Working with Factors in R

Model parameterizations, contrasts, inferences on means, etc.

Dan Hall, Director of the SCC



Department of Statistics Franklin College of Arts and Sciences

Statistical Consulting Center

Table of Contents

Introduction

The factor Class in R—Basics

Models with Factors—Parameterizations and Contrasts Example–Walking Age

Inferences on Means—The emmeans Package

Multi-factor Models

Factors and Marginal Means in Logistic Regression

Questions?

Related Resources

- Companion videos for this talk can be found here https://kaltura.uga.edu/media/t/1_cka61gmn and here https://kaltura.uga.edu/media/t/1_nkujgc63.
- A companion script, factors.R, can be found here: https://tinyurl.com/2m65myr5.

- Categorical variables are often called classification variables or factors, especially when used as explanatory variables in statistical models.
- Examples abound: sex (male, female), treatment (drug A, drug B, placebo), operating system (Windows, Linux, MacOS), etc.
- Factors are ubiquitous in data science and understanding how to use them is fundamental to the practice of statistics.
- So a discussion of factors would seem only suitable for complete novices.
- However, there are some tricky issues, especially in R where the factor object class can be quite confusing.
- Moreover, students usually learn to work with discrete explanatory variables (i.e., factors) after and less thoroughly than covariates.

- Categorical variables are often called classification variables or factors, especially when used as explanatory variables in statistical models.
- Examples abound: sex (male, female), treatment (drug A, drug B, placebo), operating system (Windows, Linux, MacOS), etc.
- Factors are ubiquitous in data science and understanding how to use them is fundamental to the practice of statistics.
- So a discussion of factors would seem only suitable for complete novices.
- However, there are some tricky issues, especially in R where the factor object class can be quite confusing.
- Moreover, students usually learn to work with discrete explanatory variables (i.e., factors) after and less thoroughly than covariates.

- Categorical variables are often called classification variables or factors, especially when used as explanatory variables in statistical models.
- Examples abound: sex (male, female), treatment (drug A, drug B, placebo), operating system (Windows, Linux, MacOS), etc.
- Factors are ubiquitous in data science and understanding how to use them is fundamental to the practice of statistics.
- So a discussion of factors would seem only suitable for complete novices.
- However, there are some tricky issues, especially in R where the factor object class can be quite confusing.
- Moreover, students usually learn to work with discrete explanatory variables (i.e., factors) after and less thoroughly than covariates.

- Categorical variables are often called classification variables or factors, especially when used as explanatory variables in statistical models.
- Examples abound: sex (male, female), treatment (drug A, drug B, placebo), operating system (Windows, Linux, MacOS), etc.
- Factors are ubiquitous in data science and understanding how to use them is fundamental to the practice of statistics.
- So a discussion of factors would seem only suitable for complete novices.
- However, there are some tricky issues, especially in R where the factor object class can be quite confusing.
- Moreover, students usually learn to work with discrete explanatory variables (i.e., factors) after and less thoroughly than covariates.

- Categorical variables are often called classification variables or factors, especially when used as explanatory variables in statistical models.
- Examples abound: sex (male, female), treatment (drug A, drug B, placebo), operating system (Windows, Linux, MacOS), etc.
- Factors are ubiquitous in data science and understanding how to use them is fundamental to the practice of statistics.
- So a discussion of factors would seem only suitable for complete novices.
- However, there are some tricky issues, especially in R where the factor object class can be quite confusing.
- Moreover, students usually learn to work with discrete explanatory variables (i.e., factors) after and less thoroughly than covariates.

- Categorical variables are often called classification variables or factors, especially when used as explanatory variables in statistical models.
- Examples abound: sex (male, female), treatment (drug A, drug B, placebo), operating system (Windows, Linux, MacOS), etc.
- Factors are ubiquitous in data science and understanding how to use them is fundamental to the practice of statistics.
- So a discussion of factors would seem only suitable for complete novices.
- However, there are some tricky issues, especially in R where the factor object class can be quite confusing.
- Moreover, students usually learn to work with discrete explanatory variables (i.e., factors) after and less thoroughly than covariates.

- In R, do you understand the factor class? What is the difference between the levels and the labels of a factor? What is the mode of a factor? How do you convert an object to or from the factor class? How do you recode a factor (e.g., change, combine, or split levels; change reference category; reorder)?
- Do you know the difference between ordered and unordered factors in R?
- Are you comfortable with alternative parameterizations of a model involving factors? Do you know how to induce different parameterizations via *contrasts* in R?
- Do you know how to get simultaneous confidence intervals for a set (or family) of means, or to test a family of contrasts and adjust those inferences for multiple comparisons?
- Do you know how to test a custom contrast among a set of means (e.g., corresponding to the levels of a factor)?

- In R, do you understand the factor class? What is the difference between the levels and the labels of a factor? What is the mode of a factor? How do you convert an object to or from the factor class? How do you recode a factor (e.g., change, combine, or split levels; change reference category; reorder)?
- Do you know the difference between ordered and unordered factors in R?
- Are you comfortable with alternative parameterizations of a model involving factors? Do you know how to induce different parameterizations via *contrasts* in R?
- Do you know how to get simultaneous confidence intervals for a set (or family) of means, or to test a family of contrasts and adjust those inferences for multiple comparisons?
- Do you know how to test a custom contrast among a set of means (e.g., corresponding to the levels of a factor)?

