STAD29: Statistics for the Life and Social Sciences

Lecture notes

Section 1

Course Outline

Course and instructor

- Lecture: Wednesday 14:00-16:00 in HW 215. Optional computer lab Monday 16:00-17:00 in BV 498.
- Instructor: Ken Butler
- Office: IC 471.
- E-mail: `butler@utsc.utoronto.ca`
- Office hours: Monday 11:00-13:00. I am often around otherwise. See if I'm in. Or make an appointment. E-mail always good.
- Course website: xxx link.
- Using Quercus for assignments/grades only; using website for everything else.

Texts

- There is no official text for this course.
- You may find "R for Data Science", **link** helpful for R background.
- I will refer frequently to my book of Problems and Solutions in Applied Statistics (PASIAS), **link**.
- Both of these resources are and will remain free.

Programs, prerequisites and exclusions

- Prerequisites:
- For undergrads: STAC32. Not negotiable.
- For grad students, a first course in statistics, and some training in regression and ANOVA. The less you know, the more you'll have to catch up!
- This course is a required part of Applied Statistics minor.
- Exclusions: **this course is not for Math/Statistics/CS majors/minors**. It is for students in other fields who wish to learn some more advanced statistical methods. The exclusions in the Calendar reflect this.
- If you are in one of those programs, you won't get program credit for this course, **or for any future STA courses you take.**

Computing

- Computing: big part of the course, **not** optional. You will need to demonstrate that you can use R to analyze data, and can critically interpret the output.
- For grad students who have not come through STAC32, I am happy to offer extra help to get you up to speed.

Assessment 1/2

- Grading: (2 hour) midterm, (3 hour) final exam. Assignments most weeks, due Tuesday at 11:59pm. Graduate students (STA 1007) also required to complete a project using one or more of the techniques learned in class, on a dataset from their field of study. Projects due on the last day of classes.
- Assessment:

	STAD29	STA 1007
Assignments	20%	20%
Midterm exam	30%	20%
Project	-	20%
Final exam	50%	40%

Assessment 2/2

- Assessments missed *with documentation* will cause a re-weighting of other assessments of same type. No make-ups.
- You **must pass the final exam** to guarantee passing the course. If you fail the final exam but would otherwise have passed the course, you receive a grade of 45.

Plagiarism

- **This link** defines academic offences at this university. Read it. You are bound by it. xxx
- Plagiarism defined (at the end) as
  The wrongful appropriation and purloining, and publication as one's own, of the ideas, or the expression of the ideas ... of another.
- The code and explanations that you write and hand in must be *yours and yours alone*.
- When you hand in work, it is implied that it is *your* work. Handing in work, with your name on it, that was actually done by someone else is an *academic offence*.
- If I am suspicious that anyone's work is plagiarized, I will take action.

Getting help

- The English Language Development Centre supports all students in developing better Academic English and critical thinking skills needed in academic communication. Make use of the personalized support in academic writing skills development. Details and sign-up information: link.
- Students with diverse learning styles and needs are welcome in this course. In particular, if you have a disability/health consideration that may require accommodations, please feel free to approach the AccessAbility Services Office as soon as possible. I will work with you and AccessAbility Services to ensure you can achieve your learning goals in this course. Enquiries are confidential. The UTSC AccessAbility Services staff are available by appointment to assess specific needs, provide referrals and arrange appropriate accommodations: (416) 287-7560 or by e-mail: `ability@utsc.utoronto.ca`.

Course material xxx

- Regression-like things
  - review of (multiple) regression
  - logistic regression (including multi-category responses)
  - survival analysis
- ANOVA-like things
  - more ANOVA
  - multivariate ANOVA
  - repeated measures
- Multivariate methods
  - discriminant analysis
  - cluster analysis
  - multidimensional scaling
  - principal components
  - factor analysis
- Miscellanea
  - time series
  - multiway frequency tables

Section 2

Review of (multiple) regression

Regression

- Use regression when one variable is an outcome (*response*, y).
- See if/how response depends on other variable(s), *explanatory*, $x_1, x_2, \ldots$.
- Can have *one* or *more than one* explanatory variable, but always one response.
- Assumes a *straight-line* relationship between response and explanatory.
- Ask: xxx
  - *is there* a relationship between y and x's, and if so, which ones?
  - what does the relationship look like?

Packages

```
library(MASS) # for Box-Cox, later
library(tidyverse)
library(broom)
```

A regression with one x

13 children, measure average total sleep time (ATST, mins) and age (years) for each. See if ATST depends on age. Data in `sleep.txt`, ATST then age. Read in data:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/sleep.txt"
sleep <- read_delim(my_url, " ")
```

```
## Parsed with column specification:
## cols(
##   atst = col_double(),
##   age = col_double()
## )
```

Check data xxx

```
glimpse(sleep)
```

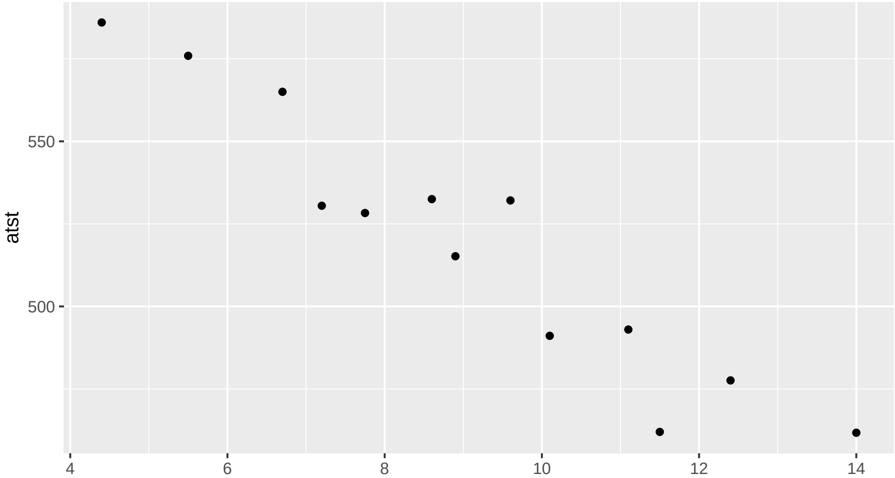
```
## Observations: 13
## Variables: 2
## $ atst <dbl> 586.00, 461.75, 491.10, 565.00, 462.…
## $ age  <dbl> 4.40, 14.00, 10.10, 6.70, 11.50, 9.6…
```

Exploratory stuff

Make scatter plot of ATST (response) vs. age (explanatory) using code overleaf:

The scatterplot

```
ggplot(sleep, aes(x = age, y = atst)) + geom_point()
```



Correlation

- Measures how well a straight line fits the data:

```
with(sleep, cor(atst, age))
```

```
## [1] -0.9515469
```

- 1 is perfect upward trend, -1 is perfect downward trend, 0 is no trend.
- This one close to perfect downward trend.
- Can do correlations of all pairs of variables:

```
cor(sleep)
```

```
##            atst        age
## atst  1.0000000 -0.9515469
## age  -0.9515469  1.0000000
```

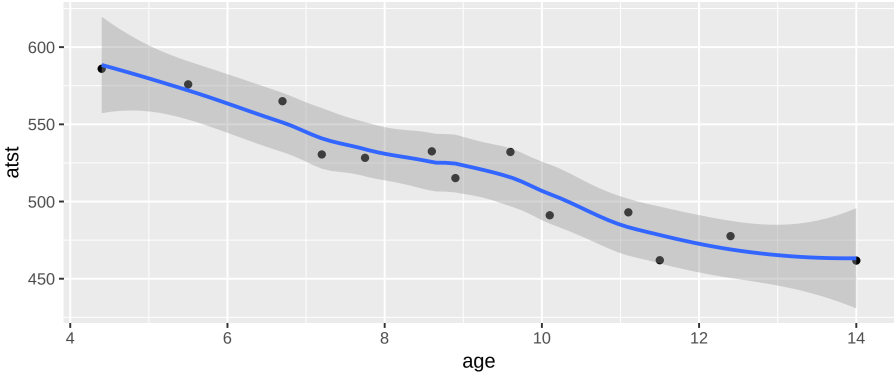
Lowess curve

- Sometimes nice to guide the eye: is the trend straight, or not?
- Idea: *lowess curve*. "Locally weighted least squares", not affected by outliers, not constrained to be linear.
- Lowess is a *guide*: even if straight line appropriate, may wiggle/bend a little. Looking for *serious* problems with linearity.
- Add lowess curve to plot using `geom_smooth`:

Plot with lowess curve

```
ggplot(sleep, aes(x = age, y = atst)) + geom_point() +
  geom_smooth()
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



The regression

Scatterplot shows no obvious curve, and a pretty clear downward trend. So we can run the regression:

```
sleep.1 <- lm(atst ~ age, data = sleep)
summary(sleep.1)
```

```
##
## Call:
## lm(formula = atst ~ age, data = sleep)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -23.011  -9.365   2.372   6.770  20.411
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  646.483     12.918   50.05 2.49e-14 ***
```

Conclusions

- The relationship appears to be a straight line, with a downward trend.
- F-tests for model as a whole and t-test for slope (same) both confirm this (P-value $5.7 \times 10^{-7} = 0.00000057$).
- Slope is -14, so a 1-year increase in age goes with a 14-minute decrease in ATST on average.
- R-squared is correlation squared (when one x anyway), between 0 and 1 (1 good, 0 bad).
- Here R-squared is 0.9054, pleasantly high.

Doing things with the regression output

- Output from regression (and eg. t-test) is all right to look at, but hard to extract and re-use information from.
- Package broom extracts info from model output in way that can be used in pipe (later):

```
tidy(sleep.1)
```

```
## # A tibble: 2 x 5
##   term        estimate std.error statistic  p.value
##   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)    646.      12.9       50.0 2.49e-14
## 2 age            -14.0      1.37     -10.3 5.70e- 7
```

```
glance(sleep.1)
```

```
## # A tibble: 1 x 11
##   r.squared adj.r.squared sigma statistic p.value    df
```

Broom part 2

```
sleep.1 %>% augment(sleep) %>% slice(1:8)
```

```
## # A tibble: 8 x 9
##     atst   age .fitted .se.fit .resid   .hat .sigma .cooksd
##    <dbl> <dbl>   <dbl>   <dbl>  <dbl>  <dbl>  <dbl>   <dbl>
## 1  586     4.4    585.    7.34   1.30 0.312    13.8 0.00320
## 2  462.   14      450.    7.68  11.8  0.341    13.0 0.319
## 3  491.   10.1    505.    3.92 -13.6  0.0887   13.0 0.0568
## 4  565     6.7    552.    4.87  12.6  0.137    13.1 0.0844
## 5  462    11.5    485.    4.95 -23.0  0.141    11.3 0.294
## 6  532.    9.6    512.    3.72  20.4  0.0801   12.0 0.114
## 7  478.   12.4    472.    5.85   5.23 0.198    13.7 0.0243
## 8  515.    8.9    522.    3.65  -6.32 0.0772   13.6 0.0105
## # … with 1 more variable: .std.resid <dbl>
```

Useful for plotting residuals against an x-variable. for week 2:

regression and multiple regression

CI for mean response and prediction intervals

Once useful regression exists, use it for prediction:

- To get a single number for prediction at a given x, substitute into regression equation, eg. age 10: predicted ATST is $646.48 - 14.04(10) = 506$ minutes.
- To express uncertainty of this prediction:
- *CI for mean response* expresses uncertainty about mean ATST for all children aged 10, based on data.
- *Prediction interval* expresses uncertainty about predicted ATST for a new child aged 10 whose ATST not known. More uncertain.
- Also do above for a child aged 5.

Intervals

- Make new data frame with these values for age

```
my.age <- c(10, 5)
ages.new <- tibble(age = my.age)
ages.new
```

```
## # A tibble: 2 x 1
##     age
##   <dbl>
## 1    10
## 2     5
```

- Feed into `predict`:

```
pc <- predict(sleep.1, ages.new, interval = "c")
pp <- predict(sleep.1, ages.new, interval = "p")
```

The intervals

Confidence intervals for mean response:

```
cbind(ages.new, pc)
```

```
##   age      fit      lwr      upr
## 1  10 506.0729 497.5574 514.5883
## 2   5 576.2781 561.6578 590.8984
```

Prediction intervals for new response:

```
cbind(ages.new, pp)
```

```
##   age      fit      lwr      upr
## 1  10 506.0729 475.8982 536.2475
## 2   5 576.2781 543.8474 608.7088
```

Comments

- Age 10 closer to centre of data, so intervals are both narrower than those for age 5.
- Prediction intervals bigger than CI for mean (additional uncertainty).
- Technical note: output from `predict` is R `matrix`, not data frame, so Tidyverse `bind_cols` does not work. Use base R `cbind`.

That grey envelope

```
ggplot(sleep, aes(x = age, y = atst)) + geom_point() +
  geom_smooth(method = "lm") +
  scale_y_continuous(breaks = seq(420, 600, 20))
```

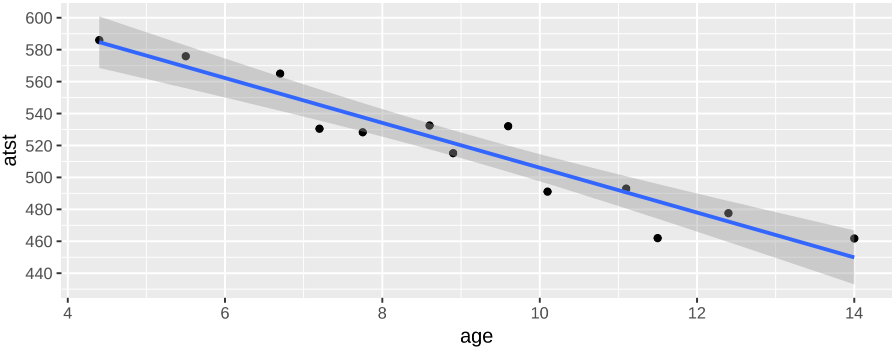


Figure 3: plot of chunk unnamed-chunk-15

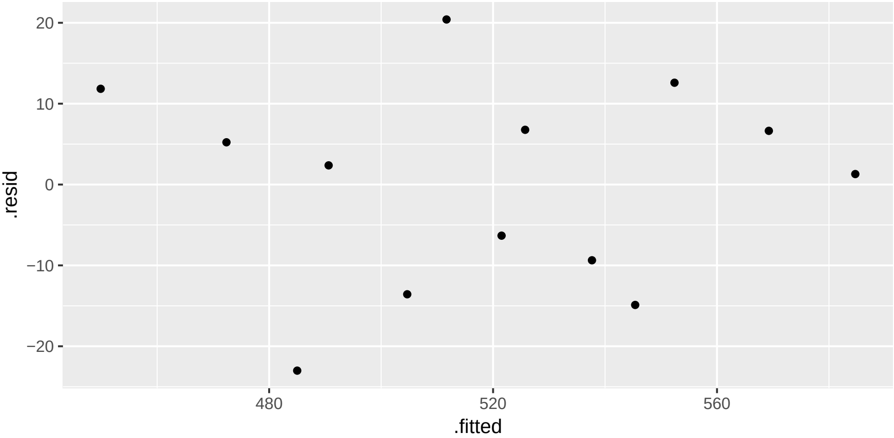
Diagnostics

How to tell whether a straight-line regression is appropriate?

- Before: check scatterplot for straight trend.
- After: plot *residuals* (observed minus predicted response) against predicted values. Aim: a plot with no pattern.

Output

```
ggplot(sleep.1, aes(x = .fitted, y = .resid)) + geom_point()
```



An inappropriate regression

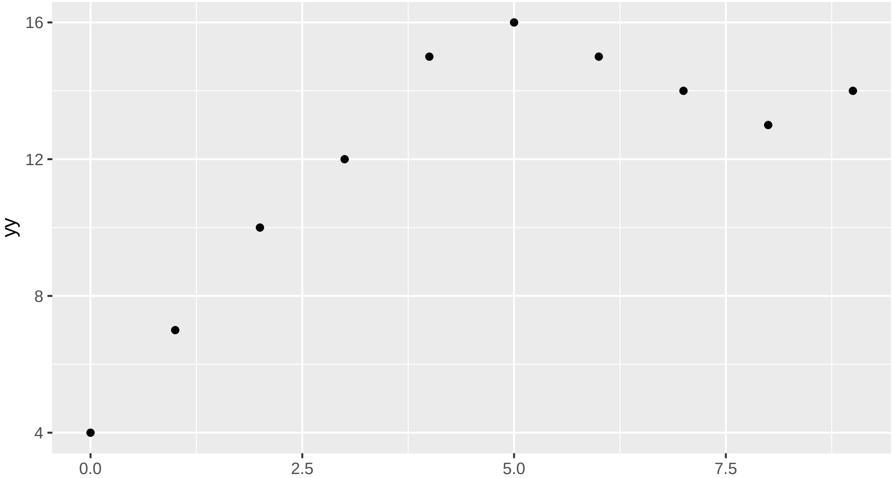
Different data:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/curvy.txt"
curvy <- read_delim(my_url, " ")
```

```
## Parsed with column specification:
## cols(
##   xx = col_double(),
##   yy = col_double()
## )
```

Scatterplot

```
ggplot(curvy, aes(x = xx, y = yy)) + geom_point()
```



Regression line, anyway

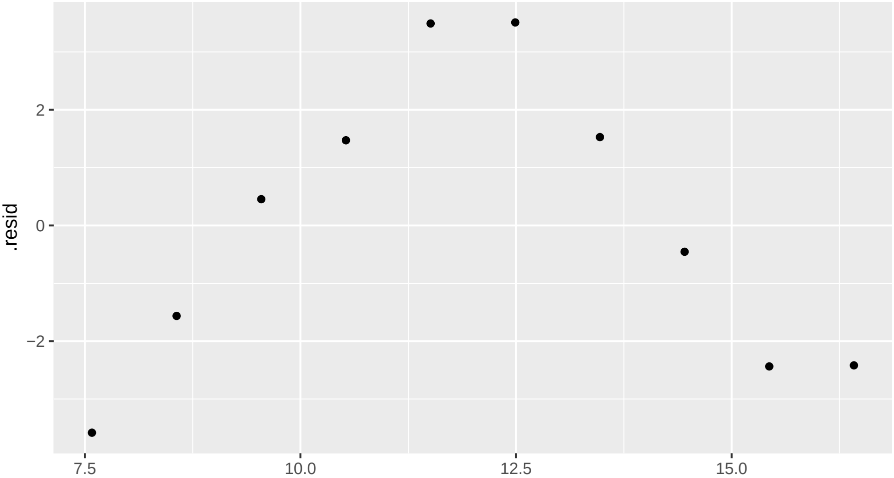
{

```
curvy.1 <- lm(yy ~ xx, data = curvy)
summary(curvy.1)
```

```
##
## Call:
## lm(formula = yy ~ xx, data = curvy)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -3.582 -2.204  0.000  1.514  3.509
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   7.5818     1.5616   4.855  0.00126 **
## xx            0.9818     0.2925   3.356  0.00998 **
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

Residual plot

```
ggplot(curvy.1, aes(x = .fitted, y = .resid)) + geom_point()
```



No good: fixing it up

- Residual plot has *curve*: middle residuals positive, high and low ones negative. Bad.
- Fitting a curve would be better. Try this:

```
curvy.2 <- lm(yy ~ xx + I(xx^2), data = curvy)
```

- Adding xx-squared term, to allow for curve.
- Another way to do same thing: specify how model *changes*:

```
curvy.2a <- update(curvy.1, . ~ . + I(xx^2))
```

Regression 2

{

```
summary(curvy.2)
```

```
##
## Call:
## lm(formula = yy ~ xx + I(xx^2), data = curvy)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -1.2091 -0.3602 -0.2364  0.8023  1.2636
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  3.90000    0.77312   5.045 0.001489 **
## xx           3.74318    0.40006   9.357 3.31e-05 ***
## I(xx^2)     -0.30682    0.04279  -7.170 0.000182 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9833 on 7 degrees of freedom
## Multiple R-squared:  0.9502, Adjusted R-squared:  0.936
## F-statistic: 66.83 on 2 and 7 DF,  p-value: 2.75e-05
```

Comments

- `xx`-squared term initely significant (P-value 0.000182), so need this curve to describe relationship.
- Adding squared term has made R-squared go up from 0.5848 to 0.9502: great improvement.
- This is a inite curve!

