STOR 664: APPLIED STATISTICS I Instructor: Richard L. Smith

Class Notes: November 29, 2022



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Class Announcements

- Take-home exam: will be set 6:00 am 9:00 pm Saturday, December 3, but with a 6-hour time limit
- Make-up exam: 12:00 pm 6:00 pm Sunday, December 4 (by prior arrangement)
- Past exams with solutions are on course webpage
- Usual Honor Code rules apply: no consulting with other class members or any outside person but me
- Review session 5:00 pm 6:00 pm Thursday, December 1 (room TBA)
- Final assignment due today (gradescope)
- Project also due today (gradescope or email)
- Office hour today: 2:00-3:00 pm (note change of usual time)
- Grades will be announced a.s.a.p. but won't be immediate (please check HW scores on gradescope)
- If I agreed to write a letter of recommendation for you and have not done so, please let me know
- Please complete CAS survey!

Chapter 8: Analysis of Designed Experiments

Basic definitions:

- Units, e.g. people, plots of land, industrial experiments
- Treatments, e.g. medical, fertilizer, temperature of an industrial process
- Blocks: other variables that affect the outcome but are not of direct interest (e.g. in medical studies, sex, age, race, prior medical condition
- Interactions arise when treatments perform better in some blocks than others

All involve *factor* (i.e. non-numeric) variables

Typically represent factors as 0-1 variables, e.g.

$$x_{ij} = \begin{cases} 1 & \text{if unit } i \text{ is at level } j \\ 0 & \text{otherwise} \end{cases}$$

Use model.matrix to see representation in R

Completely Randomized Experiments (One-Way ANOVA)

Let y_{ij} be *j*th observation on treatment *i*, $1 \le j \le n_i$, $1 \le i \le r$ $(n = \sum_{i=1}^r n_i \text{ is total sample size})$

Model $y_{ij} = \mu_i + \epsilon_{ij}$ or $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$ where $\epsilon_{ij} \sim \mathcal{N}(0, \sigma^2)$ (independent)

LSE
$$\hat{\mu}_i = \overline{y}_{i\cdot} = \frac{\sum_j y_{ij}}{n_i} = \hat{\mu} + \hat{\alpha}_i.$$

Overdetermined, need a constraint:

•
$$\sum_{i} n_i \alpha_i = 0$$
, leads to $\hat{\mu} = \frac{\sum_i \sum_j y_{ij}}{n} = \bar{y}_{..}, \ \hat{\alpha}_i = \bar{y}_{i.} - \bar{y}_{..}$

- Set $\hat{\mu} = 0$, $\hat{\alpha}_i = \bar{y}_i$.
- Fix $\alpha_1=0$, $\widehat{\mu}=\overline{y}_{1\cdot},\ \widehat{\alpha}_i=\overline{y}_{i\cdot}-\overline{y}_{1\cdot}.$
- Last one is default in R but can change this with statements like op = options(contrasts = c("contr.helmert", "contr.poly"))

ANOVA Table

$$SSTO = \sum_{i} \sum_{j} (y_{ij} - \overline{y}_{..})^{2}$$
$$= \sum_{i} \sum_{j} (y_{ij} - \overline{y}_{i.})^{2} + \sum_{i} n_{i} (\overline{y}_{i.} - \overline{y}_{..})^{2}$$
$$= SSE + SSTR$$

(DFs:) n-1 = (n-r) + (r-1)

Estimate $s^2 = \frac{SSE}{n-r}$, test the null hypothesis H_0 that all means are equal by

$$F = \frac{SSTR/(r-1)}{SSE/(n-r)} \sim F_{r-1,n-r} \text{ if } H_0 \text{ true.}$$

Reject H_0 at level α if $F > F_{r-1,n-r,1-\alpha}$ (in R: qf(1-alpha,r-1,n-r)

Testing Equality of Variances

Model $y_{ij} \sim \mathcal{N}(\mu_i, \sigma_i^2), i = 1, \dots, r, j = 1, \dots, n_i,$ test $H_0: \sigma_1^2 = \dots = \sigma_r^2$

1. Likelihood Ratio Test

Estimate
$$\hat{\sigma}_i^2 = \frac{\sum_j (y_{ij} - \bar{y}_{i\cdot})^2}{n_i}$$
, $\hat{\sigma}^2 = \frac{\sum_i \sum_j (y_{ij} - \bar{y}_{i\cdot})^2}{n}$, define

$$T = 2\log\frac{L_1}{L_0} = \sum_{i=1}^r n_i \log\frac{\hat{\sigma}^2}{\hat{\sigma}_i^2} \sim \chi_{r-1}^2 \text{ asymptotically}$$

2. Bartlett's Modification (1937)

- (a) Replace n_i by $n_i 1$, n by n r in definitions of $\hat{\sigma}_i^2$, $\hat{\sigma}^2$ and T.
- (b) Define $T' = \left\{1 + \frac{1}{3(r-1)} \sum_{i=1}^{r} \left(\frac{1}{n_i 1} \frac{1}{n-r}\right)\right\}^{-1} T$

(c) If H_0 true, $T' \sim \chi^2_{r-1}$ approximately.

