

LM, LNp. 7-1~2 → Residual Analysis: Theory

- Theory: define the **residual** for the i^{th} observation (x_i, y_i) as

$$\hat{\epsilon}_i = r_i = y_i - \hat{y}_i, \quad \hat{y}_i = \mathbf{x}_i^T \hat{\beta}$$

$\hat{\epsilon}_i$ often used to check assumptions:

\hat{y}_i contains information given by the model; r_i is the "difference" between y_i (observed) and \hat{y}_i (fitted) and contains information on possible model inadequacy.

① ϵ_i 's $\sim N(0, \sigma^2)$
 ② $E(Y) = X\beta$ is a correct mean structure

- Vector of residuals $\mathbf{r} = (r_1, \dots, r_N)^T = \mathbf{y} - \mathbf{X}\hat{\beta} = (\mathbf{I} - \mathbf{H})\mathbf{y}$

- Under the model assumption $E(\mathbf{y}) = \mathbf{X}\beta$, it can be shown that

(a) $E(\mathbf{r}) = \mathbf{0}$, $\mathbf{r} \perp \hat{\mathbf{y}}$ i.e., $X\beta$ is correct model

(b) \mathbf{r} and $\hat{\mathbf{y}}$ are independent,

Note: variance of r_i
 $\propto 1 - h_i$ (leverage) = $1 - H_{ii}$
 \propto Mahalanobis dist. btwn design pts & $\bar{\mathbf{x}}$

overall pattern individual observation (outlier)

(c) variances of r_i are nearly constant for "nearly balanced" designs.
 $\text{cov}(\mathbf{r}) = \sigma^2(\mathbf{I} - \mathbf{H})$

① $\mathbf{Y} = \mathbf{X}\beta + \epsilon = \hat{\mathbf{Y}} + \hat{\epsilon}$

② $\mathbf{Y} = \mathbf{X}_1\beta_1 + \mathbf{X}_2\beta_2 + \epsilon = (\mathbf{X}_1\beta_1 + \mathbf{H}_1\mathbf{X}_2\beta_2) + ((\mathbf{I} - \mathbf{H}_1)\mathbf{X}_2\beta_2 + \epsilon) = \hat{\mathbf{Y}}_{X_1} + \hat{\epsilon}_{X_1}$

Under fitted model: $\mathbf{Y} = \mathbf{X}_1\beta_1 + \epsilon^*$ ($\mathbf{H}_1 = \mathbf{X}_1(\mathbf{X}_1^T\mathbf{X}_1)^{-1}\mathbf{X}_1^T$)

$\sigma_x \leftrightarrow \mu_x$

Residual Plots ← LM, LNp. 7-7~9

- Plot r_i vs. \hat{y}_i (see Figure 1): It should appear as a parallel band around 0. Otherwise, it would suggest model violation. If spread of r_i increases as \hat{y}_i increases, error variance of y increases with mean of y . May need a transformation of y . (Will be explained in future lecture.)

- Plot r_i from replicates per treatment (see Figure 2): to see if error variance depends on treatment.

qualitative factor

Box plots

Note: saturated model

\hat{r} vs. predictor

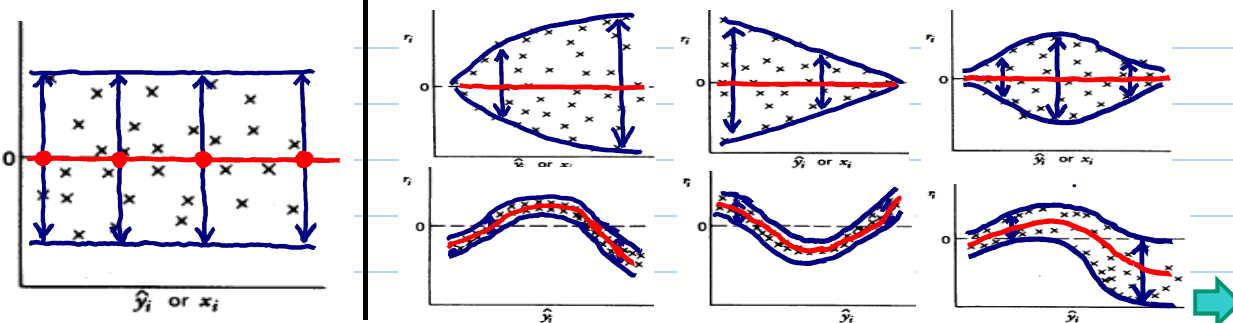
- Plot r_i vs. x_i : If not a parallel band around 0, relationship between y_i and x_i not fully captured, revise the $\mathbf{X}\beta$ part of the model.

quantitative factor

- Plot r_i vs. time sequence: to see if there is a time trend or autocorrelation over time.

