline{\Sigma}$ is symmetric, nonnegative definite. Also, suppose that $\underline{\Sigma}$ is singular. If $d=1$, this means X_1 is constant. For $d > 1$, it means $\exists \underline{x} \neq \underline{0}$ s.t. $\underline{x}^T \underline{\Sigma} \underline{x} = 0$. Or that some column is a linear combination of others. This implies that for some i , there exists

a linear combination $X_i = \sum_{j \neq i} \alpha_{ij} X_j$.

The multivariate normal random vector $\underline{X} \in \mathbb{R}^d$ can be defined as

$$\underline{X} = \underline{M} + \underline{A} \underline{N}, \quad \underline{N} = \begin{pmatrix} N_1 \\ \vdots \\ N_d \end{pmatrix}, \text{ each } N_i \sim N(0, 1).$$

It's a linear combination of standard normal. From this definition, $E[\underline{X}] = \underline{M}$. And it has covariance

$$\begin{aligned} \text{cov}(\underline{X}) &= E[\underline{A} \underline{N} (\underline{A} \underline{N})^T] = E[\underline{A} \underline{N} \underline{N}^T \underline{A}^T] \\ &= \underline{A} E[\underline{N}^T \underline{N}] \underline{A}^T = \underline{A} \underline{A}^T, \text{ so } \underline{\Sigma} = \underline{A} \underline{A}^T \end{aligned}$$

$$+ E[\underline{N} \underline{N}^T]_{ij} = E[N_i N_j] = \begin{cases} 1 & \text{if } i=j \\ 0 & \text{otherwise} \end{cases} *$$

So we have that $\underline{A} = \underline{\Sigma}^{1/2}$. Note $\underline{\Sigma}^{1/2}$ is not unique, can be acted on by orthogonal matrices, rotations. $\underline{\Sigma}^{1/2}$ can be unique if we require it to be upper-triangular.

The multivariate moment generating function is given by

$$m_{\underline{X}}(\underline{t}) = m_{\underline{X}}(t_1, \dots, t_d) = E[e^{\underline{t}^T \underline{X}}].$$

For now, assume $\underline{M} = \underline{0}$. $\underline{t}^T \underline{X} = \underline{t}^T \underline{A} \underline{N}$ is univariate normal as it is a linear combination of linear combinations of N_i , $i=1, \dots, d$. It has

$$\begin{aligned} \text{mean } 0. \quad \text{var}(\underline{t}^T \underline{A} \underline{N}) &= E[\underline{t}^T \underline{A} \underline{N} \underline{t}^T \underline{A} \underline{N}] = E[\underline{t}^T \underline{A} \underline{N} \underline{N}^T \underline{A}^T \underline{t}] \\ &= \underline{t}^T \underline{A} E[\underline{N} \underline{N}^T] \underline{A}^T \underline{t} = \underline{t}^T \underline{A} \underline{A}^T \underline{t} = \underline{t}^T \underline{\Sigma} \underline{t}. \quad \text{So, can finally show} \\ m_{\underline{X}}(\underline{t}) &= e^{\frac{1}{2} \underline{t}^T \underline{\Sigma} \underline{t}}. \quad (\text{see HW}) \end{aligned}$$

From this, we can see all you need to uniquely define \underline{X} is $\underline{M}, \underline{\Sigma}$.

9/13/23:

Let (X, Y) be bivariate normal. As we discussed before, we can write $\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \alpha_1 & 0 \\ \alpha_2 & \beta \end{pmatrix} \begin{pmatrix} N_1 \\ N_2 \end{pmatrix}$. Suppose $\text{var}(X) = \sigma_1^2$, $\text{var}(Y) = \sigma_2^2$, and $\text{cov}(X, Y) = \xi$. Then $Y = \alpha_1 N_1 + \beta N_2 \Rightarrow \sigma^2 = \text{var}(Y) = \alpha^2 + \beta^2$. And, $\xi = \text{cov}(X, Y) = E[(X-\bar{X})(Y-\bar{Y})] = E[\alpha_1 \alpha_2 N_1^2 + \alpha_1 \beta N_1 N_2] = \sigma_1 \alpha_2$.

Let $\underline{X} \in \mathbb{R}^d$ with density $f_{\underline{X}}(\underline{x})$. Let $\underline{h}: \mathbb{R}^d \rightarrow \mathbb{R}^d$ be a one-to-one transformation. Then let $\underline{Y} = \underline{h}(\underline{X}) \in \mathbb{R}^d$. If $\underline{g} = \underline{h}^{-1}$, then $\underline{X} = \underline{g}(\underline{Y})$. Let $\underline{\Sigma}(\underline{y}) \in \mathbb{R}^{d \times d}$ be the Jacobian of $\underline{g}(\underline{y})$. Then the density of \underline{Y} is given by

$$f_{\underline{Y}}(\underline{y}) = f_{\underline{X}}(\underline{g}(\underline{y})) |\det \underline{\Sigma}(\underline{y})|.$$

Let $\underline{X} \sim N_d(\underline{0}, \underline{\Sigma})$. Then we also have $\underline{X} = \underline{A} \underline{N}$. For this map to be invertible, require \underline{A} nonsingular. This true iff $\underline{\Sigma} = \underline{A}^T \underline{A}$ nonsingular. The inverse is then given by $\underline{N} = \underline{A}^{-1} \underline{X}$. It's Jacobian is then $\underline{\Sigma}(\underline{x}) = \underline{A}^{-2}$. We also know that

$$f_{\underline{N}}(\underline{n}) = \prod_{i=1}^d \frac{1}{\sqrt{2\pi}} e^{-n_i^2/2} = \frac{1}{(2\pi)^{d/2}} e^{-\underline{n}^T \underline{n}/2}.$$

Hence, we can find that

$$\begin{aligned} f_{\underline{X}}(\underline{x}) &= \frac{1}{(2\pi)^{d/2}} e^{-(\underline{A}^{-2}\underline{x})^T(\underline{A}^{-2}\underline{x})/2} \cdot |\det \underline{A}^{-1}| \\ &= \frac{1}{(2\pi)^{d/2}} e^{-\frac{1}{2} \underline{x}^T \underline{\Sigma}^{-1} \underline{x}} \cdot \frac{1}{\det(\underline{\Sigma})^{1/2}} \end{aligned}$$

Last step uses $\det(\underline{A}^{-1}) = \det(\underline{A})^{-1} = \det(\underline{\Sigma}^{1/2})^{-1} = \det(\underline{\Sigma})^{-1/2}$.

Theorem: Let $\underline{X} \in \mathbb{R}^d$, $\underline{Y} \in \mathbb{R}^m$ be uncorrelated, $\text{cov}(\underline{X}, \underline{Y}) = \underline{\underline{0}}$, such that $[\underline{X} \ \underline{Y}]^T \in \mathbb{R}^{d+m} \sim N_{d+m}(\underline{0}, \underline{\Sigma})$. Then \underline{X} and \underline{Y} are independent. In addition, each must be normal random vectors.

Note: Independence means you can separate the densities or mgfs.

Proof: Consider the covariance matrix of $[\underline{X}, \underline{Y}]^T$,

$$\underline{\Sigma} = \begin{bmatrix} \underline{\Sigma}_1 & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\Sigma}_2 \end{bmatrix}.$$

And, the mgf is given by (let $\underline{t} = [\underline{x} \ \underline{y}]^T$)

$$\begin{aligned} m_{\underline{X}+\underline{Y}}(\underline{t}) &= \exp\left(\frac{1}{2} \underline{t}^T \underline{\Sigma} \underline{t}\right) \\ &= \exp\left(\frac{1}{2} (\underline{x}^T \underline{\Sigma}_1 \underline{x} + \underline{y}^T \underline{\Sigma}_2 \underline{y})\right) \\ &= \exp\left(\frac{1}{2} \underline{x}^T \underline{\Sigma}_1 \underline{x}\right) \exp\left(\frac{1}{2} \underline{y}^T \underline{\Sigma}_2 \underline{y}\right) \end{aligned}$$

$$= m_{\underline{x}}(\underline{x}) m_{\underline{y}}(\underline{y})$$

showing that \underline{X} and \underline{Y} are independent. Proof is similar if use density.
 Note, $\underline{\Sigma}^{-1} = \begin{bmatrix} \underline{\Sigma}_x^{-1} & \underline{\Omega} \\ \underline{\Omega} & \underline{\Sigma}_y^{-1} \end{bmatrix}$. So can similarly split density function.

Theorem: Let $\underline{X}_d \sim N_d(\underline{0}, \underline{\Sigma}_d)$. Let \underline{Q} be an orthogonal matrix.

Then $\underline{Y} = \underline{Q} \underline{X} \sim N_d(\underline{0}, \underline{\Sigma}_d)$.