The residual plot now

```
ggplot(curvy.2, aes(x = .fitted, y = .resid)) + geom_point()
```

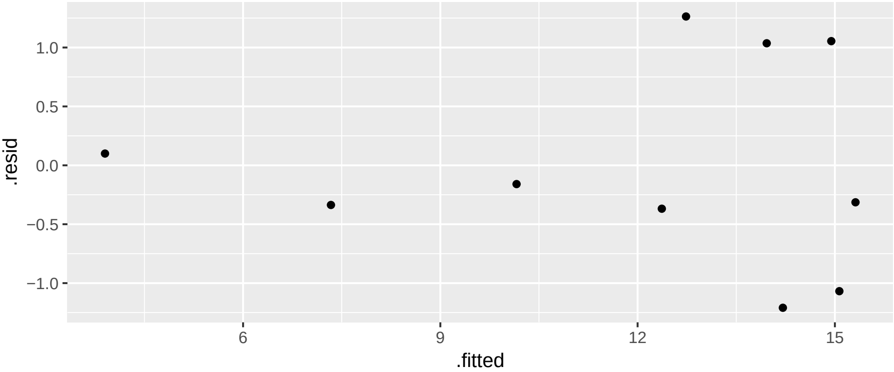


Figure 7: plot of chunk unnamed-chunk-21

Another way to handle curves

- Above, saw that changing x (adding x^2) was a way of handling curved relationships.
- Another way: change y (transformation).
- Can guess how to change y, or might be theory:
- example: relationship $y = ae^{bx}$ (exponential growth):
- take logs to get $\ln y = \ln a + bx$.
- Taking logs has made relationship linear ($\ln y$ as response).
- Or, *estimate* transformation, using Box-Cox method.

Box-Cox

- Install package `MASS` via `install.packages("MASS")` (only need to do *once*)
- Every R session you want to use something in `MASS`, type `library(MASS)`

Some made-up data

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/madeup.csv"
madeup <- read_csv(my_url)
madeup
```

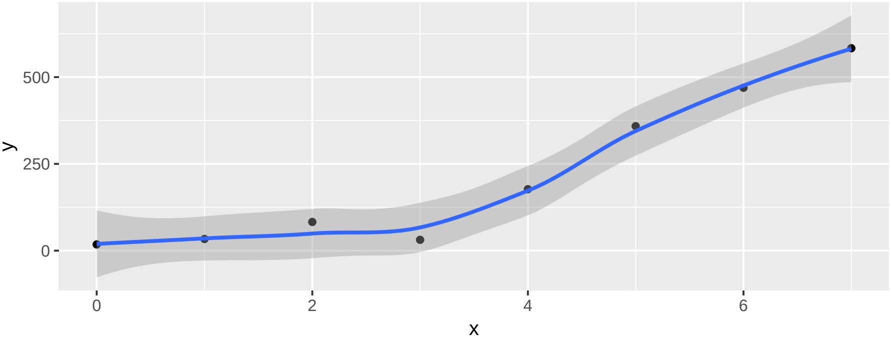
```
## # A tibble: 8 x 3
##     row     x     y
##   <dbl> <dbl> <dbl>
## 1     1     0  17.9
## 2     2     1  33.6
## 3     3     2  82.7
## 4     4     3  31.2
## 5     5     4 177.
## 6     6     5 359.
## 7     7     6 469.
## 8     8     7 583.
```

Seems to be faster-than-linear growth, maybe exponential growth.

The scatterplot: faster than linear growth

```
ggplot(madeup, aes(x = x, y = y)) + geom_point() +
  geom_smooth()
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```

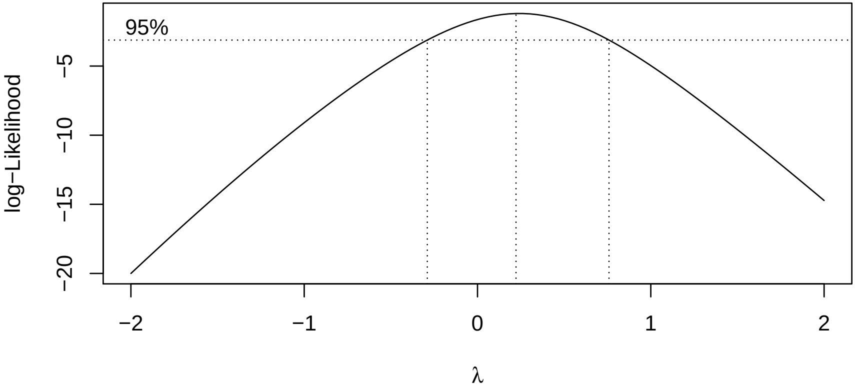


Running Box-Cox

- `library(MASS)` first.
- Feed `boxcox` a model formula with a squiggle in it, such as you would use for `lm`.
- Output: a graph (next page):

```
boxcox(y ~ x, data = madeup)
```

The Box-Cox output



Comments

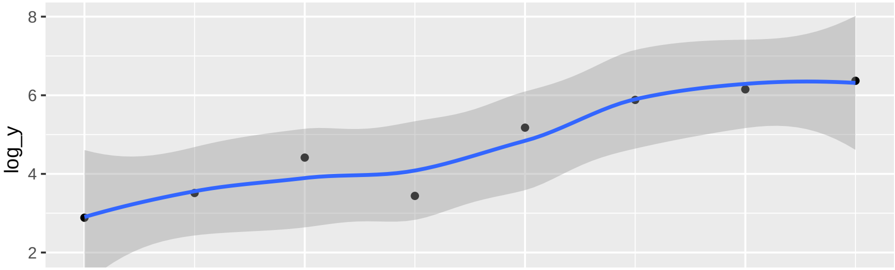
- λ (lambda) is the power by which you should transform y to get the relationship straight (straighter). Power 0 is "take logs"
- Middle dotted line marks best single value of λ (here about 0.1).
- Outer dotted lines mark 95% CI for λ, here -0.3 to 0.7, approx. (Rather uncertain about best transformation.)
- Any power transformation within the CI supported by data. In this case, log ($\lambda = 0$) and square root ($\lambda = 0.5$) good, but no transformation ($\lambda = 1$) not.
- Pick a "round-number" value of λ like $2, 1, 0.5, 0, -0.5, -1$. Here 0 and 0.5 good values to pick.

Did transformation straighten things?

- Calculate transformed y and plot against x. Here try log:

```
madeup %>%
  mutate(log_y = log(y)) %>%
  ggplot(aes(x = x, y = log_y)) + geom_point() +
  geom_smooth()
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



Regression with transformed y

```
madeup.1 <- lm(log(y) ~ x, data = madeup)
glance(madeup.1)
```

```
## # A tibble: 1 x 11
##   r.squared adj.r.squared sigma statistic p.value    df
##       <dbl>         <dbl> <dbl>     <dbl>   <dbl> <int>
## 1     0.883         0.864 0.501      45.3 5.24e-4     2
## # … with 5 more variables: logLik <dbl>, AIC <dbl>,
## #   BIC <dbl>, deviance <dbl>, df.residual <int>
```

```
tidy(madeup.1)
```

```
## # A tibble: 2 x 5
##   term        estimate std.error statistic  p.value
##   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)    2.91     0.323       8.99 0.000106
## 2 x              0.520    0.0773      6.73 0.000524
```

Multiple regression

- What if more than one x? Extra issues: % regression ex from before
- Now one intercept and a slope for each x: how to interpret?
- Which x-variables actually help to predict y?
- Different interpretations of "global" F-test and individual t-tests.
- R-squared no longer correlation squared, but still interpreted as "higher better".
- In `lm` line, add extra xs after `~`.
- Interpretation not so easy (and other problems that can occur).

Multiple regression example

Study of women and visits to health professionals, and how the number of visits might be related to other variables:

- timedrs: number of visits to health professionals (over course of study)
- phyheal: number of physical health problems
- menheal: number of mental health problems
- stress: result of questionnaire about number and type of life changes

`timedrs` response, others explanatory.

The data

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/regressx.tx
visits <- read_delim(my_url, " ")
```

```
## Parsed with column specification:
## cols(
##   subjno = col_double(),
##   timedrs = col_double(),
##   phyheal = col_double(),
##   menheal = col_double(),
##   stress = col_double()
## )
```

Check data, fit multiple regression

```
visits
```

```
## # A tibble: 465 x 5
##    subjno timedrs phyheal menheal stress
##     <dbl>   <dbl>   <dbl>   <dbl>  <dbl>
##  1      1       1       5       8    265
##  2      2       3       4       6    415
##  3      3       0       3       4     92
##  4      4      13       2       2    241
##  5      5      15       3       6     86
##  6      6       3       5       5    247
##  7      7       2       5       6     13
##  8      8       0       4       5     12
##  9      9       7       5       4    269
## 10     10       4       3       9    391
## # … with 455 more rows
```

The regression

{

```
summary(visits.1)
```

```
##
## Call:
## lm(formula = timedrs ~ phyheal + menheal + stress, data = visits)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -14.792  -4.353  -1.815   0.902  65.886
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -3.704848   1.124195  -3.296 0.001058 **
## phyheal      1.786948   0.221074   8.083  5.6e-15 ***
## menheal     -0.009666   0.129029  -0.075 0.940318
## stress       0.013615   0.003612   3.769 0.000185 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9.708 on 461 degrees of freedom
## Multiple R-squared:  0.2188, Adjusted R-squared:  0.2137
```

The slopes

Model as a whole strongly significant even though R-sq not very big (lots of data). At least one of the x's predicts `timedrs`.

"'r tidy(visits.1) "'

"' A tibble: 4 x 5 term estimate std.error statistic p.value <chr> <dbl> <dbl> <dbl> <dbl> 1 (Intercept) -3.70 1.12 -3.30 1.06e- 3 2 phyheal 1.79 0.221 8.08 5.60e-15 3 menheal -0.00967 0.129 -0.0749 9.40e- 1 4 stress 0.0136 0.00361 3.77 1.85e- 4 "'

The physical health and stress variables initely help to predict the number of visits, but *with those in the model* we don't need `menheal`. However, look at prediction of `timedrs` from `menheal` by itself:

Just menheal

{

```
visits.2 <- lm(timedrs ~ menheal, data = visits)
summary(visits.2)
```

```
##
## Call:
## lm(formula = timedrs ~ menheal, data = visits)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -13.826  -5.150  -2.818   1.177  72.513
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)   3.8159     0.8702   4.385 1.44e-05 ***
## menheal       0.6672     0.1173   5.688 2.28e-08 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
```

`menheal` by itself

- `menheal` by itself {em does} significantly help to predict `timedrs`.
- But the R-sq is much less (6.5% vs. 22%).
- So other two variables do a better job of prediction.
- With those variables in the regression (`phyheal` and `stress`), don't need `menheal` *as well*.

Investigating via correlation

Leave out first column (`subjno`):

```
visits %>% select(-subjno) %>% cor()
```

```
##           timedrs   phyheal   menheal    stress
## timedrs 1.0000000 0.4395293 0.2555703 0.2865951
## phyheal 0.4395293 1.0000000 0.5049464 0.3055517
## menheal 0.2555703 0.5049464 1.0000000 0.3697911
## stress  0.2865951 0.3055517 0.3697911 1.0000000
```

- `phyheal` most strongly correlated with `timedrs`.
- Not much to choose between other two.
- But `menheal` has higher correlation with `phyheal`, so not as much to *add* to prediction as `stress`.
- Goes to show things more complicated in multiple regression.

Residual plot (from timedrs on all)

```
ggplot(visits.1, aes(x = .fitted, y = .resid)) + geom_point()
```

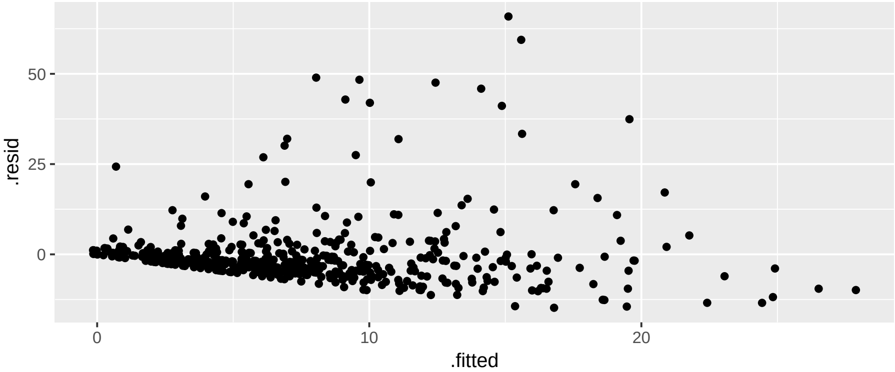
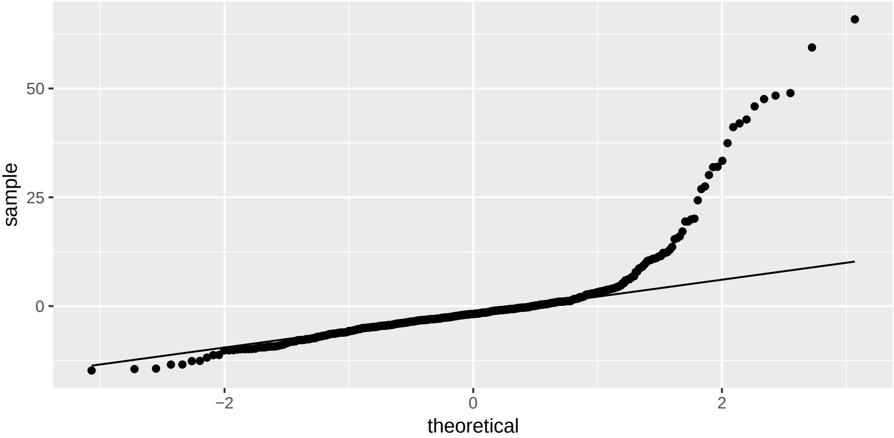


Figure 11: plot of chunk iffy8

Normal quantile plot of residuals

```
ggplot(visits.1, aes(sample = .resid)) + stat_qq() + stat_qq_l
```

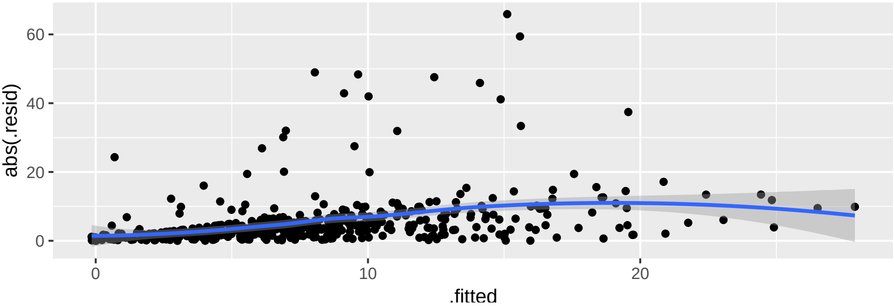


Absolute residuals

Is there trend in *size* of residuals (fan-out)? Plot *absolute value* of residual against fitted value:

```
ggplot(visits.1, aes(x = .fitted, y = abs(.resid))) +
  geom_point() + geom_smooth()
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



Comments

- On the normal quantile plot:
- highest (most positive) residuals are *way* too high
- distribution of residuals skewed to right (not normal at all)
- On plot of absolute residuals:
- size of residuals getting bigger as fitted values increase
- predictions getting more variable as fitted values increase
- that is, predictions getting *less accurate* as fitted values increase, but predictions should be equally accurate all way along.
- Both indicate problems with regression, of kind that transformation of response often fixes: that is, predict *function* of response `timedrs` instead of `timedrs` itself.

Fixing the problems

- Residuals not normal (skewed right), increase in size with fitted value.
- Sometimes residuals are *very} positive: observed a {*lot* larger than predicted.*
- *Try * transforming} response: use log or square root of response. (Note that response is {*count*, often skewed to right.)
- Try regression again, with transformed response instead of original one.
- Then check residual plot to see that it is OK now.