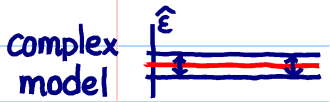
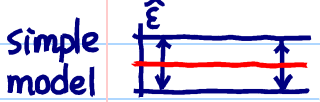
if available (or run order, measure order, ...)

null plot



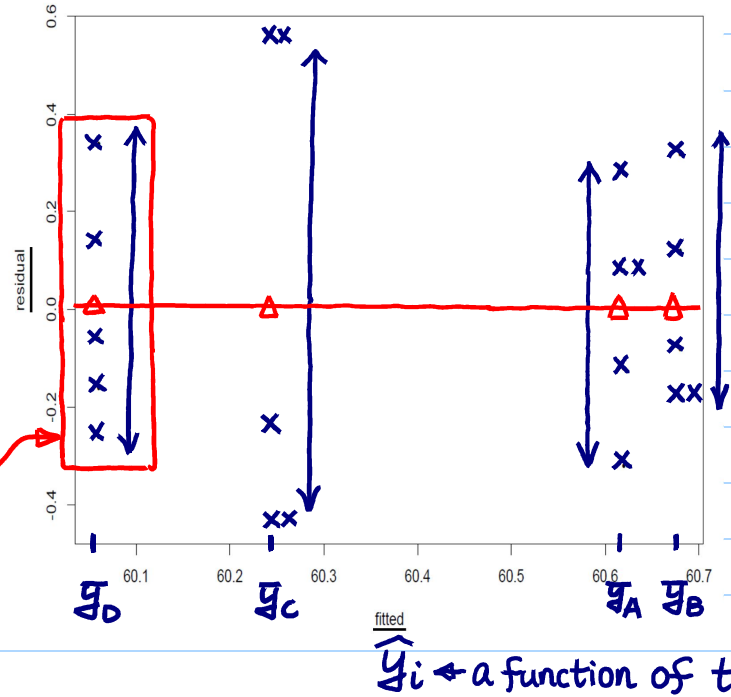


no replicate data



Plot of r_i vs. \hat{y}_i

replicates
allow "pure error" variance estimation



$\hat{y}_i \leftarrow$ a function of treatments A,B,C,D

Figure 1: r_i vs. \hat{y}_i , Pulp Experiment

LNp.1

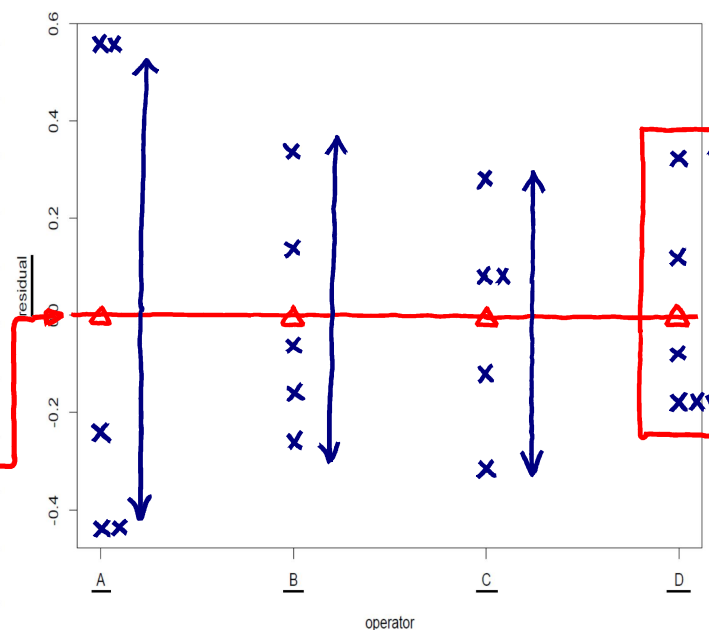


Plot of r_i vs. treatment

fitted model: saturated

Same 4 groups of residuals as in the residual plot of r_i vs. \hat{y}_i (LNp.3-24)

no need to check the trend in the mean of residuals



$$\sum_j \hat{\epsilon}_{ij} = 0 \text{ for any } i$$

$$X = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Figure 2: r_i vs. treatment, Pulp Experiment