Proof: Immediately from defn of \underline{Y} , we know it is normally distributed.
 So, $E[\underline{Y}] = E[\underline{Q} \underline{X}] = \underline{Q} E[\underline{X}] = \underline{0}$. And finally,

$$\begin{aligned} \text{cov}(\underline{Y}) &= E[\underline{Q} \underline{X} (\underline{Q} \underline{X})^T] = E[\underline{Q} \underline{X} \underline{X}^T \underline{Q}^T] \\ &= \underline{Q} E[\underline{X} \underline{X}^T] \underline{Q}^T = \underline{Q} \underline{\Sigma}_d \underline{Q}^T = \underline{Q} \underline{Q}^T = \underline{\Sigma}_d. \end{aligned}$$

Hence, we know $\underline{Y} \sim N_d(\underline{0}, \underline{\Sigma}_d)$.

Ex: $\underline{X} \sim N_d(\underline{0}, \underline{\Sigma})$, $\underline{X}_1 = \underline{A} \underline{X}$, $\underline{X}_2 = \underline{B} \underline{X}$. When are $\underline{X}_1, \underline{X}_2$ independent?
 Consider $[\underline{X}_1 \underline{X}_2]^T$, we know that this is normal as it is equal to $[\underline{A} \underline{B}]^T \underline{X}$. By previous theorem, $\underline{X}_1, \underline{X}_2$ independent iff they're uncorrelated. Well,

$$\begin{aligned} \text{cov}(\underline{X}_1, \underline{X}_2) &= E[\underline{X}_1 \underline{X}_2^T] = E[\underline{A} \underline{X} \underline{X}^T \underline{B}^T] \\ &= \underline{A} E[\underline{X} \underline{X}^T] \underline{B}^T = \underline{A} \underline{\Sigma} \underline{B}^T. \end{aligned}$$

Hence, $\underline{X}_1, \underline{X}_2$ independent iff $\underline{A} \underline{\Sigma} \underline{B}^T = \underline{0}$.

Theorem: Let \underline{P} be symmetric, idempotent, $\underline{N} \sim N_d(\underline{0}, \underline{\Sigma})$. Define $\underline{X} = \underline{P} \underline{N}$, $\underline{Y} = (\underline{\Sigma} - \underline{P}) \underline{N}$. Then \underline{X} and \underline{Y} are independent.

Proof: By previous theorem, need to show uncorrelated.

$$\text{cov}(\underline{X}, \underline{Y}) = E[\underline{P} \underline{N} \underline{N}^T (\underline{\Sigma} - \underline{P})] = \underline{P} \underline{\Sigma} (\underline{\Sigma} - \underline{P}) = \underline{0}.$$

Tests for Normality:

1) χ^2 -Test

2) Shapiro-Wiles

> Assumes iid, can't be used for residuals

3) Jarque-Bera

> Checks the first 4 moments to see if matching normal

4) Many many more

9/18/23:

Let $\underline{Y} \sim N_d(\underline{0}, \underline{\underline{I}})$, then we know a few things

First, if $\underline{\underline{A}}$ symmetric, $\underline{Y}^\top \underline{\underline{A}} \underline{Y} \sim \sum_{i=1}^d d_i N_i^2$, $d_i \geq 0$ are the eigenvalues of $\underline{\underline{A}}$.

$$\underline{Y}^\top \underline{\underline{A}} \underline{Y} = \underline{Y}^\top \underline{\underline{I}}^\top \underline{\underline{A}} \underline{\underline{I}} \underline{Y} = (\underline{\underline{I}} \underline{Y})^\top \underline{\underline{A}} (\underline{\underline{I}} \underline{Y}) \Rightarrow \underline{\underline{I}} \underline{Y} \sim N_d(\underline{0}, \underline{\underline{I}}) \Rightarrow \underline{Y} \sim N_d(\underline{0}, \underline{\underline{I}})$$

Recall that idempotent matrices have eigenvalues of 0 or 1.

Theorem: Let $\underline{\underline{A}} \in \mathbb{R}^{d \times d}$ be symmetric. Then $\underline{\underline{A}}^2 = \underline{\underline{A}} \Leftrightarrow \text{rank}(\underline{\underline{A}}) = r$ iff $\underline{\underline{A}}$ has r eigenvalues that are 1, $d-r$ that are 0.

Theorem: Let $\underline{\underline{A}} \in \mathbb{R}^{d \times d}$ be symmetric, $\underline{Y} \sim N_d(\underline{0}, \underline{\underline{I}})$. Then

$$\underline{Y}^\top \underline{\underline{A}} \underline{Y} \sim \chi_r^2 \Leftrightarrow \underline{\underline{A}}^2 = \underline{\underline{A}}, \text{rank}(\underline{\underline{A}}) = r.$$

Proof: \Leftarrow is clear. Now suppose $\underline{Y}^\top \underline{\underline{A}} \underline{Y} \sim \chi_r^2$, so $\underline{Y}^\top \underline{\underline{A}} \underline{Y} = \sum_{i=1}^r N_i^2$.

We then know that $m_{\underline{Y}^\top \underline{\underline{A}} \underline{Y}}(t) = m_{\chi_r^2}(t) = (1-2t)^{-r/2}$ on a neighborhood of $t=0$. We know that $\underline{Y}^\top \underline{\underline{A}} \underline{Y} \sim \sum_{i=1}^d d_i N_i^2$, so we also have $m_{\underline{Y}^\top \underline{\underline{A}} \underline{Y}}(t) = (1-2d_i t)^{-d_i/2}$. From these forms, we must have $d_i = 1$ for r terms, and $d_i = 0$ otherwise.

Again, let $\underline{Y} \sim N_d(\underline{0}, \underline{\underline{I}})$, and let $\underline{\underline{P}} \in \mathbb{R}^{d \times d}$ be a projection matrix with rank r . Then, by $\underline{\underline{P}}^2 = \underline{\underline{P}}$, $(\underline{\underline{I}} - \underline{\underline{P}})^2 = \underline{\underline{I}} - \underline{\underline{P}}$, $\text{range}(\underline{\underline{P}}) = \ker(\underline{\underline{I}} - \underline{\underline{P}})$

1) $\underline{Y}^\top \underline{\underline{P}} \underline{Y} \sim \chi_r^2$

(and visa-versa)

2) $\underline{Y}^\top (\underline{\underline{I}} - \underline{\underline{P}}) \underline{Y} \sim \chi_{d-r}^2$

3) $\underline{Y}^\top \underline{\underline{P}} \underline{Y}$ and $\underline{Y}^\top (\underline{\underline{I}} - \underline{\underline{P}}) \underline{Y}$ are independent.

Theorem: Let $\underline{A}, \underline{B} \in \mathbb{R}^{d \times d}$ be symmetric, $\underline{Y} \sim N_d(\underline{0}, \underline{\underline{I}})$ such that $\underline{Y}^T \underline{A} \underline{Y} = \chi_r^2$, $\underline{Y}^T \underline{B} \underline{Y} = \chi_m^2$. Then $\underline{Y}^T \underline{A} \underline{Y}$ and $\underline{Y}^T \underline{B} \underline{Y}$ are independent iff $\underline{A} \underline{B} = \underline{0}$.

Proof: By statement, \underline{A} and \underline{B} are idempotent. Suppose independence, then $\underline{Y}^T \underline{A} \underline{Y} + \underline{Y}^T \underline{B} \underline{Y} = \chi^2$. And, by factoring, this equals $\underline{Y}^T (\underline{A} + \underline{B}) \underline{Y}$. Hence, $(\underline{A} + \underline{B})$ is symmetric, idempotent, has rank $r+m$. By idempotence, $\underline{A} + \underline{B} = (\underline{A} + \underline{B})^2 = \underline{A}^2 + 2\underline{A}\underline{B} + \underline{B}^2 = \underline{A} + 2\underline{A}\underline{B} + \underline{B} \Rightarrow \underline{A}\underline{B} = \underline{0}$. For the reverse, suppose $\underline{A}\underline{B} = \underline{0}$. From that, $(\underline{A} + \underline{B})$, $\underline{A}, \underline{B}$ idempotent, getting us to the result.

Estimation Theory:

Let Y_1, Y_2, \dots, Y_n be iid random variables, suppose their distribution depends on some parameters $\underline{\theta}$. Suppose parameters $\underline{\theta}_0$ used to sample Y_1, Y_2, \dots, Y_n . How to approximate $\underline{\theta}_0$?

2) Method of Moments: Match first r moments where r is the number of unknowns

3) Least Squares: Given $E[Y] = g(\underline{\theta})$, minimize $\sum_{i=1}^n (Y_i - g(\underline{\theta}))^2$ by modifying the set of parameters

3) Least Absolute Deviation: Given median $g(\underline{\theta})$, minimize $\sum_{i=1}^n |Y_i - g(\underline{\theta})|$

o Note: ② makes sense mathematically in computing derivatives is easy, but the mean is not robust to outliers.
If data has outliers, ③ may work better

4) Maximum Likelihood Estimator:

9/20/23:

- o Let each Y_i have pdf (or pmf) $f(y, \underline{\theta})$.
- o Define $L(\underline{\theta}) = \prod_{i=1}^n f(Y_i, \underline{\theta})$, wish to find optimal $\hat{\underline{\theta}} := \arg \sup_{\underline{\theta}} L(\underline{\theta})$
- o Instead of working with likelihood function, L , work with log-likelihood, $l(\underline{\theta}) := \log(L(\underline{\theta})) = \sum_{i=1}^n \log(f(Y_i, \underline{\theta}))$, nicer to differentiate, as long as $f \neq 0$, differentiable

Ex: Consider $\text{Unif}(0, \theta)$ w/ pdf $\frac{1}{\theta} \cdot I\{0 \leq x \leq \theta\}$. Then

$$L(\theta) = \prod_{i=1}^n f(x_i, \theta) = \theta^{-n} \prod_{i=1}^n I\{0 \leq x_i \leq \theta\} = \theta^{-n} I\{\min(x) \leq \max(x) \leq \theta\}.$$

And from this form, we can see that $\hat{\theta} = \max(x)$ because $L(\theta) = 0$ for $\theta < \max(x)$, and $L(\theta) = \theta^{-n}$ for $\theta \geq \max(x)$.

