



Linear Models

STAT 551

Course Notes by Meredith Bartley



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Part One

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1. Linear Regression

- projection
- orthongonal decomposition
- Gaussian Linear Regression
- prediction (generally of \hat{y})
- different types of errors
- influence
- lack of fit
- R^2
- Multicollinearity

1.1 Projection in Euclidean Space

Monday August 22

Definition 1.1.1 — Euclidian Space. One way to think of the Euclidean plane is as a set of points satisfying certain relationships, expressible in terms of distance and angle. **Euclidean space** is an abstraction detached from actual physical locations, specific reference frames, measurement instruments, and so on.

Let Euclidian Space be denoted by \mathbb{R}^P .

$$\mathbb{R}^P = \{(x_1, \dots, x_p) : x_1 \in \mathbb{R}, \dots, x_p \in \mathbb{R}\}$$

Definition 1.1.2 — Inner Product. In linear algebra, an inner product space is a vector space with an additional structure called an inner product. This additional structure associates each pair of vectors in the space with a scalar quantity known as the inner product of the vectors. **Inner products** allow the rigorous introduction of intuitive geometrical notions such as the length of a vector or the angle between two vectors. They also provide the means of defining orthogonality between vectors (zero inner product).

Let $a \in \mathbb{R}^P, b \in \mathbb{R}^P$

$$a^T b = \sum_{i=1}^P a_i b_i$$

$$a^T b = \langle a, b \rangle$$

Definition 1.1.3 — Hilbert Space. The mathematical concept of a Hilbert space generalizes the notion of Euclidean space. It extends the methods of vector algebra and calculus from the two-dimensional Euclidean plane and three-dimensional space to spaces with any finite or infinite number of dimensions. A Hilbert space is an abstract vector space possessing the structure of an inner product that allows length and angle to be measured. Furthermore, Hilbert spaces are complete: there are enough limits in the space to allow the techniques of calculus to be used.

Hilbert Inner Product Space $\{\mathbb{R}^P, \langle a, b \rangle\}$

General Inner Product

Let $\Sigma \in \mathbb{R}^{P \times P}$ set of all $P \times P$ matrices. Assume Σ is a positive definite matrix.

$$x^T \Sigma x < 0$$

$$\forall x \in \mathbb{R}^P$$

$$x \neq 0$$

Then $a^T \Sigma b$ also satisfies the conditions for inner product.

$$a^T \Sigma b = \langle a, b \rangle_{\Sigma}$$

$$a^T b = a^T I b = \langle a, b \rangle_I$$

$\{\mathbb{R}^P, \langle, \rangle_{\Sigma}\}$ is a more general inner product space.

Linear Transformation

A matrix, $A, \in \mathbb{R}^{P \times P}$ can be viewed as linear transformation

$$T_A : \mathbb{R}^P \rightarrow \mathbb{R}^P, x \mapsto Ax$$



Bing Li will denote T_A as A .

\rightarrow means maps to for a domain.

\mapsto means maps to for a value.

\Rightarrow means implies.

If $A : \mathbb{R}^P \rightarrow \mathbb{R}^P$,

$$\ker(A) = \{x \in \mathbb{R}^P, Ax = 0\}$$

$$\text{ran}(A) = \{Ax : x \in \mathbb{R}^P\}$$

Definition 1.1.4 — Kernel. In linear algebra, the kernel, or sometimes the null space, is the set of all elements v of V for which $L(v) = 0$, where 0 denotes the zero vector in W .

In coordinate plane, think of a function that crosses the x -axis. The kernel would be all points on x where $y = 0$.

Definition 1.1.5 — Range. In coordinate plane, how much of the y axis is reached with the function? Now extend this idea to more dimensions.

A linear transformation is **idempotent** if

$$\begin{aligned} A &= A^2 \\ Ax &= A(A(x)) \\ \forall x \in \mathbb{R}^P \end{aligned}$$

If A were a number it could only be 1 or 0.

Wednesday August 24

Let $T \in \mathbb{R}^{P \times P}$ then there exists a unique operator $R \in \mathbb{R}^{P \times P}$ such that $\forall x, y \in \mathbb{R}^P$,

$$\langle x, Ty \rangle = \langle Rx, y \rangle$$

(general inner product, $a^T \Sigma b$). Aside: What this states is that if you give me any operator in the first you can find one in the second.

R is called the **adjoint operator** of T . Written as T^* , that is,

$$\langle x, Ty \rangle = \langle T^*x, y \rangle$$

Derived Facts

$$\begin{aligned} \langle x, Ty \rangle &= \langle T^*, y \rangle && \text{(by the definition)} \\ &= \langle y, T^*x \rangle && \text{(inner products the order doesn't matter)} \\ &= \langle (T^*)^*y, x \rangle && \text{(Use the definition again)} \\ &= \langle x, (T^*)^*y \rangle && \text{(swap order)} \end{aligned}$$

So, $T = (T^*)^*$.

It is easy to see in our case

$$\begin{aligned} \langle x, Ty \rangle_{\Sigma} &= x^T \Sigma Ty \\ &= x^T \Sigma T \Sigma^{-1} \Sigma y \\ &= (\Sigma^{-1} T^T \Sigma x)^T \Sigma y \\ &= \langle \Sigma^{-1} T^T \Sigma x, y \rangle_{\Sigma} \end{aligned}$$

So, $T^* = \Sigma^{-1} T^T \Sigma$ when $\Sigma = I_P$ (identity) and $T^* = T^T$.

Derived Facts

An operator is **self adjoint** if its adjoint is itself. (i.e. if $T = T^*$ or $\langle x, Ty \rangle = \langle Tx, y \rangle$). In the case of \langle, \rangle_Σ ,

$$T = \Sigma^{-1} T^T \Sigma$$

if

$$\Sigma = I_P, T = T^T$$



Self adjoint implies symmetric. It's a more general case, hence the use of Σ vs I . Useful to remember in following two Theorems

Theorem 1.1.1 If $A \in \mathbb{R}^{P \times P}$ is symmetric, then there exists **eigenvalue-eigenvector pairs**. $(\lambda_1, v_1), \dots, (\lambda_P, v_P)$ such that $v_1 \perp \dots \perp v_P$. Orthogonal basis (ONB) such that

$$A = \sum_{i=1}^P \lambda_i v_i v_i^T \text{ (spectral decomposition)}$$

More generally, if A is a linear operator in \mathcal{H} (finite dimensional inner product such as $(\mathbb{R}^P, \langle, \rangle_\Sigma)$). its eigen pair (linear operator now) (λ, v) is defined by

$$\begin{cases} Av = \lambda v \\ \langle v, v \rangle = 1 \end{cases}$$

Definition 1.1.6 — Orthogonal Basis. In the following, $(\mathbb{R}^P, \langle, \rangle_\Sigma) = \mathcal{H}$ (H for Hilbert)

ONB is defined by:

1. $v_i \perp v_j, \langle v_i, v_j \rangle = 0$
2. $\|v_i\| = 1$
3. $\text{span}\{v_1, \dots, v_P\} = \mathcal{H}$

Theorem 1.1.2 Suppose $A : \mathcal{H} \rightarrow \mathcal{H}$ is a self adjoint linear operator. Then A has eigen pairs: $(\lambda_1, v_1), \dots, (\lambda_P, v_P)$ where $\{v_1, \dots, v_P\}$ is ONB of \mathbb{R} such that

$$A = \sum_{i=1}^P \lambda_i v_i v_i^T \Sigma$$

Proof. (λ, v) is eigen pair of A , which means

$$Av = \lambda v$$

$$\langle v, v \rangle = 1$$

$$v^T \Sigma v = 1$$

Let $u = \Sigma^{\frac{1}{2}} v$.



Aside: $\Sigma^\alpha = \Sigma \lambda_i^\alpha v_i v_i^T$

Let $v = \Sigma^{-\frac{1}{2}}u$.

$$A\Sigma^{-\frac{1}{2}}u = \lambda\Sigma^{-\frac{1}{2}}u$$

$$\Sigma^{-\frac{1}{2}}u = \lambda u$$

So, (λ, v) is an eigen pair of A in $(\mathbb{R}, <, >_\Sigma) \Leftrightarrow (\lambda, u)$ '...' of $\Sigma^{\frac{1}{2}}A\Sigma^{-\frac{1}{2}}$ in $(\mathbb{R}, <, >_I)$.

Note that, A is self adjoint in $(\mathbb{R}, <, >_\Sigma)$. So, $A = \Sigma^{-1}A^T\Sigma$

$$\begin{aligned}\Sigma^{\frac{1}{2}}A\Sigma^{-\frac{1}{2}} &= \Sigma^{\frac{1}{2}}A^T\Sigma\Sigma^{-\frac{1}{2}} \\ &= \Sigma^{-\frac{1}{2}}A^T\Sigma^{\frac{1}{2}} \\ &= (\Sigma^{\frac{1}{2}}A\Sigma^{-\frac{1}{2}})^T\end{aligned}$$

Note: $\Sigma^{\frac{1}{2}}A\Sigma^{-\frac{1}{2}}$ is symmetric!! So by Theorem 1.1, $\Sigma^{\frac{1}{2}}A\Sigma^{-\frac{1}{2}} = \sum \lambda_i v_i v_i^T$ where (λ_i, v_i) eigen-pairs of $\Sigma^{\frac{1}{2}}A\Sigma^{-\frac{1}{2}}$.

That means $(\lambda_i, \Sigma^{\frac{1}{2}}v_i)$ are eigen pairs of A .

$$\text{So, } \Sigma^{\frac{1}{2}}A\Sigma^{-\frac{1}{2}} = \sum_{i=1}^P \Sigma^{\frac{1}{2}}u_i u_i^T \Sigma^{\frac{1}{2}} \Rightarrow A = \sum_{i=1}^P \lambda u_i u_i^T \Sigma$$

■

Definition 1.1.7 — Projection. If P is an operator in $(\mathbb{R}^P, <, >)$ then P is called a **projection** if it is both idempotent ($P = P^2$) and self adjoint ($P = P^*$).