- In R, do you understand the factor class? What is the difference between the levels and the labels of a factor? What is the mode of a factor? How do you convert an object to or from the factor class? How do you recode a factor (e.g., change, combine, or split levels; change reference category; reorder)?
- Do you know the difference between ordered and unordered factors in R?
- Are you comfortable with alternative parameterizations of a model involving factors? Do you know how to induce different parameterizations via *contrasts* in R?
- Do you know how to get simultaneous confidence intervals for a set (or family) of means, or to test a family of contrasts and adjust those inferences for multiple comparisons?
- Do you know how to test a custom contrast among a set of means (e.g., corresponding to the levels of a factor)?

- In R, do you understand the factor class? What is the difference between the levels and the labels of a factor? What is the mode of a factor? How do you convert an object to or from the factor class? How do you recode a factor (e.g., change, combine, or split levels; change reference category; reorder)?
- Do you know the difference between ordered and unordered factors in R?
- Are you comfortable with alternative parameterizations of a model involving factors? Do you know how to induce different parameterizations via *contrasts* in R?
- Do you know how to get simultaneous confidence intervals for a set (or family) of means, or to test a family of contrasts and adjust those inferences for multiple comparisons?
- Do you know how to test a custom contrast among a set of means (e.g., corresponding to the levels of a factor)?

- In R, do you understand the factor class? What is the difference between the levels and the labels of a factor? What is the mode of a factor? How do you convert an object to or from the factor class? How do you recode a factor (e.g., change, combine, or split levels; change reference category; reorder)?
- Do you know the difference between ordered and unordered factors in R?
- Are you comfortable with alternative parameterizations of a model involving factors? Do you know how to induce different parameterizations via *contrasts* in R?
- Do you know how to get simultaneous confidence intervals for a set (or family) of means, or to test a family of contrasts and adjust those inferences for multiple comparisons?
- Do you know how to test a custom contrast among a set of means (e.g., corresponding to the levels of a factor)?

- Do you know how to use orthogonal polynomial contrasts for ordered factors? How about when the levels of the factor are not equally spaced?
- Do you known the difference between Type I, II, III tests, their proper usage and implementation in R?
- Do you know the difference between *main effects* and *simple effects*?
- Do you know the difference between marginal means, joint means, and raw means?
- Do you know how to estimate joint and/or marginal means from a fitted model and do inferences on them properly?
- Omitting the intercept in an ANOVA model doesn't alter the model (only its parameterization), but how does it change ANOVA table F tests?

- Do you know how to use orthogonal polynomial contrasts for ordered factors? How about when the levels of the factor are not equally spaced?
- Do you known the difference between Type I, II, III tests, their proper usage and implementation in R?
- Do you know the difference between *main effects* and *simple effects*?
- Do you know the difference between marginal means, joint means, and raw means?
- Do you know how to estimate joint and/or marginal means from a fitted model and do inferences on them properly?
- Omitting the intercept in an ANOVA model doesn't alter the model (only its parameterization), but how does it change ANOVA table F tests?

- Do you know how to use orthogonal polynomial contrasts for ordered factors? How about when the levels of the factor are not equally spaced?
- Do you known the difference between Type I, II, III tests, their proper usage and implementation in R?
- Do you know the difference between *main effects* and *simple effects*?
- Do you know the difference between marginal means, joint means, and raw means?
- Do you know how to estimate joint and/or marginal means from a fitted model and do inferences on them properly?
- Omitting the intercept in an ANOVA model doesn't alter the model (only its parameterization), but how does it change ANOVA table F tests?

- Do you know how to use orthogonal polynomial contrasts for ordered factors? How about when the levels of the factor are not equally spaced?
- Do you known the difference between Type I, II, III tests, their proper usage and implementation in R?
- Do you know the difference between *main effects* and *simple effects*?
- Do you know the difference between marginal means, joint means, and raw means?
- Do you know how to estimate joint and/or marginal means from a fitted model and do inferences on them properly?
- Omitting the intercept in an ANOVA model doesn't alter the model (only its parameterization), but how does it change ANOVA table F tests?

- Do you know how to use orthogonal polynomial contrasts for ordered factors? How about when the levels of the factor are not equally spaced?
- Do you known the difference between Type I, II, III tests, their proper usage and implementation in R?
- Do you know the difference between *main effects* and *simple effects*?
- Do you know the difference between marginal means, joint means, and raw means?
- Do you know how to estimate joint and/or marginal means from a fitted model and do inferences on them properly?
- Omitting the intercept in an ANOVA model doesn't alter the model (only its parameterization), but how does it change ANOVA table F tests?

- Do you know how to use orthogonal polynomial contrasts for ordered factors? How about when the levels of the factor are not equally spaced?
- Do you known the difference between Type I, II, III tests, their proper usage and implementation in R?
- Do you know the difference between *main effects* and *simple effects*?
- Do you know the difference between marginal means, joint means, and raw means?
- Do you know how to estimate joint and/or marginal means from a fitted model and do inferences on them properly?
- Omitting the intercept in an ANOVA model doesn't alter the model (only its parameterization), but how does it change ANOVA table F tests?

• Factors in R created with factor() function.

```
(sex <- rep(c("M", "F"), each=5)) # a character vector, 5 Male, 5 Female</pre>
 [1] "M" "M" "M" "M" "M" "E" "E" "E" "E"
(sexFac \leq factor(sex))
                              # a factor
 [1] MMMMMFFFFF
                                                             a
Levels. F M
                                                              $
   • Their mode is numeric, but
      is.numeric() returns FALSE.
                                                              $0
mode(sexFac) # numeric? Really?
                                                              as
[1] "numeric"
```

• They are numeric vectors with a **levels** attribute. The elements of a factor are the indices of their levels.

attributes(sexFac)
\$lovels [1] "F" "M"
\$class [1] "factor"
as.numeric(sexFac)
[1] 2 2 2 2 2 1 1 1 1 1

is numeric(sevFac)