LNp.1

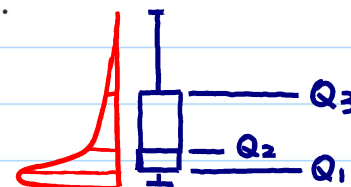
$Y_1, \dots, Y_n \text{ iid} \sim \text{cdf } F$ ← **Box-(Whisker) Plot**

- A powerful graphical display (due to Tukey) to capture the location, dispersion, skewness and extremity of a distribution. See Figure 3. ↖ LNP 27
- $Q_1 =$ lower quartile (25% quantile), $Q_3 =$ upper quartile (75% quantile), $Q_2 =$ median (50% quantile, estimate of location parameter) is the white line in the box. Q_1 and Q_3 are boundaries of the black box.
- $IQR =$ interquartile range (length of box) = $Q_3 - Q_1$: measure of dispersion.
- Minimum and maximum of observed values within

$$[Q_1 - 1.5 \times IQR, Q_3 + 1.5 \times IQR]$$

are denoted by two whiskers. Any values outside the whiskers are regarded as extreme values and displayed (possible outliers).

- If Q_1 and Q_3 are not symmetric around the median, it indicates skewness.
- Side-by-side box plots (LNP. 3-2~3) are useful to compare the difference between the distributions of several groups of data.



Box-(Whisker) Plot

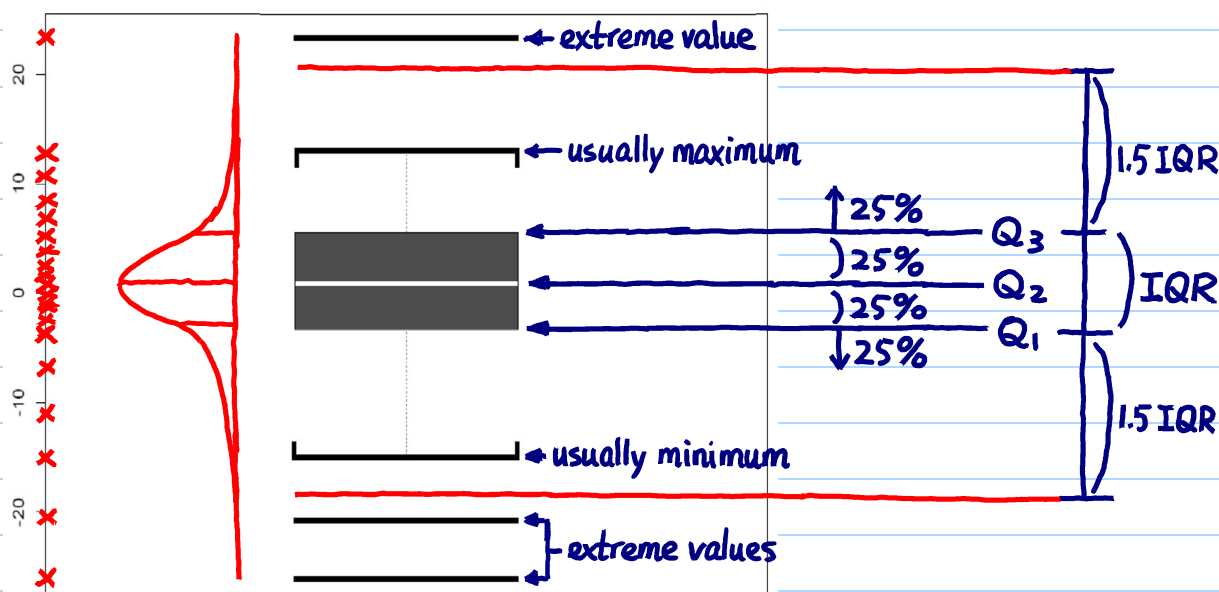


Figure 3: Box-Whisker Plot

Normal Probability Plot ← Q-Q plot (LM, LNp.7-15 ~16)

Original purpose : To test if a distribution is normal, e.g., if the residuals follow a normal distribution (see Figure 5). Q: Why need normality for error?
 can be used to identify outlier ↗ LNp.30

More powerful use in factorial experiments (discussed in Units 5 and 6).

used to identify significant effects β_i 's ← replace t-tests

- Let $r_{(1)} \leq \dots \leq r_{(N)}$ be the ordered residuals. The cumulative probability for $r_{(i)}$ is $p_i = (i - 0.5)/N$. Thus the plot of p_i vs. $r_{(i)}$ should be S-shaped as in Figure 4(a) if the errors are normal. By transforming the scale of the horizontal axis, the S-shaped curve is straightened to be a line (see Figure 4(b)).
true cdf ↗
empirical cdf ↗

• Normal probability plot of residuals :

$$\left(\Phi^{-1} \left(\frac{i - 0.5}{N} \right), r_{(i)} \right), \quad i = 1, \dots, N, \quad \Phi = \text{normal cdf.}$$

If the errors are normal, it should plot roughly as a straight line. See Figure 5.