Theorem: $\sqrt{n} (\hat{\theta} - \theta_0) \xrightarrow{(in distribution)} N\left(0, \frac{1}{I(\theta_0)}\right)$ if f smooth w.r.t. θ (not proven here)

where $I(\theta_0)$ is the Fisher information number. And no estimator can do "better" than this.

Note: MLE is relatively robust to slight changes or "mistakes". Say data is "almost" normally distributed.

Linear Models

Suppose given $(y_i, \underline{x}_i)_{i=1}^n$, \underline{x}_i observation, y_i is the result. Basic linear model given by $y_i = \underline{x}_i^\top \underline{\beta} + \varepsilon_i$, $i = 1, \dots, n$.

Let $\underline{Y} = [y_1 \dots y_n]^\top$, $\underline{X} = [\underline{x}_1 \dots \underline{x}_n]^\top$, $\underline{\varepsilon} = [\varepsilon_1 \dots \varepsilon_n]^\top$. This can be written as $\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$. Suppose \underline{X} is full rank, i.e., no observation a linear combination of another. Let $L(\underline{\beta}) = \sum_{i=1}^n (y_i - \underline{x}_i^\top \underline{\beta})^2$ in which we wish to minimize w.r.t. $\underline{\beta}$.

$$L(\underline{\beta}) = \|\underline{Y} - \underline{X}\underline{\beta}\|_2^2 = (\underline{Y} - \underline{X}\underline{\beta})^\top (\underline{Y} - \underline{X}\underline{\beta})$$

$$= \underline{Y}^\top \underline{Y} - 2\underline{X}^\top \underline{Y} \underline{\beta} + \underline{\beta}^\top \underline{X}^\top \underline{X} \underline{\beta}$$

$$\Rightarrow \frac{dL}{d\underline{\beta}} = -2\underline{X}^\top \underline{Y} + 2\underline{X}^\top \underline{X} \underline{\beta} = \underline{0}$$

$$\Rightarrow \hat{\underline{\beta}} = (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top \underline{Y}$$

$$\text{And, } \frac{d^2 L}{d\underline{\beta}^2} = 2\underline{X}^\top \underline{X} \text{ which is pos. definite.}$$

9/25/23:

Recall, $\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$, $\underline{X} \in \mathbb{R}^{n \times d}$, $\text{rank}(\underline{X}) = d$, $\underline{\varepsilon} \sim N_n(0, \sigma^2 \underline{\mathbb{I}})$, $\underline{\beta} \in \mathbb{R}^d$, $\underline{Y} \in \mathbb{R}^n$. And the least squares solution given by

$$\hat{\underline{\beta}} = (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top \underline{Y}.$$

Then, we define the fitted values as $\hat{\underline{Y}} = \underline{X}\hat{\underline{\beta}}$. Now, assume there is some "true" $\underline{\beta}_0$. Then

$$E[\hat{\underline{\beta}}] = E[(\underline{X}^\top \underline{X})^{-1} \underline{X}^\top (\underline{X}\underline{\beta}_0 + \underline{\varepsilon})]$$

$$= \underline{\beta}_0 + (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top E[\underline{\varepsilon}]$$

$$= \underline{\beta}_0.$$

And, $\text{Cov}(\hat{\underline{\beta}}) = E[\hat{\underline{\beta}}\hat{\underline{\beta}}^\top] - E[\hat{\underline{\beta}}]E[\hat{\underline{\beta}}^\top]$

$$= E[(\underline{\beta}_0 + (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top \underline{\varepsilon})(\underline{\beta}_0^\top + \underline{\varepsilon}^\top \underline{X}(\underline{X}^\top \underline{X})^{-1})] - \underline{\beta}_0 \underline{\beta}_0^\top$$

$$\begin{pmatrix} E[\underline{\varepsilon}] = 0 \\ E[\underline{\varepsilon}\underline{\varepsilon}^\top] = \sigma^2 \underline{\mathbb{I}} \end{pmatrix} = (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top \sigma^2 \underline{\mathbb{I}} \underline{X} (\underline{X}^\top \underline{X})^{-1} = \sigma^2 (\underline{X}^\top \underline{X})^{-1}$$

Gauss-Markov Theorem: (LSE is BLUE): The least squares estimate is the best linear unbiased estimator. I.e., assuming $\underline{y} = \underline{\beta}_0^\top \underline{x} + \underline{\varepsilon}$ with $\underline{\varepsilon} \sim N(0, \sigma^2)$, then given $\underline{X}, \underline{Y}$, the least squares estimate given by $\hat{\underline{\beta}} = (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top \underline{Y}$ is the unbiased linear estimator of $\underline{\beta}_0$ with minimized variance.

Proof: Let $\underline{\alpha} = \underline{C}\underline{Y}$ be another estimator. It can be written in the form $\underline{C} = (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top + \underline{D}$. Hence,

$$E[\underline{\alpha}] = E[((\underline{X}^\top \underline{X})^{-1} \underline{X}^\top + \underline{D})(\underline{X}\underline{\beta}_0 + \underline{\varepsilon})]$$

$$= E[(\underline{I} + \underline{D}\underline{X})\underline{\beta}_0] + ((\underline{X}^\top \underline{X})^{-1} \underline{X}^\top + \underline{D})E[\underline{\varepsilon}]$$

$$= E[\underline{\beta} + \underline{D}\underline{X}] \underline{\beta}_0$$

which equals $\underline{\beta}_0$ (unbiased) iff $\underline{D}\underline{X} = \underline{0}$. Finally,

$$\text{cov}(\underline{\alpha}) = E[\underline{C}\underline{Y}\underline{Y}^T\underline{C}^T] - E[\underline{C}\underline{Y}]E[\underline{Y}^T\underline{C}]$$

$$= \underline{C} E[\underline{Y}\underline{Y}^T] \underline{C}^T - \underline{C} E[\underline{Y}] E[\underline{Y}^T] \underline{C}^T$$

$$= \underline{C} \text{cov}(\underline{Y}) \underline{C}^T$$

$$= \underline{C} \sigma^2 \underline{I} \underline{C}^T$$

$$= \sigma^2 \left((\underline{X}^T \underline{X})^{-1} \underline{X}^T + \underline{D} \right) \left(\underline{X} (\underline{X}^T \underline{X})^{-1} + \underline{D}^T \right)$$

$$\stackrel{(\underline{D}\underline{X}=\underline{0})}{=} \sigma^2 \left((\underline{X}^T \underline{X})^{-1} + \underline{D} \underline{D}^T \right)$$

$$\stackrel{(\text{see above})}{=} \text{cov}(\hat{\beta}) + \sigma^2 \underline{D}^T \underline{D}.$$

And since $\underline{D}^T \underline{D}$ is positive semidefinite, $\text{cov}(\underline{\alpha})$ exceeds $\text{cov}(\hat{\beta})$ unless $\underline{D} = \underline{0}$ in which case $\underline{\alpha} = \hat{\beta}$. This could also be proven in terms of a scalar quantity of interest, $\underline{\alpha}^T \underline{\beta}_0$. We'd show that $E[\underline{\alpha}^T \hat{\beta}] = \underline{\alpha}^T E[\hat{\beta}] = \underline{\alpha}^T \underline{\beta}_0$, and that for any other estimator, $\alpha = \underline{\alpha}^T \underline{C} \underline{Y}$, $E[\alpha] = \underline{\alpha}^T \underline{\beta}_0$, and $\text{var}(\alpha) = \text{var}(\underline{\alpha}^T \hat{\beta}) + \sigma^2 \underline{\alpha}^T \underline{D}^T \underline{D} \underline{\alpha} \geq 0$.

