Analysis of Variance (ANOVA)

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MATH/STAT 571B

Module Goals:

Ch. 3 [DAE]:

Students will be able to:

- 1. Explain how to decompose total sum of squares into treatment and error sums of squares.
- 2. Conduct an analysis of variance in R including:
 - $\blacktriangleright \text{ Testing } H_0: \mu_1 = \mu_2 = \dots = \mu_a.$
 - Estimating effect sizes and interpreting in the context of the application.
 - Checking model adequacy using visual diagnostic tools.
- 3. Explain the relationship between an ANOVA and linear regression.
- 4. Estimate the sample size required to detect effects of a minimum size.

ANalysis Of VAriance (ANOVA)

ANalysis Of VAriance (ANOVA)

- We have seen several ways to compare two populations, but when we have a factor with a>2 levels, something else is required.
- ▶ The naive approach of testing all possible pairs of factor levels has two big issues:
 - The number of comparisons, $\frac{a(a-1)}{2}$, can get big quickly.
 - When we conduct multiple tests, the probability of any one of them having a type I error can be very different than the nominal level for each test.
- ► ANOVA tests the null hypothesis that the factor does not have any effect on the response.
 - ho $H_0: \mu_1 = \mu_2 = \cdots = \mu_a$ vs. $H_1: \mu_i \neq \mu_j$ for some i and j

Example: Plasma Etching Experiment¹

- An engineer is... investigating the relationship between the **RF power setting** and the **etch rate**..."
- ► "The 20 runs should be made in random order."
- ► The sample() function in R is a quick way to randomly order an index.

```
order <- sample(x = 1:20, size = 20, replace = FALSE)
order
## [1] 13 10 11 6 2 20 18 17 3 15 12 8 5 7 1 9 4 16 19 14</pre>
```

¹Section 3.1 DAE

- The read.csv() function reads comma-spaced values into a dataframe. read.table() can be used for more general tabular formats, and there are analogous functions for other data formats.
- The head()/tail() function is useful for looking at the first/last few lines of the dataframe.

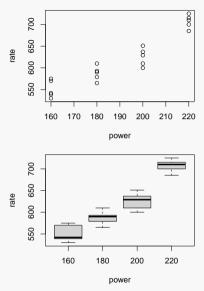
```
etching <- read.csv("etching.csv")</pre>
head(etching)
##
     power rate
      160
           575
      160
           542
## 3
      160 530
      160
           539
## 5
      160 570
## 6
      180
           565
```

► The following uses of plot() are equivalent.

```
plot(rate ~ power, data = etching)
plot(x = etching$power, y = etching$rate)
```

- ► The first uses a syntax called a "formula", which we will use for ANOVA too.
- boxplot() can be used analogously.

```
boxplot(rate ~ power, data = etching)
```



(1) Based on the figures, how much statistical evidence do you think there is for a non-zero effect of power on etching rate (none, some, a lot)?

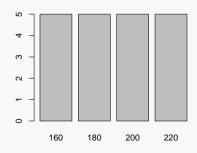
We are treating **RF power** as a categorical predictor, not a continuous one. Each level of power has its own independent etching rate.

$$y_{ij} = \mu_i + \epsilon_{ij}, \ i = 1, \dots, a; \ j = 1, \dots, n$$

The as.factor() function is a way to make this explicit for variables that could be mistakenly treated as continuous.

plot(etching\$power) etching\$power Index





ANalysis Of VAriance (ANOVA)

▶ Decomposition of sums of squares:²

$$\underbrace{SS_{T}}_{SSTO} = \underbrace{SS_{\text{Treatments}}}_{SSR} + \underbrace{SS_{E}}_{SSE}$$

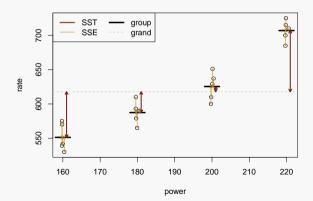
$$\sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{..})^{2} = n \sum_{i=1}^{a} (\bar{y}_{i.} - \bar{y}_{..})^{2} + \sum_{i=1}^{a} \sum_{j=1}^{n} (y_{ij} - \bar{y}_{i.})^{2}$$

This relationship is special and a consequence of using the specific estimators $\hat{\mu}_i = \bar{y}_i$, and the *squared* differences.