```
visits.3 <- lm(log(timedrs + 1) ~ phyheal + menheal + stress,
  data = visits
)
```

- `timedrs+1` because some `timedrs` values 0, can't take log of 0.
- Won't usually need to worry about this, but when response could be zero/negative, fix that before transformation.

Output

{

```
summary(visits.3)
```

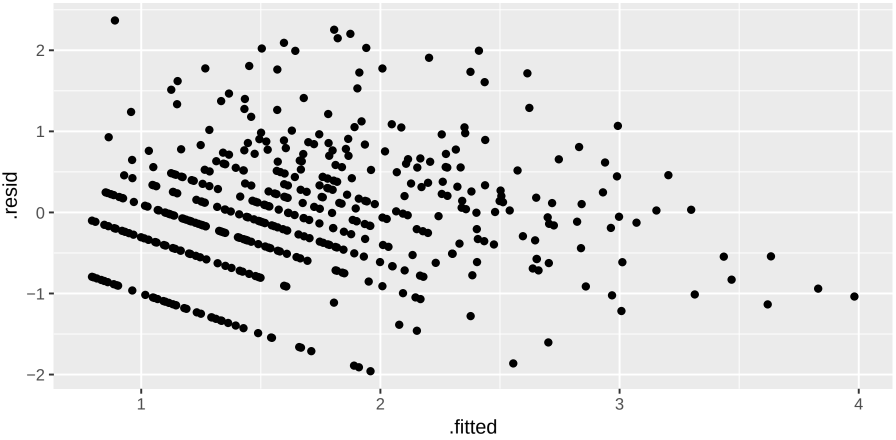
```
##
## Call:
## lm(formula = log(timedrs + 1) ~ phyheal + menheal + stress, data = visits)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.95865 -0.44076 -0.02331  0.42304  2.36797
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 0.3903862  0.0882908   4.422 1.22e-05 ***
## phyheal     0.2019361  0.0173624  11.631  < 2e-16 ***
## menheal     0.0071442  0.0101335   0.705    0.481
## stress      0.0013158  0.0002837   4.638 4.58e-06 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.7625 on 461 degrees of freedom
## Multiple R-squared:  0.3682, Adjusted R-squared:  0.3641
```

Comments

- Model as a whole strongly significant again
- R-sq higher than before (37% vs. 22%) suggesting things more linear now
- Same conclusion re `menheal`: can take out of regression.
- Should look at residual plots (next pages). Have we fixed problems?

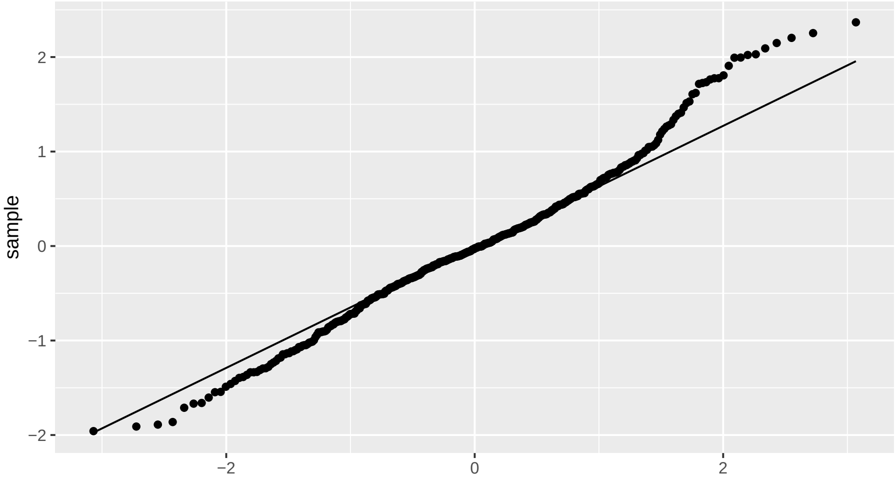
Residuals against fitted values

```
ggplot(visits.3, aes(x = .fitted, y = .resid)) +
  geom_point()
```



Normal quantile plot of residuals

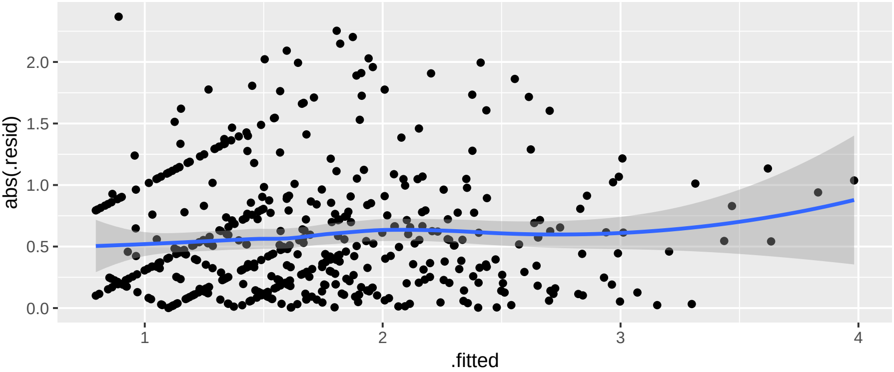
```
ggplot(visits.3, aes(sample = .resid)) + stat_qq() + stat_qq_l
```



Absolute residuals against fitted

```
ggplot(visits.3, aes(x = .fitted, y = abs(.resid))) +
  geom_point() + geom_smooth()
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```



Comments

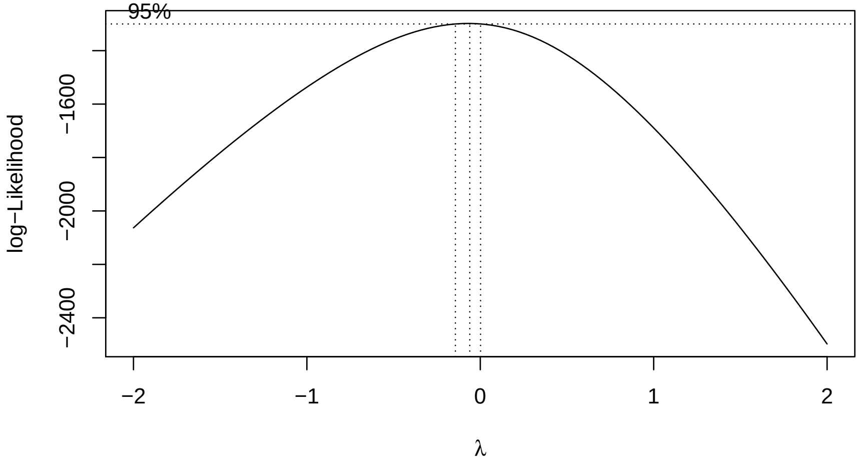
- Residuals vs. fitted looks a lot more random.
- Normal quantile plot looks a lot more normal (though still a little right-skewness)
- Absolute residuals: not so much trend (though still some).
- Not perfect, but much improved.

Box-Cox transformations

- Taking log of `timedrs` and having it work: lucky guess. How to find good transformation?
- Box-Cox again.
- Extra problem: some of `timedrs` values are 0, but Box-Cox expects all $+$. Note response for `boxcox`:

```
boxcox(timedrs + 1 ~ phyheal + menheal + stress, data = visits
```

Try 1



Comments on try 1

- Best: λ just less than zero.
- Hard to see scale.
- Focus on λ in $(-0.3, 0.1)$: {

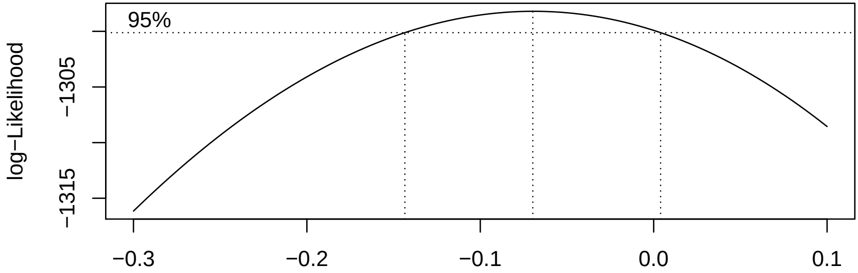
```
my.lambda <- seq(-0.3, 0.1, 0.01)
my.lambda
```

```
##  [1] -0.30 -0.29 -0.28 -0.27 -0.26 -0.25 -0.24 -0.23 -
0.22
## [10] -0.21 -0.20 -0.19 -0.18 -0.17 -0.16 -0.15 -0.14 -
0.13
## [19] -0.12 -0.11 -0.10 -0.09 -0.08 -0.07 -0.06 -0.05 -
0.04
## [28] -0.03 -0.02 -0.01  0.00  0.01  0.02  0.03  0.04  0.05
## [37]  0.06  0.07  0.08  0.09  0.10
```

}

Try 2

```
boxcox(timedrs + 1 ~ phyheal + menheal + stress,
  lambda = my.lambda,
  data = visits
)
```



Comments

- Best: λ just about -0.07.
- CI for λ about $(-0.14, 0.01)$.
- Only nearby round number: $\lambda = 0$, log transformation.
- So we made lucky guess with log before!

Testing more than one x at once

The t-tests test only whether one variable could be taken out of the regression you're looking at. To test significance of more than one variable at once, fit model with and without variables and use anova to compare fit of models: {

```
visits.5 <- lm(log(timedrs + 1) ~ phyheal + menheal + stress, data =
visits.6 <- lm(log(timedrs + 1) ~ stress, data = visits)
anova(visits.6, visits.5)
```

```
## Analysis of Variance Table
##
## Model 1: log(timedrs + 1) ~ stress
## Model 2: log(timedrs + 1) ~ phyheal + menheal + stress
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1    463 371.47
## 2    461 268.01  2    103.46 88.984 < 2.2e-16 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Results of tests

- Models don't fit equally well, so big one fits better.
- Or "taking both variables out makes the fit worse, so don't do it".
- Taking out those x's is a mistake. Or putting them in is a good idea.

The punting data

Data set `punting.txt` contains 4 variables for 13 right-footed football kickers (punters): left leg and right leg strength (lbs), distance punted (ft), another variable called "fred". Predict punting distance from other variables:

"'

left right punt fred 170 170 162.50 171 130 140 144.0 136 170 180 174.50 174 160 160 163.50 161 150 170 192.0 159 150 150 171.75 151 180 170 162.0 174 110 110 104.83 111 110 120 105.67 114 120 130 117.58 126 140 120 140.25 129 130 140 150.17 136 150 160 165.17 154

"'

Reading in

- Separated by *multiple spaces* with *columns lined up*:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/punting.txt
punting <- read_table(my_url)
```

```
## Parsed with column specification:
## cols(
##   left = col_double(),
##   right = col_double(),
##   punt = col_double(),
##   fred = col_double()
## )
```

The data

```
punting
```

```
## # A tibble: 13 x 4
##     left right  punt  fred
##    <dbl> <dbl> <dbl> <dbl>
##  1   170   170  162.   171
##  2   130   140  144    136
##  3   170   180  174.   174
##  4   160   160  164.   161
##  5   150   170  192    159
##  6   150   150  172.   151
##  7   180   170  162    174
##  8   110   110  105.   111
##  9   110   120  106.   114
## 10   120   130  118.   126
## 11   140   120  140.   129
```

Regression and output

```
punting.1 <- lm(punt ~ left + right + fred, data = punting)
summary(punting.1)
```

```
##
## Call:
## lm(formula = punt ~ left + right + fred, data = punting)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -14.9325 -11.5618  -0.0315   9.0415  20.0886
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -4.6855    29.1172  -0.161    0.876
## left          0.2679     2.1111   0.127    0.902
## right         1.0524     2.1477   0.490    0.636
```

Comments

- Overall regression strongly significant, R-sq high.
- None of the x's significant! Why?
- t-tests only say that you could take any one of the x's out without damaging the fit; doesn't matter which one.
- Explanation: look at *correlations*.

The correlations

```
cor(punting)
```

```
##           left     right      punt      fred
## left  1.0000000 0.8957224 0.8117368 0.9722632
## right 0.8957224 1.0000000 0.8805469 0.9728784
## punt  0.8117368 0.8805469 1.0000000 0.8679507
## fred  0.9722632 0.9728784 0.8679507 1.0000000
```

- *All* correlations are high: x's with `punt` (good) and with each other (bad, at least confusing).
- What to do? Probably do just as well to pick one variable, say `right` since kickers are right-footed.

Just right

{

```
punting.2 <- lm(punt ~ right, data = punting)
anova(punting.2, punting.1)
```

```
## Analysis of Variance Table
##
## Model 1: punt ~ right
## Model 2: punt ~ left + right + fred
##   Res.Df    RSS Df Sum of Sq      F Pr(>F)
## 1     11 1962.5
## 2      9 1938.2  2    24.263 0.0563 0.9456
```

} No significant loss by dropping other two variables.

Comparing R-squareds

{

```
summary(punting.1)$r.squared
```

```
## [1] 0.7781401
```

```
summary(punting.2)$r.squared
```

```
## [1] 0.7753629
```

}

Basically no difference. In regression (over), `right` significant:

Regression results

{

```r
summary(punting.2)
```

```
##
## Call:
## lm(formula = punt ~ right, data = punting)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -15.7576 -11.0611   0.3656   7.8890  19.0423
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  -3.6930    25.2649  -0.146    0.886
## right         1.0427     0.1692   6.162 7.09e-05 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 13.36 on 11 degrees of freedom
```

But...

- Maybe we got the *form* of the relationship with `left` wrong.
- Check: plot *residuals* from previous regression (without `left`) against `left`.
- Residuals here are "punting distance adjusted for right leg strength".
- If there is some kind of relationship with `left`, we should include in model.
- Plot of residuals against original variable: `augment` from `broom`.

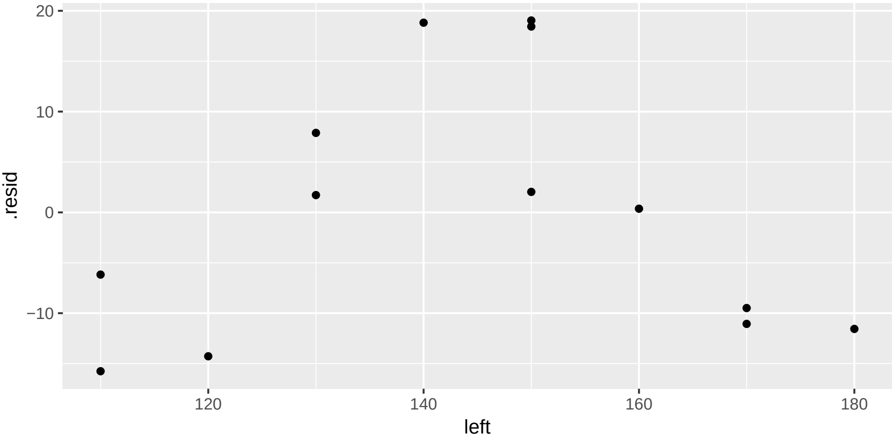
Augmenting punting.2

```
punting.2 %>% augment(punting) -> punting.2.aug
punting.2.aug %>% slice(1:8)
```

```
## # A tibble: 8 x 11
##    left right  punt  fred .fitted .se.fit  .resid   .hat
##   <dbl> <dbl> <dbl> <dbl>   <dbl>   <dbl>   <dbl>  <dbl>
## 1   170   170  162.   171    174.    5.29 -11.1   0.157
## 2   130   140  144    136    142.    3.93   1.72  0.0864
## 3   170   180  174.   174    184.    6.60  -9.49  0.244
## 4   160   160  164.   161    163.    4.25   0.366 0.101
## 5   150   170  192    159    174.    5.29  18.4   0.157
## 6   150   150  172.   151    153.    3.73  19.0   0.0778
## 7   180   170  162    174    174.    5.29 -11.6   0.157
## 8   110   110  105.   111    111.    7.38  -6.17  0.305
## # … with 3 more variables: .sigma <dbl>, .cooksd <dbl>,
## #   .std.resid <dbl>
```

Residuals against `left`

```
ggplot(punting.2.aug, aes(x = left, y = .resid)) +
  geom_point()
```



Comments

- There is a *curved* relationship with `left`.
- We should add `left`-squared to the regression (and therefore put `left` back in when we do that):

```
punting.3 <- lm(punt ~ left + I(left^2) + right,
  data = punting
)
```

Regression with `left-squared`

```
summary(punting.3)
```

```
##
## Call:
## lm(formula = punt ~ left + I(left^2) + right, data = puntin
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -11.3777  -5.3599   0.0459   4.5088  13.2669
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -4.623e+02  9.902e+01  -4.669  0.00117 **
## left         6.888e+00  1.462e+00   4.710  0.00110 **
## I(left^2)   -2.302e-02  4.927e-03  -4.672  0.00117 **
## right        7.396e-01  2.292e-01   3.227  0.01038 *
```

Comments

- This was initely a good idea (R-squared has clearly increased).
- We would never have seen it without plotting residuals from `punting.2` (without `left`) against `left`.
- Negative slope for `leftsq` means that increased left-leg strength only increases punting distance up to a point: beyond that, it decreases again.

```
## Error in FUN(X[[i]], ...): invalid 'name' argument
```

xxx

Section 3

Logistic regression (ordinal/nominal response)

Logistic regression

- When response variable is measured/counted, regression can work well.
- But what if response is yes/no, lived/died, success/failure?
- Model {*probability*} *of success.*
- *Probability must be between 0 and 1; need method that ensures this.*
- {Logistic regression} does this. In R, is a *generalized linear model* with binomial "family": `glm(ytextasciitilde x,family="binomial")`
- Begin with simplest case.

Packages

```r
library(MASS)
library(tidyverse)
library(broom)
library(nnet)
```

The rats, part 1

- Rats given dose of some poison; either live or die: \begin{small}

```
dose status
0 lived
1 died
2 lived
3 lived
4 died
5 died
```

\end{small}

- Read the data:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/rat.txt"
rats <- read_delim(my_url, " ")
```

Basic logistic regression

- Data:

```
rats
```

```
## # A tibble: 6 x 2
##    dose status
##   <dbl> <chr>
## 1     0 lived
## 2     1 died
## 3     2 lived
## 4     3 lived
## 5     4 died
## 6     5 died
```

- Make response into a factor first:

```
rats2 <- rats %>% mutate(status = factor(status))
```

- then fit model:

Output

```
summary(status.1)
```

```
##
## Call:
## glm(formula = status ~ dose, family = "binomial", data = ra
##
## Deviance Residuals:
##       1        2        3        4        5        6
##  0.5835  -1.6254   1.0381   1.3234  -0.7880  -0.5835
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)   1.6841     1.7979   0.937    0.349
## dose         -0.6736     0.6140  -1.097    0.273
##
## (Dispersion parameter for binomial family taken to be 1)
##
```

Interpreting the output

- Like (multiple) regression, get tests of significance of individual x's
- `Here not significant (only 6 observations).`
- "Slope" for dose is negative, meaning that as dose increases, probability of event modelled (survival) decreases.

Output part 2: predicted survival probs

```
p <- predict(status.1, type = "response")
cbind(rats, p)
```

```
##   dose status         p
## 1    0  lived 0.8434490
## 2    1   died 0.7331122
## 3    2  lived 0.5834187
## 4    3  lived 0.4165813
## 5    4   died 0.2668878
## 6    5   died 0.1565510
```

def

The rats, more

- More realistic: more rats at each dose (say 10).
- Listing each rat on one line makes a big data file.
- Use format below: dose, number of survivals, number of deaths.

```
dose lived died
0     10    0
1      7    3
2      6    4
3      4    6
4      2    8
5      1    9
```

- 6 lines of data correspond to 60 actual rats.
- Saved in `rat2.txt`.

These data

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/rat2.txt"
rat2 <- read_delim(my_url, " ")
```

```
## Parsed with column specification:
## cols(
##   dose = col_double(),
##   lived = col_double(),
##   died = col_double()
## )
```

```
rat2
```

```
## # A tibble: 6 x 3
##    dose lived  died
##   <dbl> <dbl> <dbl>
## 1     0    10     0
## 2     1     7     3
```

This logistic regression

```
response <- with(rat2, cbind(lived, died))
rat2.1 <- glm(response ~ dose,
  family = "binomial",
  data = rat2
)
```

- Note construction of *two-column* response, #survivals in first column, #deaths in second.
- The response variable is an R `matrix`:

```
class(response)
```

```
## [1] "matrix"
```

Output

```r
summary(rat2.1)
```

```
##
## Call:
## glm(formula = response ~ dose, family = "binomial", data =
##
## Deviance Residuals:
##       1        2        3        4        5        6
##  1.3421  -0.7916  -0.1034   0.1034   0.0389   0.1529
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)   2.3619     0.6719   3.515 0.000439 ***
## dose         -0.9448     0.2351  -4.018 5.87e-05 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Predicted survival probs

```
p <- predict(rat2.1, type = "response")
cbind(rat2, p)
```

```
##   dose lived died         p
## 1    0    10    0 0.9138762
## 2    1     7    3 0.8048905
## 3    2     6    4 0.6159474
## 4    3     4    6 0.3840526
## 5    4     2    8 0.1951095
## 6    5     1    9 0.0861238
```

def

Comments

- Significant effect of dose.
- Effect of larger dose is to decrease survival probability ("slope" negative; also see in decreasing predictions.)

Multiple logistic regression

- With more than one x, works much like multiple regression.
- Example: study of patients with blood poisoning severe enough to warrant surgery. Relate survival to other potential risk factors.
- Variables, 1=present, 0=absent:
- survival (death from sepsis=1), response
- shock
- malnutrition
- alcoholism
- age (as numerical variable)
- bowel infarction
- See what relates to death.

Read in data

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/sepsis.txt'
sepsis <- read_delim(my_url, " ")
```

```
## Parsed with column specification:
## cols(
##   death = col_double(),
##   shock = col_double(),
##   malnut = col_double(),
##   alcohol = col_double(),
##   age = col_double(),
##   bowelinf = col_double()
## )
```

def

The data

```
sepsis
```

```
## # A tibble: 106 x 6
##    death shock malnut alcohol   age bowelinf
##    <dbl> <dbl>  <dbl>   <dbl> <dbl>    <dbl>
##  1     0     0      0       0    56        0
##  2     0     0      0       0    80        0
##  3     0     0      0       0    61        0
##  4     0     0      0       0    26        0
##  5     0     0      0       0    53        0
##  6     1     0      1       0    87        0
##  7     0     0      0       0    21        0
##  8     1     0      0       1    69        0
##  9     0     0      0       0    57        0
## 10     0     0      1       0    76        0
## # … with 96 more rows
```

Fit model

```
sepsis.1 <- glm(death ~ shock + malnut + alcohol + age +
  bowelinf,
family = "binomial",
data = sepsis
)
```

Output part 1

```
tidy(sepsis.1)
```

```
## # A tibble: 6 x 5
##   term        estimate std.error statistic  p.value
##   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)  -9.75      2.54       -3.84 0.000124
## 2 shock         3.67      1.16        3.15 0.00161
## 3 malnut        1.22      0.728       1.67 0.0948
## 4 alcohol       3.35      0.982       3.42 0.000635
## 5 age           0.0922    0.0303      3.04 0.00237
## 6 bowelinf      2.80      1.16        2.40 0.0162
```

def

- All P-values fairly small
- but `malnut` not significant: remove.