↗ LNp.30

Regular and Normal Probability Plots of Normal

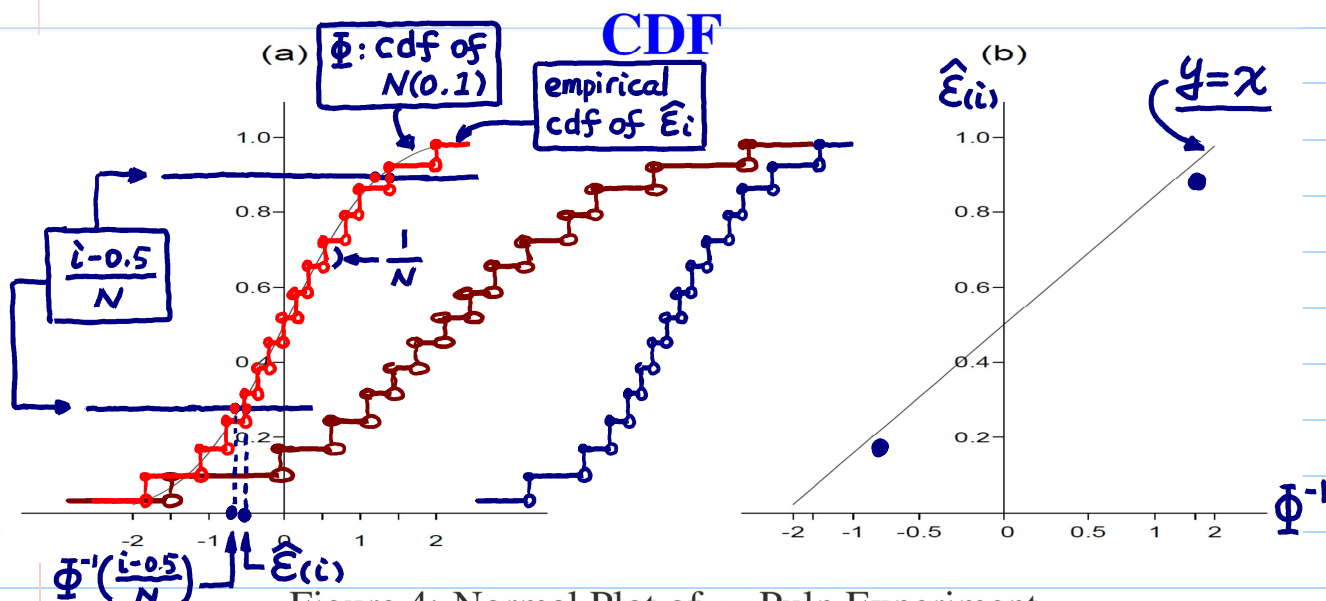


Figure 4: Normal Plot of r_i , Pulp Experiment

$$Z_1, \dots, Z_N \text{ iid } \sim N(\mu, \sigma^2)$$

$$Z_i = \sigma W_i + \mu \Leftrightarrow W_i = (Z_i - \mu) / \sigma \text{ iid } \sim N(0, 1)$$

Normal probability plot of W_i 's $\Rightarrow W_{(i)}$ vs. Φ^{-1} : $y = x$

Normal probability plot of Z_i 's $\Rightarrow Z_{(i)}$ vs. Φ^{-1} : $y = \sigma x + \mu$

