Linear Models

STAT 551

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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 $\mathbb{R}^P$.

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

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

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

$$a^T b =< a, b >$$

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 $\{\mathbb{R}^P, < a, b >\}$

General Inner Product

Let $\Sigma \in \mathbb{R}^{PxP}$ set of all PxP 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.

$$a^T \Sigma b =< a, b >_\Sigma$$

$$a^T b = a^T I b =< a, b >_I$$

$\{\mathbb{R}^P, <, >_\Sigma\}$ is a more general inner product space.

Linear Transformation

A matrix, $A, \in \mathbb{R}^{PxP}$ can be viewed as linear transformation
$T_A : \mathbb{R}^P \to \mathbb{R}^P, x \mapsto Ax$

R Bing Li will denote T_A as A.
$\to$ means maps to for a domain.
$\mapsto$ means maps to for a value.
$\Rightarrow$ means implies.

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

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

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

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

$$A = A^2$$

$$Ax = A(A(x))$$

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

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

Wednesday August 24

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

$$< x, Ty > = < Rx, y >$$

(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,

$$< x, Ty > = < T^* x, y >$$

Derived Facts

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

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

It is easy to see in our case

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

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 $< x, Ty > = < Tx, y >$). In the case of $<,>_\Sigma$,

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

if

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

R 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 $\boldsymbol{A} \in \mathbb{R}^{PxP}$ is symmetric, then there exists **eigenvalue-eigenvector pairs**. $(\lambda_1, v_1), \dots (\lambda_P, v_P)$ such that $v_1 \perp \dots \perp v_P$. Orthoginal basis (ONB) such that

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

More generally, if $\boldsymbol{A}$ is a linear operator in $\mathscr{H}$ (finite dimential inner product such as $(\mathbb{R}^P, <,>_\Sigma)$). its eigen pair (linear operator now) (λ, v) is defined by

$$\begin{cases} \boldsymbol{A}\underline{v} = \underline{\lambda v} \\ < \underline{v}, \underline{v} > = 1 \end{cases}$$

Definition 1.1.6 — Orthogonal Basis. In the following, $(\mathbb{R}^P, <,>_\Sigma) = \mathscr{H}$ (H for Hilbert)

ONB is defined by:

1. $v_i \perp v_j, < v_i, v_j > = 0$
2. $||v_i|| = 1$
3. $\text{span}\{v_1, \dots, v_P\} = \mathscr{H}$

Theorem 1.1.2 Suppose $\boldsymbol{A} : \mathscr{H} \to \mathscr{H}$ is a self adjoint linear operator. Then $\boldsymbol{A}$ 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

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

Proof. (λ, v) is eigen pair of $\boldsymbol{A}$, which means

$$\boldsymbol{A}v = \lambda v$$

$$< v, v > = 1$$

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

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

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

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

$$\begin{aligned} A\Sigma^{-\frac{1}{2}}u &= \lambda\Sigma^{-\frac{1}{2}}u \\ \Sigma^{-\frac{1}{2}}u &= \lambda u \end{aligned}$$

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.

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 ($P = P^*$).

Preposition 1.1 If A is a linear operator then $ker(A) = ran(A^*)^\perp$

Proof. Take $x \in ker(A) (\Rightarrow Ax = 0)$.
$\forall y \in ran(A^*), x \perp y$
$\Rightarrow x \perp y \forall y = A^*z, z \in \mathbb{R}^P$
Hence,

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

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

Or vice versa. ■

Friday August 26

R $\perp$ means orthogonal complement.

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

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

$$< v, w >= 0 \forall w \in \mathscr{S}$$

$$= \{v \in \mathbb{R}^P, < v, w >= 0 \forall w \in \mathscr{S}\}$$

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

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

Theorem 1.1.3 If P is a projection, then

1. $Pv = v$, $\forall v \in ran(P)$
2. $Pv = 0$, $\forall v \perp ran(P)$
3. If Q is another projections such that the $ran(Q) = ran(P)$ 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 $v \in ran(P)$. Since $P^2 = P$ (idempotent) then

$$P^2 v = Pv$$
$$\Rightarrow P^2 v - PV = 0$$
$$\Rightarrow P(Pv - v) = 0$$
$$\Rightarrow Pv - v \in ker(P)$$
$$\Rightarrow Pv - v \perp ran(P)$$
$$\Rightarrow < Pv - v, Pv - v >= 0$$
$$\Rightarrow ||Pv - v|| = 0$$
$$\Rightarrow Pv - v = 0$$
$$\Rightarrow Pv = v$$