Removing malnut

```
sepsis.2 <- update(sepsis.1, . ~ . - malnut)
tidy(sepsis.2)
```

```
## # A tibble: 5 x 5
##   term        estimate std.error statistic  p.value
##   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)  -8.89      2.32       -3.84 0.000124
## 2 shock         3.70      1.10        3.35 0.000797
## 3 alcohol       3.19      0.917       3.47 0.000514
## 4 age           0.0898    0.0292      3.07 0.00211
## 5 bowelinf      2.39      1.07        2.23 0.0260
```

def

- Everything significant now.

Comments

$

- Most of the original x's helped predict death. Only `malnut` seemed not to add anything.
- Removed `malnut` and tried again.
- Everything remaining is significant (though `bowelinf` actually became *less* significant).
- All coefficients are *positive*, so having any of the risk factors (or being older) *increases* risk of death.

Predictions from model without "malnut"

- A few chosen at random:

```
sepsis.pred <- predict(sepsis.2, type = "response")
d <- data.frame(sepsis, sepsis.pred)
myrows <- c(4, 1, 2, 11, 32)
slice(d, myrows)
```

```
##   death shock malnut alcohol age bowelinf sepsis.pred
## 1     0     0      0       0  26        0 0.001415347
## 2     0     0      0       0  56        0 0.020552383
## 3     0     0      0       0  80        0 0.153416834
## 4     1     0      0       1  66        1 0.931290137
## 5     1     0      0       1  49        0 0.213000997
```

def

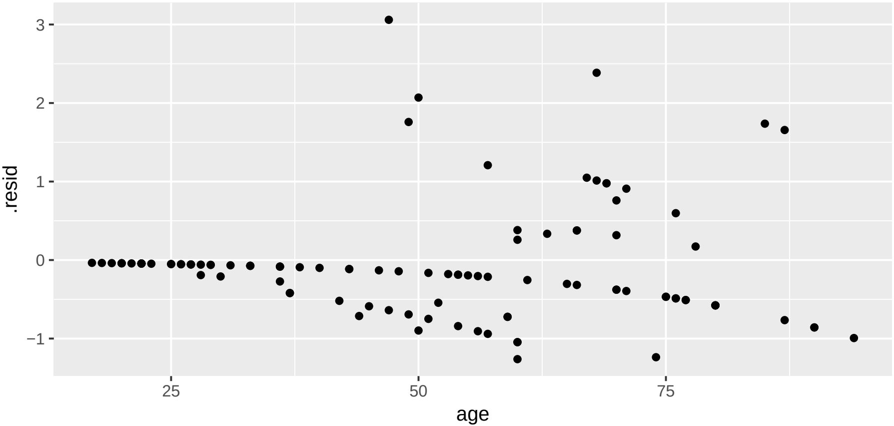
- Survival chances pretty good if no risk factors, though decreasing with age.

Assessing proportionality of odds for age

- An assumption we made is that log-odds of survival depends linearly on age.
- Hard to get your head around, but basic idea is that survival chances go continuously up (or down) with age, instead of (for example) going up and then down.
- In this case, seems reasonable, but should check:

Residuals vs. age

```
ggplot(augment(sepsis.2), aes(x = age, y = .resid)) +
  geom_point()
```



def

Probability and odds

- For probability p, odds is $p/(1-p)$. Examples:

Prob.	Odds	log-odds	in words
0.5	$0.5/0.5 = 1/1 = 1.00$	0.00	"even money"
0.1	$0.1/0.9 = 1/9 = 0.11$	-2.20	"9 to 1"
0.4	$0.4/0.6 = 1/1.5 = 0.67$	-0.41	"1.5 to 1"
0.8	$0.8/0.2 = 4/1 = 4.00$	1.39	"4 to 1 on"

- Gamblers use odds: if you win at 9 to 1 odds, get original stake back plus 9 times the stake.
- Probability has to be between 0 and 1
- Odds between 0 and infinity
- *Log*-odds can be anything: any log-odds corresponds to valid probability.

Odds ratio

- Suppose 90 of 100 men drank wine last week, but only 20 of 100 women.
- Prob of man drinking wine $90/100 = 0.9$, woman $20/100 = 0.2$.
- Odds of man drinking wine $0.9/0.1 = 9$, woman $0.2/0.8 = 0.25$.
- Ratio of odds is $9/0.25 = 36$.
- Way of quantifying difference between men and women: "odds of drinking wine 36 times larger for males than females".

Sepsis data again

- Recall prediction of probability of death from risk factors:

```
sepsis.2.tidy <- tidy(sepsis.2)
sepsis.2.tidy
```

```
## # A tibble: 5 x 5
##   term        estimate std.error statistic  p.value
##   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)  -8.89      2.32       -3.84 0.000124
## 2 shock         3.70      1.10        3.35 0.000797
## 3 alcohol       3.19      0.917       3.47 0.000514
## 4 age           0.0898    0.0292      3.07 0.00211
## 5 bowelinf      2.39      1.07        2.23 0.0260
```

- Slopes in column `estimate`.

Multiplying the odds

- Can interpret slopes by taking "exp" of them. We ignore intercept.

```
cc <- exp(sepsis.2.tidy$estimate)
data.frame(sepsis.2.tidy$term, expcoeff = round(cc, 2))
```

```
##   sepsis.2.tidy.term expcoeff
## 1        (Intercept)     0.00
## 2              shock    40.50
## 3            alcohol    24.19
## 4                age     1.09
## 5           bowelinf    10.88
```

def

- These say "how much do you *multiply* odds of death by for increase of 1 in corresponding risk factor?" Or, what is odds ratio for that factor being 1 (present) vs. 0 (absent)?

Odds ratio and relative risk

- **Relative risk** is ratio of probabilities.
- Above: 90 of 100 men (0.9) drank wine, 20 of 100 women (0.2).
- Relative risk 0.9/0.2=4.5. (odds ratio was 36).
- When probabilities small, relative risk and odds ratio similar.
- Eg. prob of man having disease 0.02, woman 0.01.
- Relative risk $0.02/0.01 = 2$. \begin{multicols}{2}
- Odds for men and for women:

```
(od1 <- 0.02 / 0.98)
```

```
## [1] 0.02040816
```

```
(od2 <- 0.01 / 0.99)
```

```
## [1] 0.01010101
```

More than 2 response categories

- With 2 response categories, model the probability of one, and prob of other is one minus that. So doesn't matter which category you model.
- With more than 2 categories, have to think more carefully about the categories: are they
- {*ordered*}*: you can put them in a natural order (like low, medium, high)*
- {nominal}: ordering the categories doesn't make sense (like red, green, blue).
- R handles both kinds of response; learn how.

Ordinal response: the miners

- Model probability of being in given category {*or lower*}.
- *Example: coal-miners often suffer disease pneumoconiosis. Likelihood of disease believed to be greater among miners who have worked longer.*
- *Severity of disease measured on categorical scale: 1 = none, 2 = moderate, 3 = severe.*
- *Data are frequencies:*

```
Exposure None Moderate Severe
5.8     98       0        0
15.0     51       2        1
21.5     34       6        3
27.5     35       5        8
33.5     32       10       9
```

Reading the data

Data in aligned columns with more than one space between, so:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/miners-tab.
freqs <- read_table(my_url)
```

```
## Parsed with column specification:
## cols(
##   Exposure = col_double(),
##   None = col_double(),
##   Moderate = col_double(),
##   Severe = col_double()
## )
```

def

The data

```
freqs
```

```
## # A tibble: 8 x 4
##   Exposure  None Moderate Severe
##      <dbl> <dbl>    <dbl>  <dbl>
## 1      5.8    98        0      0
## 2     15      51        2      1
## 3     21.5    34        6      3
## 4     27.5    35        5      8
## 5     33.5    32       10      9
## 6     39.5    23        7      8
## 7     46      12        6     10
## 8     51.5     4        2      5
```

Tidying and row proportions

```
freqs %>%
  gather(Severity, Freq, None:Severe) %>%
  group_by(Exposure) %>%
  mutate(proportion = Freq / sum(Freq)) -> miners
```

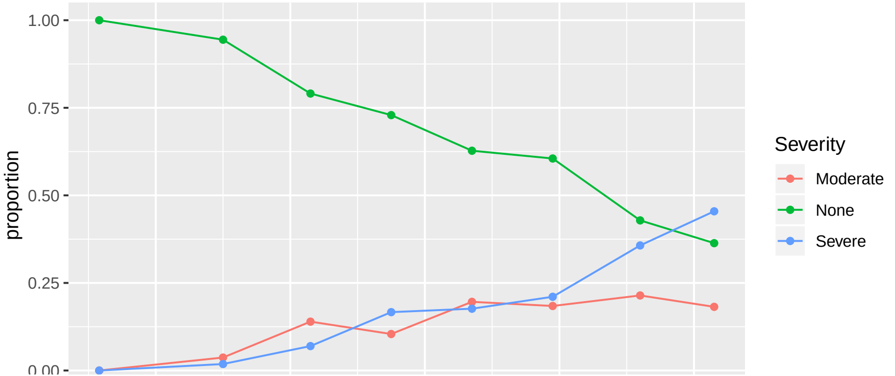
Result

```
miners
```

```
## # A tibble: 24 x 4
## # Groups:   Exposure [8]
##    Exposure Severity  Freq proportion
##       <dbl> <chr>    <dbl>      <dbl>
##  1      5.8 None        98     1
##  2     15   None        51     0.944
##  3     21.5 None        34     0.791
##  4     27.5 None        35     0.729
##  5     33.5 None        32     0.627
##  6     39.5 None        23     0.605
##  7     46   None        12     0.429
##  8     51.5 None         4     0.364
##  9      5.8 Moderate     0     0
## 10     15   Moderate     2     0.0370
## # ... with 14 more rows
```

Plot proportions against exposure

```
ggplot(miners, aes(
  x = Exposure, y = proportion,
  colour = Severity
)) + geom_point() + geom_line()
```



Reminder of data setup

“‘r miners “‘

“‘ A tibble: 24 x 4 Groups: Exposure [8] Exposure Severity Freq proportion <dbl> <chr> <dbl> <dbl> 1 5.8 None 98 1 2 15 None 51 0.944 3 21.5 None 34 0.791 4 27.5 None 35 0.729 5 33.5 None 32 0.627 6 39.5 None 23 0.605 7 46 None 12 0.429 8 51.5 None 4 0.364 9 5.8 Moderate 0 0 10 15 Moderate 2 0.0370 … with 14 more rows “‘

Creating an ordered factor

- Problem: on plot, `Severity` categories in *wrong order*.
- *In the data frame*, categories in *correct* order.
- Package `forcats` (in `tidyverse`) has functions for creating factors to specifications.
- `fct_inorder` takes levels *in order they appear in data*:

```
miners %>%
  mutate(sev_ord = fct_inorder(Severity)) -> miners
```

- To check:

```
levels(miners$sev_ord)
```

```
## [1] "None"     "Moderate" "Severe"
```

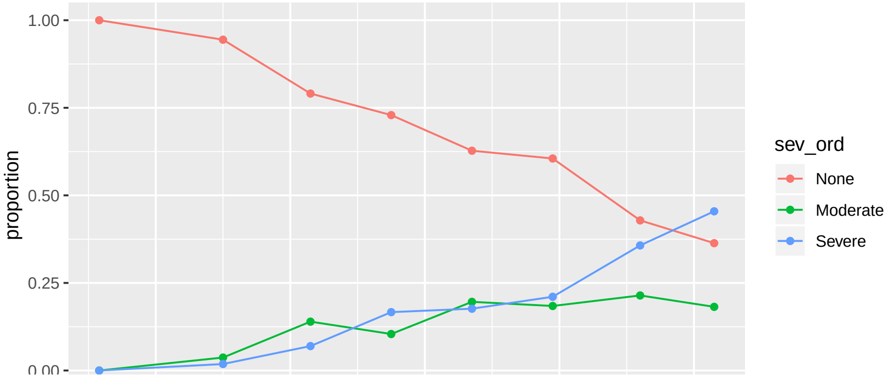
New data frame

```
miners
```

```
## # A tibble: 24 x 5
## # Groups:   Exposure [8]
##    Exposure Severity  Freq proportion sev_ord
##       <dbl> <chr>    <dbl>      <dbl> <fct>
##  1      5.8 None        98     1      None
##  2     15   None        51     0.944  None
##  3     21.5 None        34     0.791  None
##  4     27.5 None        35     0.729  None
##  5     33.5 None        32     0.627  None
##  6     39.5 None        23     0.605  None
##  7     46   None        12     0.429  None
##  8     51.5 None         4     0.364  None
##  9      5.8 Moderate     0     0      Moderate
## 10     15   Moderate     2     0.0370 Moderate
## #   with 14 more rows
```

Improved plot

```
ggplot(miners, aes(
  x = Exposure, y = proportion,
  colour = sev_ord
)) + geom_point() + geom_line()
```



Fitting ordered logistic model

Use function `polr` from package `MASS`. Like `glm`.

```
sev.1 <- polr(sev_ord ~ Exposure,
  weights = Freq,
  data = miners
)
```

def

Output: not very illuminating

```
summary(sev.1)
```

```
##
## Re-fitting to get Hessian
## Call:
## polr(formula = sev_ord ~ Exposure, data = miners, weights =
##
## Coefficients:
##           Value Std. Error t value
## Exposure 0.0959    0.01194   8.034
##
## Intercepts:
##                   Value   Std. Error t value
## None|Moderate     3.9558  0.4097      9.6558
## Moderate|Severe   4.8690  0.4411     11.0383
##
```

Does exposure have an effect?

Fit model without Exposure, and compare using anova. Note 1 for model with just intercept:

```
sev.0 <- polr(sev_ord ~ 1, weights = Freq, data = miners)
anova(sev.0, sev.1)
```

```
## Likelihood ratio tests of ordinal regression models
##
## Response: sev_ord
##      Model Resid. df Resid. Dev   Test
## 1        1       369   505.1621
## 2 Exposure       368   416.9188 1 vs 2
##      Df LR stat. Pr(Chi)
## 1
## 2     1 88.24324       0
```

def Exposure definitely has effect on severity of disease.

Another way

- What (if anything) can we drop from model with exposure?

```
drop1(sev.1, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## sev_ord ~ Exposure
##          Df    AIC    LRT  Pr(>Chi)
## <none>       422.92
## Exposure  1 509.16 88.243 < 2.2e-16 ***
## ---
## Signif. codes:
##   0 '***' 0.001 '**' 0.01 '*' 0.05
##   '.' 0.1 ' ' 1
```

- Nothing. Exposure definitely has effect.

Predicted probabilities

Make new data frame out of all the exposure values (from original data frame), and predict from that:

```
sev.new <- tibble(Exposure = freqs$Exposure)
pr <- predict(sev.1, sev.new, type = "p")
miners.pred <- cbind(sev.new, pr)
miners.pred
```

```
##   Exposure      None   Moderate     Severe
## 1      5.8 0.9676920 0.01908912 0.01321885
## 2     15.0 0.9253445 0.04329931 0.03135614
## 3     21.5 0.8692003 0.07385858 0.05694115
## 4     27.5 0.7889290 0.11413004 0.09694093
## 5     33.5 0.6776641 0.16207145 0.16026444
## 6     39.5 0.5418105 0.20484198 0.25334756
## 7     46.0 0.3879962 0.22441555 0.38758828
## 8     51.5 0.2722543 0.21025011 0.51749563
```

Comments

- Model appears to match data: as exposure goes up, prob of None goes down, Severe goes up (sharply for high exposure).
- Like original data frame, this one nice to look at but *not tidy*. We want to make graph, so tidy it.
- Also want the severity values in right order.
- Usual `gather`, plus a bit:

```
miners.pred %>%
  gather(Severity, probability, -Exposure) %>%
  mutate(sev_ord = fct_inorder(Severity)) -> preds
```

Some of the gathered predictions

```
preds %>% slice(1:15)
```

```
##    Exposure Severity probability  sev_ord
## 1       5.8     None  0.96769203     None
## 2      15.0     None  0.92534455     None
## 3      21.5     None  0.86920028     None
## 4      27.5     None  0.78892903     None
## 5      33.5     None  0.67766411     None
## 6      39.5     None  0.54181046     None
## 7      46.0     None  0.38799618     None
## 8      51.5     None  0.27225426     None
## 9       5.8 Moderate  0.01908912 Moderate
## 10     15.0 Moderate  0.04329931 Moderate
## 11     21.5 Moderate  0.07385858 Moderate
## 12     27.5 Moderate  0.11413004 Moderate
## 13     33.5 Moderate  0.16207145 Moderate
```

Plotting predicted and observed proportions

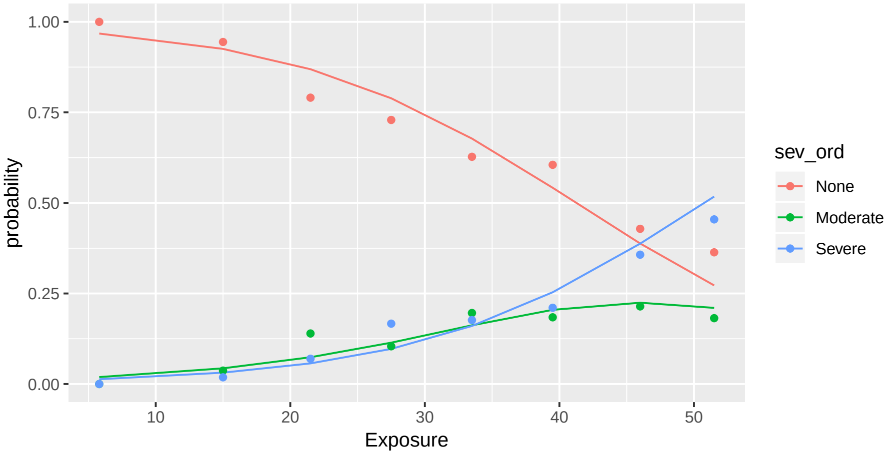
- Plot:
- predicted probabilities, lines (shown) joining points (not shown)
- data, just the points.
- Unfamiliar process: data from two *different* data frames:

```
g <- ggplot(preds, aes(
  x = Exposure, y = probability,
  colour = sev_ord
)) + geom_line() +
  geom_point(data = miners, aes(y = proportion))
```

- Idea: final `geom_point` uses data in `miners` rather than `preds`, y-variable for plot is `proportion` from that data frame, but x-coordinate is `Exposure`, as it was before, and colour is `Severity` as before. The final `geom_point` "inherits" from the first `aes` as needed.

The plot

```
g
```



mlogit.pdf

Unordered responses

- With unordered (nominal) responses, can use {*generalized logit*}.
- *Example: 735 people, record age and sex (male 0, female 1), which of 3 brands of some product preferred.*
- *Data in `mlogit.csv` separated by commas (so `read_csv` will work):*

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/mlogit.csv"
brandpref <- read_csv(my_url)
```

```
## Parsed with column specification:
## cols(
##   brand = col_double(),
##   sex = col_double(),
##   age = col_double()
## )
```

def

The data

```
brandpref
```

```
## # A tibble: 735 x 3
##    brand   sex   age
##    <dbl> <dbl> <dbl>
##  1     1     0    24
##  2     1     0    26
##  3     1     0    26
##  4     1     1    27
##  5     1     1    27
##  6     3     1    27
##  7     1     0    27
##  8     1     0    27
##  9     1     1    27
## 10     1     0    27
## # … with 725 more rows
```

Bashing into shape, and fitting model

- sex and brand not meaningful as numbers, so turn into factors:

```
brandpref <- brandpref %>%
  mutate(sex = factor(sex)) %>%
  mutate(brand = factor(brand))
```

def

- We use `multinom` from package `nnet`. Works like `polr`.

```
brands.1 <- multinom(brand ~ age + sex, data = brandpref)
```

```
## # weights:  12 (6 variable)
## initial  value 807.480032
## iter  10 value 702.976983
## final  value 702.970704
## converged
```

def

Can we drop anything?