Proposition 1.1 If A is a linear operator then $\ker(A) = \text{ran}(A^*)^\perp$

Proof. Take $x \in \ker(A) (\Rightarrow Ax = 0)$.

$$\begin{aligned}\forall y \in \text{ran}(A^*), x \perp y \\ \Rightarrow x \perp y \forall y = A^*z, z \in \mathbb{R}^P\end{aligned}$$

Hence,

$$\begin{aligned}\langle x, y \rangle &= \langle x, A^*z \rangle \\ &= \langle Ax, z \rangle \\ &= \langle 0, z \rangle \\ &= 0\end{aligned}$$

$$\begin{aligned}\Rightarrow x \perp y \\ \Rightarrow x \in \text{ran}(A^*)^\perp\end{aligned}$$

Or vice versa.

■

Friday August 26

R \perp means orthogonal complement.

$$\mathcal{S}^\perp = \{v \in \mathbb{R}^P, v \perp \mathcal{S}\}$$

$$v \perp w \forall w \in \mathcal{S}$$

$$\langle v, w \rangle = 0 \forall w \in \mathcal{S}$$

$$= \{v \in \mathbb{R}^P, \langle v, w \rangle = 0 \forall w \in \mathcal{S}\}$$

Recall, $\ker(A) = \text{ran}(A^*)^\perp$

So, if A is self adjoint then this is true and $\text{ran}(A)$ is also $\text{span}(A)$ which is the subspace spanned all columns of A .

Theorem 1.1.3 If P is a projection, then

1. $Pv = v, \forall v \in \text{ran}(P)$
 2. $Pv = 0, \forall v \perp \text{ran}(P)$
 3. If Q is another projections such that the $\text{ran}(Q) = \text{ran}(P)$ then $Q = P$. (The range determines the operator, because it is what decomposes the operator.)
- Asside: P acts like one on some spaces, and zero on orthogonal space.

Proof. 1. Let $v \in \text{ran}(P)$. Since $P^2 = P$ (idempotent) then

$$P^2v = Pv$$

$$\Rightarrow P^2v - Pv = 0$$

$$\Rightarrow P(Pv - v) = 0$$

$$\Rightarrow Pv - v \in \ker(P)$$

$$\Rightarrow Pv - v \perp \text{ran}(P)$$

$$\Rightarrow \langle Pv - v, Pv - v \rangle = 0$$

$$\Rightarrow \|Pv - v\| = 0$$

$$\Rightarrow Pv - v = 0$$

$$\Rightarrow Pv = v$$

2. If

$$v \perp \text{ran}(P)$$

$$\Rightarrow v \in \ker(P)$$

$$\Rightarrow Pv = 0$$

3. If Q is another operator with $\text{ran}(Q) = \text{ran}(P) = \mathcal{S}$ then $\forall v \in \mathcal{S}$

$$Qv = v = Pv \quad (\forall v \in \mathcal{S})$$

$$Qv = 0 = Pv$$

$$Qv = Pv \quad \forall v \in \mathcal{S}$$

$$Q = P$$

■

Theorem 1.1.4 Suppose \mathcal{S} is a subspace of \mathbb{R}^P , $R \ V_1, \dots, V_m$ is a basis of \mathcal{S} .

Let $V = (V_1, \dots, V_m) \in \mathbb{R}^{xM}$.

Then,

1. $A = V(V^T \Sigma V)^{-1} V^T \Sigma$ is a projection.

2. $\text{ran}(A) = \mathcal{S}$

Proof. 1. idempotent.

$$A^2 = V(V^T \Sigma V)^{-1} V^T \Sigma V(V^T \Sigma V)^{-1} V^T \Sigma$$

$$= V(V^T \Sigma V)^{-1} V^T \Sigma$$

$$= A$$

2. Self adjoint.

Let $x, y \in \mathbb{R}^P$

$$\begin{aligned}
 \langle x, Ay \rangle &= x^T \Sigma v (v^T \Sigma v)^{-1} v^T \Sigma y \\
 &= (v (v^T \Sigma v)^{-1} v^T \Sigma x)^T \Sigma y \\
 &= \langle Ax, y \rangle
 \end{aligned}$$

3. $\text{ran}(A) = \mathcal{S}$?Let $x \in \mathbb{R}^P$.

$$Ax = v(v^T \Sigma v)^{-1} v^T \Sigma x \in \text{span}(v) = \mathcal{S}$$

So let $x \in \mathcal{S}$,

$$x \in \text{ran}(v)$$

$$x = vy$$

for some $y \in \mathbb{R}^P$

$$= v(v^T \Sigma v)^{-1} v^T \Sigma vy$$

$$\in \text{ran}(A)$$

So, $\mathcal{S} \subseteq \text{ran}(A)$ and then $\mathcal{S} = \text{ran}(A)$. ■

We write A as $P_{\mathcal{S}}(\Sigma)$ (orthogonal projection on to \mathcal{S} with respect to Σ - product).

In the following, let $I : \mathbb{R}^P \rightarrow \mathbb{R}^P$ be the identity mapping. ($x \mapsto x$)

Let \mathcal{S} be a subspace in \mathbb{R}^P .

$$\text{Let } Q_{\mathcal{S}}(\Sigma) = I - P_{\mathcal{S}}(\Sigma)$$

Proposition 1.2 $Q_{\mathcal{S}}(\Sigma) = P_{\mathcal{S}^\perp}(\Sigma)$

Proof. Show $Q_{\mathcal{S}}(\Sigma)$ is projection.

1. Idempotent

$$\begin{aligned}
 Q_{\mathcal{S}}^2(\Sigma) &= Q_{\mathcal{S}}(\Sigma) Q_{\mathcal{S}}(\Sigma) \\
 &= (I - P_{\mathcal{S}}(\Sigma))(I - P_{\mathcal{S}}(\Sigma)) \\
 &= I - P_{\mathcal{S}}(\Sigma) - P_{\mathcal{S}}(\Sigma) + P_{\mathcal{S}} P_{\mathcal{S}} \\
 &= Q_{\mathcal{S}}(\Sigma)
 \end{aligned}$$

2. Self-adjoint

$$x, y \in \mathbb{R}^P$$

$$\begin{aligned}
 \langle x, Q_{\mathcal{S}}(\Sigma)y \rangle &= \langle x, (I - P_{\mathcal{S}}(\Sigma))y \rangle \\
 &= \langle x, y \rangle - \langle x, P_{\mathcal{S}}(\Sigma)y \rangle \\
 &= \langle x, y \rangle - \langle P_{\mathcal{S}}(\Sigma)x, y \rangle \\
 &= \langle (I - P_{\mathcal{S}}(\Sigma))x, y \rangle \\
 &= \langle Q_{\mathcal{S}}(\Sigma)x, y \rangle
 \end{aligned}$$

3. Range

$$\text{ran}(Q_{\mathcal{S}}(\Sigma)) = \mathcal{S}^\perp. \text{ Take } x \perp \mathcal{S} = \text{ran}(P_{\mathcal{S}}(\Sigma))^\perp = \ker(P_{\mathcal{S}}(\Sigma)).$$

$$\Rightarrow P_{\mathcal{S}}(\Sigma) = 0$$

$$\Rightarrow Q_{\mathcal{S}}(\Sigma)x = x - P_{\mathcal{S}}(\Sigma)x = x$$

$$X \in \text{ran}(Q_{\mathcal{S}}(\Sigma))$$

$$\Rightarrow \mathcal{S}^{\perp} \subseteq \text{ran}(Q_{\mathcal{S}}(\Sigma))$$

Take $x \in \text{ran}(Q_{\mathcal{S}}(\Sigma))$, $\forall y \in \mathcal{S} = \text{ran}(P_{\mathcal{S}}(\Sigma))$

$$y = P_{\mathcal{S}}(\Sigma)z \text{ for some } z \in \mathbb{R}^P$$

$$\langle x, y \rangle = \langle x, P_{\mathcal{S}}(\Sigma)z \rangle = \langle P_{\mathcal{S}}(\Sigma)x, z \rangle = 0$$

$$\Rightarrow x \in \mathcal{S}^{\perp}$$

$$\Rightarrow \text{ran}(Q_{\mathcal{S}}(\Sigma)) = \mathcal{S}^{\perp}$$

■

1.2 Cochran's Theorem

This section will be about the distribution of the squared norm of a projection of a Gaussian random vector.

Proposition 1.3 If A is idempotent, then its eigenvalues are either 0 or 1.

Proof. λ is eigenvalue of A .

$$\Rightarrow Av = \lambda v (||v|| = 1)$$

$$\lambda = Av = A^2v = \lambda Av = \lambda^2$$

So, λ is 0 or 1.

■

Monday August 29

Lemma 1.1 Suppose $V \sim N(0, \sigma^2 I_P)$.

P is projection with I_P - inner product. Then $V^T P V \sim \sigma^2 \chi_S^2$ where $\text{df} = \text{rank}(P)$.

Proof. P is symmetric, and it has spectral decomposition,

$$A R A^T$$

where the A 's are orthogonal and R is diagonal with diagonal entries 0 or 1.

Then,

$$A^T V \sim N_P(0, A^T (\sigma^2 I_P) A) = N_P(0, \sigma^2 I_P)$$

Let,

$$Z = R A^T V$$

then,

$$Z \sim N_P(0, \sigma^2 R^2) = N_P(0, \sigma^2 R)$$

That means among the components of Z , some are distributed as $N(0, 1)$ and the rest are zero and they are independent. So,

$$Z^T Z \sim \chi_S^2 = V^T P V$$

■

Corollary 1.2.1 Suppose $X \sim N(0, \Sigma)$. Consider the Hilbert space $(\mathbb{R}^P, \langle, \rangle_{\Sigma^{-1}})$.

$$\langle a, b \rangle_{\Sigma^{-1}} = a^T \Sigma^{-1} b$$

Let \mathcal{S} be a subspace of \mathbb{R}^P and $P_{\mathcal{S}}(\Sigma^{-1})$ be the projection onto \mathcal{S} with respect to $\langle, \rangle_{\Sigma^{-1}}$ (special case of Fisher information inner product)

Then,

$$\|P_{\mathcal{S}}(\Sigma^{-1})X\|_{\Sigma^{-1}}^2 \sim \chi_r^2$$

where $r = \dim(\mathcal{S})$.