9/27/23:

Define the residuals $\hat{\varepsilon} = \underline{Y} - \hat{\underline{Y}} = \underline{X} \underline{\beta}_0 + \underline{\varepsilon} - \underline{X} \hat{\beta} = \underline{X} \underline{\beta}_0 + \underline{\varepsilon} - \underline{X} ((\underline{X}^T \underline{X})^{-1} \underline{X}^T (\underline{X} \underline{\beta}_0 + \underline{\varepsilon}))$
 $= (\underline{I} - \underline{X} (\underline{X}^T \underline{X})^{-1} \underline{X}^T) \underline{\varepsilon} = (\underline{I} - \underline{P}) \underline{\varepsilon}$ where \underline{P} is the projection matrix of \underline{Y} onto $\hat{\underline{Y}}$. By projection properties, $(\underline{I} - \underline{P})$ is also a projector. Since $(\underline{I} - \underline{P})$ is idempotent, $\hat{\varepsilon}$ is also normal. $E[\hat{\varepsilon}] = (\underline{I} - \underline{P}) E[\underline{\varepsilon}] = \underline{0}$, and $\text{cov}(\hat{\varepsilon}) = (\underline{I} - \underline{P}) \sigma^2 \underline{I} (\underline{I} - \underline{P})^T = \sigma^2 (\underline{I} - \underline{P})$ as \underline{P} is symmetric. Hence, $\hat{\varepsilon} \sim N_n(\underline{0}, \sigma^2 (\underline{I} - \underline{P}))$. And, $\text{rank}(\underline{X}^T \underline{X}) = d$, so $\text{rank}(\underline{P}) = d$, hence, $\text{rank}(\underline{I} - \underline{P}) = n - d$, so $\hat{\varepsilon}$ really only consists of $n - d$ independent normals.

We can compute the joint distribution of $\hat{\beta}$ and $\hat{\varepsilon}$ as they are both normal. We just need the covariance matrix.

$$\begin{aligned}\text{cov}(\hat{\beta}, \hat{\varepsilon}) &= E[\hat{\beta}\hat{\varepsilon}^T] - \underbrace{E[\hat{\beta}]E[\hat{\varepsilon}^T]}_0 \\ &= E\left[\left(\underline{\beta}_0 + (\underline{X}^T\underline{X})^{-1}\underline{X}^T\underline{\varepsilon}\right)\underline{\varepsilon}^T(\underline{I} - \underline{P})^T\right] \\ &= 0 + (\underline{X}^T\underline{X})^{-1}\underline{X}^T\sigma^2\underline{I}(\underline{I} - \underline{P}) \\ &= \sigma^2(\underline{X}^T\underline{X})^{-1}\underline{X}^T(\underline{I} - \underline{X}(\underline{X}^T\underline{X})^{-1}\underline{X}^T) \\ &= 0 \Rightarrow \begin{bmatrix} \hat{\beta} \\ \hat{\varepsilon} \end{bmatrix} \sim N_{n+d}\left(\begin{bmatrix} \underline{\beta}_0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma^2(\underline{X}^T\underline{X}) & 0 \\ 0 & \sigma^2(\underline{I} - \underline{P}) \end{bmatrix}\right)\end{aligned}$$

implying that $\hat{\beta}, \hat{\varepsilon}$ are independent. And, we know that $S^2 = \frac{1}{n-d} \sum_{i=1}^d \hat{\varepsilon}_i^2 = \frac{1}{n-d} \|\hat{\varepsilon}\|^2$, which only depends on $\hat{\varepsilon}$, so, S^2 and $\hat{\beta}$ are independent.

How about $\hat{\varepsilon}^T \hat{\varepsilon}$?

$$\hat{\varepsilon}^T \hat{\varepsilon} = \hat{\varepsilon}^T (\underline{I} - \underline{P})^T (\underline{I} - \underline{P}) \hat{\varepsilon} = \hat{\varepsilon}^T (\underline{I} - \underline{P}) \hat{\varepsilon} \quad (\text{idempotent})$$

And we proved that since $(\underline{I} - \underline{P})$ is idempotent, rank $n-d$, that then $\frac{1}{\sigma^2} \hat{\varepsilon}^T (\underline{I} - \underline{P}) \hat{\varepsilon} \sim \chi_{n-d}^2 \Rightarrow \sigma^2 \hat{\varepsilon}^T \hat{\varepsilon} \sim \chi_{n-d}^2$. So from $S^2 = \frac{1}{n-d} \hat{\varepsilon}^T \hat{\varepsilon}$, $\frac{n-d}{\sigma^2} S^2 \sim \chi_{n-d}^2$. And from that $E[S^2] = \frac{\sigma^2}{n-d} \cdot (n-d) = \sigma^2$ (unbiased). We can also show that $\frac{1}{\sigma^2} (\hat{\beta} - \underline{\beta}_0)^T \underline{X}^T \underline{X} (\hat{\beta} - \underline{\beta}_0) \sim \chi_d^2$ (from $Y \sim N_0(0, \underline{\Sigma}) \Rightarrow Y^T \underline{\Sigma}^{-1} Y \sim \chi_d^2$).

Definition: The F-distribution is given by

$$F(r_1, r_2) = \frac{\chi_{r_1}^2(r_1)/r_1}{\chi_{r_2}^2(r_2)/r_2} \quad \text{with } \chi_{r_1}^2 \perp \chi_{r_2}^2$$

Then, from definition

$$\frac{(\hat{\beta} - \underline{\beta}_0)^T \underline{X}^T \underline{X} (\hat{\beta} - \underline{\beta}_0) / d}{S^2} \sim F(d, n-d)$$

Now, let $\hat{\beta}_i, \beta_{0,i}$ denote the i 'th entry of $\hat{\beta}, \underline{\beta}_0$ respectively.

Then we expect $\hat{\beta}_i - \beta_{0,i}$ to be normal with mean 0. We know $\text{cov}(\hat{\beta}) = \sigma^2 (\underline{\underline{X}}^\top \underline{\underline{X}})^{-1}$, so $\text{var}(\hat{\beta}_i) = \sigma^2 ((\underline{\underline{X}}^\top \underline{\underline{X}})^{-1})_{ii} =: \sigma^2 a_{ii}$. So $(\hat{\beta}_i - \beta_{0,i}) \sim N(0, \sigma^2 a_{ii})$, then $\frac{1}{\sigma \sqrt{a_{ii}}} (\hat{\beta}_i - \beta_{0,i}) \sim N(0, 1)$.

Definition: The t -distribution is given by

$$t(r) = \frac{N(0, 1)}{\sqrt{\chi^2(r)/r}} \quad (\text{w/ independence})$$

Then

$$\frac{\hat{\beta}_i - \beta_{0,i}}{\sqrt{a_{ii} S^2}} \sim t(n-d).$$

10/2/23:

Now, let $\varepsilon_i \sim N(0, \sigma^2)$ iid. From $y_i = \underline{x}_i^\top \underline{\beta} + \varepsilon_i$, we have $y_i \sim N(\underline{x}_i^\top \underline{\beta}, \sigma^2)$, so has density $(2\pi\sigma^2)^{-1/2} \exp\left(-\frac{1}{2}\left(\frac{y_i - \underline{x}_i^\top \underline{\beta}}{\sigma}\right)^2\right)$.

The likelihood method assigns a likelihood function

$$\begin{aligned} L(\underline{\beta}, \sigma^2) &= \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\left(\frac{y_i - \underline{x}_i^\top \underline{\beta}}{\sigma}\right)^2\right) \\ &= (2\pi\sigma^2)^{-n/2} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \underline{x}_i^\top \underline{\beta})^2\right) \\ &= (2\pi\sigma^2)^{-n/2} \exp\left(-\frac{1}{2\sigma^2} \|\underline{Y} - \underline{\underline{X}} \underline{\beta}\|_2^2\right). \end{aligned}$$

Then, the log-likelihood function, $\ell = \log(L)$, is

$$\ell(\underline{\beta}, \sigma) = -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} \|\underline{Y} - \underline{\underline{X}} \underline{\beta}\|_2^2.$$

Try to maximize $\ell \Rightarrow$ maximize L .

$$\frac{\partial \ell}{\partial \underline{\beta}} = -\frac{1}{\sigma^2} \underline{\underline{X}}^\top (\underline{Y} - \underline{\underline{X}} \underline{\beta}) = \underline{0} \Rightarrow \hat{\underline{\beta}} = (\underline{\underline{X}}^\top \underline{\underline{X}}^{-1}) \underline{\underline{X}}^\top \underline{Y}.$$

$$\frac{\partial \ell}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \|\underline{Y} - \underline{\underline{X}} \underline{\beta}\|_2^2 = 0$$

$$\Rightarrow \hat{\sigma}^2 = \frac{1}{n} \|\underline{Y} - \underline{\underline{X}} \hat{\underline{\beta}}\|_2^2$$

$$= \frac{1}{n} \sum_{i=1}^n \hat{\varepsilon}_i^2.$$

And, recall $S_n^2 = \frac{1}{n-d} \sum_{i=1}^n \hat{\epsilon}_i^2$

is an unbiased estimator for σ^2 .

The weighted least squares method, instead of minimizing $\|\underline{Y} - \underline{X}\underline{\beta}\|_2^2 = (\underline{Y} - \underline{X}\underline{\beta})^T(\underline{Y} - \underline{X}\underline{\beta})$, we try to minimize

$$S(\underline{\beta}) = (\underline{Y} - \underline{X}\underline{\beta})^T \underline{W} (\underline{Y} - \underline{X}\underline{\beta}) = \|\underline{Y} - \underline{X}\underline{\beta}\|_w^2$$

where \underline{W} is full rank, positive definite. If \underline{W} is diagonal, then this is $S(\underline{\beta}) = \sum_{i=1}^n w_i (y_i - \underline{x}_i^T \underline{\beta})^2$. Can show this is still unbiased. This can be used where the ϵ terms have different variances.