- Unfortunately `drop1` seems not to work:

```
drop1(brands.1, test = "Chisq", trace = 0)
```

```
## trying - age
```

```
## Error in if (trace) {: argument is not interpretable as log
```

- so fall back on fitting model without what you want to test, and comparing using `anova`.

Do age/sex help predict brand? 1/2

Fit models without each of age and sex:

```
brands.2 <- multinom(brand ~ age, data = brandpref)
```

```
## # weights:  9 (4 variable)
## initial  value 807.480032
## iter  10 value 706.796323
## iter  10 value 706.796322
## final  value 706.796322
## converged
```

```
brands.3 <- multinom(brand ~ sex, data = brandpref)
```

```
## # weights:  9 (4 variable)
## initial  value 807.480032
## final  value 791.861266
## converged
```

Do age/sex help predict brand? 2/2

```
anova(brands.2, brands.1)
```

```
## Likelihood ratio tests of Multinomial Models
##
## Response: brand
##         Model Resid. df Resid. Dev   Test    Df LR stat.     P
## 1         age      1466   1413.593
## 2 age + sex      1464   1405.941 1 vs 2     2 7.651236 0.02
```

```
anova(brands.3, brands.1)
```

```
## Likelihood ratio tests of Multinomial Models
##
## Response: brand
##         Model Resid. df Resid. Dev   Test    Df LR stat. Pr(C
## 1         sex      1466   1583.723
## 2 age + sex      1464   1405.941 1 vs 2     2 177.7811
```

Do age/sex help predict brand? 3/3

- age definitely significant (second `anova`)
- `sex` seems significant also (first `anova`)
- Keep both.

Another way to build model

- Start from model with everything and run step:

```
step(brands.1, trace = 0)
```

```
## trying - age
## trying - sex

## Call:
## multinom(formula = brand ~ age + sex, data = brandpref)
##
## Coefficients:
##   (Intercept)       age      sex1
## 2   -11.77469 0.3682075 0.5238197
## 3   -22.72141 0.6859087 0.4659488
##
## Residual Deviance: 1405.941
## AIC: 1417.941
```

Predictions: all possible combinations

Create data frame with various age and sex:

```
ages <- c(24, 28, 32, 35, 38)
sexes <- factor(0:1)
new <- crossing(age = ages, sex = sexes)
new
```

```
## # A tibble: 10 x 2
##       age sex
##     <dbl> <fct>
##  1    24 0
##  2    24 1
##  3    28 0
##  4    28 1
##  5    32 0
##  6    32 1
##  7    35 0
```

Making predictions

```r
p <- predict(brands.1, new, type = "probs")
probs <- cbind(new, p)
```

The predictions

```
probs
```

```
##     age sex          1          2           3
## 1    24   0 0.94795822 0.05022928 0.001812497
## 2    24   1 0.91532076 0.08189042 0.002788820
## 3    28   0 0.79313204 0.18329690 0.023571058
## 4    28   1 0.69561789 0.27143910 0.032943012
## 5    32   0 0.40487271 0.40810321 0.187024082
## 6    32   1 0.29086347 0.49503135 0.214105181
## 7    35   0 0.13057819 0.39724053 0.472181272
## 8    35   1 0.08404134 0.43168592 0.484272746
## 9    38   0 0.02598163 0.23855071 0.735467663
## 10   38   1 0.01623089 0.25162197 0.732147148
```

- Young males (`sex=0`) prefer brand 1, but older males prefer brand 3.
- Females similar, but like brand 1 less and brand 2 more.

Making a plot

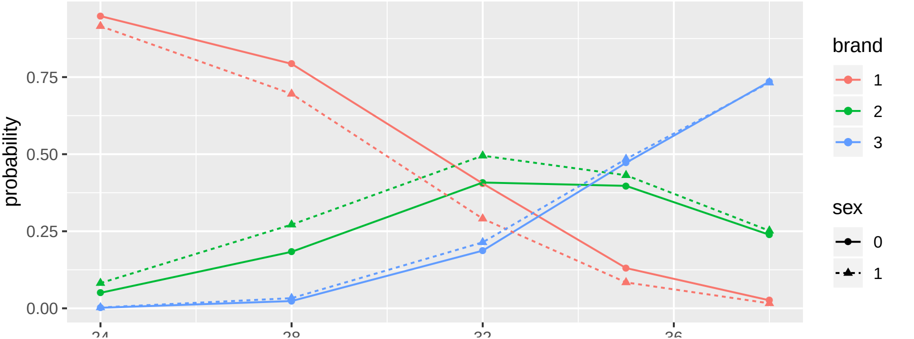
- Plot fitted probability against age, distinguishing brand by colour and gender by plotting symbol.
- Also join points by lines, and distinguish lines by gender.
- I thought about facetting, but this seems to come out clearer.
- First need tidy data frame, by familiar process:

```
probs.long <- probs %>%
  gather(brand, probability, -(age:sex))
sample_n(probs.long, 7) # 7 random rows
```

```
##   age sex brand probability
## 1  32   0     1   0.4048727
## 2  35   1     2   0.4316859
## 3  38   0     3   0.7354677
## 4  35   0     3   0.4721813
```

The plot

```
ggplot(probs.long, aes(
  x = age, y = probability,
  colour = brand, shape = sex
)) +
  geom_point() + geom_line(aes(linetype = sex))
```



Digesting the plot

- Brand vs. age: younger people (of both genders) prefer brand 1, but older people (of both genders) prefer brand 3. (Explains significant age effect.)
- Brand vs. sex: females (dashed) like brand 1 less than males (solid), like brand 2 more (for all ages). more.
- Not much brand difference between genders (solid and dashed lines of same colours close), but enough to be significant.
- Model didn't include interaction, so modelled effect of gender on brand same for each age, modelled effect of age same for each gender.

Alternative data format

Summarize all people of same brand preference, same sex, same age on one line of data file with frequency on end:

{

```
1 0 24 1
1 0 26 2
1 0 27 4
1 0 28 4
1 0 29 7
1 0 30 3
...
```

}

Whole data set in 65 lines not 735! But how?

Getting alternative data format

```
brandpref %>%
  group_by(age, sex, brand) %>%
  summarize(Freq = n()) %>%
  ungroup() -> b
b %>% slice(1:6)
```

```
## # A tibble: 6 x 4
##     age sex   brand  Freq
##   <dbl> <fct> <fct> <int>
## 1    24 0     1         1
## 2    26 0     1         2
## 3    27 0     1         4
## 4    27 1     1         4
## 5    27 1     3         1
## 6    28 0     1         4
```

Fitting models, almost the same

- Just have to remember `weights` to incorporate frequencies.
- Otherwise `multinom` assumes you have just 1 obs on each line!
- Again turn (numerical) `sex` and `brand` into factors:

```
bf <- b %>%
  mutate(sex = factor(sex)) %>%
  mutate(brand = factor(brand))
b.1 <- multinom(brand ~ age + sex, data = bf, weights = Freq)
```

```
## # weights:  12 (6 variable)
## initial  value 807.480032
## iter  10 value 702.976983
## final  value 702.970704
## converged
```

```
b.2 <- multinom(brand ~ age, data = bf, weights = Freq)
```

P-value for `sex` `identical`

```
anova(b.2, b.1)
```

```
## Likelihood ratio tests of Multinomial Models
##
## Response: brand
##        Model Resid. df Resid. Dev   Test    Df LR stat.    P
## 1        age       126   1413.593
## 2 age + sex       124   1405.941 1 vs 2     2 7.651236 0.02
```

def

Same P-value as before, so we haven't changed anything important.

Including data on plot

- Everyone's age given as whole number, so maybe not too many different ages with sensible amount of data at each:

```
b %>%
  group_by(age) %>%
  summarize(total = sum(Freq))
```

```
## # A tibble: 14 x 2
##       age total
##     <dbl> <int>
##  1     24     1
##  2     26     2
##  3     27     9
##  4     28    15
##  5     29    19
##  6     30    23
##  7     31    40
```

Comments and next

- Not great (especially at low end), but live with it.
- Need proportions of frequencies in each brand for each age-gender combination. Mimic what we did for miners:

```
b %>%
  group_by(age, sex) %>%
  mutate(proportion = Freq / sum(Freq)) -> brands
```

Checking proportions for age 32

```
brands %>% filter(age == 32)
```

```
## # A tibble: 6 x 5
## # Groups:   age, sex [2]
##     age sex   brand  Freq proportion
##   <dbl> <fct> <fct> <int>      <dbl>
## 1    32 0     1        48      0.407
## 2    32 0     2        51      0.432
## 3    32 0     3        19      0.161
## 4    32 1     1        62      0.288
## 5    32 1     2       117      0.544
## 6    32 1     3        36      0.167
```

- First three proportions (males) add up to 1.
- Last three proportions (females) add up to 1.
- So looks like proportions of right thing.

Attempting plot

- Take code from previous plot and:
- remove geom_point for fitted values
- add geom_point with correct data= and aes to plot data.

```
g <- ggplot(probs.long, aes(
  x = age, y = probability,
  colour = brand, shape = sex
)) +
  geom_line(aes(linetype = sex)) +
  geom_point(data = brands, aes(y = proportion))
```

- Data seem to correspond more or less to fitted curves:

The plot

```
g
```

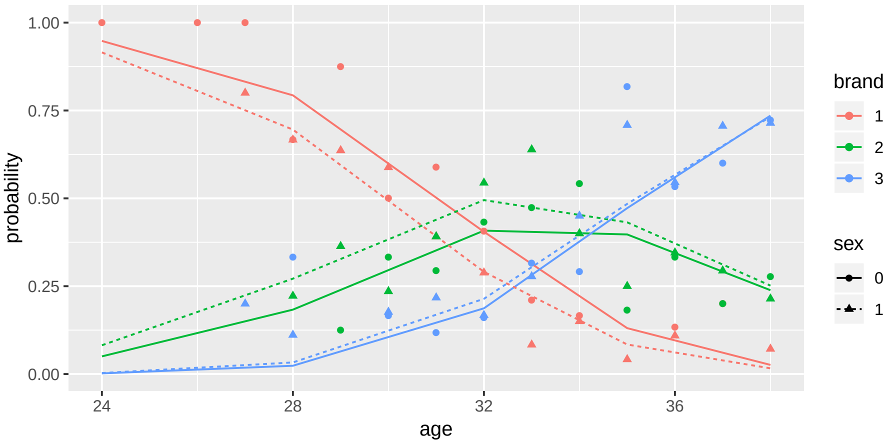


Figure 23: plot of chunk unnamed-chunk-118

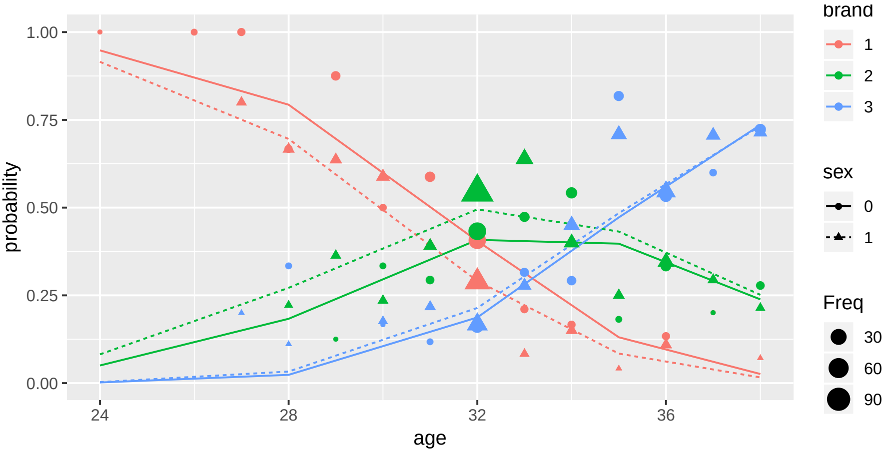
But...

- Some of the plotted points based on a lot of people, and some only a few.
- Idea: make the *size* of plotted point bigger if point based on a lot of people (in `Freq`).
- Hope that larger points then closer to predictions.
- Code:

```
g <- ggplot(probs.long, aes(
  x = age, y = probability,
  colour = brand, shape = sex
)) +
  geom_line(aes(linetype = sex)) +
  geom_point(
    data = brands,
    aes(y = proportion, size = Freq)
  )
```

The plot

```
g
```



1.00
0.75
0.50
0.25
0.00
probability
24
28
32
36
age
brand
1
2
3
sex
0
1
Freq
30
60
90

Trying interaction between age and gender

"'r b.4 <- update(b.1, . . + age:sex) "'

"' weights: 15 (8 variable) initial value 807.480032 iter 10 value 704.811229 iter 20 value 702.582802 final value 702.582761 converged "'

"'r anova(b.1, b.4) "'

"' Likelihood ratio tests of Multinomial Models Response: brand Model Resid. df Resid. Dev Test Df 1 age + sex 124 1405.941 2 age + sex + age:sex 122 1405.166 1 vs 2 2 LR stat. Pr(Chi) 1 2 0.7758861 0.678451 "'

- No evidence that effect of age on brand preference differs for the two genders. «echo=F»= pkgs = names(sessionInfo()$otherPkgs) pkgs=paste('package:', pkgs, sep = "") x=lapply(pkgs, detach, character.only = TRUE, unload = TRUE) @

Section 4

Survival analysis

Survival analysis

- So far, have seen:
- response variable counted or measured (regression)
- response variable categorized (logistic regression)

and have predicted response from explanatory variables.

- But what if response is time until event (eg. time of survival after surgery)?
- Additional complication: event might not have happened at end of study (eg. patient still alive). But knowing that patient has "not died yet" presumably informative. Such data called {*censored*}.
- *Enter* {survival analysis}, in particular the "Cox proportional hazards model".
- Explanatory variables in this context often called {*covariates*}.

Example: still dancing?

- 12 women who have just started taking dancing lessons are followed for up to a year, to see whether they are still taking dancing lessons, or have quit. The "event" here is "quit".
- This might depend on:
- a treatment (visit to a dance competition)
- woman's age (at start of study).
- Data: {

Months	Quit	Treatment	Age
1	1	0	16
2	1	0	24
2	1	0	18
3	0	0	27
4	1	0	25

About the data

- `months` and `quit` are kind of combined response:
- `Months` is number of months a woman was actually observed dancing
- `quit` is 1 if woman quit, 0 if still dancing at end of study.
- Treatment is 1 if woman went to dance competition, 0 otherwise.
- Fit model and see whether `Age` or `Treatment` have effect on survival.
- Want to do predictions for probabilities of still dancing as they depend on whatever is significant, and draw plot.

The code

- Install packages `survival` and `survminer` if not done.
- Load `survival`, `survminer`, `broom` and `tidyverse` packages, read data (column-aligned):

```
library(tidyverse)
library(survival)
library(survminer)
```

```
## Warning: package 'survminer' was built under R version 3.5.

## Warning: package 'ggpubr' was built under R version 3.5.1

## Warning: package 'magrittr' was built under R version 3.5.1
```

```
library(broom)
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/dancing.txt
dance <- read_table(my_url)
```

The data

```
dance
```

```
## # A tibble: 12 x 4
##     Months  Quit Treatment   Age
##      <dbl> <dbl>     <dbl> <dbl>
##  1       1     1         0    16
##  2       2     1         0    24
##  3       2     1         0    18
##  4       3     0         0    27
##  5       4     1         0    25
##  6       5     1         0    21
##  7      11     1         0    55
##  8       7     1         1    26
##  9       8     1         1    36
## 10      10     1         1    38
## 11      10     0         1    45
## 12      12     1         1    47
```

Examine response and fit model

- Response variable (has to be outside data frame):

```
mth <- with(dance, Surv(Months, Quit))
mth
```

```
##   [1]  1    2    2    3+  4    5   11    7    8   10   10+ 12
```

- Then fit model, predicting `mth` from explanatories:

```
dance.1 <- coxph(mth ~ Treatment + Age, data = dance)
```

def

Output looks a lot like regression

```
summary(dance.1)
```

```
## Call:
## coxph(formula = mth ~ Treatment + Age, data = dance)
##
##   n= 12, number of events= 10
##
##               coef exp(coef) se(coef)      z Pr(>|z|)
## Treatment -4.44915   0.01169  2.60929 -1.705   0.0882 .
## Age       -0.36619   0.69337  0.15381 -2.381   0.0173 *
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
##           exp(coef) exp(-coef) lower .95 upper .95
## Treatment   0.01169     85.554 7.026e-05    1.9444
```

Conclusions

- Use $\alpha = 0.10$ here since not much data.
- Three tests at bottom like global F-test. Consensus that something predicts survival time (whether or not dancer quit and how long it took).
- `Age` (definitely), `Treatment` (marginally) both predict survival time.

Model checking

- With regression, usually plot residuals against fitted values.
- Not quite same here (nonlinear model), but "martingale residuals" should have no pattern vs. "linear predictor".
- `ggcoxdiagnostics` from package `survminer` makes plot, to which we add smooth. If smooth trend more or less straight across, model OK.
- Martingale residuals can go very negative, so won't always look normal.