Proof. Let V be a basis matrix of \mathcal{S} (i.e. the col of V form basis in \mathcal{S}).

$$\begin{aligned} \|P_{\mathcal{S}}(\Sigma^{-1})X\|_{\Sigma^{-1}}^2 &= \langle P_{\mathcal{S}}(\Sigma^{-1})X, P_{\mathcal{S}}(\Sigma^{-1})X \rangle \\ &= X^T P_{\mathcal{S}}(\Sigma^{-1}) \Sigma^{-1} P_{\mathcal{S}}(\Sigma^{-1}) X \\ &= X^T (V(V^T \Sigma^{-1} V)^{-1} V^T \Sigma^{-1})^T \Sigma^{-1} (V(V^T \Sigma^{-1} V)^{-1} V^T \Sigma^{-1}) X \\ &= X^T \Sigma^{-1} V (V^T \Sigma^{-1} V)^{-1} V^T \Sigma^{-1} V (V^T \Sigma^{-1} V)^{-1} V^T \Sigma^{-1} X \\ &= (\Sigma^{-\frac{1}{2}} X)^T [\Sigma^{-\frac{1}{2}} V (V^T \Sigma^{-1} V)^{-1} (\Sigma^{-\frac{1}{2}} V)^T] (\Sigma^{-\frac{1}{2}} X) \end{aligned}$$

But,

$$\Sigma^{-\frac{1}{2}} X \sim N(0, I_P)$$

So,

$$\Sigma^{-\frac{1}{2}} V (V^T \Sigma^{-1} V)^{-1} (V^T \Sigma^{-\frac{1}{2}})^T \quad (*)$$

is a projection with respect to I_P -inner product (idempotent, self adjoint, YES).

By Lemme 1.1,

$$(*) \sim \chi_r^2$$

■

It is then easy to derive Cochran's Theorem. (see proof in Homework 1)

Theorem 1.2.2 Let $X \sim N(0, \Sigma)$ and $\mathcal{H} = \{\mathbb{R}^P, \langle, \rangle_{\Sigma^{-1}}\}$. Let $\mathcal{S}_1, \dots, \mathcal{S}_k$ be linear subspaces of \mathbb{R}^P such that $\mathcal{S}_i \perp \mathcal{S}_j$ in $\langle, \rangle_{\Sigma^{-1}}$

Let $r_i = \dim(\mathcal{S}_i)$.

Let $W_i = \|P_{\mathcal{S}_i}(\Sigma^{-1})X\|_{\Sigma^{-1}}^2$

Then,

1. $W_i \sim \chi_{r_i}^2$
2. $W_1 \perp, \dots, \perp W_k$ where \perp indicates independence.

1.3 Gaussian Linear Regresson Model

$$Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$X = \begin{pmatrix} x_{11} & \dots & x_{1P} \\ \vdots & \ddots & \vdots \\ x_{n1} & \dots & x_{nP} \end{pmatrix} \in \mathbb{R}^{n \times p}$$

Consider the linear model,

$$y = X\beta + \varepsilon$$

$$\varepsilon \sim N(0, \sigma^2 I_n)$$

where X has full column rank ($n \geq p$).

Here X is treated as fixed.

Maximum Likelihood Estimator

$$E(y) = X\beta \in \mathbb{R}^n$$

$$\text{Var}(y) = \sigma^2 I_n$$

$$y \sim N_p(X\beta, \sigma^2 I_n)$$

Multivariate Normal Density

$$y \sim N(\mu, \Sigma)$$

$$f_Y(y) = \frac{1}{(2\pi)^{\frac{n}{2}} [\det(\Sigma)]^{\frac{1}{2}}} e^{-\frac{1}{2}(y-\mu)^T \Sigma^{-1} (y-\mu)}$$

In our case,

$$\Sigma = \sigma^2 I_n$$

$$\det(\Sigma) = \det(\sigma^2 I_n) = \sigma^{2n} \det(I_n) = \sigma^{2n}$$

So,

$$f_Y(y) = \frac{1}{(2\pi)^{\frac{n}{2}} \sqrt{\sigma^{2n}}} e^{-\frac{1}{2\sigma^2} \|y-\mu\|^2}$$

To find the log likelihood and subsequently take the partial derivatives for MLE,

$$\log(f_Y(y)) = \frac{n}{2} \log(\sigma^2) - \frac{1}{2\sigma^2} \|y - \mu\|^2 = \ell(\beta, \sigma^2, y)$$

$$\frac{\partial}{\partial \beta} = \dots = -\frac{1}{2\sigma^2} 2X^T (y - X\beta) = 0$$

$$\hat{\beta} = (X^T X)^{-1} X^T Y \in \mathbb{R}^P$$

$$\frac{\partial}{\partial \sigma^2} \ell(\beta, \sigma^2, y) = \dots = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \|y - X\beta\|^2 = 0$$

$$\hat{\sigma}^2 = \frac{1}{n} \|y - X\hat{\beta}\|^2$$

In summary, the MLE for (β, σ^2) in Gaussian Linear Model are

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

$$\hat{\sigma}^2 = \frac{1}{n} \|y - X\hat{\beta}\|^2$$

Note that

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

So,

$$\hat{y} = P_{\text{span}(X)}(I_P) = P_X y$$

Now,

$$\begin{aligned}\hat{\sigma}^2 &= \frac{1}{n} \|y - \hat{y}\|^2 \\ &= \frac{1}{n} \|y - P_X y\|^2 \\ &= \frac{1}{n} \|(I_n - P_X)y\|^2 \\ &= \frac{1}{n} \|Q_X y\|^2\end{aligned}$$

where $Q_X = (I_n - P_X)$ is projection on to $\text{span}(X)^\perp$.

It turns out that $(X^T y, y^T y)$ is complete, sufficient statistic for this Gaussian linear model (see homework).

Wednesday August 31

Recall,

$$\begin{aligned}\hat{\beta} &= (X^T X)^{-1} X^T Y \\ \hat{\sigma}^2 &= \frac{1}{n} \|y - X\hat{\beta}\|^2 \\ Q_X &= I_n - P_X \\ P_X &= X(X^T X)^{-1} X^T\end{aligned}$$

Several properties,

$$E(\hat{\beta}) = \beta \quad (\text{unbiased})$$

$$\text{Var}(\hat{\beta}) = (X^T X)^{-1} X^T (\sigma^2 I_n) X (X^T X)^{-1} = \sigma^2 (X^T X)^{-1}$$

Thus,

$$\hat{\beta} \sim N(\beta, \sigma^2 (X^T X)^{-1})$$

Because P_X has rank p and Q_X has rank $(n - p)$, then

$$\|Q_X y\|^2 \sim \chi_{(n-p)}^2$$

Let's find an unbiased estimator for σ^2 (needed for UMVUE),

$$\begin{aligned} E(\hat{\sigma}^2) &= E\left(\frac{1}{n} \|Q_{xy}\|^2\right) \\ &= \frac{n-p}{n} \sigma^2 \\ E\left(\frac{n}{n-p} \hat{\sigma}^2\right) &= \tilde{\sigma}^2 \end{aligned}$$

Moreover, $\hat{\beta}$ has one-to-one transformation with

$$(X^T X)^{-1} X^T y \leftrightarrow X(X^T X)^{-1} X^T y = P_{Xy}$$

$$\begin{aligned} \text{Cov}(P_{Xy}, Q_{Xy}) &= P_X \sigma^2 I_n Q_X \\ &= \sigma^2 P_X Q_X \\ &= 0 \end{aligned}$$

$$P_{Xy} \perp\!\!\!\perp Q_{Xy} \quad (\text{due to normality})$$

$$\hat{\beta} \leftrightarrow P_{Xy}$$

$$\hat{\sigma}^2 \text{ is a function of } Q_{Xy}, \text{ so } \hat{\beta} \perp\!\!\!\perp \hat{\sigma}^2$$

In your homework, $\hat{\beta}, \hat{\sigma}^2 \leftrightarrow$ complete sufficient.

$\hat{\beta}, \tilde{\sigma}^2$ is UMVUE (Lehmann-Sheffe).

Theorem 1.3.1 — Gaussian Regression Model. Under this model:

1. $\hat{\beta}, \tilde{\sigma}^2$ UMVUE for β, σ^2
2. $\hat{\beta} \sim N(\beta, \sigma^2 (X^T X)^{-1})$
3. $(n-p) \tilde{\sigma}^2 \sim \sigma^2 \chi_{(n-p)}^2$
4. $\hat{\beta} \perp\!\!\!\perp \tilde{\sigma}^2$

1.4 Statistical Inference for β, σ^2

Suppose we want to test

$$H_0 : \beta_1 = \beta_{i0}$$

$$\text{Let } M = (X^T X)^{-1}.$$

Then,

$$\hat{\beta} \sim N(\beta, \sigma^2 M)$$

where, $M_{ii} \leftarrow (i, i)^{th}$ entry of M

Also, $\frac{(n-p)\tilde{\sigma}^2}{\sigma^2} \sim \chi_{(n-p)}^2$

$$\hat{\beta} \perp\!\!\!\perp \tilde{\sigma}^2$$

$$\frac{\hat{\beta}_i - \beta_{i0}}{\sqrt{\sigma^2 M_{ii}}} \sim N(0, 1)$$

$$\frac{\frac{\hat{\beta}_i - \beta_{i0}}{\sqrt{\sigma^2 M_{ii}}}}{\sqrt{\frac{(n-p)\tilde{\sigma}^2 / \sigma^2 \cap_{k=n}^{\infty} A_k^c}{n-p}}} \sim t_{(n-p)}$$

$$T = \frac{\hat{\beta}_i - \beta_{i0}}{\tilde{\sigma} \sqrt{M_{ii}}} \sim t_{(n-p)} = (*)$$

Reject H_0 if

$$\left| \frac{\hat{\beta}_i - \beta_{i0}}{\tilde{\sigma} \sqrt{M_{ii}}} \right| > t_{\frac{\alpha}{2}}(n-p)$$

Recall,

$$X \sim N(\mu, 1)$$

$$y \sim \chi_r^2$$

$$X \perp\!\!\!\perp y$$

$$\frac{X}{\sqrt{\frac{y}{r}}} \sim t_n(\mu)$$

Power at β_{i1}

$$\hat{\beta}_i \sim N(\beta_{i1}, \sigma^2 M_{i1})$$

So,

$$\frac{\hat{\beta}_i - \beta_{i0}}{\tilde{\sigma} \sqrt{M_{ii}}} \sim t_{(n-p)} \left(\frac{\beta_{i1} - \beta_{i0}}{\sigma \sqrt{M_{ii}}} \right)$$

(alternative distribution of T)

By this (*),

$$P(\in (-t_{\frac{\alpha}{2}}(n-p), t_{\frac{\alpha}{2}}(n-p)))$$

Convert this to put β_{i0} in between $(1 - \alpha)100$ percent C.I. for β_i .

$$(\hat{\beta}_i - t_{\frac{\alpha}{2}}(n-p) \hat{\sigma} \sqrt{M_{ii}}, \hat{\beta}_i + t_{\frac{\alpha}{2}}(n-p) \hat{\sigma} \sqrt{M_{ii}})$$

1.5 Delete One Prediction

Very useful in variable selection, cross validation, diagnostics.