2. If
$$v \perp ran(P)$$
$$\Rightarrow v \in ker(P)$$
$$\Rightarrow Pv = 0$$

3. If Q is another operator with $ran(Q) = ran(P) = \mathscr{S}$ then $\forall v \in \mathscr{S}$
$$Qv = v = Pf(\forall v \perp \mathscr{S})$$
$$Qv = 0 = Pv$$
$$Qv = Pv\forall,\ v \in \mathscr{S}$$
$$Q = P$$

■

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

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

Then,

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

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 $x, y \in \mathbb{R}^P$
   $< x, Ay > = x^T \Sigma v (v^T \Sigma v)^{-1} v^{\Sigma} y$
   $= (v(v^T \Sigma v)^{-1} v^T \Sigma x)^T \Sigma y$
   $=< Ax, y >$
3. $ran(A) = \mathscr{S}$?
   Let $x \in \mathbb{R}^P$.
   $Ax = v(v^T \Sigma v)^{-1} v^T \Sigma x \in span(v) = \mathscr{S}$
   So let $x \in \mathscr{S}$,
   $$x \in ran(v)$$
   $$x = vy$$
   for some $y \in \mathbb{R}^P$
   $$= v(v^T \Sigma v)^{-1} v^T \Sigma v y$$
   $\in ran(A)$
   So, $\mathscr{S} \subseteq ran(A)$ and then $\mathscr{S} = ran(A)$.

■

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

In the following, let $I : \mathbb{R}^P \to \mathbb{R}^P$ be the identity mapping. ($x \mapsto x$)
Let $\mathscr{S}$ be a subspace in $\mathbb{R}^P$.
Let $Q_{\mathscr{S}}(\Sigma) = I - P_{\mathscr{S}}(\Sigma)$

Proprosition 1.2 $Q_{\mathscr{S}}(\Sigma) = P_{\mathscr{S}^{\perp}}(\Sigma)$

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

1. *Idempotent*
   $Q^2_{\mathscr{S}}(\Sigma) = Q_{\mathscr{S}}(\Sigma) Q_{\mathscr{S}}(\Sigma)$
   $= (I - P_{\mathscr{S}}(\Sigma))(I - P_{\mathscr{S}}(\Sigma))$
   $= I - P_{\mathscr{S}}(\Sigma) - P_{\mathscr{S}}(\Sigma) + P_{\mathscr{S}} P_{\mathscr{S}}$
   $= Q_{\mathscr{S}}(\Sigma)$
2. *Self-adjoint*
   $$x, y \in \mathbb{R}^P$$
   $< x, Q_{\mathscr{S}}(\Sigma) y > =< x, (I - P_{\mathscr{S}}(\Sigma)) y >$
   $=< x, y > - < x, P_{\mathscr{S}}(\Sigma)) y >$
   $=< x, y > - < P_{\mathscr{S}}(\Sigma)) x, y >$
   $=< (I - P_{\mathscr{S}}(\Sigma)) x, y >$
   $=< Q_{\mathscr{S}}(\Sigma) x, y >$
3. *Range*
   $ran(Q_{\mathscr{S}}(\Sigma)) = \mathscr{S}^{\perp}$. Take $x \perp \mathscr{S} = ran(P_{\mathscr{S}}(\Sigma))^{\perp} = ker(P_{\mathscr{S}}(\Sigma))$.

$$\Rightarrow P_{\mathscr{S}}(\Sigma) = 0$$
$$\Rightarrow Q_{\mathscr{S}}(\Sigma)x = x - P_{\mathscr{S}}(\Sigma)x = x$$
$$X \in ran(Q_{\mathscr{S}}(\Sigma))$$
$$\Rightarrow \mathscr{S}^{\perp} \subseteq ran(Q_{\mathscr{S}}(\Sigma))$$

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

$$y = P_{\mathscr{S}}(\Sigma)z \text{ for some } z \in \mathbb{R}^P$$
$$< x, y >=< x, P_{\mathscr{S}}(\Sigma)z >=< P_{\mathscr{S}}(\Sigma)x, z >= 0$$
$$\Rightarrow x \in \mathscr{S}^{\perp}$$
$$\Rightarrow ran(Q_{\mathscr{S}}(\Sigma)) = \mathscr{S}^{\perp}$$

■

1.2 Cochran's Theorem

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

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

Proof. λ is eigenvalue of A.