• Can specify the levels and, optionally, labels to print in place of levels. Specifying levels can be useful to put them in a desired order and for other reasons.

sexFac # levels alphabetically ordered by default

[1] M M M M M F F F F F Levels: F M

(sexFac.MF <- factor(sex,levels=c("M","F"), labels=c("Male","Female"))) #set diff't order</pre>

[1] Male Male Male Male Female Female Female Female Female Female Levels: Male Female

table(sexFac) # a freq distribution for sexFac

sexFac F M 5 5

table(sexFac.MF) # note the difference in the order of levels

sexFac.MF Male Female 5 5

- Use meaningful levels or, if not, use labels!
- Specifying levels induces an ordering, but that doesn't mean the factor is an *ordered* factor.
- An ordered factor is a special type of factor.
 - Order of levels stored with object.
 - min(), max() <, > can be used to compare ordered factors.
 - More importantly, we may wish to parameterize ordered factors differently than unordered factors in models.

```
opin <- c(-1,0,-1,1,-1)
(opinFac <- factor(opin,levels=-1:1,labels=c("disagree","neutral","agree")))</pre>
```

[1] disagree neutral disagree agree disagree Levels: disagree neutral agree

(opinOrd <- factor(opin,levels=-1:1,labels=c("disagree","neutral","agree"),ordered=TRUE))</pre>

[1] disagree neutral disagree agree disagree Levels: disagree < neutral < agree

max(opinOrd) # max(opinFac) gives error

[1] agree Levels: disagree < neutral < agree</pre>

[1] 1 2 2 1 3

- Until recently, read.table(), data.frame(), etc. automatically coerced character vectors into factors, unless option stringsAsFactors set to FALSE.
 - Thankfully, as of R 4.0.0, this behavor has been changed.
- A categorical variable is sometimes more conveniently manipulated as a factor, other times as a non-factor (e.g., numeric or character).
 - Keep two versions (e.g., keep both opin and opinFac).
- Be careful turning a factor into a "non-factor".

Recoding factors

Many good tools in forcats package (part of tidyverse).

- Collapsing levels:
 - fct_collapse().
- Expanding (adding) levels:
 - fct_expand().
- Dropping levels:
 - fct_drop().
- Re-ordering levels:
 - fct_inorder(), fct_infreq(), fct_inseq(), fct_relevel(),
 fct_reorder(), fct_rev(), fct_shift().
- Combine levels based on frequency of occurrence:
 - fct_lump_min(), fct_lump_prop(), fct_lump_n(), fct_lump_lowfreq().
- Recode levels:
 - fct_recode() (can be used to collapse levels).
- Create a factor from combination of levels of two factors:
 - fct_cross().
- Examples in script, factors.R.

- Presentation focuses on linear models, but extends to GLMs, others.
- Linear models with factors are known as ANOVA and ANCOVA models.
- Such models can be equivalently formulated in multiple ways depending on how the factor(s) are handled.
 - These alternative approaches are different parameterizations of a model, not different models.

Example—One-way ANOVA Model:

• Two common parameterizations:

Cell means version: $y_{ij} = \mu_i + e_{ij}$ Effects version: $y_{ij} = \mu + \alpha_i + e_{ij}$

- μ_i s are treatment means.
- α_i s are treatment effects up/down from a constant μ .

Cell means version: $y_{ij} = \mu_i + e_{ij}$ Effects version: $y_{ij} = \mu + \alpha_i + e_{ij}$,

i = 1, ..., g (treatments), $j = 1, ..., n_i$ (replicates). Suppose g = 4.

- Models are equivalent. Four means for 4 treatments.
- Effects model is *overparameterized*. It captures 4 means with 5 parameters: $\mu, \alpha_1, \alpha_2, \alpha_3, \alpha_4$.
 - One parameter is redundant.
 - Redundancy does not have to be removed, but R always does.
 - Redundancy can be removed in several different ways. We could:
 - set $\mu = 0$ (becomes the cell means model)
 - set $\alpha_1 = 0$ (μ becomes mean in trt 1)
 - set $\alpha_i = 0$ for any *i* (μ becomes mean in trt *i*)
 - constrain $\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 = 0$ (μ becomes mean of the trt means, or grand mean).
 - Choices yield different parameterizations of the same model.
 - In R, choice is controlled via *contrasts*.

- R uses contrasts (contrast matrices) applied to each factor to avoid overparameterization.
 - *contrast matrices* is a misnomer. Should be called *coding matrices* (as in Venables' codingMatrices package).
- Contrast matrices remove parameter redundancy by coding the columns of the *model matrix* corresponding to a factor so they are not linearly dependent with the column for the constant term μ .
- R "contrast" functions implement these recodings:
 - contr.treatment(g,i): equivalent to setting $\alpha_i = 0$.
 - Primary argument g is number of levels of the factor.
 - ▶ Default value of i is 1.
 - contr.SAS(g) is wrapper for contr.treatment(g,g)
 - contr.sum(g): equivalent to "sum-to-zero" constraint, $\sum_i \alpha_i = 0$.
 - contr.helmert(g): parameters become (orthogonal) contrasts b/w 2nd and 1st level, b/w 3rd level and avg of levels 1 & 2, etc.
 - contr.poly(g): parameterizes ordered factor effects in terms of orthogonal polynomial contrasts (linear effect, quadratic effect,...,g 1st order effect).

How do I set the contrasts for the factors in my model?