Prediction: $\hat{y} = X\hat{\beta} = P_X y$

But this has a drawback as it favors overfitting. Projecting onto larger spaces will always decrease the norm, $\|Q_X y\|^2$. (This can decrease errors which would cause you to think it's better, even though it's not.)

To prevent overfitting, try to be objective, withhold y_i when predicting y_i (inverse of a matrix, rank 1 perpendicular)

Theorem 1.5.1 — Theorem 1.7. Suppose $A \in \mathbb{R}^{P \times P}$ is a symmetric, nonsingular matrix. and $v \in \mathbb{R}^P$.

Then,

$$(A \pm vv^T)^{-1} = A^{-1} \pm \frac{A^{-1}vv^T A^{-1}}{1 \pm v^T A^{-1}v}$$

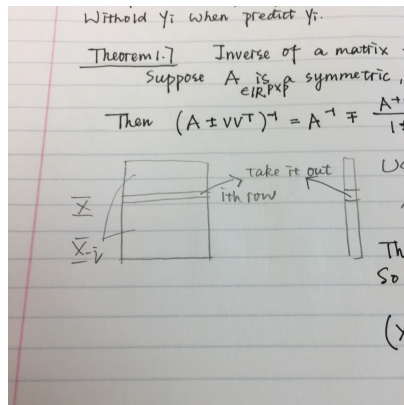


Figure 1.1: Theorem 1.7 Visualization

Use what is left to compute $\hat{\beta}_{-i}$.

$$\hat{\beta}_{-i} = (X_{-i}^T X_{-i})^{-1} X_{-i}^T y_{-i}$$

This can be expanded in simple sum, so that you don't have to do n regressions.

$$\begin{aligned}
(X_{-i}^T X_{-i})^{-1} &= (X^T X - X_i X_i^T)^{-1} \\
&= A^{-1} + \frac{A^{-1} v v^T A^{-1}}{1 - v^T A^{-1} v} \\
&= (X^T X)^{-1} + \frac{(X^T X)^{-1} X_i X_i^T (X^T X)^{-1}}{1 - X_i^T M X_i} \\
X_i^T M X_i &= X_i^T (X^T X)^{-1} \\
&= (P_x)_{ii} \\
&= P_i
\end{aligned}$$

$$\begin{aligned}
\hat{\beta}_i &= (X^T X - X_i X_i^T)^{-1} (X^T y - X_i y_i) \\
&= [M + \frac{M X_i X_i^T M}{1 - P_i}] (X^T y - X_i y_i) \\
&= M X^T y + \frac{M X_i X_i^T M X^T y}{1 - P_i} - M X_i y_i - \frac{M X_i X_i^T M X_i y_i}{1 - P_i} \\
&= \dots \\
&= \hat{\beta} - \frac{M X_i}{1 - P_i} (y_i - X_i^T \hat{\beta})
\end{aligned}$$


Delete-one regression.

$$X_i \hat{\beta}_{-i} = \hat{y}_i - \frac{P_i}{1 - P_i} (y_i - \hat{y}_i)$$

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Delete- one error

$$y_i - \hat{y}_i^{(-i)}$$

 Recall, you want to leave out y^i so you don't overfit.

The above is equivalent to

$$\begin{aligned}
&y_i - X_i^T \hat{\beta}_{-i} \\
&y_i - \hat{y}_i - \frac{P_i}{1 - P_i} (y_i - \hat{y}_i) \\
&(y_i - \hat{y}_i) (1 - \frac{P_i}{1 - P_i}) \\
&\frac{1}{1 - P_i} (y_i - \hat{y}_i)
\end{aligned}$$

Delete-one cross validation

$$\sum_{i=1}^n (y_i - \hat{y}_i^{(-i)})^2$$

This method is not affected by over fitting.

The following is often used for "tuning" or variable selection (i.e. penalty, bandwidth, regularization, etc). $\sum_{i=1}^n \frac{1}{(1-P_i)^2} (y_i - \hat{y}_i)^2$

Note: we will come back to variable selection later.

$$\beta = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_n \end{pmatrix}$$

$$A \subseteq \{1, \dots, P\}$$

Cross validation of A minimizes over $A \in 2^{\{1, \dots, P\}}$. Best cross validation set.

1.6 Residuals

- Residual

$$\hat{e}_i = y_i - \hat{y}_i$$

- Standardized Residual

$$\text{Var}(\hat{e}_i) = \text{Var}(y_i - \hat{y}_i) = \text{Var}((Q_X)_{ii} y_i)$$

$$= ((Q_X)_{ii} y_i) \sigma^2$$

$$= (1 - P_i) \sigma^2$$

$$sd(\hat{e}_i) = \sqrt{1 - P_i} \sigma$$

$$\hat{sd}(\hat{e}_i) = \sqrt{1 - P_i} \tilde{\sigma}$$

$$\tilde{\sigma} = \frac{\sum_{i=1}^n (y_i - \hat{y}_i^{(-i)})^2}{n - p}$$

- Standardized residual

$$E_i^* = \frac{\hat{e}_i}{\tilde{\sigma} \sqrt{1 - P_i}}$$

- Prediction Error Sum of Squares (PRESS) Residual

$$y_i - \hat{y}_i^{(-i)} = \frac{1}{1 - P_i} \hat{e}_i = \hat{e}_{iP}$$

$$\hat{e}_{iP} \sim N(0, \frac{\sigma^2}{1 - P_i})$$

- Standardized PRESS Error

$$\frac{\hat{e}_{iP}}{\tilde{\sigma} / \sqrt{1 - P_i}} = \frac{\frac{1}{1 - P_i} \hat{e}_i}{\tilde{\sigma} (\sqrt{1 - P_i})} = \frac{\hat{e}_i}{\tilde{\sigma} (\sqrt{1 - P_i})} = E_i^*$$

1.7 Influence and Cook's Distance

Definition 1.7.1 — Influence. The difference between predictions with and without a data point.

$$\hat{y}_i - \hat{y}_i^{(-i)}$$

$$\hat{y}_i - \hat{y}_i^{(-i)}$$

$$X_i \hat{\beta} - X_i \hat{\beta}_{-i}$$

$$\begin{aligned} &\propto \|X_i \hat{\beta} - X_i \hat{\beta}_{-i}\|^2 \\ &= (X(\hat{\beta} - \hat{\beta}_{-i}))^T (X(\hat{\beta} - \hat{\beta}_{-i})) \\ &= (\hat{\beta} - \hat{\beta}_{-i})^T X^T X (\hat{\beta} - \hat{\beta}_{-i}) \end{aligned}$$

Recall,

$$\hat{\beta}_{-i} - \hat{\beta} = -\frac{MX_i(y_i - \hat{y}_i)}{1 - P_i} = -\frac{MX_i \hat{e}_i}{1 - P_i}$$

$$\|X_i \hat{\beta} - X_i \hat{\beta}_{-i}\|^2 =$$

=

Cook's Distance (Technometrics, 1976?)

$$\left\| \frac{\hat{y} - \hat{y}^{(-i)}}{\tilde{\sigma}^2} \right\|^2 = \frac{|i \hat{e}_i|^2}{(1 - P_i)^2 \tilde{\sigma}^2}$$

Definition 1.7.2 — Cook's Distance. Cook's distance measures the influence of the i^{th} observation.

1.8 Orthogonal Decomposition

Recall, \mathbb{R}^n is Euclidean Space.

\mathcal{S} is a subspace ($\mathcal{S} \leq \mathbb{R}^n$)

R \leq is subspace
 \subseteq is a subset

For

$$\mathcal{S}_1 \leq \mathcal{S}_1 \mathcal{S}_2 \leq \mathcal{S}$$

$$\mathcal{S}_1 + \mathcal{S}_2 = \{x + y : x \in \mathcal{S}_1, y \in \mathcal{S}_2\}$$

Suppose $\mathcal{S}_1, \mathcal{S}_2 \leq \mathcal{S}$,

$$\mathcal{S}_1 + \mathcal{S}_2 = \mathcal{S}, \mathcal{S}_1 \perp \mathcal{S}_2$$

then,

$$\{\mathcal{S}_1, \mathcal{S}_2\}$$

is called an orthogonal decomposition of \mathcal{S}

In this case,

$$\mathcal{S}_1 \oplus \mathcal{S}_2 = \mathcal{S}$$

More generally,

Definition 1.8.1 — Orthogonal Decomposition (O.D.). Let $\mathcal{S}_1, \dots, \mathcal{S}_k$ be subspaces of \mathcal{S} such that

$$1. \mathcal{S}_1, \dots, \mathcal{S}_k = \{v_1 + \dots + v_k : v_1 \in \mathcal{S}_1, \dots, v_k \in \mathcal{S}_k\}$$

$$2. \mathcal{S}_i \perp \mathcal{S}_j \quad \forall i \neq j$$

Then, $\{\mathcal{S}_1, \mathcal{S}_2, \dots, \mathcal{S}_k\}$ is an **orthogonal decomposition** of \mathcal{S} . We may write $\mathcal{S} = \mathcal{S}_1 \oplus \mathcal{S}_2 \oplus \dots \oplus \mathcal{S}_k$.