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

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

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 $V^T PV \sim \sigma^2 \chi^2_S$ where df = rank(P).

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

$$ARA^T$$

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

Then,

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

Let,

$$Z = RA^T V$$

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 distributied as N(0, 1) and the rest are zero and they are independant. So,

$$Z^T Z \sim \chi^2_S = V^T PV$$

■

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

$$< a,b >_{\Sigma^{-1}} = a^T \Sigma^{-1} b$$

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

Then,

$$||P_{\mathscr{S}}(\Sigma^{-1})x||^2_{\Sigma^{-1}} \sim \chi^2_r$$

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

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

$$\begin{aligned}
||P_{\mathscr{S}}(\Sigma^{-1})X||^2_{\Sigma^{-1}} &=< P_{\mathscr{S}}(\Sigma^{-1})X, P_{\mathscr{S}}(\Sigma^{-1})X > \\
&= X^T P_{\mathscr{S}}(\Sigma^{-1})\Sigma^{-1} P_{\mathscr{S}}(\Sigma^{-1})X \\
&= X^T (V(V^T\Sigma^{-1}V)^{-1}V^T\Sigma^{-1})^T \Sigma^{-1}(V(V^T\Sigma^{-1}V)^{-1}V^T\Sigma^{-1})X \\
&= X^T\Sigma^{-1}V(V^T\Sigma^{-1}V)^{-1}v^T\Sigma^{-1}V(V^T\Sigma^{-1}V)^{-1}V^T\Sigma^{-1})X \\
&= (\Sigma^{-\frac{1}{2}}X)^T[\Sigma^{-\frac{1}{2}}V(V^T\Sigma^{-1}V)^{-1}(\Sigma^{-\frac{1}{2}}V)^T](\Sigma^{-\frac{1}{2}}X)
\end{aligned}$$

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 repect to I_P-inner producted (idempotent, self adjoint, YES).

By Lemme 1.1,

$$(*) \sim \chi^2_r$$

.

■

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

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

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

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

Then,

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

1.3 Gaussian Linear Regresson Model

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

$$X = \begin{pmatrix} x_{11} & \dots & x_{1P} \\ \vdots & \ddots & \vdots \\ x_{n1} & \dots & x_{np} \end{pmatrix} \in \mathbb{R}^{nxp}$$

Consider the linear model,

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

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

where X has full comlumn rank ($n \geq p$).
Here X is treated as fixed

- Maximum Likelihood Estimator

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

$$Var(y) = \sigma^2 I_n$$

$y \sim N_p(X\beta, \sigma^2 I_n$
Multivariate normal density

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

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

In our case,

$$\Sigma = \sigma I_n$$

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

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

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

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

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

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

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

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, $\hat{y} = P_{span(x)}(I_P) = P_X$.

Now,

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

where $(I_n - P_X)$ is projection on to $span(X)^{\perp}$.
It turns out that $(X^T y, y^T y)$ is complete, sufficient statistic for this Gaussian linear model.
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,
$E(\hat{\beta}) = B$ (unbiased)
$Var(\hat{\beta}) = (X^T X)^{-1} X^T \sigma^2 I_n X (X^T X)^{-1} = \sigma^2 (X^T X)^{-1}$
$\hat{\beta} \sim N(\beta, \sigma^2 (X^T X)^{-1})$

Because P_x has rank p and Q_x has rank $(n-p)$, then

$$||Q_x y||^2 \sim \chi^2_{(n-p)}$$

Let's find an unbiased estimator for σ^2

$$\begin{aligned}
E(\hat{\sigma^2}) &= E(\frac{1}{n}||Q_x y||^2) \\
&= \frac{n-p}{n}\sigma^2 \\
E(\frac{n}{n-p}\hat{\sigma^2}) &= \sigma^2
\end{aligned}$$

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

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

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

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

$\hat{\beta} \leftrightarrow P_{Xy}$
$\hat{\sigma^2}$ is a funciton of Q_{Xy}, 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. $(n-p)\tilde{\sigma^2} \sim \sigma^2 \chi^2_{(n-p)}$
4. $\hat{\beta} \perp\!\!\!\perp \tilde{\sigma^2}$

1.4 Statistical Inference for β, σ^2

Suppose we want to test
$H_0 : \beta_1 = \beta_{i0}$
Let $M = (X^T X)^{-1}$.