²with alternate notation from Kutner et al. (2004). ALRM.

ANalysis Of VAriance (ANOVA)

- ▶ Decomposition of sums of squares: $SS_T = SS_{\text{Treatments}} + SS_E$
- If $\frac{SS_{\text{Treatments}}/(a-1)}{SS_E/(N-a)}$ is large, then there is more variation *between* the estimated effects than *within* them.
- We have a ratio of two sums of squares, so we should expect an F sampling distribution.



▶ The ANOVA table³ output and p-value for H_0 is easy to get with R.

(2) What is the MSE?

³Compare with Table 3.4 in DAE.

Example: Plasma Etching Experiment (INCORRECT!)

- ► This code gives the wrong answer!
- ▶ **RF power** is mistakenly treated as continuous factor with a single overall trend.

(3) What is something about the summary output that would let you know something was not right?

ANOVA as linear regression

ightharpoonup An alternative way to denote the model $y_{ij} = \mu_i + \epsilon_{ij}$ is

$$y_{ij} = x_{1ij}\mu_1 + x_{2ij}\mu_2 + \dots + x_{aij}\mu_a + \epsilon_{ij}$$
$$x_{kij} = \begin{cases} 1, k = i \\ 0, k \neq i \end{cases}$$

Let $\mu_i = \beta_i$, $\mathbf{x}'_{ij} = (0 \dots 0 \underbrace{1}_i 0 \dots 0)$, $\boldsymbol{\beta'} = (\beta_1, \dots, \beta_a)$

$$y_{ij} = \mathbf{x}'_{ij}\boldsymbol{\beta} + \epsilon_{ij}$$

Using full matrix notation:

$$\mathbf{y} = \mathbf{X}\boldsymbol{eta} + \boldsymbol{\epsilon}, \quad \mathbf{X}_{N imes a} = \begin{pmatrix} \mathbf{x}_{11} \\ \mathbf{x}_{12} \\ \vdots \\ \mathbf{x}_{an} \end{pmatrix}, \quad \boldsymbol{\epsilon} \sim \mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_N)$$

ANOVA as linear regression: Plasma Etching Experiment

- ► The function lm() fits a linear regression model using least squares.
- The summary output includes the overall test of a relationships between at least one predictor and the response, which is equivalent to the ANOVA approach.

```
fit_lm <- lm(rate ~ as.factor(power), data = etching)</pre>
summary(fit lm)
## Call:
## lm(formula = rate ~ as.factor(power), data = etching)
## Coefficients:
##
                     Estimate Std. Error t value Pr(>|t|)
## (Intercept) 551.200 8.169 67.471 < 2e-16 ***
## as.factor(power)180 36.200 11.553 3.133 0.00642 **
## as.factor(power)200 74.200 11.553 6.422 8.44e-06 ***
## as.factor(power)220 155.800 11.553 13.485 3.73e-10 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 18.27 on 16 degrees of freedom
## Multiple R-squared: 0.9261, Adjusted R-squared: 0.9122
## F-statistic: 66.8 on 3 and 16 DF, p-value: 2.883e-09
```

ANOVA as linear regression: Plasma Etching Experiment

- ► The standard linear regression assigns the intercepts to one category and estimates the differences between that reference category and all others.
- ▶ In this case the reference category is for **RF power** = 160W.⁴

$$y_{ij} = \underbrace{\mu_1 + \alpha_i}_{\mu_i} + \epsilon_{ij}, \ \alpha_i = \mu_i - \mu_1$$

⁴Verify results with Example 3.3 on p. 79 of DAE.