Round-robin test data

| Laboratory i | n_i | Mean | S.D. | S_i | \widehat{lpha}_i | S.E. |
|--------------|-------|-------|------|---------|--------------------|------|
| 1 | 5 | 102.1 | 48.1 | 9254.44 | | |
| 2 | 9 | 92.8 | 8.3 | 551.12 | | |
| 3 | 4 | 97.2 | 8.6 | 221.88 | | |
| 4 | 5 | 79.9 | 9.2 | 338.56 | | |
| 5 | 5 | 87.0 | 4.8 | 92.16 | | |
| 6 | 5 | 93.1 | 5.5 | 121.00 | | |
| 7 | 5 | 82.2 | 4.4 | 77.44 | | |
| 8 | 6 | 54.9 | 1.9 | 18.05 | | |
| 9 | 5 | 94.0 | 8.3 | 275.56 | | |
| 10 | 5 | 90.4 | 2.2 | 19.36 | | |
| 11 | 5 | 84.7 | 5.7 | 129.96 | | |

p-value for equality of variances: 1.3×10^{-12} p-value for equality of means: 0.0007

Round-robin test data

| Laboratory i | n_i | Mean | S.D. | S_i | \widehat{lpha}_i | S.E. |
|--------------|-------|------|------|--------|--------------------|------|
| | | | | | | |
| 2 | 9 | 92.8 | 8.3 | 551.12 | | |
| 3 | 4 | 97.2 | 8.6 | 221.88 | | |
| 4 | 5 | 79.9 | 9.2 | 338.56 | | |
| 5 | 5 | 87.0 | 4.8 | 92.16 | | |
| 6 | 5 | 93.1 | 5.5 | 121.00 | | |
| 7 | 5 | 82.2 | 4.4 | 77.44 | | |
| 8 | 6 | 54.9 | 1.9 | 18.05 | | |
| 9 | 5 | 94.0 | 8.3 | 275.56 | | |
| 10 | 5 | 90.4 | 2.2 | 19.36 | | |
| 11 | 5 | 84.7 | 5.7 | 129.96 | | |

p-value for equality of variances: 0.05 p-value for equality of means: 7×10^{-13}

Round-robin test data

| Laboratory i | n_i | Mean | S.D. | S_i | \widehat{lpha}_i | S.E. |
|--------------|-------|------|------|--------|--------------------|------|
| | | | | | | |
| 2 | 9 | 92.8 | 8.3 | 551.12 | 3.62 | 2.06 |
| 3 | 4 | 97.2 | 8.6 | 221.88 | 8.02 | 3.28 |
| 4 | 5 | 79.9 | 9.2 | 338.56 | -9.28 | 2.90 |
| 5 | 5 | 87.0 | 4.8 | 92.16 | -2.18 | 2.90 |
| 6 | 5 | 93.1 | 5.5 | 121.00 | 3.92 | 2.90 |
| 7 | 5 | 82.2 | 4.4 | 77.44 | -6.98 | 2.90 |
| | | | | | | |
| 9 | 5 | 94.0 | 8.3 | 275.56 | 4.82 | 2.90 |
| 10 | 5 | 90.4 | 2.2 | 19.36 | 1.22 | 2.90 |
| 11 | 5 | 84.7 | 5.7 | 129.96 | -4.48 | 2.90 |

p-value for equality of variances: 0.18 p-value for equality of means: 0.003

Conclusions

- We threw out Lab 1 because the SD seemed obviously wrong

 either Bartlett or Likelihood Ratio test decisively rejects
 hypothesis of equal variances
- We then threw out Lab 8 because the mean was discrepant
 F-test decisively rejects hypothesis of equal means
- Among the rest, estimated treatment effect is significantly positive for Lab 3, negative for Labs 4 and 7
- However we could develop the last point in more detail with more formal multiple comparisons procedures — Least Significant Differences, Tukey test for pairwise differences, Scheffé test for contrasts (assuming equal variances)