Then,

$$\hat{\beta} \sim N(\beta_i 0, \sigma^2 M_{ii})$$

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

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

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

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

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

Reject H_0 if

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

Recall,
$X \sim N(\mu, 1)$ $y \sim \chi^2_r$ $X \perp\!\!\!\perp y$
$\frac{X}{\sqrt{\frac{y}{r}}} \sim t_n(\mu)$

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 distrabution 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 $\beta_{i.}$.

$$(\hat{\beta}_1 - t_{\frac{n}{2}(n-p)}\hat{\sigma}\sqrt{M_{ii}}, \hat{\beta}_1 + t_{\frac{n}{2}(n-p)}\hat{\sigma}\sqrt{M_{ii}})$$

1.5 Delete One Prediciton

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. Projectioning 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 Suppose $A \in \mathbb{R}^{PxP}$ is a symmetric, nonsingular matrix. and $v \in \mathbb{R}^P$.
Then,

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

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

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

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

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

R 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

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

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

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

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

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

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

- Standardized residual

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

- Prediction Error Sum of Squares (PRESS) Residual

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

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

- Standardized PRESS Error

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

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?)

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

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

1.8 Orthogonal Decomposition

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

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

R $\leq$ is subspace
$\subseteq$ is a subset

For
$\mathscr{S}_1 \leq \mathscr{S}_1\mathscr{S}_2 \leq \mathscr{S}$

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

Suppose $\mathscr{S}_1, \mathscr{S}_2 \leq \mathscr{S}$,
$\mathscr{S}_1 + \mathscr{S}_2 = \mathscr{S}$, $\mathscr{S}_1 \perp \mathscr{S}_2$
then,

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

is called an orthogonal decomposition of $\mathscr{S}$

In this case,

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

More generally,

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

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

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

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

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

$$v_1 + \cdots + v_k$$

, where $v_1 \in \mathscr{S}_1, \ldots v_k \in \mathscr{S}_k$.

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

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

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

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

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

Proposition 1.7 - Orthogonal Decomposition and Projection Consider a Hilbert Space, $\mathscr{H} = \{\mathbb{R}^n, <,>_A\}$,

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

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

2. If $\mathscr{S} \leq \mathscr{H}, \ldots, \mathscr{S}_k \leq \mathscr{H}$, and $\mathscr{S}_1 \perp \cdots \perp \mathscr{S}_k$, then

$$P_{\mathscr{S}_1, \oplus \cdots \oplus \mathscr{S}_k}(A) = P_{\mathscr{S}_1}(A) + \cdots + P_{\mathscr{S}_k}(A)$$

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

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

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

Let $\mathscr{H} = \{<,>_{\Sigma^{-1}}\}$. Suppose $\mathscr{S}_1, \ldots \mathscr{S}_k, \mathscr{S} \leq \mathscr{H}$ such that $\mathscr{S} = \mathscr{S}_1 \oplus \cdots \oplus \mathscr{S}_k$.

Let

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

Then,

1. $w = w_1 + \cdots + w_k$
2. $w_1 \perp\!\!\!\perp \ldots \perp\!\!\!\perp w_k$
3. $w_i \sim \chi^2_{r_i}$
   $w \sim \chi^2_r$
   where r_i is the $dim(\mathscr{S}_i)$, r is the $dim(\mathscr{S})$, and $r = r_1 + \cdots + r_k$.

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.*

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

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,

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

So, let N denote a full sample size.

$$N = m_1 + \cdots + m_n$$

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

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

So,

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

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

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

$$H_O : E(y_i) = 1_{m_i} X_i^T \beta$$
$$H_1 : E(y_i) = 1_{m_i} \mu_i$$

We are testing whether the arbitrary means, $\mu_1, \dots \mu_n$ sit on the same line.

2. ANOVA (1-way)

2.1 Overview

- General linear models
- Scheffe's simulteaneous confidence
- Singular decomposition
- Non Gaussian error

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

- $\bar{X}_{\substack{\vdots \\ i}} - \bar{X}_{\substack{\vdots \\ i}}$

5. Random Effects Model

5.1 Overview

II

Part Two

6. Basic Concepts

6.1 Overview

7. Estimation

7.1 Overview

8. Inference

8.1 Overview

- deviance <-> sum of squares

9. Residuals

9.1 Overview

10. Cetegorical Prediction

10.1 Overview

11. Some Important GLM

11.1 Overview

12. Multivariate GLM

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Part Three

13. Principle Componant Analysis

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14. Canonical Correlation Analysis

14.1 Overview

15. Independent Componant Analysis

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