

Review

X : design matrix

y : output

b : estimated model parameters

also

Φ : design matrix of "features"

where

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \phi_1(x_1) & \phi_2(x_1) & \dots & \phi_p(x_1) \\ \vdots & \vdots & & \vdots \\ \phi_1(x_n) & \phi_2(x_n) & \dots & \phi_p(x_n) \end{bmatrix} \begin{bmatrix} b_1 \\ \vdots \\ b_p \end{bmatrix}$$

Least squares estimate (soln to both LS & ML)

$$b = (X'X)^{-1} X'y \quad (\text{error-free})$$

Estimated fitted values & residuals

$$\hat{y} = Xb \Rightarrow \hat{y} = HY \quad \text{where } H = X(X'X)^{-1}X'$$

residuals

$$e = (I - H)Y$$

and

$$\text{cov}(e) = (I - H) \text{cov}(Y) (I - H)'$$

where if $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$, $\text{cov}(Y) = \sigma^2 I$

and

$$\text{cov}(e) = \sigma^2 (I - H)$$

when we don't know σ^2 we replace it with MSE to yield

$$s^2 \{e\} = \text{MSE}(I - H)$$

$$\text{rank} \left(I - \frac{1}{n} J \right) = \overbrace{\text{rank}(I)}^n - \overbrace{\text{rank} \left(\frac{1}{n} J \right)}^1$$

iff $I - \frac{1}{n} J$ sym. & idempotent

$$\begin{aligned} \left[I - \frac{1}{n} J \right] \left[I - \frac{1}{n} J \right] &= I - \frac{2}{n} J + \frac{1}{n^2} J J \\ &= I - \frac{2}{n} J + \frac{1}{n^2} \begin{bmatrix} n & & & \\ & \ddots & & \\ & & \ddots & \\ & & & n \end{bmatrix} \\ &= I - \frac{1}{n} J \quad \square \end{aligned}$$

$$\text{rank} \left(H - \frac{1}{n} J \right) = \overbrace{\text{rank}(H)}^p - \overbrace{\text{rank} \left(\frac{1}{n} J \right)}^1$$

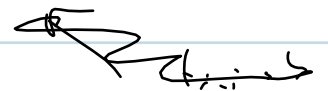
iff $H - \frac{1}{n} J$ sym. & idempotent

$$\begin{aligned} \left[H - \frac{1}{n} J \right] \left[H - \frac{1}{n} J \right] &= \cancel{H - \frac{2}{n} H J - \frac{1}{n} J H + \frac{1}{n^2} J J} \\ &= \cancel{H - \frac{2}{n} H J - \frac{1}{n} J H} \\ &= H - \frac{1}{n} H J - \frac{1}{n} J H + \frac{1}{n^2} J J \\ &= H + \frac{1}{n} J - \frac{1}{n} (H J + J H) \\ &= H + \frac{1}{n} J - \frac{2}{n} H J \end{aligned}$$

$$\begin{aligned} (J' H')' &= (J H)' = H' J' \\ &= H J \end{aligned}$$

~~$\Rightarrow J = H H' J$~~ ~~$(X' X)^{-1} X' Y$~~

symmetrisch & idempotent



ANOVA Sums of squares and Mean squares

$$SSTO = Y' \left[I - \frac{1}{n} J \right] Y$$

$$df = \text{rank} \left(I - \frac{1}{n} J \right) = n - 1$$

$$SSE = Y' (I - H) Y$$

$$df = \text{rank} (I - H) = n - p \quad (\text{if design matrix full col. rank})$$

$$SSR = Y' \left(H - \frac{1}{n} J \right) Y$$

$$df = \text{rank} \left(H - \frac{1}{n} J \right) = p - 1$$

Where we define the mean squares as before (by dividing by df)

$$MSR = SSR / p - 1$$

$$MSE = SSE / n - p$$

$$E[MSE] = \sigma^2$$

$$E[MSR] = \sigma^2 + f(b) \quad \leftarrow \text{positive function of model params}$$

ANOVA table for general linear regression model:

	SS	df	MS
Regression	SSR	p - 1	MSR = SSR / p - 1
Error	SSE	n - p	MSE = SSE / n - p
Total	SSTO	n - 1	

F-test for regression relation

To choose between the alternatives

$$H_0: \beta_1 = \beta_2 = \dots = \beta_{p-1} = 0$$

$$H_a: \text{not all } \beta_k \text{ (} k=1, \dots, p-1 \text{) equal zero}$$

we use the test statistic

$$F^* = MSR / MSE$$

The decision rule to control type I error at α is

$$\text{If } F^* \leq F(1 - \alpha; p - 1, n - p) \text{ conclude } H_0$$

$$\text{else if } F^* > F(1 - \alpha; p - 1, n - p) \text{ " } H_a$$

Standard normal

$$\frac{b_k - \beta_k}{S\{b_k\}} = \frac{b_k - \beta_k}{\sigma\{b_k\}} \div \frac{S\{b_k\}}{\sigma\{b_k\}}$$

