

Model 1: no interactions

(Slide for design matrix)

$$\vec{Y} = X\vec{\beta} + \vec{\varepsilon}$$

$$X_{8 \times (1+3)}$$

-1 low level
+1 high level

$$\vec{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}$$

$2\beta_1$: Effect of
changing temp.
from low to
high level
etc.

Note: orthogonal columns

$$X^T X = n I$$

8

Consequence:

$$\hat{\beta} = (X^T X)^{-1} X^T \vec{Y} = \frac{1}{n} X^T \vec{Y} \quad (\text{estimator})$$

Estimates:

$$\hat{\beta} = \frac{1}{n} X^T \vec{y} \quad \hat{\beta}_0 = \frac{1}{n} \sum y_i = \bar{y}$$

$$\hat{\beta}_1 = \frac{1}{n} \left(\sum_{i=1}^4 y(\text{temp high lev}) - \sum_{i=5}^8 y(\text{temp low lev}) \right)$$

$$\Rightarrow 2\hat{\beta}_1 = \bar{y}_{\text{temp high}} - \bar{y}_{\text{temp low}}$$

$$\hat{\beta} \sim \text{MVN}(\vec{\beta}, \underbrace{\sigma^2 (X^T X)^{-1}}_{\frac{\sigma^2}{n} I})$$

$$\frac{\sigma^2}{n} I$$



independent
 $\hat{\beta}$ -s

→ simplifies interpretation

→ maximizes precision (min. variance)

same var ← all estimates.

Plot 95% ellipsoids

○ $\begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} \sim \text{MVN}(\vec{0}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix})$

◇ $\begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} \sim \text{MVN}(\vec{0}, \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix})$

SLIDE: Two runs

R model summary

Temp: $\hat{\beta}_1 = -2.831$ $2\hat{\beta}_1 = -5.662$

main effects plot ?

How good is the model?

Some repetition

$$S = 28.3$$

$$R^2 = 0.384$$

$$F = 2.493$$

$$s^2 = \frac{SSE}{n-k-1} = \frac{SSE}{12} \rightarrow SSE = 12 \cdot s^2 = \approx 4610$$

$\uparrow \quad \uparrow$
16 3

$$F = \frac{SSR / 3}{SSE / 12} \rightarrow SSR = F \cdot 3 \cdot \frac{SSE}{12} \approx 5990$$

$$SST = SSR + SSE = 15600$$

$$R^2 = \frac{SSR}{SST} \approx 0.38$$

→ Lots of variation in Y not explained by the model (SSR) but left to ε (SSE)

→ Not a very good model for "removal efficiency".

Model 2: interactions

Wast (skip indices)

two factor interactions

$$Y = \mu + T + C + pH + T \cdot C + T \cdot pH + C \cdot pH$$

$$+ T \cdot C \cdot pH + \varepsilon$$

three factor interaction.

$$\vec{Y} = X \vec{\beta} + \vec{\varepsilon}$$

$$\vec{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_{12} \\ \beta_{13} \\ \beta_{23} \\ \beta_{123} \end{pmatrix}$$

main effects

interaction effects

→ slide: X

Note Tmp: Conc → multiply-

→ Slide: model summary

Note: $\hat{\beta}_1 = -2.831$ (as before → all columns orthogonal)

Better model?

$$S = 4.606$$

$$R^2 = 0.9891$$

SST same (15600)

$$\sum (y_i - \bar{y})^2$$

~~Typ~~ SSE ≈ 170 (9610)

$$SSR = 15430$$

model has clearly improved.

Main effect + interaction effect

Plots

$$\hat{\beta}_2 \approx -11$$

conc.

$$\hat{\beta}_{23} \approx 23$$

conc. x
pH

↑ ?

moving from
low to high:

reduce efficiency 22%

If pH low level :

$$2(\hat{\beta}_2 + \hat{\beta}_{23}(-1)) = 2(-11 - 23) = -68\%$$

lower
efficiency
at high
concentration
compared
to low.

If pH high level

$$2(\hat{\beta}_2 + \hat{\beta}_{23}(+1)) = 2(-11 + 23) = 24\%$$

improved
efficiency
high conc.
vs low.

Blocking

One of the effects will
be confounded / aliased with lab.

Choose carefully → often 3-factor
interaction.

Example: Drug dosage

fractional factorial design.

6 drugs, 2 levels

$$2^6 = 64 \text{ combinations.}$$

Too many experiments.

$$2^{6-1} = 32 \text{ runs OK.}$$

which?

Defining rel: $ABCDEF = I$

↳ where 6-factor interaction is I .

(look back to block).

Consequence

$$A = BCDEF$$

$$AB = CDEF$$

$$ABC = DEF$$

main effect
aliased with
5-factor int
two factor int
aliased with
4-factor int.

No tests of sign. but sums of squares.
why it makes sense:

$$SST = SSR + SSE$$

$$SSR = \vec{Y}^T (H - \frac{1}{n} \vec{J}) \vec{Y}$$

$$\frac{1}{n} \vec{J} \vec{Y} = \hat{\beta}_{0j} \vec{1}$$

$$H \vec{Y} = X \underbrace{(X^T X)^{-1} X^T}_{\substack{\text{here} \\ \frac{1}{n} I}} \vec{Y} = X \underbrace{\frac{1}{n} X^T \vec{Y}}_{\hat{\beta}}$$

$$\begin{aligned} \vec{Y}^T (X \hat{\beta} - \hat{\beta}_{0j} \vec{1}) &= n \hat{\beta}^T \hat{\beta} - n \hat{\beta}_0^2 \\ &= n \hat{\beta}_1^2 + n \hat{\beta}_2^2 + \dots \end{aligned}$$

Variance explained by factor A:

$$\frac{n \hat{\beta}_1^2}{SST}$$