Normal Probability Plot : Pulp Experiment

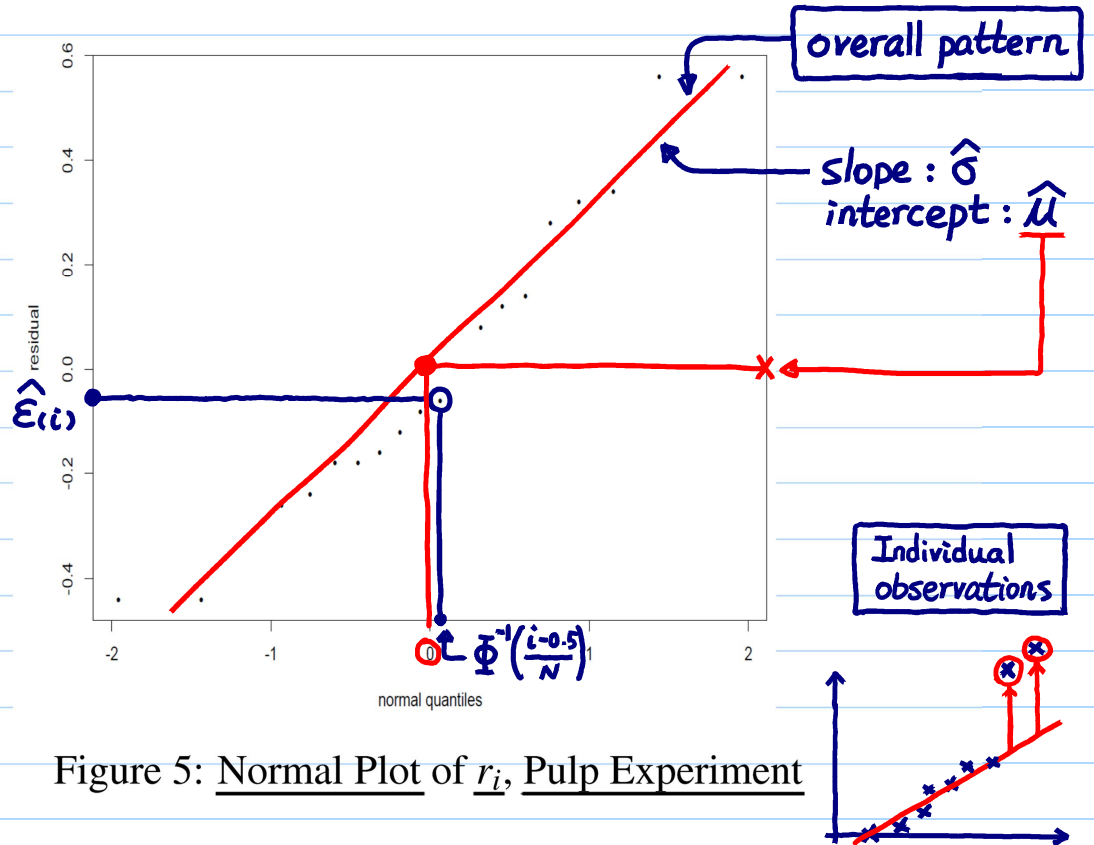


Figure 5: Normal Plot of r_i , Pulp Experiment

❖ Reading: textbook, 2.6

Pulp Experiment Revisited

LNp.1

- Compare the 2 scenarios
- (S1) plant has only 4 operators (or only interested in these 4 operators)

effects of operators

τ_i 's: parameters (unknown fixed values)

after sampling & conditioning

interest: difference btwn the 4 specific τ_i 's

cf.

(S2) 4 operators randomly sampled from a

before sampling

large population of operators

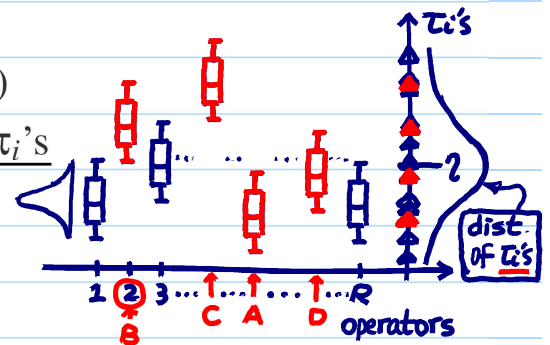
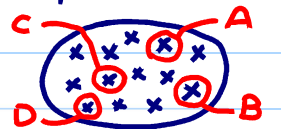
τ_i 's: random variables

$\mu_i = E(y_{ij})$

interest: difference btwn all operators in this population

Q: Are A, B, C, D a representative sample of the population?

population



- In the pulp experiment the effects τ_i are called fixed effects because the interest was in comparing the four specific operators in the study. If these four operators were chosen randomly from the population of operators in the plant, the interest would usually be in the variation among all operators in the population. Because the observed data are from operators randomly selected from the population, the variation among operators in the population is referred to as random effects. conditioned on these 4 operators

One-way random effects model (REM \leftarrow cf. \rightarrow FEM) : fixed effect model

FEM in LNp.3-4&3-8 $\xrightarrow{cf.}$ $y_{ij} = \eta + \tau_i + \epsilon_{ij}$ $\xrightarrow{cf.}$ whole- & sub-plot errors in LNp.4-47~48

$y_{ij} \sim N(\eta, \sigma_\tau^2 + \sigma^2)$

where ϵ_{ij} 's: independent error terms with $N(0, \sigma^2)$,
 τ_i 's: independent $N(0, \sigma_\tau^2)$,
 and τ_i and ϵ_{ij} are independent (Why? Give an example.);
 σ^2 and σ_τ^2 are the two variance components of the model. **check Σ^***

The variance among operators in the population is measured by σ_τ^2 .