ANOVA as linear regression: Plasma Etching Experiment

ightharpoonup The following formula can be used to get the the effects τ_i in the model⁵

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

$$\mu_i = \mu + \tau_i = \alpha_i + \mu_1 \implies \tau_i = \alpha_i + \mu_1 - \mu$$

(4) What indices (integers) should go in the blanks to calculate the point estimate for τ_3 (**RF power** = 200W)?

```
coef(fit_lm)[__] + coef(fit_lm)[__] - mean(etching$rate)
## as.factor(power)200
## 7.65
```

⁵eq. 3.2 in DAE; example 3.3 on p.79

Model Adequacy Checking

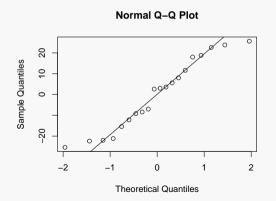
Model Adequacy Checking

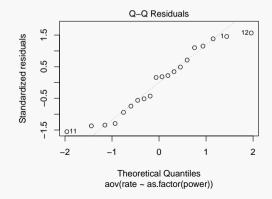
- Recall our modeling assumptions:
 - 1. ϵ_{ij} are normally distributed with
 - 2. constant variance, σ^2 , and
 - 3. are mutually independent.
- Define residuals $e_{ij}=y_{ij}-\hat{y}_{ij}$, where $\hat{y}_{ij}=\hat{\mu}_i=ar{y}_{i.}$
- $ightharpoonup e_{ij}$ are therefore also mean-zero normal (but *not* independent).
- Residuals should be **structureless**: no obvious patterns, and no correlation related to time/space/other indices.

Model Adequacy Checking: Normality

A QQ-plot with a normal reference distribution ("normal probability plot" in DAE) is a good way to visually evaluate the assumption of normality.

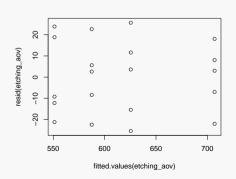
```
qqnorm(resid(etching_aov))
qqline(resid(etching_aov))
plot(etching_aov, which = 2)
```



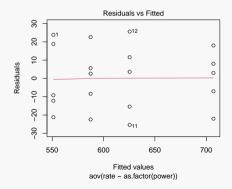


Model Adequacy Checking: Constant Variances

- Plotting residuals on the vertical axis against various other variables on the horizontal axis can reveal structure/patterns that conflict with model assumptions.
- ▶ No obvious signs of heteroskedasticity from these figures.



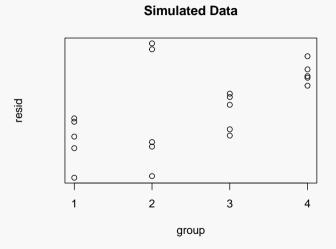
plot(etching_aov, which = 1)



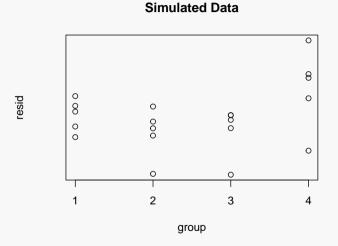
Model Adequacy Checking: Constant Variances

- Visual diagnostics are often sufficient, but formal tests for model assumptions are sometimes available.
- ▶ Bartlett's test is based on a statistic with a sampling distribution that is approximately chi-square if normality can be assumed.
- ▶ The modified Levene test is robust to the assumption of normality.

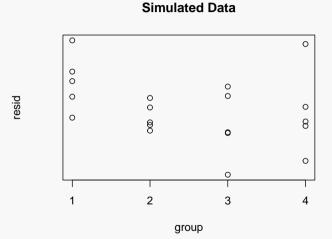
```
bartlett.test(rate ~ as.factor(power), data = etching)
##
   Bartlett test of homogeneity of variances
##
## data: rate by as.factor(power)
## Bartlett's K-squared = 0.43349. df = 3. p-value = 0.9332
library(car)
## Loading required package: carData
leveneTest(rate ~ as.factor(power), data = etching)
## Levene's Test for Homogeneity of Variance (center = median)
##
        Df F value Pr(>F)
## group 3 0.1959 0.8977
##
     16
```



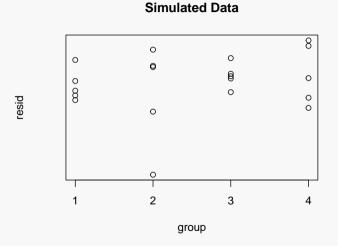
(5) Do you see evidence of heteroskedasticity (non-constant variance)?