- contrasts() function can query or change contrasts for a factor.
- There's a system option that sets contrasts to be used for unordered and ordered factors unless otherwise specified.

```
options("contrasts")
$contrasts
        unordered
                             ordered
"contr.treatment"
                        "contr.polv"
sexFac <- factor(rep(c("M", "F"), each=5)) # 5 Male, 5 Female</pre>
contrasts(sexFac) # returns the contrasts used by default
  М
F 0
M 1
# Change to sum-to-zero contrasts:
contrasts(sexFac) \leq contr.sum(2) # 2 because sexFac has 2 levels
op <- options(contrasts=c("contr.SAS", "contr.poly")) # change contrasts option & store previous value in op
ageFac <- factor(rep(c("Adult", "Child"), times=5)) # A.C.A.C....</pre>
contrasts(ageFac) # returns the contrasts used by default
      Adult.
Adult.
Child
          0
options(op) # restore defaults
```

How do I set the contrasts for the factors in my model?

• Many model-fitting functions have a contrasts= option.

```
Call:
lm(formula = rnorm(10) - sexFac + ageFac, contrasts = list(sexFac = "contr.treatment",
    ageFac = "contr.SAS"))
Coefficiente:
```

(Intercept) sexFacM ageFacAdult -0.2043 0.3771 -0.1152

In linear models, any of the standard inferences (tests, confidence intervals) we would wish to perform can be done in any parameterization of the model.

- Some parameterizations more convenient for some purposes than others, but the parameterization does not limit what we can do.
- Parameterization is essentially arbitrary, but that does not mean it doesn't matter.
- We do need to understand the parameterization we are working in.
- For Type III tests on main effects to be constructed correctly (e.g., by Anova() in car package) in models with interactions for unbalanced data, must use contr.sum().

Example–Walking Age

- Infants randomized to 4 treatments to stimulate a walking response in newborns:
 - control, no exercise, passive exercise, active exercise.
- Response is the age (in mos.) when child first began to walk.
- See factors.R and video linked here.

Highlights:

- Note the default choices made when reading data, setting up factors.
- One-way ANOVA model fitted with aov(), a wrapper for lm().
 - Fitted model object has two classes **aov** and **lm**.
 - Default summary for **aov** object is an ANOVA table. Parameter estimates less important. Parameterization is arbitrary.
- Treatment means and comparisons among them of main interest.
- Lots of parameterizations considered for group, the treatment factor.
 - A parameterization can be chosen so that (regression) coefficients of the model are quantities of interest.
- For an ordered factor, parameterization in terms of polynomial contrasts or consecutive differences may be appealing.
 - Use scores= option in contr.poly() for unequally spaces factor levels.

Example–Walking Age

Highlights (continued):

- Models with different parameterizations all give same ANOVA table, ${\cal F}$ test for group.
 - Exception is when model lacks an intercept. Then
 - ▶ the choice of contrast matrix (factor coding) does not matter,
 - regression parameters are treatment means,
 - \blacktriangleright and ANOVA table F test differs. Now it tests that all means are equal to 0, an uninteresting hypothesis!
 - Default calculation of R^2 is incorrect when model lacks an intercept.
- Regardless of parameterization, **emmeans** package can be used to estimate means and do inferences on them.
 - emmeans() function can give means and confidence intervals for them.
 - contrast() function (not contrasts()!) can estimate and test contrasts among means.

Inferences on Means—The emmeans Package

- An ANOVA model is a framework for inference on the effects of factors. Usually, want to do inference on the treatment means.
 - We do model-based inference.
- In one-way model, basic question is, Are all treatment means the same?
- Just a starting point. If not all equal,
 - which ones differ and by how much?
 - point estimates and intervals for each treatment mean;
 - Usually want inference on several quantities. How do we control type I error for all these inferences?
- Extremely useful tools for these tasks in the emmeans package.

Inferences on Means—The emmeans Package

The emmeans Package:

- Gives estimates of treatment means, associated SEs, and CIs based on a fitted model.
 - In a multifactor model, can get
 - ▶ joint means (at combinations of levels of the factors),
 - ▶ or marginal means (at each level of one factor, averaging over others).
- Can estimate, give CIs for, and test hypotheses on contrasts and other linear combinations of means.
- Implements multiplicity adjustments to control type I error rate/simultaneous coverage probability when doing multiple inferences.
- Can plot means and associated CIs, including interaction plots in multi-factor models.
- Works with a variety of different model classes (lms and aovs, mlms, glms, lmerMods, glmerMods, gam's, many others).
- Based on LSMEANS statement in SAS (package originally called lsmeans).

Inferences on Means—The emmeans Package

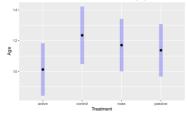
Example—Walking Age

walk.m1 <- aov(age-group,data=walkdata)
(walk.m1.emm <- emmeans(walk.m1,specs= ~ group,adjust="bonferroni"))</pre>

group	emmean	SE	df	lower.CL	upper.CL
active	10.1	0.619	19	8.42	11.8
control	12.3	0.678	19	10.48	14.2
noex	11.7	0.619	19	10.00	13.4
passive	11.4	0.619	19	9.67	13.1

Confidence level used: 0.95 Conf-level adjustment: bonferroni method for 4 estimates

plot(walk.mi.emm,horizontal=F,xlab="Age",ylab="Treatment")+ggtitle("Treatment mean estimates and 95% CIs, Walking Age Exp't")



Treatment mean estimates and 95% CIs, Walking Age Exp't

Inferences on Means—The emmeans Package

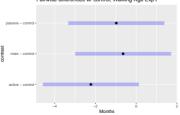
Example—Walking Age (Continued)