Two-way ANOVA Without Interactions

$$y_{ij} = \mu + \alpha_i + \beta_j + \epsilon_{ij}, \ 1 \le i \le r, \ 1 \le j \le c.$$

Assume $\sum_{i} \alpha_{i} = \sum_{j} \beta_{j} = 0$ (but default in R is $\alpha_{1} = \beta_{1} = 0$) Equality of treatments H_{0} : $\alpha_{1} = \ldots = \alpha_{r} = 0$ Equality of blocks H'_{0} : $\beta_{1} = \ldots = \beta_{c} = 0$ Typically, H_{0} is of interest but H'_{0} is not

ANOVA decomposition:

$$\sum_{i} \sum_{j} (y_{ij} - \bar{y}_{..})^{2} = \sum_{i} \sum_{j} (y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})^{2} + c \sum_{i} (\bar{y}_{i.} - \bar{y}_{..})^{2} + r \sum_{j} (\bar{y}_{.j} - \bar{y}_{..})^{2}$$

$$= \sum_{i} \sum_{j} (y_{ij} - \hat{\mu} - \hat{\alpha}_{i} - \hat{\beta}_{j})^{2} + c \sum_{i} \hat{\alpha}_{i}^{2} + r \sum_{j} \hat{\beta}_{j}^{2},$$

$$SSTO = SSE + SSTR + SSB$$

$$rc - 1 = (r - 1)(c - 1) + (c - 1) + (r - 1)$$

F test for H_0 :

$$\frac{SSTR/(c-1)}{SSE/((r-1)(c-1))} \sim F_{c-1,(r-1)(c-1)} \text{ if } H_0 \text{ true.}$$

Two-way ANOVA With Interactions

Assume t > 1 observations for each treatment-block pair

 $y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \epsilon_{ijk}, \ 1 \le i \le r, \ 1 \le j \le c, \ 1 \le k \le t.$

Assume $\sum_{i} \alpha_{i} = \sum_{j} \beta_{j} = 0$, $\sum_{j} \gamma_{ij} = 0$ for each i, $\sum_{i} \gamma_{ij} = 0$ for each j. $\hat{\mu} = \bar{y}_{\dots}$, $\hat{\alpha}_{i} = \bar{y}_{i\dots}$, $\hat{\beta}_{j} = \bar{y}_{\cdot j \cdot}$, $\hat{\gamma}_{ij} = \bar{y}_{ij \cdot}$.

ANOVA decomposition becomes

$$SSTO = SSE + SSI + SSTR + SSB$$

$$rct - 1 = rc(t - 1) + (r - 1)(c - 1) + (c - 1) + (r - 1)$$

F test for no treatment effect:

$$\frac{SSTR/(c-1)}{SSE/(rc(t-1))} \sim F_{c-1,rc(t-1)} \text{ if no treatment effect}$$

$$\frac{SSI/((r-1)(c-1))}{SSE/(rc(t-1))} \sim F_{(r-1)(c-1),rc(t-1)} \text{ if no interaction}.$$

What if t = 1?

Tukey's 1DF Test for Additivity

Consider model

$$y_{ij} = \mu + \alpha_i + \beta_j + \theta \alpha_i \beta_j + \epsilon_{ij}, \ 1 \le i \le r, \ 1 \le j \le c.$$
Assume $\sum_i \alpha_i = \sum_j \beta_j = 0$, test $H_0: \ \theta = 0$ against $H_1: \ \theta \ne 0.$
Define $z_{ij} = y_{ij} - \bar{y}_{i} - \bar{y}_{\cdot j} + \bar{y}_{\cdot \cdot}$, then model
$$z_{ij} = \theta a_i b_j + e_{ij}, \ e_{ij} \text{ random error}, a_i, b_j \text{ known s.t. } \sum_i a_i = \sum_j b_j = 0.$$
Estimate $\hat{\theta} = \frac{\sum_i \sum_j z_{ij} a_i b_j}{\sum_i a_i^2 \cdot \sum_j b_j^2} = \frac{\sum_i \sum_j y_{ij} a_i b_j}{\sum_i a_i^2 \cdot \sum_j b_j^2}, \ \text{Var}(\hat{\theta}) = \frac{\sigma^2}{\sum_i a_i^2 \cdot \sum_j b_j^2}.$

Under
$$H_0$$
, $\frac{\hat{\theta}^2 \sum_i a_i^2 \sum_j b_j^2}{\sigma^2} = \frac{(\sum_i \sum_j y_{ij} a_i b_j)^2}{\sigma^2 \sum_i a_i^2 \sum_j b_j^2} \sim \chi_1^2$.