(6) Do you see evidence of heteroskedasticity (non-constant variance)?



(7) Do you see evidence of heteroskedasticity (non-constant variance)?



(8) Do you see evidence of heteroskedasticity (non-constant variance)?

Effect on inference?

Repeat the following 5000 times:

- 1. Simulate data from null model with $\sigma_1^2 = \sigma_3^2 = 10^2$ and $\sigma_2^2 = \sigma_4^2 = 20^2$.
- 2. Compute ANOVA-based p-value (which assumes common variance).

Then:

- 3. Determine proportion of times H_0 was incorrectly rejected at level $\alpha = 0.05$.
- 4. Compare to nominal type I error rate.

(9) Is our test too liberal (rejects too often) or too conservative (fails to reject too often)?

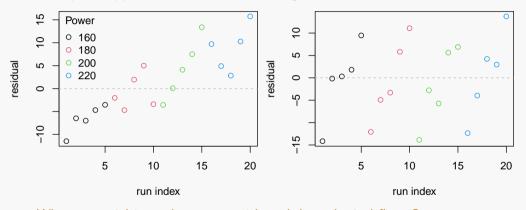
Model Adequacy Checking: Independence

- "If data have been collected on any other variables that might possibly affect the response, the residuals should be plotted against these variables."
- Example: Suppose the order of the etchings had not been randomized and the experimenter had done all runs for each power level together. Confounding effects could invalidate the independence assumption, and structure would likely be visible in the residuals plotted against run order.

⁶Ch. 3.4.4 DAE

Model Adequacy Checking: Independence

Example: Suppose the order of the etchings had not been randomized...



(10) What potential issue do you see with each hypothetical figure?

Non-independence can be very hard to adequately address.

Remedial Measures: Transformations of Response

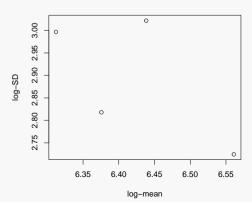
- One easy to implement remedial measure that can address heterogeneity is a transformation of the response.
- ightharpoonup Common transformations to try: \sqrt{y} , $\log(y)$, 1/y
- Remember that effects must be interpreted for transformed response.
- Plotting $\log(\bar{y}_{i.})$ on the horizontal axis and $\log(S_i)$ on the vertical axis can (sometimes) help with the choice of transformation.

```
sds <- aggregate(rate ~ power, data = etching, FUN = sd)
sds
## power rate
## 1  160 20.01749
## 2  180 16.74216
## 3  200 20.52559
## 4  220 15.24795
means <- aggregate(rate ~ power, data = etching, FUN = mean)</pre>
```

Remedial Measures: Transformations of Response

- Plotting $\log(\bar{y}_{i.})$ on the horizontal axis and $\log(S_i)$ on the vertical axis can (sometimes) help with the choice of transformation.
- $y^* = y^{1-\text{slope}}$

```
par(mar = c(4, 4, 1, 1))
plot(log(means$rate), log(sds$rate), xlab = "log-mean", ylab = "log-SD")
```



Remedial Measures: Non-parametric Inference

- Non-parametric tests generally trade some power for a relaxation of assumptions.
- If parametric assumptions are in fact valid, then non-parametric inference is usually **conservative** (sometimes VERY conservative).
- **Kruskal–Wallis** is a non-parametric test for $H_0: \mu_1 = \cdots = \mu_a$: No assumption of normality.
- ▶ Based on *ranks* instead of raw observations.
- ightharpoonup Overall F-test is fairly robust to assumptions, especially under a balanced design, but other aspects of analysis may not be.

```
kruskal.test(rate ~ as.factor(power), data = etching)
##
## Kruskal-Wallis rank sum test
##
## data: rate by as.factor(power)
## Kruskal-Wallis chi-squared = 16.907, df = 3, p-value = 0.0007386
```