REM:
 (1) $E(Y) = \eta \mathbf{1}$
 (2) $cov(y_{11}, y_{12}) = cov(\eta + \tau_1 + \epsilon_{11}, \eta + \tau_1 + \epsilon_{12}) = \sigma_\tau^2$
 $cov(y_{11}, y_{21}) = cov(\eta + \tau_1 + \epsilon_{11}, \eta + \tau_2 + \epsilon_{21}) = 0$

FEM: y_{ij} indep. $N(\eta + \tau_i, \sigma^2)$
 (1) $E(Y) = X\beta \leftarrow \eta + \tau_i$
 (2) $cov(Y) = \sigma^2 I$

Σ^* relationship btwn Y & X
 $\Sigma^* = \sigma_\tau^2 \mathbf{1}\mathbf{1}^T + \sigma^2 I$
 $\Sigma^* = \sigma_\tau^2 \begin{bmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \dots & 1 \end{bmatrix} + \sigma^2 \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix}$

$Y = \begin{bmatrix} y_{11} \\ \vdots \\ y_{1n_1} \\ y_{21} \\ \vdots \\ y_{2n_2} \\ \vdots \\ y_{k1} \\ \vdots \\ y_{kn_k} \end{bmatrix}$

One-way Random Effects Model: ANOVA \leftarrow cf. \rightarrow $H_0: \sigma_\tau^2 = 0$ in LNp.4-63

In the following, assume $n_1 = \dots = n_k = n$.
 The null hypothesis for the FEM:
 $H_0: \tau_1 = \dots = \tau_k$
 should be replaced by $H_0^*: \sigma_\tau^2 = 0$.
 Under H_0^* , the F-test and the ANOVA table in LNp. 3-6 still holds.

$Y \sim N(\eta \mathbf{1}, \Sigma^*)$

Ω (dim = k) $\text{span}\{\mathbf{1}\} = \omega$ (dim = 1)

P_0, P_1, P_2 : projection matrix onto $\Omega, \Omega^\perp, \omega, \omega^\perp$

Ω^\perp, Ω : different eigenspace of Σ^*
 $\sigma^2, n\sigma_\tau^2 + \sigma^2$: eigenvalue (exercise, use the vectors in LNp.3-4)

Reason: under H_0^* ,
 (under H_0^*) $SSTr \sim \sigma^2 \chi_{k-1}^2$,
 and
 (under H_0^* & H_A^*) $SSE \sim \sigma^2 \chi_{N-k}^2$,
 and they are independent.
 Therefore the F-test has the distribution $F_{k-1, N-k}$ under H_0^* .

$E(P_0 Y) = P_0 \eta \mathbf{1} = \eta \mathbf{1}$
 $E(P_1 Y) = E(P_2 Y) = 0$

$SSTr = \|P_1 Y\|^2 = \sum_i n (\bar{y}_i - \bar{y}_..)^2 \sim (n\sigma^2 + \sigma^2) \chi_{k-1}^2$
 $\sqrt{n} \bar{y}_i = \sqrt{n} (\eta + \tau_i + \bar{\epsilon}_i) \stackrel{iid}{\sim} N(\sqrt{n}\eta, n\sigma^2 + \sigma^2)$
 $\bar{y}_.. = \bar{y}_i$ **check LNp.36**

$SSE = \|P_2 Y\|^2 = \sum_i \sum_j (y_{ij} - \bar{y}_i)^2 \sim \sigma^2 \chi_{N-k}^2$
 $\sim \sigma^2 \chi_{n-1}^2$ $k(n-1)$

$cov(P_1 Y, P_2 Y) = P_1 cov(Y) P_2^T = P_1 \Sigma^* P_2^T = 0$
 columns of P_1 & P_2 are eigenvectors of Σ^* & $P_1 P_2 = 0$

ANOVA Tables ($n_i = n$)