Martingale residual plot for dance data

```
ggcoxdiagnostics(dance.1) + geom_smooth(se = F)
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```

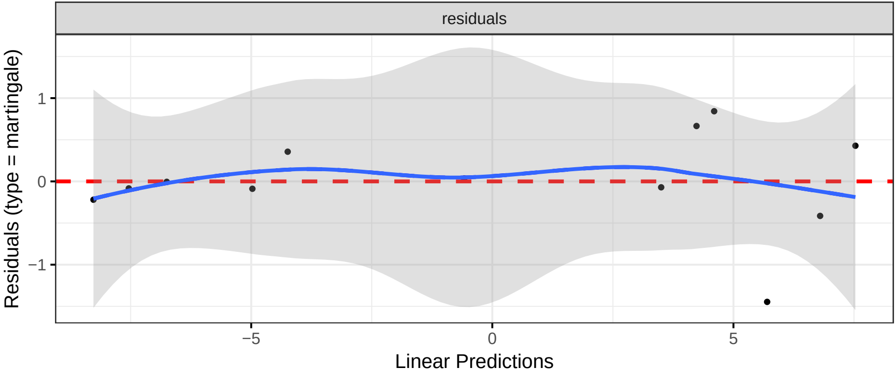


Figure 25: plot of chunk unnamed-chunk-128

Predicted survival probs

The function we use is called `survfit`, though actually works rather like `predict`. First create a data frame of values to predict from. We'll do all combos of ages 20 and 40, treatment and not, using `crossing` to get all the combos:

```
treatments <- c(0, 1)
ages <- c(20, 40)
dance.new <- crossing(Treatment = treatments, Age = ages)
dance.new
```

```
## # A tibble: 4 x 2
##   Treatment   Age
##       <dbl> <dbl>
## 1         0    20
## 2         0    40
## 3         1    20
## 4         1    40
```

The predictions

One prediction *for each time* for each combo of age and treatment:

```
s <- survfit(dance.1, newdata = dance.new, data = dance)
summary(s)
```

```
## Call: survfit(formula = dance.1, newdata = dance.new, data
##
##  time n.risk n.event survival1 survival2 survival3 surviva
##     1     12       1  8.76e-01  1.00e+00  9.98e-01      1.0
##     2     11       2  3.99e-01  9.99e-01  9.89e-01      1.0
##     4      8       1  1.24e-01  9.99e-01  9.76e-01      1.0
##     5      7       1  2.93e-02  9.98e-01  9.60e-01      1.0
##     7      6       1 2.96e-323  6.13e-01  1.70e-04      0.9
##     8      5       1  0.00e+00  2.99e-06  1.35e-98      0.8
##    10      4       1  0.00e+00  3.61e-20  0.00e+00      0.5
##    11      2       1  0.00e+00  0.00e+00  0.00e+00      0.0
##    12      1       1  0.00e+00  0.00e+00  0.00e+00      0.0
```

Conclusions from predicted probs

- Older women more likely to be still dancing than younger women (compare "profiles" for same treatment group).
- Effect of treatment seems to be to increase prob of still dancing (compare "profiles" for same age for treatment group vs. not)
- Would be nice to see this on a graph. This is `ggsurvplot` from package `survminer`:

```
g <- ggsurvplot(s, conf.int = F)
```

Plotting survival probabilities

```
g
```

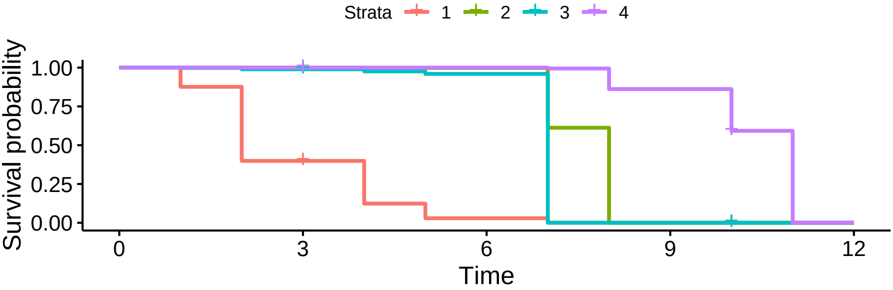
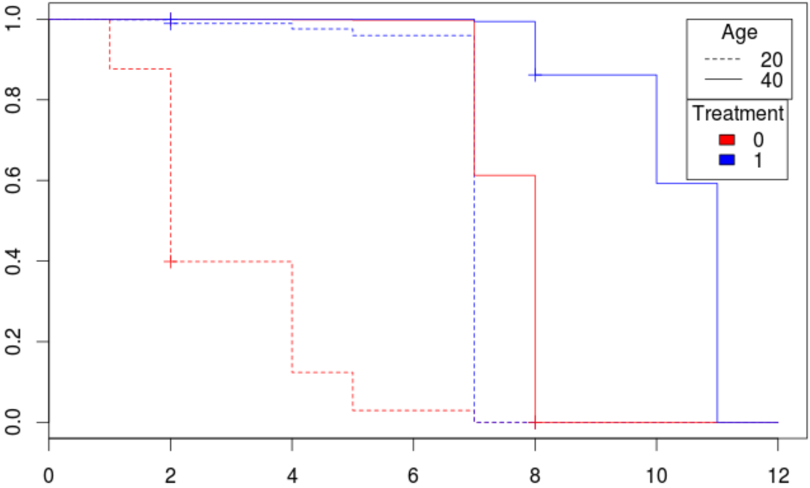


Figure 26: plot of chunk unnamed-chunk-134

Stratum	Age	Treatment
1	20	no

Discussion



A more realistic example: lung cancer

- When you load in an R package, get data sets to illustrate functions in the package.
- One such is `lung`. Data set measuring survival in patients with advanced lung cancer.
- Along with survival time, number of "performance scores" included, measuring how well patients can perform daily activities.
- Sometimes high good, but sometimes bad!
- Variables below, from the help file data set (`?lung`).

The variables

Format

inst:	Institution code
time:	Survival time in days
status:	censoring status 1=censored, 2=dead
age:	Age in years
sex:	Male=1 Female=2
ph.ecog:	ECOG performance score (0=good 5=dead)
ph.karno:	Karnofsky performance score (bad=0-good=100) rated by physician
pat.karno:	Karnofsky performance score as rated by patient
meal.cal:	Calories consumed at meals
wt.loss:	Weight loss in last six months

Uh oh, missing values

```
lung %>% slice(1:16)
```

```
##    inst time status age sex ph.ecog ph.karno pat.karno meal
## 1     3  306      2  74   1       1       90       100
## 2     3  455      2  68   1       0       90        90
## 3     3 1010      1  56   1       0       90        90
## 4     5  210      2  57   1       1       90        60
## 5     1  883      2  60   1       0      100        90
## 6    12 1022      1  74   1       1       50        80
## 7     7  310      2  68   2       2       70        60
## 8    11  361      2  71   2       2       60        80
## 9     1  218      2  53   1       1       70        80
## 10    7  166      2  61   1       2       70        70
## 11    6  170      2  57   1       1       80        80
## 12   16  654      2  68   2       2       70        70
## 13   11  728      2  68   2       1       90        90
```

A closer look

```
summary(lung)
```

```
##       inst            time            status           age
##  Min.    : 1.00   Min.    :   5.0   Min.    :1.000   Min.    :3
##  1st Qu.: 3.00   1st Qu.: 166.8   1st Qu.:1.000   1st Qu.:5
##  Median :11.00   Median : 255.5   Median :2.000   Median :6
##  Mean   :11.09   Mean   : 305.2   Mean   :1.724   Mean   :6
##  3rd Qu.:16.00   3rd Qu.: 396.5   3rd Qu.:2.000   3rd Qu.:6
##  Max.   :33.00   Max.   :1022.0   Max.   :2.000   Max.   :8
##  NA's   :1
##     ph.ecog          ph.karno        pat.karno         meal
##  Min.   :0.0000   Min.    : 50.00   Min.    : 30.00   Min.
24.000
##  1st Qu.:0.0000   1st Qu.: 75.00   1st Qu.: 70.00   1st Qu.
##  Median :1.0000   Median : 80.00   Median : 80.00   Median
##  Mean   :0.9515   Mean    : 81.94   Mean    : 79.96   Mean
```

Remove any obs with any missing values

```
cc <- complete.cases(lung)
lung %>% filter(cc) -> lung.complete
lung.complete %>%
  select(meal.cal:wt.loss) %>%
  head(10)
```

```
##    meal.cal wt.loss
## 1      1225      15
## 2      1150      11
## 3       513       0
## 4       384      10
## 5       538       1
## 6       825      16
## 7       271      34
## 8      1025      27
## 9      2600      60
## 10     1150      -5
```

Check!

```
summary(lung.complete)
```

```
##       inst            time            status            age
##  Min.   : 1.00   Min.   :   5.0   Min.   :1.000   Min.   :3
##  1st Qu.: 3.00   1st Qu.: 174.5   1st Qu.:1.000   1st Qu.:5
##  Median :11.00   Median : 268.0   Median :2.000   Median :6
##  Mean   :10.71   Mean   : 309.9   Mean   :1.719   Mean   :6
##  3rd Qu.:15.00   3rd Qu.: 419.5   3rd Qu.:2.000   3rd Qu.:7
##  Max.   :32.00   Max.   :1022.0   Max.   :2.000   Max.   :8
##     ph.ecog          ph.karno        pat.karno          meal
##  Min.   :0.0000   Min.   : 50.00   Min.   : 30.00   Min.
24.000
##  1st Qu.:0.0000   1st Qu.: 70.00   1st Qu.: 70.00   1st Qu.
##  Median :1.0000   Median : 80.00   Median : 80.00   Median
##  Mean   :0.9581   Mean   : 82.04   Mean   : 79.58   Mean
##  3rd Qu.:1.0000   3rd Qu.: 90.00   3rd Qu.: 90.00   3rd Qu.
```

Model 1: use everything except inst

```
str(lung.complete)
```

```
## 'data.frame':    167 obs. of  10 variables:
##  $ inst     : num  3 5 12 7 11 1 7 6 12 22 ...
##  $ time     : num  455 210 1022 310 361 ...
##  $ status   : num  2 2 1 2 2 2 2 2 2 2 ...
##  $ age      : num  68 57 74 68 71 53 61 57 57 70 ...
##  $ sex      : num  1 1 1 2 2 1 1 1 1 1 ...
##  $ ph.ecog  : num  0 1 1 2 2 1 2 1 1 1 ...
##  $ ph.karno : num  90 90 50 70 60 70 70 80 80 90 ...
##  $ pat.karno: num  90 60 80 60 80 80 70 80 70 100 ...
##  $ meal.cal : num  1225 1150 513 384 538 ...
##  $ wt.loss  : num  15 11 0 10 1 16 34 27 60 -5 ...
```

def

```
resp <- with(lung.complete, Surv(time, status == 2))
lung.1 <- coxph(resp ~ . - inst - time - status
```

summary of model 1: too tiny to see!

```
summary(lung.1)
```

```
## Call:
## coxph(formula = resp ~ . - inst - time - status, data = lu
##
##   n= 167, number of events= 120
##
##                  coef  exp(coef)   se(coef)      z Pr(>|z|)
## age         1.080e-02  1.011e+00  1.160e-02  0.931  0.35168
## sex        -5.536e-01  5.749e-01  2.016e-01 -2.746  0.00603
## ph.ecog     7.395e-01  2.095e+00  2.250e-01  3.287  0.00101
## ph.karno    2.244e-02  1.023e+00  1.123e-02  1.998  0.04575
## pat.karno -1.207e-02  9.880e-01  8.116e-03 -1.488  0.13685
## meal.cal    2.835e-05  1.000e+00  2.594e-04  0.109  0.91298
## wt.loss    -1.420e-02  9.859e-01  7.766e-03 -1.828  0.06748
## ---
```

Overall significance

The three tests of overall significance:

```
glance(lung.1)[c(4, 6, 8)]
```

```
## # A tibble: 1 x 3
##   p.value.log p.value.sc p.value.wald
##         <dbl>      <dbl>        <dbl>
## 1    0.000205   0.000193     0.000271
```

def All strongly significant. *Something* predicts survival.

Coefficients for model 1

```
tidy(lung.1) %>% select(term, p.value) %>% arrange(p.value)
```

```
## # A tibble: 7 x 2
##   term       p.value
##   <chr>        <dbl>
## 1 ph.ecog    0.00101
## 2 sex        0.00603
## 3 ph.karno   0.0457
## 4 wt.loss    0.0675
## 5 pat.karno  0.137
## 6 age        0.352
## 7 meal.cal   0.913
```

def

- Model as a whole significant (strongly)
- sex and `ph.ecog` definitely significant

Model 2

```r
lung.2 <- update(lung.1, . ~ . - age - pat.karno - meal.cal)
tidy(lung.2) %>% select(term, p.value)
```

```
## # A tibble: 4 x 2
##   term      p.value
##   <chr>       <dbl>
## 1 sex      0.00409
## 2 ph.ecog  0.000112
## 3 ph.karno 0.101
## 4 wt.loss  0.108
```

def

- Compare with first model:

```r
anova(lung.2, lung.1)
```

```
## Analysis of Deviance Table
```

Model 3, and last

Take out ph.karno and wt.loss as well.

```
lung.3 <- update(lung.2, . ~ . - ph.karno - wt.loss)
tidy(lung.3) %>% select(term, estimate, p.value)
```

```
## # A tibble: 2 x 3
##   term    estimate  p.value
##   <chr>      <dbl>    <dbl>
## 1 sex       -0.510 0.00958
## 2 ph.ecog    0.483 0.000266
```

```
anova(lung.3, lung.2)
```

```
## Analysis of Deviance Table
##  Cox model: response is  resp
##  Model 1: ~ sex + ph.ecog
##  Model 2: ~ sex + ph.ecog + ph.karno + wt.loss
##    loglik  Chisq Df P(>|Chi|)
```

Commentary

- OK (just) to take out those two covariates.
- Both remaining variables strongly significant.
- Effect on survival time:
- Higher value of `sex` (female) has *negative* effect on event (death).
- Higher value of `ph.ecog` has *positive* effect on death.
- i. e. being female or having lower `ph.ecog` score has positive effect on survival.
- Picture?

Plotting survival probabilities

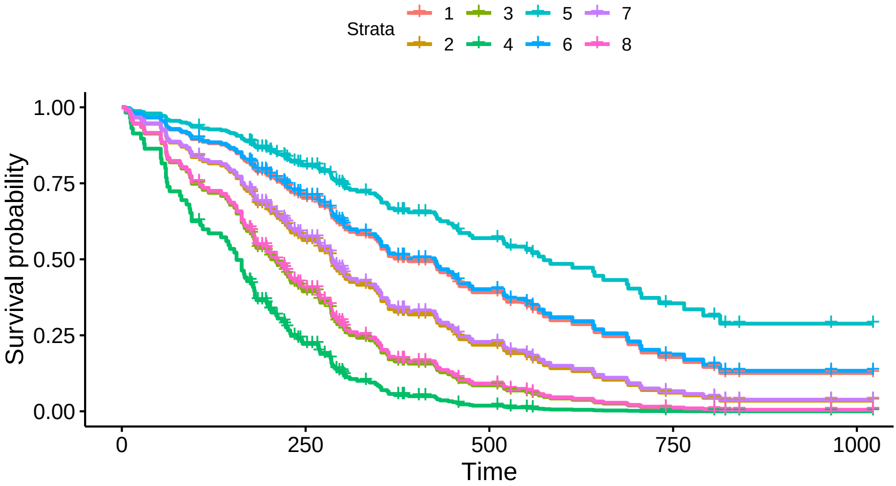
- Create new data frame of values to predict for, then predict:

```
sexes <- c(1, 2)
ph.ecogs <- 0:3
lung.new <- crossing(sex = sexes, ph.ecog = ph.ecogs)
lung.new
```

```
## # A tibble: 8 x 2
##     sex ph.ecog
##   <dbl>   <int>
## 1     1       0
## 2     1       1
## 3     1       2
## 4     1       3
## 5     2       0
## 6     2       1
## 7     2       2
```

The plot

```
ggsurvplot(s, conf.int = F)
```



Discussion of survival curves

- Best survival is teal-blue curve, stratum 5, females with (`ph.ecog`) score 0.
- Next best: blue, stratum 6, females with score 1, and red, stratum 1, males score 0.
- Worst: green, stratum 4, males score 3.
- For any given `ph.ecog` score, females have better predicted survival than males.
- For both genders, a lower score associated with better survival.
- `sex` coeff in model 3 negative, so being higher `sex` value (female) goes with *less* hazard of dying.
- `ph.ecog` coeff in model 3 positive, so higher `ph.ecog` score goes with *more* hazard of dying
- Two coeffs about same size, so being male rather than female

Martingale residuals for this model

```
ggcoxdiagnostics(lung.3) + geom_smooth(se = F)
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```

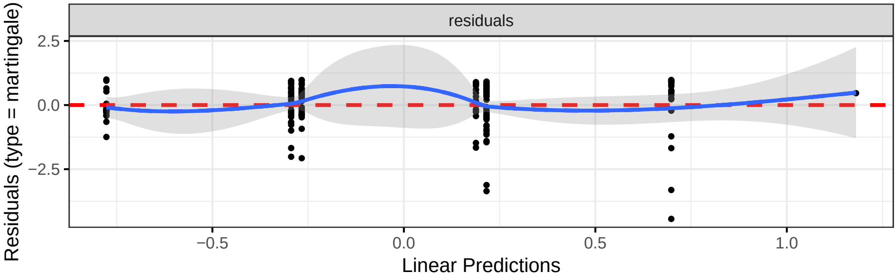


Figure 27: plot of chunk unnamed-chunk-150

No problems here.

When the Cox model fails

- Invent some data where survival is best at middling age, and worse at high *and* low age:

```
age <- seq(20, 60, 5)
survtime <- c(10, 12, 11, 21, 15, 20, 8, 9, 11)
stat <- c(1, 1, 1, 1, 0, 1, 1, 1, 1)
d <- tibble(age, survtime, stat)
y <- with(d, Surv(survtime, stat))
```

- Small survival time 15 in middle was actually censored, so would have been longer if observed.