Proposition 1.5 If $\mathcal{S}_1, \dots, \mathcal{S}_k$ is an O.D. of \mathcal{S} , then any $v \in \mathcal{S}$ can be uniquely written as

$$v_1 + \dots + v_k$$

, where $v_1 \in \mathcal{S}_1, \dots, v_k \in \mathcal{S}_k$.

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Definition 1.8.2 — Direct Difference. Let $\mathcal{S}_1 \leq \mathcal{S}_2 \leq \mathbb{R}^n$. Then,

$$\mathcal{S}_2 \cap \mathcal{S}_1^\perp \equiv \mathcal{S}_2 \ominus \mathcal{S}_1$$

is called **direct difference**. This is almost the same as orthogonal complement, except it is within \mathcal{S}_2 .

Proposition 1.6 If $\mathcal{S}_1 \leq \mathcal{S}_2$, then

$$\mathcal{S}_2 = \mathcal{S}_1 \oplus (\mathcal{S}_2 \ominus \mathcal{S}_1)$$

Proposition 1.7 - Orthogonal Decomposition and Projection Consider a Hilbert Space, $\mathcal{H} = \{\mathbb{R}^n, \langle, \rangle_A\}$,

1. If $\mathcal{S} \leq \mathcal{S}_1 \perp \mathcal{S}_2$ in \mathcal{H} , then

$$P_{\mathcal{S}_1}(A)P_{\mathcal{S}_2}(A) = 0$$

2. If $\mathcal{S} \leq \mathcal{H}, \dots, \mathcal{S}_k \leq \mathcal{H}$, and $\mathcal{S}_1 \perp \dots \perp \mathcal{S}_k$, then

$$P_{\mathcal{S}_1 \oplus \dots \oplus \mathcal{S}_k}(A) = P_{\mathcal{S}_1}(A) + \dots + P_{\mathcal{S}_k}(A)$$

3. If $\mathcal{S}_1 \leq \mathcal{S}_2 \leq \mathbb{R}^n$, then

$$P_{\mathcal{S}_2 \ominus \mathcal{S}_1}(A) = P_{\mathcal{S}_2}(A) - P_{\mathcal{S}_1}(A)$$

Theorem 1.8.1 — Generalization of the earlier Cochran's Theorem. Suppose $X \sim N(0, \Sigma)$ where $\Sigma \in \mathbb{R}^{n \times n}$ is positive definite.

Let $\mathcal{H} = \{\langle, \rangle_{\Sigma^{-1}}\}$. Suppose $\mathcal{S}_1, \dots, \mathcal{S}_k, \mathcal{S} \leq \mathcal{H}$ such that $\mathcal{S} = \mathcal{S}_1 \oplus \dots \oplus \mathcal{S}_k$.

Let

$$w_i = \|P_{\mathcal{S}_i}(\Sigma^{-1})X\|_{\Sigma^{-1}}^2$$

$$w = \|P_{\mathcal{S}}(\Sigma^{-1})X\|_{\Sigma^{-1}}^2$$

Then,

$$1. w = w_1 + \dots + w_k$$

$$2. w_1 \perp \dots \perp w_k$$

$$3. w_i \sim \chi_{r_i}^2$$

$$w \sim \chi_r^2$$

where r_i is the $\dim(\mathcal{S}_i)$, r is the $\dim(\mathcal{S})$, and $r = r_1 + \dots + r_k$.

Notation 1.1. We use \oplus for spaces. We can also use \oplus function to stack up matrices. Let A_1, \dots, A_k be matrices with arbitrary dimensions.

$$A_1 \oplus \dots \oplus A_k = \begin{pmatrix} A_1 & \dots & 0 \\ & \ddots & \\ 0 & \dots & A_k \end{pmatrix}$$

1.9 Lack of Fit Test

Goodness of Fit

At each x_i you have multiple observations, say y_{i1}, \dots, y_{im_i} . In this case, you may test to see if a linear model, $y_i = x_i^T \beta + \varepsilon_i$, is the correct choice for fitting the data. In general, lack of fit refers to testing whether any (linear, generalized, etc) model is adequately describing the data.

Denote

$$y_i = \begin{pmatrix} y_{i1} \\ \vdots \\ y_{im_i} \end{pmatrix}$$

$$1_{m_i} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$$

$$X = \begin{pmatrix} X_1^T \\ \vdots \\ X_m^T \end{pmatrix}$$

Assume

$$y_{ij} = X_i^T \beta + \varepsilon_{ij}$$

where $\varepsilon \sim^{iid} N(0, \sigma^2)$.

The point is that you have $y_{i1} \dots y_{jm}$ for each X_i .

In matrix form,

$$(1_{m_1} \oplus \dots \oplus 1_{m_n})X\beta + \varepsilon$$

So, let N denote a full sample size.

$$N = m_1 + \dots + m_n$$

this is a special case of linear model, except the design matrix is structured $(1_{m_1} \oplus \dots \oplus 1_{m_n})X$ instead of X . So the formula for MLE (and so on) is the same.

$$X \leftrightarrow (1_{m_1} \oplus \dots \oplus 1_{m_n})X$$

So,

$$\hat{\beta} = ((1_{m_1} \oplus \dots \oplus 1_{m_n})X)^T ((1_{m_1} \oplus \dots \oplus 1_{m_n})X)^{-1} [(1_{m_1} \oplus \dots \oplus 1_{m_n})X]^T y$$

$$\begin{aligned}
\hat{y} &= (1_{m_1} \oplus \cdots \oplus 1_{m_n})X\hat{\beta} \\
&= (1_{m_1} \oplus \cdots \oplus 1_{m_n})X[(1_{m_1} \oplus \cdots \oplus 1_{m_n})X]^T[(1_{m_1} \oplus \cdots \oplus 1_{m_n})X]^{-1}[(1_{m_1} \oplus \cdots \oplus 1_{m_n})X]^T y \\
&= (1_{m_1} \oplus \cdots \oplus 1_{m_n})X[X^T \begin{pmatrix} m_1 & \cdots & 0 \\ & \ddots & \\ 0 & \cdots & m_n \end{pmatrix} X]^{-1}X^T(1_{m_1} \oplus \cdots \oplus 1_{m_n})
\end{aligned}$$

So, in linear model with replication we have our hypotheses for lack of fit test,

$$H_0 : E(y_i) = 1_{m_i}X_i^T \beta$$

$$H_1 : E(y_i) = 1_{m_i}\mu_i$$

We are testing whether the arbitrary means, μ_1, \dots, μ_n sit on the same line.

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Under H_1 ,

$$y = (1_{m_1} \oplus \cdots \oplus 1_{m_n}) \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_n \end{pmatrix} + \varepsilon$$

So the \hat{y} under this model,

$$\hat{y}_{H_1} = P_{1_{m_1} \oplus \cdots \oplus 1_{m_n}} y = (1_{m_1} \oplus \cdots \oplus 1_{m_n}) \begin{pmatrix} m_1 & & \\ & \ddots & \\ & & m_n \end{pmatrix} (1_{m_1} \oplus \cdots \oplus 1_{m_n})^T y$$

but under H_0 ,

$$\hat{y}_{H_0} = P_{(1_{m_1} \oplus \cdots \oplus 1_{m_n})X} y$$

$$\mathcal{S}_1 = \text{span}\{(1_{m_1} \oplus \cdots \oplus 1_{m_n})X\} \quad (\text{p-dim})$$

$$\mathcal{S}_2 = \text{span}\{(1_{m_1} \oplus \cdots \oplus 1_{m_n})\} \quad (\text{n-dim})$$

$$\mathcal{S}_3 = \mathbb{R}^N \quad (N = m_1 + \cdots + m_n)$$

$$\mathcal{S}_1 \leq \mathcal{S}_2 \leq \mathcal{S}_3$$

R Above used the fact that $\text{span}(AB) \subseteq \text{span}(A)$

Lemma 1.1 If $\mathcal{S}_1 \leq \mathcal{S}_2 \leq \mathcal{S}_3$ then

1. $\mathcal{S}_3 \ominus \mathcal{S}_2 \leq \mathcal{S}_3 \ominus \mathcal{S}_1$
2. $(\mathcal{S}_3 \ominus \mathcal{S}_1) \ominus \mathcal{S}_2 = \mathcal{S}_3 \ominus \mathcal{S}_2$
3. $(\mathcal{S}_3 \ominus \mathcal{S}_1) = (\mathcal{S}_3 \ominus \mathcal{S}_2) \oplus (\mathcal{S}_2 \ominus \mathcal{S}_1)$

Go back to lack of fit,

$$(\mathcal{S}_3 \ominus \mathcal{S}_1) = (\mathcal{S}_3 \ominus \mathcal{S}_2) \oplus (\mathcal{S}_2 \ominus \mathcal{S}_1)$$

$$P_{\mathcal{S}_3 \ominus \mathcal{S}_1} y = P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y + P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y \quad (\text{Orthogonal Decomposition})$$

$$\|P_{\mathcal{S}_3 \ominus \mathcal{S}_1} y\|^2 = \|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2 + \|P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y\|^2$$

$$\dim(\mathcal{S}_2 \ominus \mathcal{S}_1) = n - p$$

$$\dim(\mathcal{S}_3 \ominus \mathcal{S}_2) = N - n$$

Now,

$$E(P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y) = P_{\mathcal{S}_3 \ominus \mathcal{S}_2} E(y) = P_{\mathcal{S}_3 \ominus \mathcal{S}_2} \mu = 0$$

But,

$$\mu = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_n \end{pmatrix} \in \mathcal{S}_2$$

and,

$$(1_{m_1} \oplus \cdots \oplus 1_{m_n}) \underline{\mu}$$

$$\text{Var}(P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y) = P_{\mathcal{S}_3 \ominus \mathcal{S}_2} \text{Var}(y) P_{\mathcal{S}_3 \ominus \mathcal{S}_2} = \sigma^2 P_{\mathcal{S}_3 \ominus \mathcal{S}_2}^2 = \sigma^2 P_{\mathcal{S}_3 \ominus \mathcal{S}_2}$$

We know that $y \sim N(\mu, \sigma^2 I_n)$. So,

$$P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y \sim N(0, \sigma^2 P_{\mathcal{S}_3 \ominus \mathcal{S}_2})$$