Differentiating, find $\hat{\underline{\beta}} = (\underline{X}^T \underline{W} \underline{X})^{-1} \underline{X}^T \underline{W} \underline{Y}$.

Ex: Let $y_i = \underline{x}_i^T \underline{\beta} + \epsilon_i$ for $i = 1, \dots, n$ with $\epsilon_i \sim N(0, \sigma_{\epsilon_i}^2)$, independent, but not identically distributed. Then, should weight $w_i \propto \frac{1}{\sigma_{\epsilon_i}^2}$, so let $w_i = \frac{1}{\sigma_{\epsilon_i}^2}$. This way, each $w_i (y_i - \underline{x}_i^T \underline{\beta})^2 = \left(\frac{y_i - \underline{x}_i^T \underline{\beta}}{\sqrt{w_i}}\right)^2 \sim (N(0, 1))^2$.

Ex: Similarly, if $\epsilon \sim N_n(0, \Sigma)$, then choose $\underline{W} = \Sigma^{-1}$.

10/4/23:

In weighted LS, $\hat{\underline{\beta}} = (\underline{X}^T \underline{W} \underline{X})^{-1} \underline{X}^T \underline{Y}$. So

$$\mathbb{E}[\hat{\underline{\beta}}] = (\underline{X}^T \underline{W} \underline{X})^{-1} \underline{X}^T \underline{W} \mathbb{E}[\underline{X} \underline{\beta} + \epsilon] = \underline{\beta} + \underline{0} = \underline{\beta}.$$

And,

$$\text{cov}(\hat{\underline{\beta}}) = \text{cov}((\underline{X}^T \underline{W} \underline{X})^{-1} \underline{X}^T \underline{W} \epsilon)$$

$$= (\underline{X}^T \underline{W} \underline{X})^{-1} \underline{X}^T \underline{W} \mathbb{E}[\epsilon \epsilon^T] \underline{W}^T \underline{X} (\underline{X}^T \underline{W} \underline{X})^{-1}$$

$$= (\underline{X}^T \underline{W} \underline{X})^{-1} \underline{X}^T \underline{W} \Sigma \underline{W}^T \underline{X} (\underline{X}^T \underline{W} \underline{X})^{-1}$$

What is the distribution of $\hat{\underline{\beta}}$? Since $\epsilon \sim N_n(0, \Sigma)$,

$$\hat{\underline{\beta}} \sim N_d(\underline{\beta}, (\underline{X}^T \underline{V} \underline{X})^{-1} \underline{V} \underline{V} (\underline{X}^T \underline{V} \underline{X})^{-1}).$$

The location + scale family is as follows. Suppose we have a random variable X with density $f_0(t)$, called the mother density. Then define the scale $\sigma > 0$, and location $M \in \mathbb{R}$. Then define $Y = M + \sigma X$. We can find the density of Y to be $f_Y(t) = \frac{1}{\sigma} f_0\left(\frac{t-M}{\sigma}\right)$.

Now, suppose we have the linear model $y_i = \underline{x}_i^T \underline{\beta} + \varepsilon_i$. Suppose ε_i ~ location/scale. We know $M = E[y_i] = \underline{x}_i^T \underline{\beta}$. Then, if we don't know σ^2 , variance of ε_i , generate likelihood function

$$L(\underline{\beta}, \sigma) = \prod_{i=1}^n \frac{1}{\sigma} f_0\left(\frac{y_i - \underline{x}_i^T \underline{\beta}}{\sigma}\right)$$

$$\Rightarrow l(\underline{\beta}, \sigma) = -n \log(\sigma) + \sum_{i=1}^n \log\left(f_0\left(\frac{y_i - \underline{x}_i^T \underline{\beta}}{\sigma}\right)\right)$$

We wish to maximize l w.r.t. $\underline{\beta}, \sigma$. For shorthand, we define $\rho(x) = \log(f_0(x))$, and $e_i(\underline{b}) = t - \underline{x}_i^T \underline{b}$. Note that if $f_0 \sim N(0, 1)$, $\rho(x) = \frac{1}{2}x^2$. The solution to this are called the M-estimators.

10/18/23:

In hypothesis testing, we have some $\underline{X} \sim f(\underline{x}, \underline{\theta})$, $\underline{\theta} \in \Theta$. We form the null hypothesis $\underline{\theta} \in \Theta_0$, versus the alternative hypothesis $\underline{\theta} \in \Theta_a$ with $\Theta_0 \cup \Theta_a \subseteq \Theta$ and $\Theta_0 \cap \Theta_a = \emptyset$. We wish to either reject the null, H_0 , or fail to reject H_0 . We form a rejection region, C . If $\underline{x} \in C$, we reject H_0 , if $\underline{x} \notin C$, we do not reject H_0 . The power function is defined as

$$\pi_C(\underline{\theta}) = P[\underline{x} \in C | \underline{\theta} = \underline{\theta}]$$

Two types of errors possible

- 1) Type I Error: We reject H_0 when H_0 is correct
- 2) Type II Error: We fail to reject H_0 when H_0 is incorrect.

We would like to bound

$$\max_{\hat{\theta} \in \Theta_0} \pi_c(\hat{\theta}) = \max_{\hat{\theta} \in \Theta_0} P[\underline{X} \in C | \hat{\theta} = \theta] \leq \alpha.$$

I.e., we would like to bound how likely we reject given the null is true, bounding type I errors.

Ex: X_1, \dots, X_n iid $N(\mu, 1)$. Wish to test $H_0: \mu = \mu_0$ versus $H_a: \mu > \mu_0$. So $\Theta_0 = \{\mu_0\}$, $\Theta_a = \{\mu: \mu > \mu_0\}$, $\Theta = \mathbb{R}$. Now, must form a rejection region. Clearly, it will take the form of $C = \{x: x > c\}$, and see if $\bar{X} \in C$. We know $\bar{X} \sim N(\mu, \frac{1}{n})$. Under H_0 , $\bar{X} \sim N(\mu_0, \frac{1}{n})$. We can compute the power function

$$\pi_c(\mu_0) = P[\bar{X} > c | \bar{X} \sim N(\mu_0, \frac{1}{n})]$$

$$= P[N(0, 1) > \sqrt{n}(c - \mu_0)]$$

$$= 1 - \Phi(\sqrt{n}(c - \mu_0)) \stackrel{\text{set}}{=} \alpha$$

and then use a computer to approximate c . Note that then the probability of rejection given H_0 is true is α , i.e., α is the probability of a type I error. Can see from this,

$$\lim_{\mu \rightarrow \infty} \pi_c(\mu) = 1 \quad \text{and} \quad \lim_{\substack{\mu \rightarrow \infty \\ (\epsilon < c > \mu)}} \pi_c(\mu) \text{ given } \mu > \mu_0 = 1.$$

We could create another test for $\text{median}(\underline{X}) \geq a$. Which is better? Turns out the first is better, as \bar{X} is the maximum likelihood estimator for μ .

Now, instead, let H_0 be $M \leq M_0$, H_a be $M > M_0$.

want $\alpha = \max_{M \leq M_0} \pi_C(M)$ which occurs at $M = M_0$, so get same analysis as before.

So $\alpha = \pi_C(M_0) = 1 - \Phi(\frac{\bar{X}_n - c}{\sigma/\sqrt{n}})$ again.

10/23/23:

Given rejection regions C and D, we say C is better than D if $\pi_C(\theta) \geq \pi_D(\theta) \quad \forall \theta \in \Theta_a$, i.e., for every possible observation under the alternative hypothesis, we are more (or equally) likely to reject.

Ex: X_1, \dots, X_n iid Poisson(λ). Wish to test $H_0: \lambda \geq \lambda_0$ vs $H_a: \lambda < \lambda_0$ with λ_0 given. We know $E[X_i] = \lambda$. \bar{X}_n is a good estimator for $\lambda = E[X_i]$. So, intuitively, define rejection as $\bar{X} \leq c$. Then, for a size of α ,

$$\alpha = \sup_{\lambda \geq \lambda_0} \pi_C(\lambda)$$

$$= \sup_{\lambda \geq \lambda_0} P[\bar{X} \leq c \mid \lambda].$$

We know $\sum_{i=1}^n X_i \sim \text{Pois}(n\lambda)$, so $n\bar{X} \sim \text{Pois}(n\lambda)$. So

$$\alpha = \sup_{\lambda \geq \lambda_0} P[\text{Pois}(n\lambda) \leq nc]$$

$$= P[\text{Pois}(n\lambda_0) \leq nc]$$

$$= \sum_{x=0}^{nc} \frac{(n\lambda_0)^x e^{-n\lambda_0}}{x!}.$$

Ex: X_1, \dots, X_n iid $N(\mu, \sigma^2)$ with μ, σ^2 unknown, wish to test $H_0: \mu = \mu_0$ vs. $H_a: \mu \neq \mu_0$. We call σ^2 a nuisance parameter as it doesn't appear in the null or alternative. We will reject H_0

when $|\bar{X} - \mu|$ is large. We don't know σ^2 , so approximate it with S^2 . So, we will reject when $\frac{|\bar{X} - \mu|}{S/\sqrt{n}} \geq c$. We know this is distributed

as $t(n-1)$. So this hypothesis test becomes a t -test.