Practical Interpretation

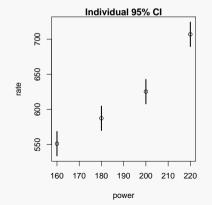
Group Effects

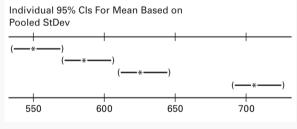
- ► The predict() method in R is very useful in many contexts.
- ► Takes two arguments:
 - object: fitted model (e.g., etching_aov)
 - newdata: dataframe with columns exactly named to match model variables

```
pred_data <- data.frame(power = c(160, 180, 200, 220))</pre>
effects CI <- predict(etching aov, newdata = pred data, interval = "confidence")
effects CI
      fit lwr
                         upr
## 1 551.2 533.8815 568.5185
## 2 587.4 570.0815 604.7185
## 3 625.4 608.0815 642.7185
## 4 707.0 689.6815 724.3185
 (11) Why do you think the follow code throws an error?
pred data <- data.frame(power = c(160, 180, 200, 220, 240))
```

effects CI <- predict(etching_aov, newdata = pred_data, interval = "confidence")</pre>

Group Effects: Figures





DAE p.104

Comparing Pairs of Treatment Means

- ► "Snooping"⁷ through the results to find standout groups has to be done carefully.
- Significant" differences are often interpreted with respect to individual error rates, but in fact should be interpreted with respect to **experimentwise** error rates.
- There are several methods for addressing the issue of "multiple comparisons" such as:
 - Fisher's Least Significant Difference
 - Bonferroni correction
 - Tukey's Honest Significant Difference

⁷In my experience, this term generally always has a negative connotation.

Fisher's Least Significant Difference

- \triangleright Do a bunch of pairwise t-tests (without pooling variances).
- ▶ Does **NOT** control experimentwise error rate!

```
t.test(rate ~ power, data = etching[etching$power %in% c(160, 180), ], conf.level = 0.99)
## Welch Two Sample t-test
##
## data: rate by power
## t = -3.1018, df = 7.7575, p-value = 0.01519
t.test(rate ~ power, data = etching[etching$power %in% c(160, 200), ], conf.level = 0.99)
## t = -5.787, df = 7.995, p-value = 0.0004122
t.test(rate ~ power, data = etching[etching$power %in% c(180, 200), ], conf.level = 0.99)
## t = -3.2079, df = 7.6894, p-value = 0.01313
t.test(rate ~ power, data = etching[etching$power %in% c(180, 220), ], conf.level = 0.99)
## t = -11.81, df = 7.9311, p-value = 2.601e-06
t.test(rate ~ power, data = etching[etching$power %in% c(200, 220), ], conf.level = 0.99)
## t = -7.136, df = 7.3842, p-value = 0.0001454
```

Fisher's Least Significant Difference

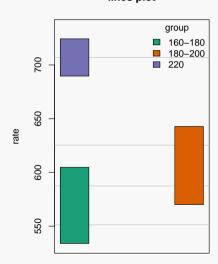
Pair	p-value
160-180	0.015
160-200	0.00041
180-200	0.013
180-220	0.0000026
200-220	0.00015

- (12) Why do we not need to see the p-value for the pair 160-220?
- (13) How would you "collect" these four levels based on the p-values?

"Lines plot": A useful qualitative figure?

- Popularized by SAS, these plots give a qualitative visualization groups means by whether or not they are significantly different from each other.
- No simple implementation in R.
 - Maybe for good reason? The SAS ones *look* quantitative, but they're really not.
- Plot is based on a particular method for pairwise comparisons (e.g., Fisher's LSD).
- ► Version to the right uses extremes of CIs for each level in collection.
 - No sound statistical basis for doing this that I know of.
 - Code is a little clunky.^a

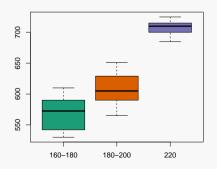
lines plot



^abut available upon request

"Lines plot"

A simpler to code and probably equally effective version.