Similarly,

$$E(P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y) = P_{\mathcal{S}_2 \ominus \mathcal{S}_1} E(y)$$

which under H_0 is,

$$P_{\mathcal{S}_2 \ominus \mathcal{S}_1} (1_{m_1} \oplus \cdots \oplus 1_{m_n}) X \beta = 0$$

$$\text{Var}(P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y) = \sigma^2 P_{\mathcal{S}_2 \ominus \mathcal{S}_1}$$

$$P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y \sim N(0, \sigma^2 P_{\mathcal{S}_2 \ominus \mathcal{S}_1})$$

By Chochran's Theorem:

Under H_0 ,

$$\|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2 \sim \chi_{(N-n)}^2$$

$$\|P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y\|^2 \sim \chi_{(n-p)}^2$$

$$\|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2 \perp\!\!\!\perp \|P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y\|^2$$

So our lack of fit test is:

$$\frac{||P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y||^2 / (n-p)}{||P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y||^2 / (N-n)} \sim F_{n-p, N-n}$$

1.10 Explicit Intercept

We now apply this $\mathcal{S}_1, dots$ argument to another problem: special linear model.

$$y_i = \alpha + \beta^T X_i + \varepsilon_i \quad i = 1, \dots, n$$

$$y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

$$X = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix}$$

$$\varepsilon = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}$$

$$Y = 1_n \alpha + X \beta + \varepsilon = (1_n X) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} + \varepsilon = U \eta + \varepsilon$$

$$\text{Let } P_{1_n} = 1_n (1_n^T 1_n)^{-1} 1_n^T = \frac{1_n 1_n^T}{n}.$$

$$\text{Note that for all } a = \begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix} \in \mathbb{R}^n,$$

$$P_{1_n} a = \frac{1_n 1_n^T a}{n} = 1_n \bar{a}, \quad \bar{a} = \frac{1}{n} \sum_{i=1}^n a_i$$

which is a mean projection. (?)

$$Q_{1_n} = I_n - P_{1_n} \quad (\text{projection on } 1_n^\perp)$$

$$Q_{1_n} a = \begin{pmatrix} a_1 - \bar{a} \\ \vdots \\ a_n - \bar{a} \end{pmatrix}$$

Decompose X:

$$X = P_{1_n} X + Q_{1_n} X$$

$$U \eta = 1_n \alpha + X \beta = 1_n \alpha + P_{1_n} X \beta + Q_{1_n} X \beta = 1_n \left(\alpha + \frac{1_n^T X \beta}{n} \right) + Q_{1_n} X \beta = (1_n Q_{1_n} X) \begin{pmatrix} \alpha^* \\ \beta \end{pmatrix} = (1_n Q_{1_n} X) \eta^* = U^* \eta^*$$

So we do least squares of

$$(y - U^* \eta^*)^T (y - U^* \eta^*)$$

and minimize this over all $\eta^* \in \mathbb{R}^{P \times 1}$

$$\hat{\eta}^* = (U^{*T} U^*) U^{*T} y$$

$$U^{*T} U^* = \begin{pmatrix} 1_n^T \\ (Q_{1_n} X)^T \end{pmatrix} (1_n Q_{1_n} X) = \begin{pmatrix} 1_n^T 1_n & Q_{1_n} X 1_n \\ 1_n^T Q_{1_n} X & Q_{1_n} X Q_{1_n} X \end{pmatrix} = \begin{pmatrix} n & 0 \\ 0 & X^T Q_{1_n} X \end{pmatrix}$$

$$\hat{\eta}^* = \begin{pmatrix} n^{-1} & 0 \\ 0 & (X^T Q_{1_n} X)^{-1} \end{pmatrix} \begin{pmatrix} 1_n \\ (Q_{1_n} X)^T \end{pmatrix} y$$

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So

$$\hat{\alpha}^* = n^{-1} 1_n^T y$$

$$\hat{\beta} = (X^T Q X)^{-1} X^T Q y$$

$$\hat{\alpha} = n^{-1} 1_n^T y - n^{-1} X^T \hat{\beta}^*$$

For statistical inference, we want to make a decomposition of \mathbb{R}^n .

Let, $\mathcal{S}_1 = \text{span}(1_n)$, $\mathcal{S}_2 = \text{span}(1_n, X)$, $\mathcal{S}_3 = \mathbb{R}^n$.

Then,

$$(\mathcal{S}_3 \ominus \mathcal{S}_1) = (\mathcal{S}_3 \ominus \mathcal{S}_2) \oplus (\mathcal{S}_2 \ominus \mathcal{S}_1)$$

Then,

$$\|P_{\mathcal{S}_3 \ominus \mathcal{S}_1} y\|^2 = \|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2 + \|P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y\|^2$$

Or,

$$SSTotal = SSE_{Error} + SS_{Regression}$$

We may compute these terms,

$$\begin{aligned} P_{\mathcal{S}_3 \ominus \mathcal{S}_1} &= P_{\mathcal{S}_3} - P_{\mathcal{S}_1} \\ &= I_n - \frac{1_n 1_n^T}{1_n^T 1_n} \\ &= Q_{1_n} \\ \mathcal{S}_2 \ominus \mathcal{S}_1 &= \text{span}(Q_{1_n} X) \\ P_{\mathcal{S}_2 \ominus \mathcal{S}_1} &= Q X (X^T Q X)^{-1} Q X^T \\ P_{\mathcal{S}_3 \ominus \mathcal{S}_2} &= Q - Q X (X^T Q X)^{-1} X^T Q \end{aligned}$$

By Cochran's Theorem, (these are orthogonalized projections, etc),

$$\begin{aligned} \|P_{\mathcal{S}_3 \ominus \mathcal{S}_1} y\|^2 &\sim \chi^2(n-1) \\ \|P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y\|^2 &\sim \chi^2_{(p-1)} \\ \|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2 &\sim \chi^2_{(n-p-1)} \end{aligned}$$



$$\dim(\mathcal{S}_3) = n$$

$$\dim(\mathcal{S}_2) = p + 1 \quad \dim(\mathcal{S}_3) = 1$$

We also know that these are all independent of each other. So we can test regression effect with the following hypothesis:

$$H_0 : \beta = 0$$

$$\frac{\|P_{\mathcal{S}_2 \ominus \mathcal{S}_1} y\|^2 / (p-1)}{\|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2 / (n-p-1)} = \frac{y^T QX(X^T QX)^{-1} QX^T y / (p-1)}{y^T (Q - QX(X^T QX)^{-1} X^T Q) y / (n-p-1)} \sim F_{p-1, n-p-1}$$

Distributions

$$\hat{\beta}(X^T QX)^{-1} X^T Qy$$

$$E(\hat{\beta}) = (X^T QX)^{-1} X^T Q(1_n \alpha + X\beta) = (X^T QX)^{-1} X^T QX\beta = \beta$$

$$\text{Var}(\hat{\beta}) = (X^T QX)^{-1} X^T Q(\sigma^2 I_n) QX(X^T QX)^{-1} = \sigma^2 (X^T QX)^{-1}$$

$$\hat{\alpha} = \hat{\alpha}^* - X^T \hat{\beta}$$

Because $\hat{\beta}$ is a function of Qy and $\hat{\alpha}^*$ is a function of $P_{1_n} y$ (and these are orthogonal to each other and thus by normality also independent).

$$\text{Var}(\hat{\alpha}) = \text{Var}(\hat{\alpha}^*) + \text{Var}(\bar{X}^T \hat{\beta}) = \text{Var}(\bar{y}) + \text{Var}(\bar{X}^T \hat{\beta}) = \frac{\sigma^2}{n} + \sigma^2 \bar{X}^T (X^T QX)^{-1} \bar{X}$$

$$\hat{\alpha} \sim N\left(\alpha, \frac{\sigma^2}{n} + \sigma^2 \bar{X}^T (X^T QX)^{-1} \bar{X}\right)$$

$$\text{Cov}(\hat{\alpha}, \hat{\beta}) = \text{Cov}(\hat{\alpha}^* - \bar{X}^T \hat{\beta}, \hat{\beta})$$

$$= -\bar{X}^T \text{Var}(\hat{\beta})$$

$$= -\bar{X}^T \sigma^2 (X^T QX)^{-1}$$

$$\begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix} \sim N\left[\begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \begin{pmatrix} \frac{\sigma^2}{n} + \sigma^2 \bar{X}^T (X^T QX)^{-1} \bar{X} & -\sigma^2 \bar{X}^T (X^T QX)^{-1} \bar{X} \\ -\sigma^2 \bar{X}^T (X^T QX)^{-1} \bar{X} & \frac{\sigma^2}{n} + \sigma^2 \bar{X}^T (X^T QX)^{-1} \bar{X} \end{pmatrix}\right]$$

Estimate σ^2

$$\|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2 = \sum_{i=1}^n (y_i - \hat{\alpha} - \hat{\beta}^T X_i)^2 \sim \sigma^2 \chi_{n-p-1}^2$$

So,

$$E(\|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2) = \sigma^2 (n-p-1)$$

Thus,

$$\hat{\sigma}^2 = \frac{\|P_{\mathcal{S}_3 \ominus \mathcal{S}_2} y\|^2}{n-p-1}$$

Theorem 1.10.1 Under the explicit intercept model,

1. $(\hat{\alpha}, \hat{\beta}, \hat{\sigma}^2)$ is UMVUE of $(\alpha, \beta, \sigma^2)$ by Lehmann-Sheffe.