Neyman-Pearson Lemma: Given $\underline{X} \sim f(\underline{x}; \underline{\theta})$, wish to test $H_0: \underline{\theta} = \underline{\theta}_0$ vs. $H_a: \underline{\theta} = \underline{\theta}_a$ with $\underline{\theta}_0 \neq \underline{\theta}_a$. Then, defining the rejection region

$$C = \left\{ \underline{x} : \frac{f(\underline{x}; \underline{\theta}_0)}{f(\underline{x}; \underline{\theta}_a)} \leq c \right\},$$

it is optimal in the sense that $\pi_c(\underline{\theta}_a) \geq \pi_{c^*}(\underline{\theta}_a)$ for any other rejection region C^* for a fixed size α with

$$\alpha = \pi_c(\underline{\theta}_0) = \pi_{c^*}(\underline{\theta}_0).$$

The quantity $f(\underline{x}; \underline{\theta}_0) / f(\underline{x}; \underline{\theta}_a)$ is the likelihood ratio.

The generalized likelihood method with $H_0: \underline{\theta} \in \Theta_0$, $H_a: \underline{\theta} \in \Theta_a$, calls to reject H_0 if

$$\frac{\sup_{\underline{\theta} \in \Theta_0} f(\underline{x}; \underline{\theta})}{\sup_{\underline{\theta} \in \Theta_a} f(\underline{x}; \underline{\theta})} \leq c.$$

Alternatively, can reject by the likelihood ratio

$$\lambda(\underline{x}) = \frac{\sup_{\underline{\theta} \in \Theta_0} f(\underline{x}; \underline{\theta})}{\sup_{\underline{\theta} \in \Theta_0 \cup \Theta_a} f(\underline{x}; \underline{\theta})} \leq c \quad (\leq 1).$$

It is very tricky to solve for c in terms of a size α , so instead use the rule to reject if $-2 \log(\lambda(\underline{x})) \geq \alpha$.

Under H_0 , we have $-2 \log(\lambda(\underline{x})) \sim \chi^2(r)$, $r = \dim(\Theta_0 \cup \Theta_a) - \dim(\Theta_0)$.

Ex: X_1, \dots, X_n i.i.d $N(\mu, 1)$. Wish to test $H_0: \mu \leq \mu_0$ vs $H_a: \mu > \mu_0$. The likelihood is given by

$$f(\underline{x}; \mu) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(x_i - \mu)^2} = (2\pi)^{-n/2} e^{-\frac{1}{2} \sum_{i=1}^n (x_i - \mu)^2}.$$

Now, to find the likelihood ratio, first we already know

$$\max_{\mu} f(\underline{x}; \mu) = f(\underline{x}, \bar{x}).$$

Additionally, f has a unique maximizer, so

$$\max_{M \in M_0} f(\underline{x}; M) = \begin{cases} \bar{X} & M_0 \geq \bar{X} \\ M_0 & \text{otherwise} \end{cases} = \min(M_0, \bar{X}).$$

Hence, we can compute the likelihood ratio

$$\lambda(\underline{x}) = \frac{f(\underline{x}; \min(M_0, \bar{X}))}{f(\underline{x}; \bar{X})}$$

which equals one when $\bar{X} \leq M_0$. Recall, we reject when $\lambda(\underline{x})$ is small, i.e., \bar{X} is large relative to M_0 . This makes sense with respect to definition of H_0, H_a . Going back to log,

$$-2 \log(\lambda(\underline{x})) \sim \chi_r^2 \quad \text{with } r = \dim(\Theta_0 \cup \Theta_a) - \dim(\Theta_0) = 1 - 1 = 0$$

so this method doesn't work.

10/25/23:

Consider the model $\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$, $\underline{Y} \in \mathbb{R}^n$, $\underline{X} \in \mathbb{R}^{n \times p}$ with rank p , $\underline{\beta} \in \mathbb{R}^p$, $\underline{\varepsilon} \sim N_n(0, \sigma^2 \mathbb{I})$. Let $\underline{A} \in \mathbb{R}^{q \times p}$ with $\text{rank}(\underline{A}) = q$, and $\underline{c} \in \mathbb{R}^q$. We wish to estimate $\underline{\beta}$ under the restriction $\underline{A}\underline{\beta} = \underline{c}$.

We introduce Lagrange multipliers, so we wish to minimize

$$g(\underline{\beta}, \underline{\lambda}) = \|\underline{Y} - \underline{X}\underline{\beta}\|_2^2 + (\underline{A}\underline{\beta} - \underline{c})^\top \underline{\lambda}.$$

$$\frac{dg}{d\underline{\lambda}}(\hat{\underline{\beta}}_H, \hat{\underline{\lambda}}_H) = \underline{A}\hat{\underline{\beta}}_H - \underline{c} = \underline{0} \Rightarrow \underline{A}\hat{\underline{\beta}}_H = \underline{c},$$

$$\frac{dg}{d\underline{\beta}}(\hat{\underline{\beta}}_H, \hat{\underline{\lambda}}_H) = -2\underline{X}^\top \underline{Y} + 2\underline{X}^\top \underline{X}\hat{\underline{\beta}}_H + \underline{A}^\top \hat{\underline{\lambda}}_H = \underline{0}$$

$$\Rightarrow \hat{\underline{\beta}}_H = (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top \underline{Y} - \frac{1}{2} (\underline{X}^\top \underline{X})^{-1} \underline{A}^\top \hat{\underline{\lambda}}_H$$

$$\Rightarrow \underline{c} = \underline{A}\hat{\underline{\beta}}_H = \underline{A}\underline{\beta} - \frac{1}{2} \underline{A}(\underline{X}^\top \underline{X})^{-1} \underline{A}^\top \hat{\underline{\lambda}}_H$$

$$\Rightarrow \hat{\underline{\lambda}}_H = 2(\underline{A}(\underline{X}^\top \underline{X})^{-1} \underline{A}^\top)^{-1} (\underline{A}\hat{\underline{\beta}} - \underline{c})$$

$$\Rightarrow \hat{\underline{\beta}}_H = \hat{\underline{\beta}} - (\underline{\underline{X}}^T \underline{\underline{X}})^{-1} \underline{\underline{A}}^T (\underline{\underline{A}} (\underline{\underline{X}}^T \underline{\underline{X}})^{-1} \underline{\underline{A}}^T)^{-1} (\underline{\underline{A}} \hat{\underline{\beta}} - \underline{\underline{c}})$$

where $\hat{\underline{\beta}}$ is the standard least squares solution. Since this is a linear operator on $\hat{\underline{\beta}}$, we must have that $\hat{\underline{\beta}}_H$ is also normal. Now,

$$E[\hat{\underline{\beta}}_H] = \hat{\underline{\beta}} - (\dots)(\underline{\underline{A}} \hat{\underline{\beta}} - \underline{\underline{c}})$$

$$= \hat{\underline{\beta}} \quad \text{if } \underline{\underline{A}} \hat{\underline{\beta}} = \underline{\underline{c}}.$$

Note if $\underline{\underline{A}} \hat{\underline{\beta}} \neq \underline{\underline{c}}$ (even though $\underline{\underline{A}} \hat{\underline{\beta}}_H = \underline{\underline{c}}$), then this is not an unbiased estimator for $\underline{\beta}$. Next, we could solve for the covariance matrix of $\hat{\underline{\beta}}_H$, but it will be ugly. An interesting question is to compare

$$RSS = \| \underline{Y} - \underline{\underline{X}} \hat{\underline{\beta}} \|_2^2 \text{ and } RSS_H = \| \underline{Y} - \underline{\underline{X}} \hat{\underline{\beta}}_H \|_2^2.$$

It is clear that $RSS \leq RSS_H$ since the "H" problem is constrained.

10/30/23:

We previously showed that

$$\| \underline{Y} - \underline{\underline{X}} \underline{\beta} \|_2^2 = \| \underline{Y} - \underline{\underline{X}} \hat{\underline{\beta}} \|_2^2 + \| \underline{\underline{X}} (\hat{\underline{\beta}} - \underline{\beta}) \|_2^2.$$

Setting $\underline{\beta} = \hat{\underline{\beta}}_H$,

$$\| \underline{Y} - \underline{\underline{X}} \hat{\underline{\beta}}_H \|_2^2 = \| \underline{Y} - \underline{\underline{X}} \hat{\underline{\beta}} \|_2^2 + \| \underline{\underline{X}} (\hat{\underline{\beta}} - \hat{\underline{\beta}}_H) \|_2^2$$

or, written in words:

$$RSS_H = RSS + \| \underline{\underline{X}} (\hat{\underline{\beta}} - \hat{\underline{\beta}}_H) \|_2^2.$$

Can derive that

$$\frac{(RSS_H - RSS)/q}{RSS/(n-p)} = \frac{(\underline{\underline{A}} \hat{\underline{\beta}} - \underline{\underline{c}}) (\underline{\underline{A}} (\underline{\underline{X}}^T \underline{\underline{X}})^{-1} \underline{\underline{A}})^{-1} (\underline{\underline{A}} \hat{\underline{\beta}} - \underline{\underline{c}}) / q}{S^2} \sim F(q, n-p)$$

$(q = \text{rank}(\underline{\underline{A}}))$

So, can use an F-test to investigate RSS_H vs RSS.