Bonferroni

- Controls experimentwise error rate, but can be very conservative.
- $> 0.01/6 \approx 0.00167$

Pair	p-value
160-180	0.015
160-200	0.00041
180-200	0.013
180-220	0.0000026
200-220	0.00015

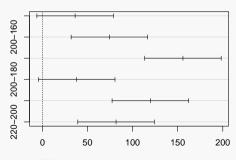
(14) How would our conclusions change about pairwise differences after using Bonferroni correction?

Tukey's HSD

Controls experimentwise error rate and less conservative than Bonferroni.

```
etching hsd <- TukeyHSD(etching aov,
                                                plot(etching hsd)
                         conf.level = 0.99)
etching_hsd
##
     Tukey multiple comparisons of means
##
       99% family-wise confidence level
##
   $`as.factor(power)`
            diff
                        1 wr
                                  upr
                                          p adj
            36.2
                  -6.21498
                             78.61498 0.0294279
   180-160
   200-160
                  31,78502, 116,61498, 0,0000455
   220-160 155.8 113.38502 198.21498 0.0000000
   200-180
            38.0
                  -4.41498
                             80.41498 0.0215995
   220-180 119.6
                  77, 18502, 162, 01498, 0, 0000001
   220-200
           81.6 39.18502 124.01498 0.0000146
```

99% family-wise confidence level



Differences in mean levels of as.factor(power)

Dunnett's procedure

- For comparing means to a single control level (DAE p.101).
- Implemented in DescTools package: DunnettTest()
- Demo: scrutinizing packages
 - ► Version: fine-grain numbering suggests regular maintenance
 - ▶ Published: within the last year or two is best
 - ► Author: recognize anyone? many authors sometimes a good sign. Google them :)
 - ▶ URL: sometimes gives more info about package and team
 - Vignettes: good sign if these exist and are carefully prepared

Contrasts

- More general comparing group means, we might be interested in comparing linear combinations of group means.
- Example: $H_0: \frac{\mu_1 + \mu_2}{2} = \frac{\mu_3 + \mu_4}{2}$
 - Equivalent representation: $\mu_1 + \mu_2 \mu_3 \mu_4 = \sum_{i=1}^4 c_i \mu_i = \mathbf{c}' \boldsymbol{\mu} = 0$ where $\mathbf{c}' = (1, 1, -1, -1)$
- When $\sum_{i=1}^{a} c_i = 0$, this is called a contrast.

Scheffé's Method

- Controls experimentwise error rate for all contrasts.
- More conservative than Tukey's HSD for pairwise means only.
- $C = \sum_{i=1}^{a} c_i \bar{y}_{i.}$
- ightharpoonup Compare |C| to $S_C\sqrt{(a-1)F_{lpha,a-1,N-a}}$

```
c <- c(1, -1, 0, 0)
means <- aggregate(rate ~ power, data = etching, FUN = mean)
ybars <- means$rate
C <- sum(c * ybars)
S_C <- sqrt(sigma(etching_aov)^2 * sum(c^2 / 5))
C
## [1] -36.2
S_C * sqrt(3 * qf(1 - 0.01, 3, 16))
## [1] 46.03492</pre>
```

Power Analysis: Determining Sample Size

Determining Sample Size

- ► Heuristic: Run a hypothetical experiment + analysis and see how it goes.
- Brute force:
 - Simulate many (thousands, maybe much more) hypothetical data sets,
 - analyze each one,
 - compute proportion of data sets for which type II error occurs.
 - Adjust sample size until satisfactory power is reached.
- To avoid all the computation, need to know sampling distribution under particular alternative hypothesis (often "non-central" distributions).