2.

$$\begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix} \sim N \left[\begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \begin{pmatrix} \frac{\sigma^2}{n} + \sigma^2 \bar{X}^T (X^T Q X)^{-1} \bar{X} & -\sigma^2 \bar{X}^T (X^T Q X)^{-1} \bar{X} \\ -\sigma^2 \bar{X}^T (X^T Q X)^{-1} \bar{X} & \frac{\sigma^2}{n} + \sigma^2 \bar{X}^T (X^T Q X)^{-1} \bar{X} \end{pmatrix} \right]$$

3. $(n-p-1)\hat{\sigma}^2 \sim \sigma^2 \chi_{(n-p-1)}^2$

4. $\begin{pmatrix} \hat{\alpha} \\ \hat{\beta} \end{pmatrix} \perp \hat{\sigma}^2$

1.11 R^2

Proportion of Sum of Squares (SS) explained by regression (i.e. by β).

$$R^2 = \frac{SSR}{SST} = \frac{||P_{\mathcal{J}_2 \ominus \mathcal{J}_1} y||^2}{||P_{\mathcal{J}_3 \ominus \mathcal{J}_1} y||^2}$$

But we know that,

$$R^2 = \frac{||P_{\mathcal{J}_2 \ominus \mathcal{J}_1} y||^2}{||P_{\mathcal{J}_2 \ominus \mathcal{J}_1} y||^2 + ||P_{\mathcal{J}_3 \ominus \mathcal{J}_2} y||^2} = \frac{SSR}{SSR + SSE} = \frac{SSR/SSE}{SSR/SSE + 1}$$

$$F = \frac{SSR/p}{SSE/(n-p-1)} = \frac{(n-p-1)}{p} \frac{SSR}{SSE}$$

$$\frac{SSR}{SSE} = \frac{p}{(n-p-1)} F$$

$$R^2 = \frac{\alpha F}{\alpha F + 1}$$

where $\alpha = \frac{p}{n-p-1}$

This is how we compute the null distribution of R^2 .

1.12 Multicollinearity

Wednesday September 14

$$y = C_1 \beta_1 + \dots + C_p \beta_p$$

$$X = (C_1, \dots, C_p) = \begin{pmatrix} X_1^T \\ \vdots \\ X_n^T \end{pmatrix}$$

In an extreme case, multicollinearity simply means that the C_1, \dots, C_p are linearly dependent. In this case β is not identifiable.

We have C_1, C_2, C_3 .

$$C_1 = a$$

$$C_2 = 2a$$

$$C_3 = b$$

$$\begin{aligned} y &= a\beta_1 + 2a\beta_2 + b\beta_3 + \varepsilon \\ &= a(\beta_1 + 2\beta_2) + b\beta_3 + \varepsilon \end{aligned}$$

β_1 & β_2 cannot be split.

In the less extreme case, $X^T X$ is nearly singular, meaning it has small eigenvalues. In this case, although β is identifiable, they have large variance. For example, if $C_1 = aC_2$ then β_1, β_2 have large variance which means your parameterization is not good. So may define new parameterization.

$$\gamma_1 = \beta_1 + 2\beta_2$$

$$\gamma_2 = \beta_3$$

If you run regression against these then the variance would be 'normal'.

So, how to weed out redundant variables? One way Variance Inflation Factor (VIF) which for each $i = 1, 2, \dots, p$ regresses C_i on $\{C_1, \dots, C_p \setminus C_i\}$ then you get R^2 for this regression call it R_i^2 .

If C_i is redundant then R_i^2 would be close to 1.

$$VIF_i = \frac{1}{1 - R_i^2}$$

1.13 Variable Selection

$$y = C_1\beta_1 + \dots + C_p\beta_p + \varepsilon$$

Some of these β 's are zero.

Let us define an active set of parameters,

$$A_0 = \{i : \beta_i \neq 0\}$$

To estimate A_0 is the goal of variable selection.

Mallow's C_p criterion

The fundamental issue is variable selection, penalty - penalizing the number of parameters, so you cannot use something like $y - \hat{y}$ as criterion. The more variables you have the smaller $\|\hat{y} - y\|^2$ is. So we want to penalize the number of parameters in a reasonable way.

Let any subset $A \subset \{1, \dots, p\}$,

$$X_A = \{C_i : i \in A\}$$

Notation 1.2. While we often use X for iid variables (a vector), but here X is a matrix and X_i were referring to its columns. We've changed X_i to C_i to better reflect that we are dealing with columns of X .

So, $A = \{1, 3, 5\}$,

$$X_A = \begin{pmatrix} C_1 \\ C_3 \\ C_5 \end{pmatrix}$$

Let P_{X_A}, Q_{X_A} be the projection on to $\text{span}(X_A)$, $\text{span}(X_A)^\perp$. For example,

$$P_{X_A} = X_A (X_A^T X_A)^{-1} X_A^T$$

Let $\mu = E(y) = X\beta = X_{A_0}\beta_{A_0}$.

Mallow says we minimize

$$\frac{E\|P_A y - \mu\|^2}{\sigma^2}$$

among all $A \subset \{1, \dots, p\}$.

But we do not know what σ^2 or μ are. If so, we would already know A_0 . We must estimate these.

$$E\|P_{X_A} y - \mu\|^2 = \text{tr}(E(P_{X_A} y - \mu)(P_{X_A} y - \mu)^T)$$

$$\begin{aligned} E(P_{X_A} y - \mu)(P_{X_A} y - \mu)^T &= E[(P_{X_A} y - P_{X_A} \mu) + (P_{X_A} \mu - \mu)][(P_{X_A} y - \mu) + (P_{X_A} \mu - \mu)]^T \\ &= \text{expand, two terms are zero} \\ &= E(P_{X_A} y - P_{X_A} \mu)(P_{X_A} y - P_{X_A} \mu) + (P_{X_A} \mu - \mu)(P_{X_A} \mu - \mu)^T \\ &= \text{Var}(P_{X_A} y) \\ &= P_{X_A} \sigma^2 I_n P_{X_A} = \sigma^2 P_{X_A} \\ &= \text{tr}(\sigma^2 P_{X_A} + Q_{X_A} \mu \mu^T Q_{X_A}) \\ &= \sigma * 2\text{tr}(P_{X_A}) + \text{tr}(Q_{X_A} \mu \mu^T Q_{X_A}) \\ &= \sigma^2 (\#(A)) + \text{tr}(\mu^T Q_{X_A} \mu) \end{aligned}$$

$$\Rightarrow E \frac{\|P_{X_A} y - \mu\|^2}{\sigma^2} = \#(A) + \frac{\text{tr}(\mu^T Q_{X_A} \mu)}{\sigma^2}$$

Now let's estimate $\frac{\mu^T Q_{X_A} \mu}{\sigma^2}$.

Recall, if U is a random vector with multivariate normal distribution so

$$E(U) = e$$

$$\text{Var}(U) = Q_{X_A}$$

$$U^T U \sim \chi_{(\text{rank}(Q)_{X_A})}^2(\|e\|^2)$$

Also, $W \sim \chi_{(r)}^2(\delta)$ where $E(W) = r + \delta$.

Go back to our problem of estimating $\frac{\mu^T Q_{X_A} \mu}{\sigma^2}$.

What about $y^T Q_{X_A} y$? We know that

$$E\left(\frac{Q_{X_A} y}{\sigma}\right) = \frac{Q_{X_A} \mu}{\sigma}$$

and

$$\text{Var}\left(\frac{Q_{X_A} y}{\sigma}\right) = \frac{1}{\sigma^2} Q_{X_A} \sigma^2 I_n = 0$$

So,

$$\frac{Q_{X_A} y}{\sigma} \sim N\left(\frac{Q_{X_A} \mu}{\sigma}, 0\right)$$

So

$$\left(\frac{Q_{X_A} y}{\sigma}\right)^T \left(\frac{Q_{X_A} y}{\sigma}\right) \sim \chi_{(n-\#(A))}^2\left(\left(\frac{Q_{X_A} \mu}{\sigma}\right)^T \left(\frac{Q_{X_A} \mu}{\sigma}\right)\right) = \chi_{(n-\#(A))}^2\left(\frac{\mu^T Q_{X_A} \mu}{\sigma^2}\right)$$

Thus,

$$E\left(\frac{y^T Q_{X_A} y}{\sigma^2}\right) = n - \#(A) + \frac{\mu^T Q_{X_A} \mu}{\sigma^2}$$

Which, if you subtract over the n and $\#(A)$ you get an unbiased estimator of $\frac{\mu^T Q_{X_A} \mu}{\sigma^2}$. But σ^2 is still unknown, but we use full model,

$$\hat{\sigma}^2 = \frac{y^T Q_{X_A} y}{n - p}$$

Now we can estimate $\frac{\mu^T Q_{X_A} \mu}{\sigma^2}$ by

$$\frac{y^T Q_{X_A} y}{\frac{y^T Q_{X_A} y}{n-p}} - n + 2\#(A) = (n-p) \frac{y^T Q_{X_A} y}{y^T Q_{X_A} y} - n + 2\#(A)$$

So to recap,

$$E\left(\frac{\|P_{X_A} y - \mu\|^2}{\sigma^2}\right) = (n-p) \frac{y^T Q_{X_A} y}{y^T Q_{X_A} y} - n + 2\#(A)$$

Friday September 16

Akaike/Bayesian Information Criteria (AIC/BIC)

Suppose we have some generic (i.e. not related to the design/covariance in regression context) X_1, \dots, X_n , a sample of independent random vectors with joint density $f_\theta(x_1, \dots, x_n)$.

$$\theta \in \Theta \subset \mathbb{R}^P$$

$$\theta = \begin{pmatrix} \theta_1 \\ \vdots \\ \theta_P \end{pmatrix}$$

Let $M_0 \subset \{1, \dots, P\}$ be the true active set, that is $\{i : \theta_i \neq 0\} = M_0$. Also, let $M_0 \subset \{1, \dots, P\}$. We want to recover the true active set M_0 .

Let Θ_M be the parameter space, corresponding to M .

$$\Theta_M = \{\theta \in \Theta : \theta_i = 0 \text{ if } i \notin M\}$$

Of course we also have Θ_{M_0} .

for each $M \subset \{1, \dots, P\}$ define,

$$L_M = \sup_{\theta \in M} f_{\theta}(x_1, \dots, x_n)$$

Then,

$$\text{AIC}(M) = -2 \log L_M + 2(\#M)$$

$$\text{BIC}(M) = -2 \log L_M + (\log n)(\#M)$$

Use them

$$\hat{M} = \arg \min \{\text{AIC}(M) : M \in 2^{\{1, \dots, P\}}\}$$

$$\hat{M} = \arg \min \{\text{BIC}(M) : M \in 2^{\{1, \dots, P\}}\}$$

When P is large, this is called **forward backward selection** instead of **Best Set Selection**.