Tukey's 1DF Test for Additivity, Page 2

ANOVA decomposition

$$\sum_{i} \sum_{j} z_{ij}^2 = \sum_{i} \sum_{j} (z_{ij} - \hat{\theta} a_i b_j)^2 + \hat{\theta}^2 \sum_{i} a_i^2 \sum_{j} b_j^2,$$

$$SSI = SSIE + SSG,$$

$$(r-1)(c-1) = (rc-r-c) + 1.$$

Calculations show SSG, SSIE are statistically independent (not trivial). Hence, if H_0 true,

$$\frac{SSG}{SSIE/(rc-r-c)} \sim F_{1,rc-r-c} \qquad (*)$$

Now comes the key step: All this is true for any choices of a_i , b_j , therefore, in particular, it's true if we take $a_i = \hat{\alpha}_i$, $b_j = \hat{\beta}_j$.

With this substitution, (*) gives an exact test.

Fisher's data on barley varieties

| Place | Year | Manchuria | Svansota | Velvet | Trebi | Peatland | Row Mean |
|----------|------|-----------|----------|--------|---------|----------|----------|
| 1 | 1931 | 81.0 | 105.4 | 119.7 | 109.7 | 98.3 | 102.82 |
| 1 | 1932 | 80.7 | 82.3 | 80.4 | 87.2 | 84.2 | 82.96 |
| 2 | 1931 | 146.6 | 142.0 | 150.7 | 191.5 | 145.7 | 155.30 |
| 2 | 1932 | 100.4 | 115.5 | 112.2 | 147.7 | 108.1 | 116.78 |
| 3 | 1931 | 82.3 | 77.3 | 78.4 | 131.3 | 89.6 | 91.78 |
| 3 | 1932 | 103.1 | 105.1 | 116.5 | 139.9 | 129.6 | 118.84 |
| 4 | 1931 | 119.8 | 121.4 | 124.0 | 140.8 | 124.8 | 126.16 |
| 4 | 1932 | 98.9 | 61.9 | 96.2 | 125.5 | 75.7 | 91.64 |
| 5 | 1931 | 98.9 | 89.0 | 69.1 | 89.3 | 104.1 | 90.08 |
| 5 | 1932 | 66.4 | 49.9 | 96.7 | 61.9 | 80.3 | 71.04 |
| 6 | 1931 | 86.9 | 77.1 | 78.9 | 101.8 | 96.0 | 88.14 |
| 6 | 1932 | 67.7 | 66.7 | 67.4 | 91.8 | 94.1 | 77.54 |
| Col Mean | | 94.392 | 91.133 | 99.183 | 118.200 | 102.542 | 101.09 |

Two models considered here:

- 1. Two-way ANOVA with interactions, t = 2 observations for each treatment-place combination (but ignoring possible year to year variation)
- 2. Treat each place \times year combination as a block, so we have 5 treatments, 12 blocks, 1 observation for each treatmentplace combination, but apply Tukey test for interaction

ANOVA Table for 2-way model with interactions (F-ratio for SSI is 0.48, not significant)

| SOURCE | SUM OF SQUARES | D.F. | MEAN SQUARE |
|--------|----------------|------|--------------|
| SST | 5309.97 | 4 | 1327.5 |
| SSB | 21220.90 | 5 | 4244.2 |
| SSI | 4433.02 | 20 | 221.7 |
| SSE | 13768.46 | 30 | 458.9 |
| Total | 44732.35 | 59 | F-ratio 2.89 |

ANOVA Table for Tukey's 1-DF test (F-ratio for SSG is 3.27, p=0.077)

| SOURCE | SUM OF SQUARES | D.F. | MEAN SQUARE |
|--------|----------------|------|--------------|
| SST | 5309.97 | 4 | 1327.5 |
| SSB | 31913.32 | 11 | 2901.2 |
| SSG | 531.09 | 1 | 531.1 |
| SSIE | 6977.97 | 43 | 162.3 |
| Total | 44732.35 | 59 | F-ratio 8.18 |



Plot of residuals vs. fitted values for barley data, 2-way model without interactions

Conclusions

- First model inadequate ignores year to year variation, which masks the treatment effect.
- Second model seems OK Tukey test accepts hypothesis of no interaction but the treatment effect *is* significant.
- However there are other possible models, e.g. model year effect explicitly as a 3-way ANOVA; make either the block effect or the interaction (or both) a random effect.
- Could also use Tukey multiple comparisons procedure to determine which pairwise treatment differences are significant.