Fit Cox model

"'r y.1 <- coxph(y age, data = d) summary(y.1) "'

"' Call: coxph(formula = y age, data = d) n= 9, number of events= 8 coef exp(coef) se(coef) z Pr(>|z|) age 0.01984 1.02003 0.03446 0.576 0.565 exp(coef) exp(-coef) lower .95 upper .95 age 1.02 0.9804 0.9534 1.091 Concordance= 0.545 (se = 0.105) Likelihood ratio test= 0.33 on 1 df, p=0.6 Wald test = 0.33 on 1 df, p=0.6 Score (logrank) test = 0.33 on 1 df, p=0.6 "'

Martingale residuals

```
ggcoxdiagnostics(y.1) + geom_smooth(se = F)
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```

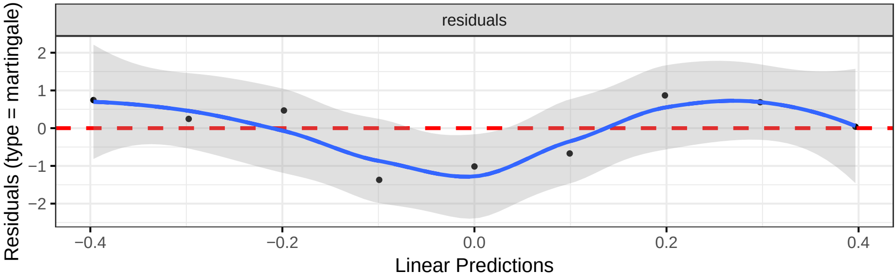


Figure 28: plot of chunk unnamed-chunk-153

Down-and-up indicates incorrect relationship between age and survival. Add

Attempt 2

```
y.2 <- coxph(y ~ age + I(age^2), data = d)
summary(y.2)
```

```
## Call:
## coxph(formula = y ~ age + I(age^2), data = d)
##
##   n= 9, number of events= 8
##
##                 coef exp(coef)  se(coef)      z Pr(>|z|)
## age        -0.380184  0.683736  0.241617 -1.573   0.1156
## I(age^2)    0.004832  1.004844  0.002918  1.656   0.0977 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
##
##          exp(coef) exp(-coef) lower .95 upper .95
## age         0.6837     1.4626    0.4258     1.098
## I(age^2)    1.0048     0.9952    0.9991     1.011
```

Martingale residuals this time

```
ggcoxdiagnostics(y.2) + geom_smooth(se = F)
```

```
## `geom_smooth()` using method = 'loess' and formula 'y ~ x'
```

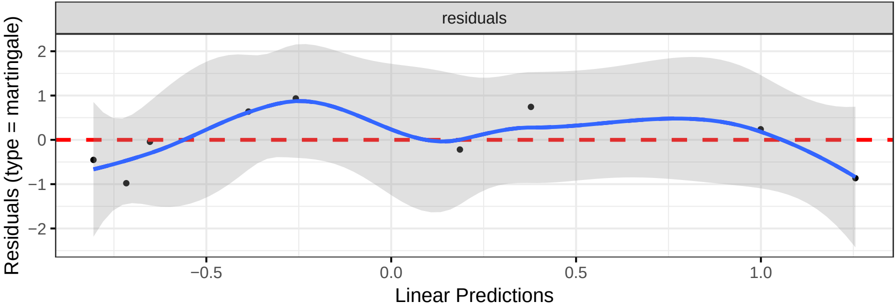


Figure 29: plot of chunk unnamed-chunk-155

Section 5

Analysis of variance

Analysis of variance

- Analysis of variance used with:
- counted/measured response
- categorical explanatory variable(s)
- that is, data divided into groups, and see if response significantly different among groups
- or, see whether knowing group membership helps to predict response.
- Typically two stages:
- F-test to detect *{any} differences among/due to groups*
- *if F-test significant, do* {multiple comparisons} to see which groups significantly different from which.
- Need special multiple comparisons method because just doing (say) two-sample t-tests on each pair of groups gives too big a chance of

Packages

These:

```r
library(tidyverse)
library(broom)
```

Example: Pain threshold and hair colour

- Do people with different hair colour have different abilities to deal with pain?
- Men and women of various ages divided into 4 groups by hair colour: light and dark blond, light and dark brown.
- Each subject given a pain sensitivity test resulting in pain threshold score: higher score is higher pain tolerance.
- 19 subjects altogether.

The data

In `hairpain.txt`:

“‘ “‘

hair pain lightblond 62 lightblond 60
lightblond 71 lightblond 55
lightblond 48 darkblond 63
darkblond 57 darkblond 52 darkblond
41 darkblond 43 lightbrown 42
lightbrown 50 lightbrown 41
lightbrown 37 darkbrown 32
darkbrown 39 darkbrown 51
darkbrown 30 darkbrown 35

Summarizing the groups

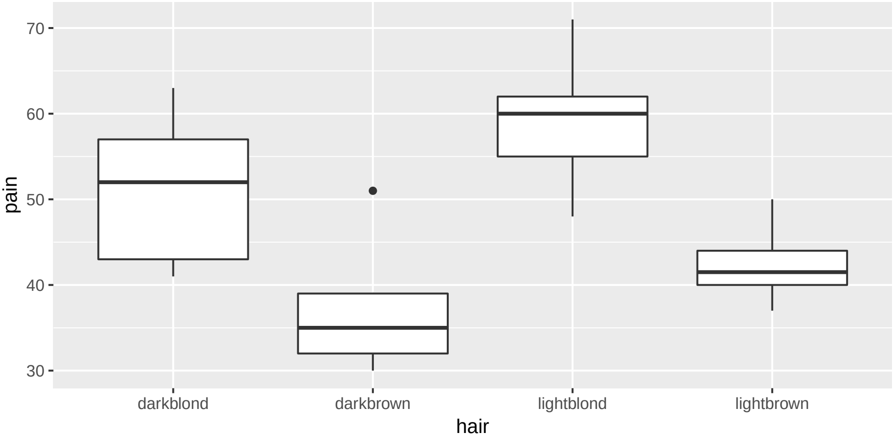
```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/hairpain.tx
hairpain <- read_delim(my_url, " ")
```

```
## Parsed with column specification:
## cols(
##   hair = col_character(),
##   pain = col_double()
## )
```

```
hairpain %>%
  group_by(hair) %>%
  summarize(
    n = n(),
    xbar = mean(pain),
    s = sd(pain)
  )
```

Boxplot

```
ggplot(hairpain, aes(x = hair, y = pain)) + geom_boxplot()
```



Assumptions

- Data should be:
- normally distributed within each group
- same spread for each group
- `darkbrown` group has upper outlier (suggests not normal)
- `darkblond` group has smaller IQR than other groups.
- But, groups *small*.
- Shrug shoulders and continue for moment.

Testing equality of SDs

- via **Levene's test** in package car:

```
car::leveneTest(pain ~ hair, data = hairpain)
```

```
## Warning in leveneTest.default(y = y, group = group, ...): g
## Levene's Test for Homogeneity of Variance (center = median)
##       Df F value Pr(>F)
## group  3  0.3927   0.76
##       15
```

- No evidence (at all) of difference among group SDs.
- Possibly because groups *small*.

Analysis of variance

```
hairpain.1 <- aov(pain ~ hair, data = hairpain)
summary(hairpain.1)
```

```
##             Df Sum Sq Mean Sq F value  Pr(>F)
## hair         3   1361   453.6   6.791 0.00411 **
## Residuals   15   1002    66.8
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

- P-value small: the mean pain tolerances for the four groups are *not* all the same.
- Which groups differ from which, and how?

Multiple comparisons

- Which groups differ from which? Multiple comparisons method. Lots.
- Problem: by comparing all the groups with each other, doing many tests, have large chance to (possibly incorrectly) reject H_0 : groups have equal means.
- 4 groups: 6 comparisons (1 vs 2, 1 vs 3, …, 3 vs 4). 5 groups: 10 comparisons. Thus 6 (or 10) chances to make mistake.
- Get "familywise error rate" of 0.05 (whatever), no matter how many comparisons you're doing.
- My favourite: Tukey, or "honestly significant differences": how far apart might largest, smallest group means be (if actually no differences). Group means more different: significantly different.

Tukey

- TukeyHSD:

{

```
TukeyHSD(hairpain.1)
```

```
##   Tukey multiple comparisons of means
##     95% family-wise confidence level
##
## Fit: aov(formula = pain ~ hair, data = hairpain)
##
## $hair
##                           diff        lwr        upr     p adj
## darkbrown-darkblond   -13.8 -28.696741  1.0967407 0.0740679
## lightblond-darkblond    8.0  -6.896741 22.8967407 0.4355768
## lightbrown-darkblond   -8.7 -24.500380  7.1003795 0.4147283
## lightblond-darkbrown   21.8   6.903259 36.6967407 0.0037079
## lightbrown-darkbrown    5.1 -10.700380 20.9003795 0.7893211
## lightbrown-lightblond -16.7 -32.500380 -0.8996205 0.0366467
```

def }

The old-fashioned way

- List group means in order
- Draw lines connecting groups that are *not* significantly different:

```
darkbrown lightbrown  darkblond lightblond
37.4      42.5       51.2       59.2
-------------------------
---------------
```

- `lightblond` significantly higher than everything except `darkblond` (at $\alpha = 0.05$).
- `darkblond` in middle ground: not significantly less than `lightblond`, not significantly greater than `darkbrown` and `lightbrown`.
- More data might resolve this.
- Looks as if blond-haired people do have higher pain tolerance, but not

Some other multiple-comparison methods

- Work any time you do k tests at once (not just ANOVA).
- **Bonferroni**: multiply all P-values by k.
- **Holm**: multiply smallest P-value by k, next-smallest by $k-1$, etc.
- **False discovery rate**: multiply smallest P-value by $k/1$, 2nd-smallest by $k/2$, ..., i-th smallest by k/i.
- Stop after non-rejection.

Example

- P-values 0.005, 0.015, 0.03, 0.06 (4 tests all done at once) Use $\alpha = 0.05$.
- Bonferroni:
- Multiply all P-values by 4 (4 tests).
- Reject only 1st null.
- Holm:
- Times smallest P-value by 4: $0.005 * 4 = 0.020 < 0.05$, reject.
- Times next smallest by 3: $0.015 * 3 = 0.045 < 0.05$, reject.
- Times next smallest by 2: $0.03 * 2 = 0.06 > 0.05$, do not reject. Stop.

...Continued

- With P-values 0.005, 0.015, 0.03, 0.06:
- False discovery rate:
- Times smallest P-value by 4: $0.005 * 4 = 0.02 < 0.05$: reject.
- Times second smallest by $4/2$: $0.015 * 4/2 = 0.03 < 0.05$, reject.
- Times third smallest by $4/3$: $0.03 * 4/3 = 0.04 < 0.05$, reject.
- Times fourth smallest by $4/4$: 0.06*4/4=0.06>0.05, do not reject. Stop.

pairwise.t.test

“‘r attach(hairpain) pairwise.t.test(pain, hair, p.adj = ”none”) “‘

“‘ Pairwise comparisons using t tests with pooled SD data: pain and hair darkblond darkbrown lightblond darkbrown 0.01748 - - lightblond 0.14251 0.00075 - lightbrown 0.13337 0.36695 0.00817 P value adjustment method: none “‘

“‘r pairwise.t.test(pain, hair, p.adj = ”holm”) “‘

“‘ Pairwise comparisons using t tests with pooled SD data: pain and hair darkblond darkbrown lightblond darkbrown 0.0699 - - lightblond 0.4001 0.0045 - lightbrown 0.4001 0.4001 0.0408 P value adjustment method: holm “‘

“‘r pairwise.t.test(pain, hair, p.adj = ”fdr”) “‘

“‘ Pairwise comparisons using t tests with pooled SD data: pain and hair darkblond darkbrown lightblond darkbrown 0.0350 - - lightblond 0.1710 0.0045 - lightbrown 0.1710 0.3670 0.0245 P value adjustment method: fdr “‘

“‘r pairwise.t.test(pain, hair, p.adj = ”bon”) “‘

“‘ Pairwise comparisons using t tests with pooled SD data: pain and hair darkblond darkbrown lightblond darkbrown 0.1049 - - lightblond 0.8550 0.0045 - lightbrown 0.8002 1.0000 0.0490 P value adjustment method: bonferroni “‘

Comments

- P-values all adjusted upwards from "none".
- Required because 6 tests at once.
- Highest P-values for Bonferroni: most "conservative".
- Prefer Tukey or FDR or Holm.
- Tukey only applies to ANOVA, not to other cases of multiple testing.

Rats and vitamin B

- What is the effect of dietary vitamin B on the kidney?
- A number of rats were randomized to receive either a B-supplemented diet or a regular diet.
- Desired to control for initial size of rats, so classified into size classes `lean` and `obese`.
- After 20 weeks, rats' kidneys weighed.
- Variables:
- Response: `kidneyweight` (grams).
- Explanatory: `diet`, `ratsize`.
- Read in data:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/vitaminb.tx
vitaminb <- read_delim(my_url, " ")
```

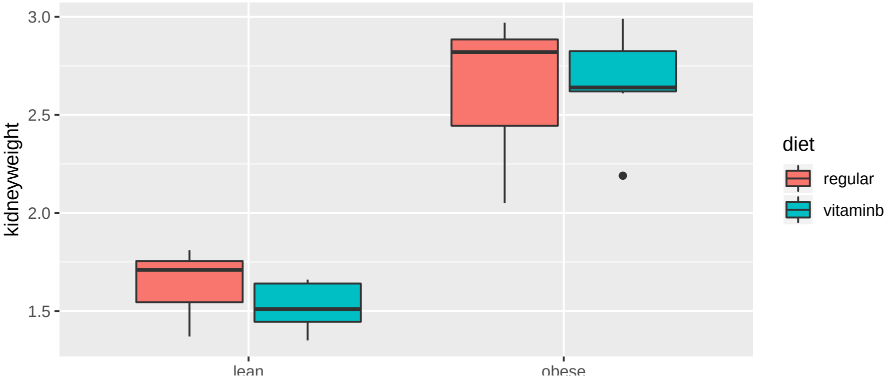
The data

```
vitaminb
```

```
## # A tibble: 28 x 3
##    ratsize diet     kidneyweight
##    <chr>   <chr>           <dbl>
##  1 lean    regular          1.62
##  2 lean    regular          1.8 
##  3 lean    regular          1.71
##  4 lean    regular          1.81
##  5 lean    regular          1.47
##  6 lean    regular          1.37
##  7 lean    regular          1.71
##  8 lean    vitaminb         1.51
##  9 lean    vitaminb         1.65
## 10 lean    vitaminb         1.45
## # … with 18 more rows
```

Grouped boxplot

```
ggplot(vitaminb, aes(
  x = ratsize, y = kidneyweight,
  fill = diet
)) + geom_boxplot()
```



What's going on?

- Calculate group means:

```
summary <- vitaminb %>%
  group_by(ratsize, diet) %>%
  summarize(mean = mean(kidneyweight))
summary
```

```
## # A tibble: 4 x 3
## # Groups:   ratsize [2]
##   ratsize diet      mean
##   <chr>   <chr>    <dbl>
## 1 lean    regular   1.64
## 2 lean    vitaminb  1.53
## 3 obese   regular   2.64
## 4 obese   vitaminb  2.67
```

- Rat size: a large and consistent effect.

ANOVA with interaction

```
vitaminb.1 <- aov(kidneyweight ~ ratsize * diet,
  data = vitaminb
)
summary(vitaminb.1)
```

```
##              Df Sum Sq Mean Sq F value   Pr(>F)    
## ratsize       1  8.068   8.068 141.179 1.53e-11 ***
## diet          1  0.012   0.012   0.218    0.645    
## ratsize:diet  1  0.036   0.036   0.638    0.432    
## Residuals    24  1.372   0.057                     
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

Significance/nonsignificance as we expected. Note no significant interaction (can be removed).

Interaction plot

- Plot mean of response variable against one of the explanatory, using other one as groups. Start from summary:

```
g <- ggplot(summary, aes(
  x = ratsize, y = mean,
  colour = diet, group = diet
)) +
  geom_point() + geom_line()
```

- For this, have to give *both* `group` and `colour`.

The interaction plot

```
g
```

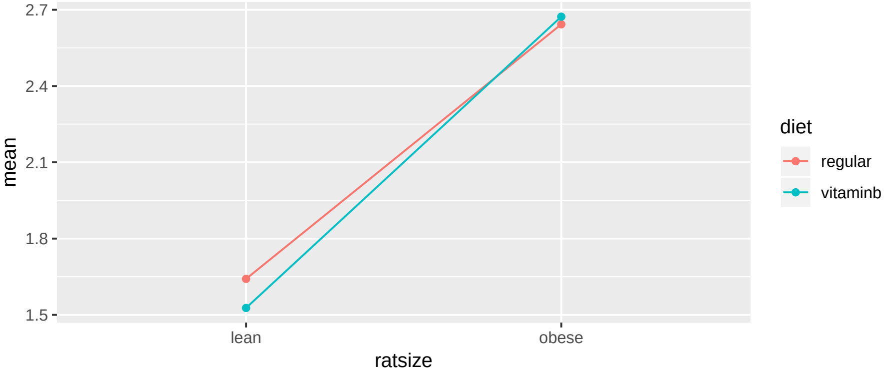


Figure 32: plot of chunk unnamed-chunk-169

Take out interaction

```
vitaminb.2 <- update(vitaminb.1, . ~ . - ratsize:diet)
summary(vitaminb.2)
```

```
##             Df Sum Sq Mean Sq F value   Pr(>F)
## ratsize      1  8.068   8.068 143.256 7.59e-12 ***
## diet         1  0.012   0.012   0.221    0.643
## Residuals   25  1.408   0.056
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

- No Tukey for `diet`: not significant.
- No Tukey for `ratsize`: only two sizes, and already know that obese rats have larger kidneys than lean ones.
- Bottom line: diet has no effect on kidney size once you control for size of rat.

The auto noise data

In 1973, the President of Texaco cited an automobile filter developed by Associated Octel Company as effective in reducing pollution. However, questions had been raised about the effects of filter silencing. He referred to the data included in the report (and below) as evidence that the silencing properties of the Octel filter were at least equal to those of standard silencers.

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/autonoise.t
autonoise <- read_table(my_url)
```

```
## Parsed with column specification:
## cols(
##   noise = col_double(),
##   size = col_character(),
##   type = col_character(),
##   side = col_character()
## )
```

The data

```
autonoise
```

```
## # A tibble: 36 x 4
##    noise size  type  side 
##    <dbl> <chr> <chr> <chr>
##  1   840 M     Std   R    
##  2   770 L     Octel L    
##  3   820 M     Octel R    
##  4   775 L     Octel R    
##  5   825 M     Octel L    
##  6   840 M     Std   R    
##  7   845 M     Std   L    
##  8   825 M     Octel L    
##  9   815 M     Octel L    
## 10   845 M     Std   R    
## # … with 26 more rows
```

Making boxplot

- Make a boxplot, but have combinations of filter type and engine size.
- Use grouped boxplot again, thus:

```
g <- autonoise %>%
  ggplot(aes(x = size, y = noise, fill = type)) +
  geom_boxplot()
```

The boxplot

```
g
```

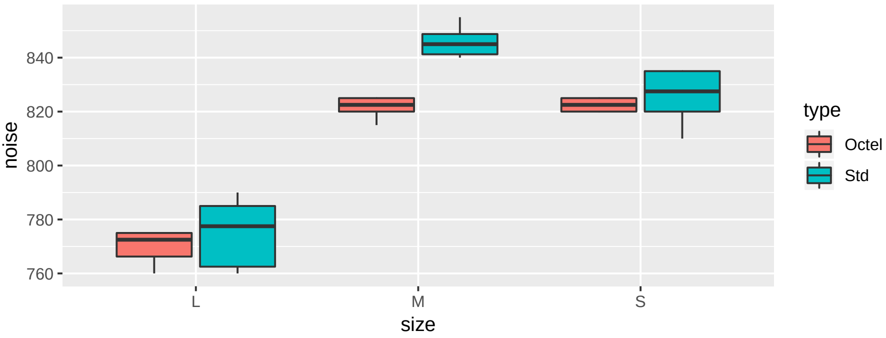


Figure 33: plot of chunk unnamed-chunk-174

- Difference in engine noise between Octel and standard is larger for

ANOVA

```
autonoise.1 <- aov(noise ~ size * type, data = autonoise)
summary(autonoise.1)
```

```
##             Df Sum Sq Mean Sq F value   Pr(>F)    
## size         2  26051   13026 199.119  < 2e-16 ***
## type         1   1056    1056  16.146 0.000363 ***
## size:type    2    804     402   6.146 0.005792 ** 
## Residuals   30   1962      65                     
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

- The interaction is significant, as we suspected from the boxplots.
- The within-group spreads don't look very equal, but only based on 6 obs each.

Tukey: ouch!