Dunnett intervals and tests for each pairwise diff with control
(for 1-tailed tests, 1-sided intervals add argument: side="<");
(diffsVSControl <- contrast(valk.m.lemm,method="trt.vs.ctrl",refe"control",infer=c(TRUE,TRUE),adjust="dunnettx"))</pre>

contrast	estimate	SE	df	lower.CL	upper.CL	t.ratio	p.value
active - control	-2.225	0.918	19	-4.58	0.133	-2.423	0.0670
noex - control	-0.642	0.918	19	-3.00	1.716	-0.699	0.8013
passive - control	-0.975	0.918	19	-3.33	1.383	-1.062	0.5854

Confidence level used: 0.95 Conf-level adjustment: dunnettx method for 3 estimates P value adjustment: dunnettx method for 3 tests

plot(diffsVsControl,xlab="Months")+ggtitle("Pairwise differences w/ control, Walking Age Exp't")



Pairwise differences w/ control, Walking Age Exp't

Inferences on Means—The emmeans Package

Example—Walking Age. Custom Contrasts:

levels(walkdata\$group)

[1] "active" "control" "noex" "passive"

```
# contrast to compare exercise absent groups to exercise present groups:
exerciseContrast -c(1,-1,-1,1)/2 #avg of control & nose v. avg of others
contrast(valk.mi.emm_method=list(exerciseContrast),inferre(T,T)) #infer asks for interval and test
```

 contrast
 estimate
 SE df lower.CL upper.CL t.ratio
 p.value

 c(0.5, -0.5, -0.5, 0.5)
 -1.28
 0.634
 19
 -2.61
 0.0485
 -2.016
 0.0581

Confidence level used: 0.95

test(contrast(walk.m1.emm,method=list(exerciseContrast,c(1,0,0,-1),c(0,1,-1,0))),joint=TRUE) # joint F test (same as main effect test)

df1 df2 F.ratio p.value 3 19 2.142 0.1285

anova(walk.m1)

Analysis of Variance Table

Response: age Df Sum Sq Mean Sq F value Pr(>F) group 3 14.778 4.9259 2.1422 0.1285 Residuals 19 43.690 2.2995

Multi-factor Models

Example—Soybean Weeds

An experiment in a randomized complete block design (RCBD) was conducted to study effects of soybean variety and herbicide use on weed biomass.

- Trt factors: Variety (16 levs); Herbicide (never, @2 wks, @4 wks).
- Blocking factor: Location (Rosemount, St.Paul)

All 16*3=48 treatments randomized to plots in each location.

- Do herbicide effects differ across varieties (interaction).
- If not, what are herbicide effects (*main effects*, averaged over variety).
- If so, what are herbicide effects for each variety (*simple effects*).

Potentially interested in two types of means:

- Joint means for each of the 48 treatments.
- Marginal means for each level of herbicide (avg'd over variety).
- Marginal means for each variety (avg'd over herbicide).

Multi-factor Models

Example—Soybean Weeds (continued)

Model:

$$y_{ijk} = \underbrace{\mu + \alpha_i + \beta_j + \gamma_{ij} + \tau_k}_{\equiv \mu_{ijk}} + e_{ijk}, \quad i = 1, ..., 16; j = 1, 2, 3; k = 1, 2.$$

- Joint means: $\bar{\mu}_{ij}$.
- Marginal means:
 - $\bar{\mu}_{i\cdots}$ mean for *i*th variety,
 - $\bar{\mu}_{\cdot j}$ mean for *j*th level of herbicide.
- In fact, all these means are averaged over block (marginal, in a sense).
- Estimates of above quantities obtained from the fitted model.

Multi-factor Models

Model-based Means vs. Raw Means:

- Raw means (Soybean Weeds example):
 - Joint: \bar{y}_{ij} . (simple avg of data in i, jth treatment).
 - Marginal: $\bar{y}_{i..}$ and $\bar{y}_{.j.}$ (simple avg of data at each level of a factor).
- These ignore the model (a bad idea).
 - The model "adjusts for" nuisance variables (e.g., the blocking factor). We want our estimates to reflect such adjustments!
- Sometimes model-based estimates of means and raw means agree, but not in general (e.g., unbalanced designs).
 - Even when they agree, inferences typically don't agree.
- Validate the model and then use it as a framework for inference!

Multi-factor Models—Soybean Weeds (continued)

Examine the data and fit the model:

str(weedDat) # returns structure of the data frame containing the data.

'data.frame': 96 obs. of 7 variables: \$ variety: chr "Parker" "Lambert" "M89-792" "Sturdy" ... \$ weeds : num 750 870 1090 1110 1150 1210 1330 1630 1660 2210 ... \$ herb : num 2 2 2 2 2 2 2 2 2 2 2 2 ... \$ loc : chr "R" "R" "R" "R" "R" \$ locFac : Factor w/ 2 levels "Rosemount", "St.Paul": 1 1 1 1 1 1 1 1 1 1 1 ... \$ herbFac: Factor w/ 3 levels "none", "2 weeks",..: 2 2 2 2 2 2 2 2 2 2 ... \$ varFac : Factor w/ 3 levels "none", "2 weeks",..: 2 9 16 14 5 10 11 7 1 ...

weeds.m1 <- aov(weeds-locFac+varFac+herbFac+varFac:herbFac,data=weedDat)
summary(weeds.m1)</pre>

 Df
 Sum Sq
 Mean Sq
 F value
 Pr(>F)

 locFac
 1
 50634150
 50634150
 42.453
 4.45e-08

 varFac
 15
 25587029
 1705602
 1.430
 0.173

 herbFac
 2
 85183540
 42591770
 35.710
 3.71e-10

 varFac: herbFac
 30
 2242627
 747555
 0.627
 0.912

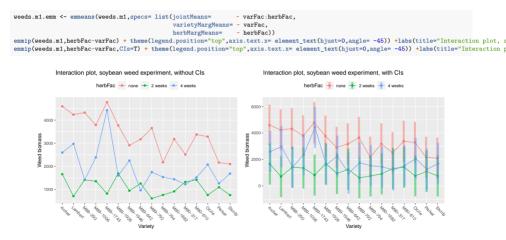
 Residuals
 47
 56057750
 1192718
 --- ---

 --- Signif. codes:
 0 ****
 0.001 '**'
 0.05 ','
 0.1 ' '
 1

- Very little evidence of interaction.