Specialized to Gaussian Linear Regression Model

Here there is no variable selection,

$$\theta = \begin{pmatrix} \beta \\ \sigma^2 \end{pmatrix}$$

$$\Theta \subset \mathbb{R}^{P+1} \text{ (M is in } \Theta)$$

$$\beta \in B$$

$$\text{subset } \mathbb{R}^P \text{ (A is in B)}$$

In our case,

$$y \sim N(X_A \beta_A, \sigma^2 I_n)$$

where $A \subseteq B$ which is where β is.

Note we are again using the notation $X_A = \{C_i : i \in \beta\}$ and that

$$\#A + 1 = \#M$$

If A is an active set of β then $M = A \cup \{p+1\}$ is the active set of θ because σ^2 is always active.

But $L_M = ?$

Recall, MLE for β is (under A),

$$\hat{\beta}_A = (X_A^T X_A)^{-1} X_A^T y$$

$$\hat{\sigma}_A^2 = \frac{y^T Q_{X_A} y}{n}$$

So the likelihood at $(\hat{\beta}_A, \hat{\sigma}_A^2)$,

$$\begin{aligned} f_{\hat{\theta}_A}(x_1, \dots, x_n) &= \frac{1}{(2\pi)^{\frac{n}{2}} \det(\hat{\sigma}_A^2 I_n)} e^{-\frac{1}{2\hat{\sigma}_A^2} \|y - X_A \hat{\beta}_A\|^2} \\ &= L_M = \dots e^{-\frac{1}{2\hat{\sigma}_A^2} \|y - X_A \hat{\beta}_A\|^2} \\ &= \dots e^{-\frac{1}{2\hat{\sigma}_A^2} \|y - X_A (X_A^T X_A)^{-1} X_A^T y\|^2} \\ &= \dots e^{-\frac{1}{2\hat{\sigma}_A^2} \|y - P_{X_A} y\|^2} \\ &= \dots e^{-\frac{n}{2} \left\| \frac{y^T Q_{X_A} y}{n} \right\|^2} \\ L_M &= \frac{1}{(2\pi)^{\frac{n}{2}} \left(\frac{y^T Q_{X_A} y}{n} \right)^{\frac{n}{2}}} e^{-\frac{n}{2}} \\ \log L_M &= -\frac{n}{2} \log(2\pi) - \frac{n}{2} \log\left(\frac{y^T Q_{X_A} y}{n}\right) - \frac{n}{2} \end{aligned}$$

$$\text{AIC}(A) = -2 \log L_M + 2(\#M) =$$

It is equivalent to minimize,

$$n \dots$$

For BIC, replace $2(\#A + 1)$ by $(\log n)(\#A + 1)$.

Variable Selection Consistency

(as opposed to estimation consistency)

You have data, $(X_1, \dots, X_n) = \mathcal{X}$ (again, generic X, not in regression context). An estimator,

$$\mathcal{X} \rightarrow \Theta$$

Variable selection,

$$\hat{A} : \mathcal{X} \rightarrow 2^{\{1, \dots, P\}}$$

that is to say,

$$(x_1, \dots, x_n) \mapsto M$$

Definition 1.13.1 — Variable Selector Consistency. A variable selector, \hat{A} is said to be **consistent** if

$$P(\hat{A} = A_0) \rightarrow 1$$

where A_0 is the true action set.

Next, BIC in variable selection consistency.

Ordering of sequences, $\{a_n\}, \{b_n\}$ 2 sequences in \mathbb{R} , positive...

Notation 1.3 (Asymptotic Order of Magnitude). $a_n \prec b_n$ if $\frac{a_n}{b_n} \rightarrow 0$ as $n \rightarrow \infty$.

- **Example 1.1**
- $a_n \prec 1 \Leftrightarrow a_n \rightarrow 0$
 - $a_n \prec n \Leftrightarrow \frac{a_n}{n} \rightarrow 0$

$$a_n \succ 1$$

$$\Rightarrow 1 \prec a_n$$

- **Example 1.2**
- $\Rightarrow \frac{1}{a_n} \rightarrow 0$
 - $\Rightarrow a_n \rightarrow \infty$

- $n^{\frac{1}{2}}$

The symbol \sim means both \prec and \succ .

Monday September 19

Lemma 1.3

Under some regularity conditions (identifiability, smoothness of log likelihood, support doesn't depend on parameters, ...) then

1. $\Theta_{M_0} \subseteq \Theta_M$

$$2(\log L_M - \log L_{M_0}) \rightarrow^{\mathcal{D}} \chi^2_{(\#M - \#M_0)}$$

Here, recall,

$$L_M = \sup_{\theta \in \Theta} f_{\theta}(x_1, \dots, x_n)$$

2. If $\Theta_M \subseteq \Theta_{M_0}$ then,

$$n^{-1} 2(\log L_M - \log L_{M_0}) \rightarrow^P 2(\sup_{\theta \in \Theta} E \log f_{\theta}(x_1, \dots, x_n) - E \log f_{\theta_0}(x_1, \dots, x_n))$$

Moreover, if $M \subset M_0$ then

$$\lim_{n \rightarrow \infty} (2(\sup_{\theta \in \Theta} E \log f_{\theta}(x_1, \dots, x_n) - E \log f_{\theta_0}(x_1, \dots, x_n))) < 0$$

Theorem 1.13.1 Let $BIC(M) = -2 \log L_M + (cn)(\#M)$ where $1 \prec c(n) \prec n$. This generalizes BIC so that $c(n)$ replaces $\log(n)$ but still converges slower than n (as does \log).

Let $\hat{M} = \arg \min_{M \in \{1, 2, \dots, p\}} BIC(M)$ then

$$P(\hat{M} = M_0) = 1$$

Proof. Consider the difference,

$$BIC(M) - BIC(M_0) = 2(\log L_{M_0} - \log L_M) + c(n)(\#M - \#M_0)$$

We want to show (with probability going to 1) that

$$BIC(M) - BIC(M_0) > 0 \quad \forall M \neq M_0$$

Case 1 $M \supset M_0$

Then $c(n)(\#M - \#M_0) \rightarrow \infty$

Meanwhile, $2(\log L_{M_0} - \log L_M) = O_p(1)$.

R Fact. If $U_n = O_p(1)$, $\alpha_n \rightarrow \infty$ then

$$P(U_n + \alpha_n > 0) \rightarrow 1$$

So,

$$P(BIC(M) - BIC(M_0)) \rightarrow 1$$

Case 2 $M \subseteq M_0$

$n^{-1}2(\log L_{M_0} - \log L_M) \rightarrow c(n) > 0$

R Fact. $n^{-1}U_n \rightarrow c > 0$, $\alpha_n \prec n$ and $n^c \prec n$ then

$$P(U_n + \alpha_n > 0) \rightarrow 1$$

So again,

$$P(BIC(M) - BIC(M_0)) \rightarrow 1$$

Thus, $P(BIC(M))$ is uniquely minimized at $M_0) \rightarrow 1$.

■

1.14 Non iid Linear Regression

Suppose

$$y = X\beta + \varepsilon$$

where $\varepsilon \sim N(0, \sigma^2 \Sigma)$ with arbitrary but known matrix $\Sigma > 0$.

Then MLE for $\hat{\beta}$ is

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

MLE for $\hat{\sigma}^2$ is

$$\hat{\sigma}^2 = \|Q_X(\Sigma^{-1})y\|^2 / n$$

But remember $\|Q_X(\Sigma^{-1})y\|_{\Sigma^{-1}}^2 \sim \sigma^2 \chi_{n-p}^2$, so now we have

$$E(\|Q_X(\Sigma^{-1})y\|_{\Sigma^{-1}}^2) = \sigma^2(n-p)$$

so the unbiased estimator is,

$$\tilde{\sigma}^2 = \frac{\|Q_X(\Sigma^{-1})y\|_{\Sigma^{-1}}^2}{n-p}$$

Theorem 1.14.1 Under $y = X\beta + \varepsilon$ with ε as above, we have

1. $\hat{\beta}, \hat{\sigma}^2$ are UMVUE
2. $\hat{\beta} \sim N(\beta, \sigma^2(x^T \Sigma^{-1} X)^{-1})$
3. $\hat{\sigma}^2 \sim \sigma^2(n-p)^{-1} \chi_{n-p}^2$
4. $\hat{\sigma}^2 \perp\!\!\!\perp \hat{\beta}$

All theories developed previously for $\varepsilon \sim N(0, \sigma^2 I_n)$ can be generalized here in a straightforward manner.

2. General Linear Hypothesis & Simultaneous Conf

2.1 General Linear Model

Definition 2.1.1 — General Linear Models. General Linear Models are the same as linear Gaussian Model, except it is stated in a coordinate-free or geometric way.

Let $\mathcal{S} \leq \mathbb{R}^N$.

A general linear model gives,

$$y \sim N(\mu, \sigma^2 I_N)$$

where $\mu \in \mathcal{S}$.

If we take X to be a basis matrix of \mathcal{S} , that is $\text{span}(X) = \mathcal{S}$, then we have

$$y = \mu X + \varepsilon = X\beta + \varepsilon$$

the same as before. (because $\mu \in \mathcal{S}, \text{span}(x) = \mathcal{S} \Rightarrow \mu = X\beta \text{ for some } \beta$)

The MLE can be derived in a similar way.

3. Mutiway ANOVA

3.1 Overview

- Orthogonal design
- Additive 2 way ANOVA
- simultaneous intervals
- nonadditive
- decomposition of sum of squares
- Latin square
- nested design

4. Nonorthogonal Design

4.1 Overview

- $\bar{X}_j - \bar{X}_i$



5. Random Effects Model

5.1 Overview



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6. Basic Concepts

6.1 Overview



7. Estimation

7.1 Overview

8. Inference

8.1 Overview

- deviance \leftrightarrow sum of squares



9. Residuals

9.1 Overview



10. Categorical Prediction

10.1 Overview



11. Some Important GLM

11.1 Overview



12. Multivariate GLM

12.1 Overview



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13. Principle Component Analysis

13.1 Overview



14. Canonical Correlation Analysis

14.1 Overview



15. Independent Component Analysis

15.1 Overview

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