11/1/23:

Given ordinary linear model $\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$, $\underline{\beta} \in \mathbb{R}^p$, $\underline{X} \in \mathbb{R}^{n \times p}$ full rank (p), $\underline{Y} \in \mathbb{R}^n$, $\underline{\varepsilon} \sim N_n(0, \sigma^2 \mathbb{I})$. Then, given $\underline{A} \in \mathbb{R}^{q \times p}$ rank (q), $\underline{c} \in \mathbb{R}^q$, and test $H_0: \underline{A}\underline{\beta} = \underline{c}$ vs $H_a: H_0$ not true.

Recall the likelihood function

$$f(\underline{\beta}, \sigma^2) = (2\pi\sigma^2)^{-n/2} e^{-\frac{1}{2\sigma^2} \|\underline{Y} - \underline{X}\underline{\beta}\|_2^2}.$$

The likelihood ratio is then given by

$$\frac{\max_{\underline{A}\underline{\beta}=\underline{c}} f(\underline{\beta}, \sigma^2)}{\max_{\underline{\beta}, \sigma^2} f(\underline{\beta}, \sigma^2)} = \frac{\max_{\underline{A}\underline{\beta}=\underline{c}} f(\underline{\beta}, \sigma^2)}{f(\hat{\underline{\beta}}, \hat{\sigma}^2)}$$

where $\hat{\underline{\beta}} = (\underline{X}^\top \underline{X})^{-1} \underline{X}^\top \underline{Y}$, $\hat{\sigma}^2 = \frac{1}{n} \|\underline{Y} - \underline{X}\hat{\underline{\beta}}\|_2^2$. Now, using def of $\hat{\sigma}^2$,

$$f(\hat{\underline{\beta}}, \hat{\sigma}^2) = (2\pi\hat{\sigma}^2)^{-n/2} e^{-n/2}.$$

Now, we also solved for the constrained $\hat{\underline{\beta}}_H$, and $\hat{\sigma}_H^2 = \frac{1}{n} \|\underline{Y} - \underline{X}\hat{\underline{\beta}}_H\|_2^2$, so

$$f(\hat{\underline{\beta}}_H, \hat{\sigma}_H^2) = (2\pi\hat{\sigma}_H^2)^{-n/2},$$

hence,

$$\lambda_{LR} = \frac{\max_{\underline{A}\underline{\beta}=\underline{c}} f(\underline{\beta}, \sigma^2)}{\max_{\underline{\beta}, \sigma^2} f(\underline{\beta}, \sigma^2)} = \left(\frac{\hat{\sigma}^2}{\hat{\sigma}_H^2} \right)^{n/2}.$$

We reject H_0 if $\lambda_{LR} = (\hat{\sigma}^2/\hat{\sigma}_H^2)^{n/2}$ is small, i.e., $\hat{\sigma}_H^2/\hat{\sigma}^2$ large, i.e., $\frac{\hat{\sigma}_H^2 - \hat{\sigma}^2}{\hat{\sigma}^2}$ large, i.e., $\frac{RSS_H - RSS}{RSS}$ large (we know $RSS_H \geq RSS$).

Ex: 2 samples: $U_i = M_1 + \varepsilon_i$, $i = 1, \dots, n_1$, $V_i = M_2 + \eta_i$, $i = 1, \dots, n_2$, with ε_i, η_i iid $N(\mu, \sigma^2)$. Wish to test $H_0: M_1 = M_2$ against $H_a: M_1 \neq M_2$. Set up linear model

$$\underline{Y} = \begin{bmatrix} U_1 \\ \vdots \\ U_{n_1} \\ V_1 \\ \vdots \\ V_{n_2} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \vdots & \vdots \\ 1 & 0 \\ 0 & 1 \\ \vdots & \vdots \\ 0 & 1 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \end{bmatrix} + \underline{\varepsilon} = \underline{X}\underline{\beta} + \underline{\varepsilon}.$$

And, wish to test if

$$\underline{\underline{A}} \underline{\underline{\beta}} = \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \end{bmatrix} = \underline{\underline{O}} = \underline{\underline{c}}.$$

So, we first calculate that $\underline{\underline{x}}^T \underline{\underline{x}} = \begin{bmatrix} n_1 & 0 \\ 0 & n_2 \end{bmatrix}$, so
 $(\underline{\underline{x}}^T \underline{\underline{x}})^{-1} = \begin{bmatrix} 1/n_1 & 0 \\ 0 & 1/n_2 \end{bmatrix}$. Next, without restriction,

$$\begin{bmatrix} \hat{M}_1 \\ \hat{M}_2 \end{bmatrix} = \hat{\underline{\underline{\beta}}} = (\underline{\underline{x}}^T \underline{\underline{x}})^{-1} \underline{\underline{x}}^T \underline{\underline{y}} = \begin{bmatrix} \bar{U} \\ \bar{V} \end{bmatrix}.$$

Next, define $\tilde{M} = \frac{1}{n_1+n_2} \left(\sum_{i=1}^{n_1} U_i + \sum_{i=1}^{n_2} V_i \right)$. From former work,

$$\begin{aligned} \text{RSS}_H - \text{RSS} &= (\underline{\underline{A}} \hat{\underline{\underline{\beta}}} - \underline{\underline{c}})^T (\underline{\underline{A}} (\underline{\underline{x}}^T \underline{\underline{x}})^{-1} \underline{\underline{A}}^T) (\underline{\underline{A}} \hat{\underline{\underline{\beta}}} - \underline{\underline{c}}) \\ &= (\bar{U} - \bar{V}) \left([1 \ -1] \begin{bmatrix} 1/n_1 & 0 \\ 0 & 1/n_2 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \right)^{-1} (\bar{U} - \bar{V}) \\ &= (\bar{U} - \bar{V})^2 \left(\frac{1}{n_1} + \frac{1}{n_2} \right)^{-1}. \end{aligned}$$

Now, under H_0 , $\bar{U} - \bar{V} \sim N(M_1 - M_2, \frac{\sigma^2}{n_1} + \frac{\sigma^2}{n_2}) = N(0, \sigma^2(\frac{1}{n_1} + \frac{1}{n_2}))$.
 Hence, $\frac{1}{\sigma^2}(\bar{U} - \bar{V})^2 \left(\frac{1}{n_1} + \frac{1}{n_2} \right)^{-1} \sim \chi^2_2$. Additionally, we know that

$$\text{RSS} = \|\underline{\underline{y}} - \underline{\underline{x}} \hat{\underline{\underline{\beta}}}\|_2^2 = (n_1 + n_2) \hat{\sigma}^2, \text{ so}$$

$$\frac{\text{RSS}_H - \text{RSS}}{\text{RSS}} = \frac{(\bar{U} - \bar{V}) \left(\frac{1}{n_1} + \frac{1}{n_2} \right)^{-1}}{(n_1 + n_2) \hat{\sigma}^2}$$

test if this value is large.

If the previous problem is extended to 3 variables, U_i, V_i, Z_i , then it is more common to use ANOVA w/ 3 populations.

Now, consider the model $y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$. We can define the R^2 value as

$$R^2 = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2} = \frac{(\sum_{i=1}^n (y_i - \bar{y})(x_i - \bar{x}))^2}{\sum_{i=1}^n (y_i - \bar{y})^2 \sum_{i=1}^n (x_i - \bar{x})^2}$$

which can be interpreted as a correlation between y_i, x_i if each are random.
 Or, interpreted as a ratio of the model's (β_0, β_1 's) impact to that of just the mean (β_0, β_1 not in model).

11/6/23:

Resampling:

- 1) Jackknife provides a simulation based method to estimate σ (unknown)
- 2) Bootstrap computes the density function of a statistic

Lemma: Let X_1, \dots, X_n be iid r.v.s with cdf $F(x)$. Define the empirical density function, $F_n(t) = \frac{1}{n} \sum_{i=1}^n I[X_i \leq t]$.

Then,

- 1) $F_n(t) \xrightarrow{\text{P}} F(t)$ for all t
- 2) $\sup_t |F_n(t) - F(t)| \xrightarrow{\text{P}} 0$

"Proof": The first statement falls out of the law of large numbers because $E[I[X_i \leq t]] = 1 \cdot P[X_i \leq t] = F(t)$. The second statement is the Fundamental Theorem of Statistics.