Multi-factor Models—Soybean Weeds (continued)

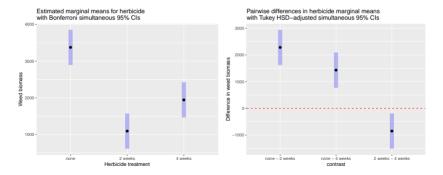
Get estimated means from the model and plot the non-significant interaction:



Multi-factor Models—Soybean Weeds (continued)

Comparisons among marginal means are reasonable with no interaction.

Bonferroni-adjusted CIs for each herbicide marginal mean: plot(summary(weeds.ml.emm%herbMargMeans,adjust="bonferroni"),horizontal=FALSE) + labs(x="Weed bionass",y="Herbicide treatment",itile="Estimated marginal means for herbicide\nuith Bonferroni simultaneous 95% CIs") # Tukey HSD adjusted confidence intervals for each pairwise difference in marginal herbicide means: plot(contrast(weeds.ml.emm%herbMargMean,method="pairwise"), horizontal=FALSE) + geom_Vlime(xintercept=0,color="red",linetype=2) + labs(x="Difference in weed biomass",itle="Pairwise differences in herbicide marginal means\nuith Tukey HSD-adjusted simultaneous 95% CIs")

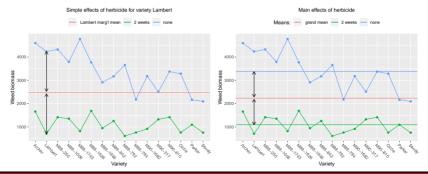


Multi-factor Models—Simple vs. Main Effects.

An "effect" in this context: for each level of a factor, the deviation up or down from the mean across all levels of the factor.

- Simple effects are in terms of joint means. E.g., differences among levels of herbicide within each variety.
- Main effects are in terms of marginal means. E.g., differences among marginal means of herbicide averaged over variety.

To simplify, suppose only 2 herbicide levels: none, 2 weeks.



Multi-factor Models—Simple Effects and Effect Slices

In presence of significant interaction, main effects (usually) not appropriate.

- Interaction implies simple effects differ, so main effect tests and comparisons of marginal means are too simplistic. They simplify or even distort the true story.
- Instead, test hypothesis of no simple effects of one factor at each level of the other (i.e., tests of **effect slices**),
- and/or use joint means to make specific comparisons across levels of one factor within each level of the other.

Soybean Weeds. Herbicide effects sliced by variety:

```
ts <- test(contrast(weeds.m1.emm$jointMeans,simple="herbFac"),joint=TRUE)
ts[1:3,] # first 3 of 16 tests</pre>
```

 varFac
 df1
 df2
 F.ratio
 p.value
 note

 1
 Archer
 2
 47
 3.770
 0.030312283
 d

 4
 Lambert
 2
 47
 5.350
 0.008065586
 d

 7
 M88-250
 2
 47
 4.733
 0.013403684
 d

Multi-factor Models—Simple Effects and Effect Slices

In the presence of interaction, testing effect slices is an appropriate alternative to testing main effects.

- In the Soybean Weed example, that replaces a single 2-df test by 16 tests. Doesn't that inflate Type I error rate?
- Yes! So apply some multiplicity adjustment.

Here we use p.adjust() function to add p-values adjusted by

- Holm's method (controls familywise error rate), and
- Benjamini-Hochberg method (controls false discovery rate).

ts%fdr_adjpval <- format.pval(p.adjust(ts%p.value,method="fdr"),digits=3,eps=.0001)
ts%holm_adjpval <- format.pval(p.adjust(ts%p.value,method="holm"),digits=3,eps=.0001)
ts[1:6], # first 6 of 16 tests</pre>

	varFac	df1	df2	F.ratio	p.value	note	fdr_adjpval	holm_adjpval
1	Archer	2	47	3.770	0.0303122833	d	0.0970	0.3637
4	Lambert	2	47	5.350	0.0080655864	d	0.0645	0.1210
7	M88-250	2	47	4.733	0.0134036844	d	0.0715	0.1877
10	M89-1006	2	47	2.505	0.0925044831	d	0.1693	0.9067
13	M89-1743	2	47	8.047	0.0009876509	d	0.0158	0.0158
16	M89-1926	2	47	2.527	0.0906722193	d	0.1693	0.9067

For data from experiments with crossed treatment factors, we typically include main effects and all interactions among the factors.

- E.g., the Soybean Weed example, herbicide is crossed with variety.
 - We include herbFac, varFac and herbFac:varFac to assess whether factors interact and, if not, how each factor alone affects the mean response.

We **do not** test interaction and, if not significant, drop it and re-fit.

• The model reflects the design, allowing means for every treatment. It's a framework for inference on all questions about how treatment means differ.

But in a model that allows for interaction, how do we test main effects? When data are unbalanced, there is more than one answer to that question!

- Type I (sequential) tests
- Type II tests
- Type III tests

- Type I: model is built up one term at a time and significance of each effect is relative to the previous model that lacked that term.
 - This approach rarely tests interesting hypotheses on main effects.
- Type II: the significance of an effect is based on how much it improves a $hierarchical\ model^1$ that lacks the effect.
 - Each effect is tested based on adjusting for all other effects of the same order and higher order effects not containing the effect.
 - For main effects in an unbalanced two-way model, this tests a null hypothesis defined in terms of a weighted average of treatment means, weighted by relative sample sizes.
 - Unless sensible to average over factor levels in proportion to their sample sizes², this is unappealing.