Simulation: DAE Example 3.10 p.107

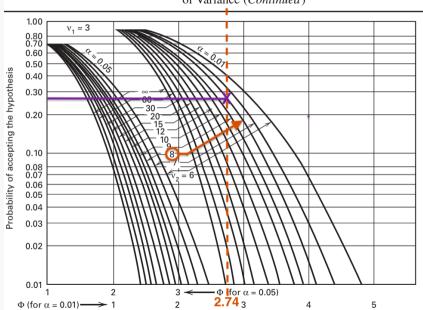
- Desired power (probability of detecting difference) is 0.90.
- Hypothetical group means $\mu_1=575, \mu_2=600, \mu_3=650, \mu_4=675$ and variance $\sigma=25.$
- Maximum error type I rate of $\alpha = 0.01$.

```
n < -3
mus \leftarrow c(mu1 = 575, mu2 = 600, mu3 = 650, mu4 = 675)
alpha <- 0.01
sigma <- 25
typeII <- sapply(1:2000, function(i){</pre>
  sim_data <- data.frame(power = as.factor(rep(mus, rep(n, 4))),</pre>
                           rate = c(sapply(mus, function(mu) rnorm(n, mu, sd = sigma))))
  sim_aov <- aov(rate ~ power, data = sim_data)</pre>
  summary(sim_aov)[[1]]$`Pr(>F)`[1] < alpha</pre>
})
mean(typeII)
## [1] 0.7495
```

Simulation: DAE Example 3.10 p.107

```
n < -4
typeII <- sapply(1:2000, function(i){
  sim_data <- data.frame(power = as.factor(rep(mus, rep(n, 4))),</pre>
                           rate = c(sapply(mus, function(mu) rnorm(n, mu, sd = sigma))))
  sim_aov <- aov(rate ~ power, data = sim_data)</pre>
  summary(sim_aov)[[1]]$`Pr(>F)`[1] < alpha</pre>
})
mean(typeII)
## [1] 0.9545
n < -5
typeII <- sapply(1:2000, function(i){</pre>
  sim data <- data.frame(power = as.factor(rep(mus, rep(n, 4))),
                           rate = c(sapply(mus, function(mu) rnorm(n, mu, sd = sigma))))
  sim aov <- aov(rate ~ power, data = sim data)</pre>
  summary(sim aov)[[1]]$`Pr(>F)`[1] < alpha</pre>
})
mean(typeII)
## [1] 0.9975
```

V Operating Characteristic Curves for the Fixed Effects Model Analysis of Variance (Continued)



Power calculations in R

```
power.anova.test(groups = 4, n = 4, between.var = var(mus),
                 within.var = sigma^2, sig.level = 0.01)
##
##
        Balanced one-way analysis of variance power calculation
##
##
            groups = 4
##
                 n = 4
##
       between.var = 2083.333
##
        within.var = 625
##
         sig.level = 0.01
##
             power = 0.9621239
##
## NOTE: n is number in each group
```

Details

Exactly one of the parameters groups, n, between.var, power, within.var, and sig.level must be passed as NULL, and that parameter is determined from the others. Notice that sig.level has non-NULL default so NULL must be explicitly passed if you want it computed.

Power calculations in R

```
power.anova.test(groups = 4, between.var = var(mus),
                 within.var = sigma^2, sig.level = 0.01, power = 0.90)
##
##
        Balanced one-way analysis of variance power calculation
##
##
            groups = 4
                 n = 3.520243
##
##
       between.var = 2083.333
##
      within.var = 625
         sig.level = 0.01
##
##
            power = 0.9
##
## NOTE: n is number in each group
```

Simulation: DAE example bottom p. 107

- ▶ Want to reject the null if *any two levels* differ by at least 75
- Move creation of mus inside the *apply() function so that they are generated randomly each time.

Simulation: Maximum difference of 2

```
typeII <- sapply(1:2000, function(i){</pre>
  n < -6
  mus \leftarrow c(mu1 = 525, mu2 = 600, mu3 = runif(1, 525, 600), mu4 = runif(1, 525, 600))
  alpha <- 0.01
  sigma <- 25
  sim data <- data.frame(power = as.factor(rep(mus, rep(n, 4))),
                           rate = c(sapply(mus, function(mu) rnorm(n, mu, sd = sigma))))
  sim_aov <- aov(rate ~ power, data = sim_data)</pre>
  summary(sim_aov)[[1]]$`Pr(>F)`[1] < alpha</pre>
})
mean(typeII)
## [1] 0.9665
```

- ightharpoonup Conclusion: at least n=6 required (agrees with DAE).
- Simulation approach admits lots of flexibility in hypothetical scenarios.