- We can apply the same ANOVA and F-test in the fixed effects case for analyzing data.
 - same test statistic
 - same null dist

ANOVA table (FEM) in LNp.3-6

Source	d.f.	SS	MS
treatment	$k - 1$	$SSTr$	$MSTr = \frac{SSTr}{k-1}$
residual	$N - k$	SSE	$MSE = \frac{SSE}{N-k}$
total	$N - 1$		

different \leftarrow cf. $E(MS)$ in LNp.3-6

Under $H_0^* UH_0^*$

Under H_0^* , $\sigma_\tau^2 = 0$
 $E(MSTr) = \sigma^2$

ANOVA result (FEM) in LNp.3-7

Pulp Experiment				
Source	d.f.	SS	MS	E(MS)
treatment	3	1.34	0.447	$\sigma^2 + 5\sigma_\tau^2$
residual	16	1.70	0.106	σ^2
total	19	3.04		

- However, we need to compute the expected mean squares under the alternative of $\sigma_\tau^2 > 0$,
 - for sample size determination, and
 - to estimate the variance components. (σ_τ^2 & σ^2)

Expected Mean Squares for Treatments

- Equation (1) holds independent of σ_τ^2 ,

(LNp.3-33) $\sigma^2 \chi_{N-k}^2 \sim$

$$E(MSE) = E\left(\frac{SSE}{N-k}\right) = \sigma^2$$

$SSE/N-k$: an unbiased estimator of σ^2

SSE only contains information of error var. component σ^2 (1)

- Under the alternative: $\sigma_\tau^2 > 0$, and for $n_i = n$,

(LNp.3-33) $(n\sigma_\tau^2 + \sigma^2) \chi_{k-1}^2 \sim$

$$E(MSTr) = E\left(\frac{SSTr}{k-1}\right) = \sigma^2 + n\sigma_\tau^2$$

$$E\left(\frac{\frac{SSTr}{k-1} - \frac{SSE}{N-k}}{n}\right) = \sigma_\tau^2$$

an unbiased estimator of σ_τ^2 (2)

- For unequal n_i 's, n in (2) is replaced by

$$n' = \frac{1}{k-1} \left[\sum_{i=1}^k n_i - \frac{\sum_{i=1}^k n_i^2}{\sum_{i=1}^k n_i} \right]$$

(exercise) use (o) in LNp.3-33

$SSTr$ contains information about factor var. component σ_τ^2 error var. component σ^2

(cf. $E(SSTr)$ of FEM in LNp.3-6)



$y_{ij} = \tau + \tau_i + \epsilon_{ij}$

Proof of (2)

$z_1, \dots, z_k \stackrel{i.i.d.}{\sim} N(\mu, \sigma^2)$
 $\frac{\sum_{i=1}^k (z_i - \bar{z})^2}{\sigma^2} \sim \chi_{k-1}^2$
 $\Rightarrow \sum_{i=1}^k (z_i - \bar{z})^2 \sim \sigma^2 \chi_{k-1}^2$

$\frac{\tau + \tau_i + \bar{\epsilon}_i - \tau - \bar{\tau} - \bar{\epsilon}_{..}}{\bar{y}_i - \bar{y}_{..}} = (\tau_i - \bar{\tau}) + (\bar{\epsilon}_i - \bar{\epsilon}_{..})$

LNp 3-5

$E(SSTr) = \sum_{i=1}^k n (\bar{y}_i - \bar{y}_{..})^2$
 $= n \left\{ \sum_{i=1}^k (\tau_i - \bar{\tau})^2 + \sum_{i=1}^k (\bar{\epsilon}_i - \bar{\epsilon}_{..})^2 + 2 \sum_{i=1}^k (\bar{\epsilon}_i - \bar{\epsilon}_{..})(\tau_i - \bar{\tau}) \right\}$

The cross product term has mean 0 (because τ and ϵ are independent). It can be shown that

$E\left(\sum_{i=1}^k (\tau_i - \bar{\tau})^2\right) = (k-1)\sigma_\tau^2$ and $E\left(\sum_{i=1}^k (\bar{\epsilon}_i - \bar{\epsilon}_{..})^2\right) = \frac{(k-1)\sigma^2}{n}$
 (iid $N(0, \sigma_\tau^2)$ average of τ_i 's) (iid $N(0, \sigma^2/n)$ average of $\bar{\epsilon}_i$'s)