¹Hierarchy principle: interactions aren't allowed unless subordinate effects also included. ²Might be sensible if replication is proportional to population prevalence so that factor levels aren't equally relevant to the population.

- Type III: significance of an effect is based on its effect when dropped from the model.
 - For main effects in a two-way model, equivalent to testing if the marginal means for the factor are all equal.
 - But the previous interpretation only applies when sum-to-zero constraints are used to parameterize the model!
 - Otherwise, the type 3 tests will be nonsensical.

In R,

- anova(fittedModel) and summary(fittedModel) give Type I tests.
 - Often inappropriate and can be very different from Types II and III.
- For Types II and III use Anova(fittedModel,type=) from car package.
- Type III is usually the right choice for experimental data, **but must use sum-to-zero constraints** when fitting the model.

Soybean Weed Example:

- Suppose varieties 3-16 in Rosemount and 1-14 in St.Paul.
 - This gives an unbalanced design with different treatments in each block.

```
# Fit the model to the unblanaced data. All 3 modelsbelow are equivalent.
# Important to use 3rd one for Type III tests
weeds.mla.un <- aov(weeds-locFac+varFac+herbFac,data=weedDat.un)
weeds.mla.un <- aov(weeds-locFac+varFac+herbFac,data=weedDat.un,contrasts=list(locFac=contr.sum,varFac=contr.sum,herbFac=contr.sum))
# Type I tests depend on the order of the terms in the formula within the aov() function (not good)).
anova(weeds.ml.un) anova(weeds.ml.un)</pre>
```

```
Analysis of Variance Table
Response: weeds
                  Sum Sq Mean Sq F value
              Df
                                              Pr(>F)
locFac
               1 43545600 43545600 48.5258 4.226e-08 ***
varFac
              15 24332306 1622154 1.8077
                                             0.07408
herbFac
               2 70519779 35259889 39 2925 1 130e-09 ***
varFac:herbFac 30 32559288 1085310 1.2094
                                            0.29245
              35 31407928 897369
Residuals
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Analysis of Variance Table
Response: weeds
              Df
                   Sum Sg Mean Sg F value
                                              Pr(>F)
varFac
              15 37275633 2485042 2 7693 0 006504 **
herbFac
               2 70519779 35259889 39 2925 1 130e-09 ***
locFac
                1 30602272 30602272 34 1022 1 256e-06 ***
varFac-herbFac 30 32559288 1085310 1 2094 0 292454
Residuals
              35 31407928 897369
```

Soybean Weed Example (continued):

Type III tests: Anova(weeds.m1b.un,type=3)

Anova Table (Type III tests)

Response: weeds Sum Sg Df F value Pr(>F) (Intercept) 364844813 1 406.5715 < 2.2e-16 *** locFac 30602272 1 34 1022 1 256e-06 *** varFac 24332306 15 1 8077 0 07408 herbFac 61967112 2 34 5271 5 238e-09 *** varFac:herbFac 32559288 30 1 2094 0 29245 Regiduale 31407928 35 Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Type III tests with wrong type of contrasts give garbage results, but no warnings, so must know what you are doing!: Anova(weeds.m1.un,type=3) # WRONG!

Anova Table (Type III tests)

 Response: weeds
 Sum Sq Df F value
 Pr(>F)

 (Intercept)
 53572721
 1
 59.6997
 4.523e-09

 locFac
 30602272
 1
 34.1022
 1.256e-06

 varFac
 29292533
 15
 2.1752
 0.02904
 *

 herbFac
 8992300
 2
 5.0104
 0.01220 *
 varFac:herbFac
 32559288
 30
 1.2094
 0.29245

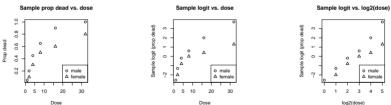
 Residuals
 31407928
 35
 --- Signif. codes:
 0 '***'
 0.001 '**'
 0.05 '.'
 0.1 ' '
 1

Factors and Marginal Means in Logistic Regression

A logistic regression example—Tobacco Budworms

		doseFac	1	2	4	8	16	32	
sexFac	deadFac								
Male	No		19	16	11	7	2	0	
	Yes		1	4	9	13	18	20	
Female	No		20	18	14	10	8	4	
	Yes		0	2	6	10	12	16	

Plot (a)



Plot (b)

Plot (c)

A main effects model: y_{ij} 's indep, $y_{ij} \sim Bin(20, \pi_{ij})$

$$\operatorname{logit}(\pi_{ij}) = \underbrace{\mu + \alpha_i + \beta_j}_{\equiv \eta_{ij}}, \quad i = 1, 2; j = 1, ..., 6$$

bud.mainmod <- glm(cbind(dead,alive)-sexFac+doseFac,data=budworm,family=binomial(link="logit"),contrasts=list(doseFac=contr.poly))
gof(bud.mainmod) # adequate fit</pre>

D = 5.0128, df = 5, P(>D) = 0.4143176 X2 = 3.7014, df = 5, P(>X2) = 0.5931545

```
# Test main effects with LR tests:
Anova(bud.mainmod,type=2,test.statistic="LR") # don't use anova()!
```

Analysis of Deviance Table (Type II tests)

Response: cbind(dead, alive) LR Chiag Df Pr(>Chiag) sexFac 10.14 1 0.001451 ** doseFac 113.79 5 < 2.2e-16 *** ---Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Marginal means of the linear predictor:

- Avg log odds of of death for sex *i*, averaged over dose: $\bar{\eta}_{i} = \frac{1}{6}(\eta_{i1} + \dots + \eta_{i6}).$
- Avg log odds of death at dose j, averaged over sex: $\bar{\eta}_{ij} = \frac{1}{2}(\eta_{1j} + \eta_{2j})$.