Now, from the above lemma, a few facts:

- 1) $n F_n(t) = \sum_{i=1}^n I[X_i \leq t] \sim \text{Binomial}(n, F(t))$
- 2) $\sqrt{n} (F_n(t) - F(t)) = \frac{n F_n(t) - n F(t)}{\sqrt{n}} \xrightarrow{D} N(0, F(t)(1-F(t)))$

due to normalization & variance of Bernoulli(p) = $\text{Binom}(1, p)$ is $p(1-p)$.

- 3) $\sqrt{n} \sup_t |F_n(t) - F(t)| \xrightarrow{D} \text{Kolmogorov-Smirnov}$

Lemma: Let X_1, \dots, X_n iid with cdf F . Let X be a random variable where X is one of X_1, \dots, X_n selected uniformly randomly. We know that (assuming each X_i not equal), $P[X = X_i | X_1, \dots, X_n] = \frac{1}{n}$, and $E[X | X_1, \dots, X_n] = \bar{X}$. Additionally, $P[X \leq t | X_1, \dots, X_n] = F_n(t)$.

Back to model $Y = X\beta + \varepsilon$, and test $H_0: \beta \in \Theta_0$ vs $H_a: \beta \notin \Theta_0$. Wish to find a statistic Δ_n s.t. $\Delta_n \xrightarrow{D} \xi$ under H_0 , and $\Delta_n \xrightarrow{\text{P}} \infty$ under H_a .

(cdf of Δ_n) (cdf of ξ)

Note, $\Delta_n \xrightarrow{D} \xi \Rightarrow G_n(t) \rightarrow G(t)$ for all t except for on set of measure zero.
And for a test of size α , wish to choose c_n s.t.

$$\alpha = 1 - G_n(c_n) = P[\xi \geq c_n] \approx P[\Delta_n \geq c_n].$$

Bootstrap procedure: (Efron Bootstrap 1970's, Stanford):

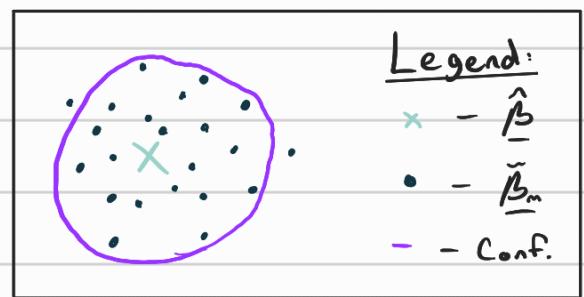
- 1) Estimate $\hat{\beta}_H$ to be a constrained regression solution ($\hat{\beta}_H \in \Theta_0$)
- 2) Generate residuals $\hat{\varepsilon} = \underline{Y} - \underline{X}\hat{\beta}_H$. (without is negligible for n large)
- 3) Sample i_1, \dots, i_k from $\{1, \dots, n\}$ with replacement
- 4) Compute $\tilde{\Delta}_{k,m}$ from $\hat{y}_{i_j} = \underline{X}^T \hat{\beta}_H, j=1, \dots, k$, for $m=1, \dots, M$.
- 5) $\frac{1}{M} \sum_{m=1}^M I[\tilde{\Delta}_{k,m} \leq t] \approx G(t)$ (approximate cdf)

11/8/23:

Consider the same model $\underline{Y} = \underline{X}\underline{\beta} + \underline{\varepsilon}$ with $\underline{\beta} \in \mathbb{R}^n$. We wish to find a confidence set with $1-\alpha$ coverage for $\underline{\beta}$. Let $\hat{\beta}$ be the LSE for $\underline{\beta}$, and define $\hat{\varepsilon} = \underline{Y} - \underline{X}\hat{\beta}$. Then, for $m=1, \dots, M$, sample from the data, and generate the bootstrapped LSE $\tilde{\beta}_m, \tilde{\varepsilon}_m$.

Next, we create a cloud which contains $(1-\alpha)\%$ of the $\tilde{\beta}_m$'s.

Note: This region is not unique, its shape / what is included or excluded is up to the statistician.



11/13/23:

Consider the same set-up as before. We can use Tikhonov regularization or ridge regularization, to generate a ridge estimator $\hat{\beta}_{\text{ridge}}$.

$$L(\underline{\beta}) = \|\underline{Y} - \underline{X}\underline{\beta}\|_2^\alpha + 2\|\underline{\beta}\|_2^\alpha$$

$$= \underline{Y}^T \underline{Y} - 2\underline{\beta}^T \underline{X}^T \underline{Y} + \underline{\beta}^T \underline{X}^T \underline{X} \underline{\beta} + \lambda \underline{\beta}^T \underline{\beta}$$

$$\Rightarrow \frac{dL(\underline{\beta})}{d\underline{\beta}} = -2\underline{X}^T \underline{Y} + 2\underline{X}^T \underline{X} \underline{\beta} + 2\lambda \underline{\beta} = 0$$

$$\Rightarrow \hat{\underline{\beta}}_{\text{ridge}} = (\underline{X}^T \underline{X} + \lambda \underline{I})^{-1} \underline{X}^T \underline{Y}.$$

Note, the ridge estimator is biased, $E[\hat{\underline{\beta}}_{\text{ridge}}] \neq \underline{\beta}$ (for $\lambda \neq 0$). We can rewrite it as

$$\hat{\underline{\beta}}_{\text{ridge}} = (\underline{X}^T \underline{X} + \lambda \underline{I})^{-1} (\underline{X}^T \underline{X}) \underline{\beta} = \underline{C} \underline{\beta}.$$

So, we see

$$\hat{\underline{\beta}}_{\text{ridge}} \sim N_d(\underline{C} \underline{\beta}, \sigma^2 \underline{C}^T (\underline{X}^T \underline{X})^{-1} \underline{C}).$$

The mean squared error, MSE, is defined to be

$$MSE(\hat{\underline{\beta}}) = E\left[\|\hat{\underline{\beta}} - \underline{\beta}\|_2^2\right].$$

Can show that $MSE(\hat{\underline{\beta}}_{\text{ridge}}) < MSE(\hat{\underline{\beta}})$ for $0 < \lambda < 1$.

Ex: $\underline{Y} = \underline{X} \underline{\beta} + \underline{\varepsilon}$, $H_0: \underline{\beta} = \underline{\beta}_0$ vs $H_a: \underline{\beta} \neq \underline{\beta}_0$. We wish to find a test based on $\hat{\underline{\beta}}_{\text{ridge}}$.

$$\text{We have that } \frac{(\hat{\underline{\beta}}_{\text{ridge}} - \underline{C} \underline{\beta}_0)^T \underline{W} (\hat{\underline{\beta}}_{\text{ridge}} - \underline{C} \underline{\beta}_0) / \rho}{S^2} \sim F(\rho, n-\rho)$$

$$\text{where } S^2 = \frac{1}{n-\rho} \|\underline{Y} - \underline{X} \hat{\underline{\beta}}\|_2^2, \quad \underline{W} = (\underline{C}^T (\underline{X}^T \underline{X})^{-1} \underline{C})^{-1},$$

so can do a two-sided test with this.

For a lasso regularization, we consider the loss function

$$L(\underline{\beta}) = \|\underline{Y} - \underline{X} \underline{\beta}\|_2^2 + \lambda \|\underline{\beta}\|_1$$

where $\|\underline{\beta}\|_1 = \sum_{i=1}^p |\beta_i|$. Lasso shrinks small coordinates to zero while ridge shrinks all coordinates towards (but not to) zero. So lasso leads to a sparse model.

11/20/23:

Differentiating,

$$\frac{d \underline{L}}{d \underline{\beta}} = -2 \underline{\underline{X}}^T \underline{Y} + 2 \underline{\underline{X}}^T \underline{\underline{X}} \underline{\beta} + \lambda \text{sign}(\underline{\beta}).$$

We then will assume the inputs are normalized, i.e., $\underline{\underline{X}}^T \underline{\underline{X}} = \underline{\underline{I}}$
assump.

$$= -2 \underline{\underline{X}}^T \underline{Y} + 2 \underline{\beta} + \lambda \text{sign}(\underline{\beta}).$$

We can write the i^{th} component as

$$\sum_{j=1}^n (-2x_{ij}y_j) + 2\beta_i + \lambda \text{sign}(\beta_i) = 0$$
$$\Rightarrow \beta_i = \begin{cases} \frac{\sum_{j=1}^n x_{ij}y_j - \frac{\lambda}{2}}{2}, & \frac{\sum_{j=1}^n x_{ij}y_j - \frac{\lambda}{2}}{2} > 0 \\ \frac{\lambda}{2} - \sum_{j=1}^n x_{ij}y_j, & \frac{\lambda}{2} - \sum_{j=1}^n x_{ij}y_j < 0 \\ 0, & \text{otherwise} \end{cases}$$

The elastic net or garotte method mixes the above two:

$$\underline{L}(\underline{\beta}) = \|\underline{Y} - \underline{\underline{X}} \underline{\beta}\|_2^2 + \lambda \|\underline{\beta}\|_2^2 + \mu \|\underline{\beta}\|_1.$$