Therefore

$E(SSTr) = \frac{n(k-1)\sigma_\tau^2}{n} + (k-1)\sigma^2 \xrightarrow{cf.} In FEM (LNp. 3-6)$
 $E(MSTr) = E\left(\frac{SSTr}{k-1}\right) = \sigma^2 + n\sigma_\tau^2$
 $E(SSTr) = n \cdot \sum_i (\tau_i - \bar{\tau})^2 + (k-1)\sigma^2$



Variance components: estimation of σ^2 and σ_τ^2

- From equations (1) and (2) in LNp. 3-35, we obtain the following unbiased estimates of the variance components:

Same as the $\hat{\sigma}^2$ in FEM

$\hat{\sigma}^2 = MSE$ and $\hat{\sigma}_\tau^2 = \frac{MSTr - MSE}{n}$
 (Note: $\sigma_\tau^2 \geq 0$)

Note that $\hat{\sigma}_\tau^2 \geq 0$ if and only if $MSTr \geq MSE$, which is equivalent to $F \geq 1$. Therefore a negative variance estimate $\hat{\sigma}_\tau^2$ occurs only if the value of the F statistic is less than 1. Obviously the null hypothesis H_0 is not rejected when

$E(F_{n_1, n_2}) = \frac{n_2}{n_2 - 2}$

$F \leq 1$. Since variance cannot be negative, a negative variance estimate is replaced by 0. This does not mean that σ_τ^2 is zero. It simply means that there is not enough information in the data to get a good estimate of σ_τ^2 . not "accept H_0 "

$H_0: \sigma_\tau^2 = 0$

- For the pulp experiment, $n = 5$, $\hat{\sigma}^2 = 0.106$, $\hat{\sigma}_\tau^2 = (0.447 - 0.106)/5 = 0.068$, i.e., sheet-to-sheet variance (within same operator) is 0.106, which is about 50% higher than operator-to-operator variance 0.068.

Implications on process improvement: try to reduce the two sources of variation, also considering costs.

a property of operator population

check graph in LNp 3-31

Estimation of Overall Mean η ← the only fixed effect in REM

- In REM, η , the population mean, is often of interest.

From $E(y_{ij}) = \eta$, we use the estimate

the intercept parameter in FEM is usually of no interest

In FEM, $E(y_{ij}) = \mu_i = \tau + \tau_i$

For balanced data, GLS = OLS

same as the $\hat{\eta}$ in FEM under sum coding, but in the case of FEM $\tau = (\mu_1 + \dots + \mu_k) / k$

- $Var(\hat{\eta}) = Var(\bar{\tau} + \bar{\epsilon}_{..}) = \frac{\sigma_{\tau}^2}{k} + \frac{\sigma^2}{N}$, where $N = \sum_{i=1}^k n_i$.

$\hat{\eta} = \bar{y}_{..} = \tau + \bar{\tau}_{.} + \bar{\epsilon}_{..} \sim N(\tau, \sigma^2/k + \sigma^2/N) \rightarrow = E(MSTr)$

pivotal quantity $\frac{\bar{y}_{..} - \tau}{se(\hat{\eta})}$

For $n_i = n$, $Var(\hat{\eta}) = \frac{\sigma_{\tau}^2}{k} + \frac{\sigma^2}{nk} = \frac{1}{nk} (\sigma^2 + n\sigma_{\tau}^2)$.

$se(\hat{\eta}) = \sqrt{\frac{MSTr}{nk}}$

Using (2) in LNp.3-35, $\frac{MSTr}{nk}$ is an unbiased estimate of $Var(\hat{\eta})$.

Confidence interval for η : $\bar{y}_{..}$ and $MSTr$ are indep. (LNp 33)

$SSTr \sim (\sigma^2 + n\sigma_{\tau}^2) \chi_{k-1}^2$

estimate \pm (critical value) \times s.e. (estimate)

$\hat{\eta} \pm t_{k-1, \frac{\alpha}{2}} \sqrt{\frac{MSTr}{nk}}$

In FEM (under sum coding) C.I. for τ :

$\bar{y}_{..} \pm t_{N-k, \frac{\alpha}{2}} \sqrt{\frac{MSE}{N}}$

- In the pulp experiment, $\hat{\eta} = 60.40$, $MSTr = 0.447$, and the 95% confidence interval for η is

$SSE \sim \sigma^2 \chi_{N-k}^2$

compare REM and Split-plot design (LNp 4-45~66, future lecture)

$60.40 \pm 3.182 \sqrt{\frac{0.447}{5 \times 4}} = [59.92, 60.88]$

❖ Reading: textbook, 2.5