(bud.mainmod.emm <- emmeans(bud.mainmod,adjust="bonferroni",specs= list(doseMargMeans= ~ doseFac,sexMargMeans= ~ sexFac)))

\$doseMargMeans

doseFac	emmean	SE	df	asymp.LCL	asymp.UCL
1	-3.799	1.019	Inf	-6.488	-1.110
2	-1.837	0.455	Inf	-3.038	-0.636
4	-0.549	0.339	Inf	-1.443	0.345
8	0.325	0.332	Inf	-0.550	1.200
16	1.173	0.378	Inf	0.176	2.170
32	2.313	0.538	Inf	0.893	3.733

Results are averaged over the levels of: sexFac Results are given on the logit (not the response) scale. Confidence level used: 0.95 Conf-level adjustment: bonferroni method for 6 estimates

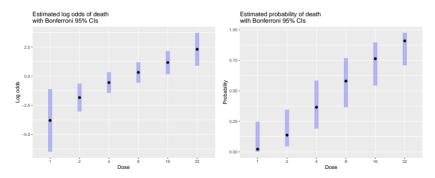
\$sexMargMeans

sexFac	emmean	SE	df	asymp.LCL	asymp.UCL
Male	0.149	0.285	lnf	-0.49	0.788
Female	-0.940	0.293	Inf	-1.60	-0.284

Results are averaged over the levels of: doseFac Results are given on the logit (not the response) scale. Confidence level used: 0.95 Conf-level adjustment: bonferroni method for 2 estimates

Plots of the marginal means for doseFac on log odds and probability scales (note the type= argument):

plot(bud.mainmod.emm%doseMargMeans,adjust="bonferroni",horizontal=FALSE.ylab="Dose",xlab="Log odds",type="link") +
ggtitle("Estimated log odds of death/nuith Bonferroni 95% CIs")
plot(Dud.mainmod.emm%doseMargMeans,adjust="bonferroni",horizontal=FALSE,ylab="Dose",xlab="Probability",type="response") +
ggtitle("Estimated probability of death/nuith Bonferroni 95% CIs")



Contrasts in marginal means:

- Doses are evenly spaced on the log₂ scale. Suppose we wish to test that dose effects on log odds of death are linear on that scale (recall plots).
 - Because we coded doseFac with contr.poly() contrasts, the coefficients for this factor can tell us whether linear, higher-order effects are significant:

arm::display(bud.mainmod,detail=TRUE) # briefer summary than given by summary() function

```
glm(formula = cbind(dead, alive) ~ sexFac + doseFac, family = binomial(link = "logit"),
   data = budworm, contrasts = list(doseFac = contr.poly))
            coef.est coef.se z value Pr(>|z|)
(Intercept) 0.15
                             0.52
                                     0.60
                      0.29
sexFacFemale -1.09
                      0.35
                             -3.09
                                     0.00
                            6.60
doseFac.L
             4.84
                      0.73
                                    0.00
doseFac.0
            -0.64
                      0.66
                             -0.97
                                    0.33
          0.45
doseFac C
                      0.54
                            0.82
                                    0.41
          0.01
doseFac^4
                      0.44
                            0.03
                                     0.98
doseFac^5
            -0.01
                      0.36
                             -0.04
                                     0.97
 n = 12, k = 7
 residual deviance = 5.0, null deviance = 124.9 (difference = 119.9)
```

• With this coding of doseFac, we can test nonlinear dose effects with joint test of the last 4 coefficients of the model. Or, under any parameterization, we can do the test on the marginal means.³

```
# Wald test that nonlinear effects of dose are null, computed two different ways:
coef.names <- names(coef(bud.mainmod)); lht(bud.mainmod,coef.names[-c(1:3]]) # lht stands for linear hypothesis test. From car package.
Linear hypothesis test
Hypothesis:
doseFac: 0 = 0
doseFac' 4 = 0
doseFac' 5 = 0
Model 1: restricted model
Model 2: cbind(dead, alive) - sexFac + doseFac
Res.Df Df Chisq Pr(>Chisq)
1 9
2 5 4 1.4684 0.8322
```

test(contrast(bud.mainmod.emm\$doseMargMeans,method=as.data.frame(contr.poly(6)[,-1])),joint=T) # F test w/ inf df equiv to chisq test above

df1 df2 F.ratio p.value 4 Inf 0.367 0.8322

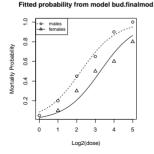
³This is a Wald test, which is asymptotically equivalent to a likelihood ratio test. LRTs have somewhat better properties, so an LRT would be a better choice here and is easy to implement as anova(update(bud.mainmod,.~sexFac+ldose),bud.mainmod,test="LRT").

Conclusion:

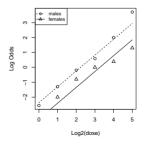
• log odds of death are linear in $\log_2(\mathrm{dose})$ with different intercepts for each sex:

$$logit(\pi_{ij}) = \alpha_i + \beta \log_2(dose).$$

bud.finalmod <- update(bud.mainmod,.~0+sexFac+ldose)</pre>



Fitted log odds from model bud.finalmod



Questions?

Questions?

Thanks

- If you need assistance with R or with any statistical design or analysis task, please contact the SCC.
 - www.stat.uga/consulting
- We can help!

Thank you!