Cochran's Thm

$$\frac{\chi^2 (n-p)}{n-p}$$

Note: $\frac{S^2\{b_k\}}{\sigma^2\{b_k\}} = \frac{MSE \cdot (X'X)^{-1}_{kk}}{\sigma^2 (X'X)^{-1}_{kk}} =$

$$\frac{SSE / (n-p)}{\sigma^2}$$

so $\frac{b_k - \beta_k}{S\{b_k\}} \sim \frac{Z}{\sqrt{\frac{\chi^2 (n-p)}{n-p}}}$ independent as well, also by Cochran's Thm.

i.e.

$$\frac{b_k - \beta_k}{S\{b_k\}} \sim t(n-p)$$

Inferences about regression-params

$$\begin{aligned} E[b] &= E[(X'X)^{-1} X'Y] = (X'X)^{-1} X' E[Y] \\ &= (X'X)^{-1} X'X\beta \\ &= \beta \end{aligned}$$

$$\begin{aligned} \text{cov}[b] &= \text{cov}[(X'X)^{-1} X'Y] \\ &= (X'X)^{-1} X' \text{cov}[Y] X (X'X)^{-1} \\ &= \sigma^2 (X'X)^{-1} \end{aligned}$$

$$s^2 \{b\} = \text{MSE} \cdot (X'X)^{-1}$$

Interval estimation of β_k

We can derive

$$\frac{b_k - \beta_k}{s\{b_k\}} \sim t(n-p), \quad k=0, 1, \dots, p-1$$

Hence the confidence limits for β_k with $1-\alpha$ confidence coefficient are:

$$b_k \pm t(1-\alpha/2; n-p) s\{b_k\}$$

Tests for β_k

To test

$$H_0: \beta_k = 0$$

$$H_a: \beta_k \neq 0$$

we may use

$$t^* = \frac{b_k}{s\{b_k\}}$$

and the decision-rule

if $|t^*| \leq t(1-\alpha/2; n-p)$ conclude H_0
else H_a

What does this mean?

Bonferroni: joint confidence intervals can be used to test ~~select~~ multiple multiple coeffs simultaneously.

Interval Estimation of $E\{Y_n\}$

The mean response to be estimated is

$$E\{Y_n\} = X_n' \beta$$

the estimate of this quantity is

$$\hat{Y}_n = X_n' b$$

This estimator is unbiased

$$E\{\hat{Y}_n\} = E\{X_n' b\} = X_n' \beta = E\{Y_n\}$$

The variance of this estimator is

$$s^2\{\hat{Y}_n\} = X_n' \sigma^2 \{b\} X_n$$

$$= \sigma^2 X_n' (X'X)^{-1} X_n$$

when σ^2 unknown we replace it as usual with MSE

$$\Rightarrow s^2\{\hat{Y}_n\} = \text{MSE} (X_n' (X'X)^{-1} X_n)$$

The confidence limits $(1-\alpha)$ for $E\{Y_n\}$ are

$$\hat{Y}_n \pm t(1-\alpha/2; n-p) s\{\hat{Y}_n\}$$

Prediction of New Observation $Y_{n(\text{new})}$

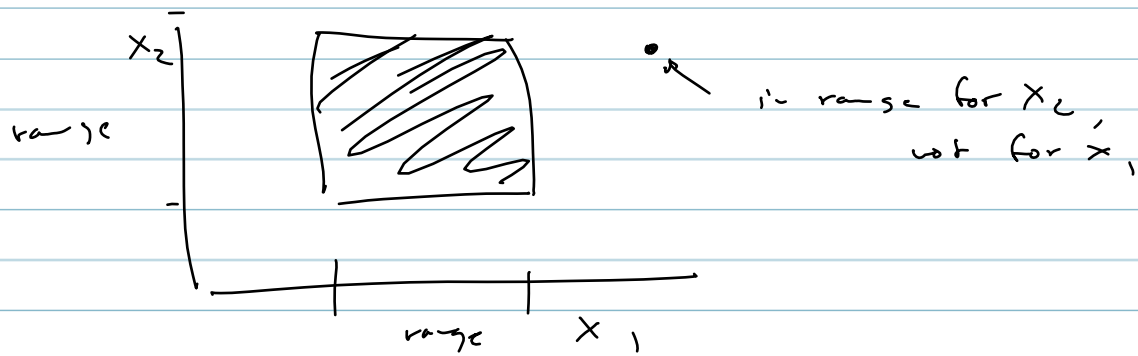
Same as in 1-d case, extra variance

$$\hat{Y}_n \pm t(1-\alpha/2; n-p) s\{\text{pred}\}$$

where

$$\begin{aligned} s^2\{\text{pred}\} &= \text{MSE} + s^2\{\hat{Y}_n\} \\ &= \text{MSE} (1 + X_n' (X'X)^{-1} X_n) \end{aligned}$$

Note Hidden Extrapolations



Meaning of response surface
(take partial derivatives of Y w.r.t. X_1, X_2, \dots)

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n$$