```
autonoise.2 <- TukeyHSD(autonoise.1)
autonoise.2$`size:type`
```

```
##                        diff        lwr       upr            p
## M:Octel-L:Octel  51.6666667  37.463511  65.869823 6.033496e
11
## S:Octel-L:Octel  52.5000000  38.296844  66.703156 4.089762e
11
## L:Std-L:Octel     5.0000000  -9.203156  19.203156 8.890358e
01
## M:Std-L:Octel    75.8333333  61.630177  90.036489 4.962697e
14
## S:Std-L:Octel    55.8333333  41.630177  70.036489 9.002910e
12
## S:Octel-M:Octel   0.8333333 -13.369823  15.036489 9.999720e
01
```

Interaction plot

- This time, don't have summary of mean noise for each size-type combination.
- One way is to compute summaries (means) first, and feed into `ggplot` as in vitamin B example.
- Or, have `ggplot` compute them for us, thus:

```
g <- ggplot(autonoise, aes(
  x = size, y = noise,
  colour = type, group = type
)) +
  stat_summary(fun.y = mean, geom = "point") +
  stat_summary(fun.y = mean, geom = "line")
```

Interaction plot

```
g
```

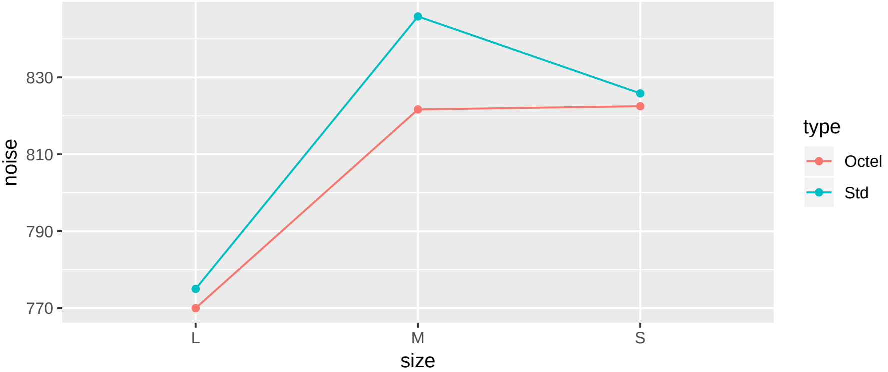
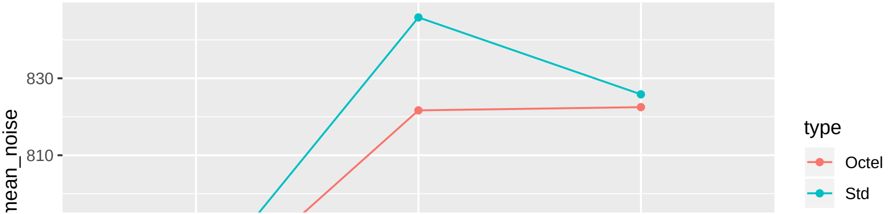


Figure 34: plot of chunk unnamed-chunk-178

If you don't like that...

...then compute the means first, in a pipeline:

```
autonoise %>%
  group_by(size, type) %>%
  summarize(mean_noise = mean(noise)) %>%
  ggplot(aes(
    x = size, y = mean_noise, group = type,
    colour = type
  )) + geom_point() + geom_line()
```



Simple effects for auto noise example

- In auto noise example, weren't interested in all comparisons between car size and filter type combinations.
- Wanted to demonstrate (lack of) difference between filter types *for each car type*.
- These are called **simple effects** of one variable (filter type) conditional on other variable (car type).
- To do this, pull out just the data for small cars, compare noise for the two filter types. Then repeat for medium and large cars. (Three one-way ANOVAs.)

Do it using dplyr tools

- Small cars:

```
autonoise %>%
  filter(size == "S") %>%
  aov(noise ~ type, data = .) %>%
  summary()
```

```
##             Df Sum Sq Mean Sq F value Pr(>F)
## type         1   33.3   33.33   0.548  0.476
## Residuals   10  608.3   60.83
```

- No filter difference for small cars.
- For Medium, change `S` to `M` and repeat.

Simple effect of filter type for medium cars

{

```
autonoise %>%
  filter(size == "M") %>%
  aov(noise ~ type, data = .) %>%
  summary()
```

```
##             Df Sum Sq Mean Sq F value   Pr(>F)
## type         1 1752.1  1752.1   68.93 8.49e-06 ***
## Residuals   10  254.2    25.4
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

}

- There *is* an effect of filter type for medium cars. Look at means to investigate: {

```
autonoise %>%
  filter(size == "M") %>%
```

Medium and large cars

- Octel filters produce *less* noise for medium cars.
- Large cars:

```
autonoise %>%
  filter(size == "L") %>%
  aov(noise ~ type, data = .) %>%
  summary()
```

```
##             Df Sum Sq Mean Sq F value Pr(>F)
## type         1     75      75   0.682  0.428
## Residuals   10   1100     110
```

- No significant difference again.
- Or use `glance` from `broom`:

```
autonoise %>%
  filter(size == "L") %>%
```

All at once, using split/apply/combine

The "split" part:

```
autonoise %>%
  group_by(size) %>%
  nest()
```

```
## # A tibble: 3 x 2
##   size  data
##   <chr> <list>
## 1 M     <tibble [12 × 3]>
## 2 L     <tibble [12 × 3]>
## 3 S     <tibble [12 × 3]>
```

Now have *three* rows, with the data frame for each size encoded as *one element* of this data frame.

Apply

- Write function to do aov on a data frame with columns `noise` and `type`, returning P-value:

```
aov_pval <- function(x) {
  noise.1 <- aov(noise ~ type, data = x)
  gg <- glance(noise.1)
  gg$p.value
}
```

- Test it:

```
autonoise %>%
  filter(size == "L") %>%
  aov_pval()
```

```
## [1] 0.428221
```

- Check.

Combine

- Apply this function to each of the nested data frames (one per engine size):

```
autonoise %>%
  group_by(size) %>%
  nest() %>%
  mutate(p_val = map_dbl(data, ~ aov_pval(.)))
```

```
## # A tibble: 3 x 3
##   size  data                   p_val
##   <chr> <list>                 <dbl>
## 1 M     <tibble [12 × 3]> 0.00000849
## 2 L     <tibble [12 × 3]> 0.428
## 3 S     <tibble [12 × 3]> 0.476
```

- `map_dbl` because `aov_pval` returns a decimal number (a `dbl`). Investigate what happens if you use `map` instead.

Tidy up

- The data column was stepping-stone to getting answer. Don't need it any more:

```
simple_effects <- autonoise %>%
  group_by(size) %>%
  nest() %>%
  mutate(p_val = map_dbl(data, ~ aov_pval(.))) %>%
  select(-data)
simple_effects
```

```
## # A tibble: 3 x 2
##   size        p_val
##   <chr>       <dbl>
## 1 M      0.00000849
## 2 L      0.428
## 3 S      0.476
```

Simultaneous tests

- When testing simple effects, doing several tests at once. (In this case, 3.)
- Have to adjust P-values for this. Eg. Holm:

```
simple_effects %>%
  arrange(p_val) %>%
  mutate(multiplier = 4 - row_number()) %>%
  mutate(p_val_adj = p_val * multiplier)
```

```
## # A tibble: 3 x 4
##   size        p_val multiplier p_val_adj
##   <chr>       <dbl>      <dbl>     <dbl>
## 1 M      0.00000849          3 0.0000255
## 2 L      0.428               2 0.856
## 3 S      0.476               1 0.476
```

* No change in rejection decisions.

Confidence intervals

- Perhaps better way of assessing simple effects: look at *confidence intervals* rather than tests.
- Gives us sense of accuracy of estimation, and thus whether non-significance might be lack of power: "absence of evidence is not evidence of absence".
- Works here because *two* filter types, using `t.test` for each engine type.
- Want to show that the Octel filter is equivalent to or better than the standard filter, in terms of engine noise.

Equivalence and noninferiority

- Known as "equivalence testing" in medical world. A good read: link. Basic idea: decide on size of difference δ that would be considered "equivalent", and if CI entirely inside $\pm\delta$, have evidence in favour of equivalence.
- We really want to show that the Octel filters are "no worse" than the standard one: that is, equivalent *or better* than standard filters.
- Such a "noninferiority test" done by checking that `upper limit` of CI, new minus old, is *less* than δ. (This requires careful thinking about (i) which way around the difference is and (ii) whether a higher or lower value is better.)

CI for small cars

Same idea as for simple effect test:

```
autonoise %>%
  filter(size == "S") %>%
  t.test(noise ~ type, data = .) %>%
  .[["conf.int"]]
```

```
## [1] -14.517462   7.850795
## attr(,"conf.level")
## [1] 0.95
```

CI for medium cars

```
autonoise %>%
  filter(size == "M") %>%
  t.test(noise ~ type, data = .) %>%
  .[["conf.int"]]
```

```
## [1] -30.75784 -17.57549
## attr(,"conf.level")
## [1] 0.95
```

CI for large cars

```
autonoise %>%
  filter(size == "L") %>%
  t.test(noise ~ type, data = .) %>%
  .[["conf.int"]]
```

```
## [1] -19.270673   9.270673
## attr(,"conf.level")
## [1] 0.95
```

Or, all at once: split/apply/combine

```
ci_func <- function(x) {
  tt <- t.test(noise ~ type, data = x)
  tt$conf.int
}
cis <- autonoise %>%
  group_by(size) %>%
  nest() %>%
  mutate(ci = map(data, ~ ci_func(.))) %>%
  unnest(ci)
```

“‘r cis “‘

“‘ A tibble: 6 x 2 size ci <chr> <dbl> 1 M -30.8 2 M -17.6 3 L -19.3 4 L 9.27 5 S -14.5 6 S 7.85 “‘

* Function to get CI of difference in noise means for types of filter on input

* Group by ‘size‘, nest (mini-df per size)

* Calculate CI for each thing in ‘data‘ (ie. each ‘size‘). ‘map‘: CI is two numbers long

* ‘unnest‘ ‘ci‘ column to see two

CIs and noninferiority test

- Suppose we decide that a 20 dB difference would be considered equivalent. (I have no idea whether that is reasonable.)
- Intervals:

```
cis %>%
  mutate(hilo = rep(c("lower", "upper"), 3)) %>%
  spread(hilo, ci)
```

```
## # A tibble: 3 x 3
##   size  lower  upper
##   <chr> <dbl>  <dbl>
## 1 L     -19.3   9.27
## 2 M     -30.8 -17.6
## 3 S     -14.5   7.85
```

\begin{tabular}{lrr}

Contrasts in ANOVA

- Sometimes, don't want to compare *all* groups, only *some* of them.
- Might be able to specify these comparisons ahead of time; other comparisons of no interest.
- Wasteful to do ANOVA and Tukey.

Example: chainsaw kickback

- From link.
- Forest manager concerned about safety of chainsaws issued to field crew. 4 models of chainsaws, measure “kickback” (degrees of deflection) for 5 of each:

```
 A  B  C  D
-----------
42 28 57 29
17 50 45 29
24 44 48 22
39 32 41 34
43 61 54 30
```

- So far, standard 1-way ANOVA: what differences are there among models?

chainsaw kickback (2)

- But: models A and D are designed to be used at home, while models B and C are industrial models.
- Suggests these comparisons of interest:
- home vs. industrial
- the two home models A vs. D
- the two industrial models B vs. C.
- Don't need to compare *all* the pairs of models.

What is a contrast?

- Contrast is a linear combination of group means.
- Notation: μ_A for (population) mean of group A, and so on.
- In example, compare two home models: $H_0 : \mu_A - \mu_D = 0$.
- Compare two industrial models: $H_0 : \mu_B - \mu_C = 0$.
- Compare average of two home models vs. average of two industrial models: $H_0 : \frac{1}{2}(\mu_A + \mu_D) - \frac{1}{2}(\mu_B + \mu_C) = 0$ or $H_0 : 0.5\mu_A - 0.5\mu_B - 0.5\mu_C + 0.5\mu_D = 0$.
- Note that coefficients of contrasts add to 0, and right-hand side is 0.

Contrasts in R

- Comparing two home models A and D ($\mu_A - \mu_D = 0$):

```
c.home <- c(1, 0, 0, -1)
```

- Comparing two industrial models B and C ($\mu_B - \mu_C = 0$):

```
c.industrial <- c(0, 1, -1, 0)
```

- Comparing home average vs. industrial average ($0.5\mu_A - 0.5\mu_B - 0.5\mu_C + 0.5\mu_D = 0$):

```
c.home.ind <- c(0.5, -0.5, -0.5, 0.5)
```

Orthogonal contrasts

- What happens if we multiply the contrast coefficients one by one?

```
c.home * c.industrial
```

```
## [1] 0 0 0 0
```

```
c.home * c.home.ind
```

```
## [1]  0.5  0.0  0.0 -0.5
```

```
c.industrial * c.home.ind
```

```
## [1]  0.0 -0.5  0.5  0.0
```

- in each case, the results **add up to zero**. Such contrasts are called **orthogonal**.

Orthogonal contrasts (2)

- Compare these:

```
c1 <- c(1, -1, 0)
c1
```

```
## [1]  1 -1  0
```

```
c2 <- c(0, 1, -1)
c2
```

```
## [1]  0  1 -1
```

```
c1 * c2
```

```
## [1]  0 -1  0
```

Does not add up to zero, so c1 and c2 are *not* orthogonal.

- Orthogonal contrasts are much easier to deal with.
- Can use non-orthogonal contrasts, but much more trouble (and beyond

Starting the analysis

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/chainsaw.tx
chain.wide <- read_table(my_url)
```

```
## Parsed with column specification:
## cols(
##   A = col_double(),
##   B = col_double(),
##   C = col_double(),
##   D = col_double()
## )
```

```
chain.wide
```

```
## # A tibble: 5 x 4
##       A     B     C     D
##   <dbl> <dbl> <dbl> <dbl>
## 1    42    28    57    29
```

Tidying

Need all the kickbacks in *one* column:

```
chain <- gather(chain.wide, model, kickback, A:D,
  factor_key = T
)
```

Starting the analysis (2)

The proper data frame, displayed in two pieces:

“‘r chain “‘

“‘ A tibble: 10 x 2 model kickback <fct> <dbl> 1 A 42 2 A 17 3 A 24 4 A 39 5 A 43 6 B 28 7 B 50 8 B 44 9 B 32 10 B 61 “‘

“‘r chain “‘

“‘ A tibble: 10 x 2 model kickback <fct> <dbl> 1 C 57 2 C 45 3 C 48 4 C 41 5 C 54 6 D 29 7 D 29 8 D 22 9 D 34 10 D 30 “‘

Setting up contrasts

```
m <- cbind(c.home, c.industrial, c.home.ind)
m
```

```
##      c.home c.industrial c.home.ind
## [1,]      1            0        0.5
## [2,]      0            1       -0.5
## [3,]      0           -1       -0.5
## [4,]     -1            0        0.5
```

```
contrasts(chain$model) <- m
```

ANOVA as regression

Now run ANOVA *as if regression*: {

```
chain.1 <- lm(kickback ~ model, data = chain)
summary(chain.1)
```

```
##
## Call:
## lm(formula = kickback ~ model, data = chain)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -16.00  -7.10   0.60   6.25  18.00
##
## Coefficients:
##                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)         38.450      2.179  17.649 6.52e-12 ***
## modelc.home          2.100      3.081   0.682  0.50524
## modelc.industrial   -3.000      3.081  -0.974  0.34469
## modelc.home.ind    -15.100      4.357  -3.466  0.00319 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 9.743 on 16 degrees of freedom
## Multiple R-squared:  0.4562, Adjusted R-squared:  0.3542
```

Conclusions

```
tidy(chain.1) %>% select(term, p.value)
```

```
## # A tibble: 4 x 2
##   term                p.value
##   <chr>                 <dbl>
## 1 (Intercept)        6.52e-12
## 2 modelc.home        5.05e- 1
## 3 modelc.industrial  3.45e- 1
## 4 modelc.home.ind    3.19e- 3
```

- Two home models not sig. diff. (P-value 0.51)
- Two industrial models not sig. diff. (P-value 0.34)
- Home, industrial models *are* sig. diff. (P-value 0.0032).

Means by model

- The means:

```
chain %>%
  group_by(model) %>%
  summarize(mean.kick = mean(kickback)) %>%
  arrange(desc(mean.kick))
```

```
## # A tibble: 4 x 2
##   model mean.kick
##   <fct>     <dbl>
## 1 C          49
## 2 B          43
## 3 A          33
## 4 D          28.8
```

- Home models A & D have less kickback than industrial ones B & C.
- Makes sense because industrial users should get training to cope with

Section 6

Analysis of covariance

Analysis of covariance

- ANOVA: explanatory variables categorical (divide data into groups)
- traditionally, analysis of covariance has categorical x's plus one numerical x ("covariate") to be adjusted for.
- `lm` handles this too.
- Simple example: two treatments (drugs) (`a` and `b`), with before and after scores.
- Does knowing before score and/or treatment help to predict after score?
- Is after score different by treatment/before score?

Data

Treatment, before, after:

‘‘‘ ‘‘‘

a 5 20 a 10 23 a 12 30 a 9 25 a 23 34 a 21 40 a 14 27 a 18 38 a 6 24 a 13 31 b 7 19 b 12 26 b 27 33 b 24 35 b 18 30 b 22 31 b 26 34 b 21 28 b 14 23 b 9 22

Packages

tidyverse and broom:

```
library(tidyverse)
```

```
## Attaching packages  tidyverse 1.2.1

## ggplot2 3.1.1           purrr   0.3.2
## tibble  2.1.1           dplyr   0.8.0.1
## tidyr   0.8.3.9000      stringr 1.4.0
## readr   1.3.1           forcats 0.3.0

## Warning: package 'ggplot2' was built under R version 3.5.3

## Warning: package 'tibble' was built under R version 3.5.3

## Warning: package 'tidyr' was built under R version 3.5.3

## Warning: package 'readr' was built under R version 3.5.2

## Warning: package 'purrr' was built under R version 3.5.3
```

Making a plot

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/ancova.txt'
prepost <- read_delim(my_url, " ")
```

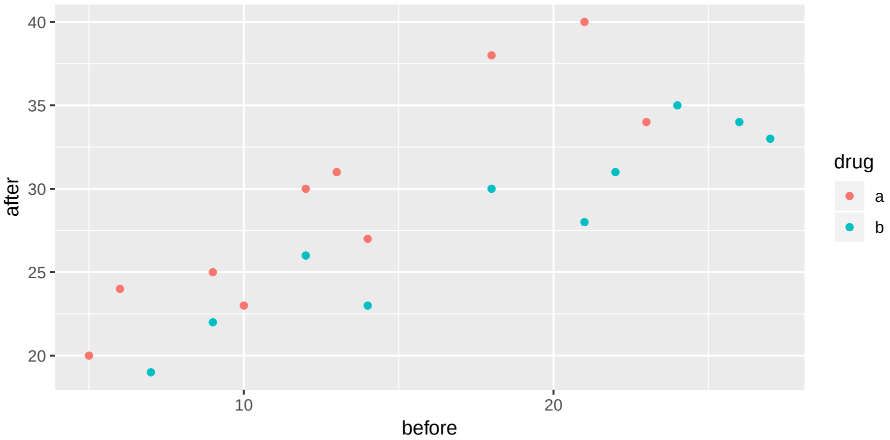
```
## Parsed with column specification:
## cols(
##   drug = col_character(),
##   before = col_double(),
##   after = col_double()
## )
```

```
glimpse(prepost)
```

```
## Observations: 20
## Variables: 3
## $ drug   <chr> "a", "a", "a", "a", "a", "a", "a", "a", "a",
## $ before <dbl> 5, 10, 12, 9, 23, 21, 14, 18, 6, 13, 7, 12,
## $ after  <dbl> 20, 23, 30, 25, 34, 40, 27, 38, 24, 31, 19,
```

The plot

```
g
```



def

Comments

```
g
```

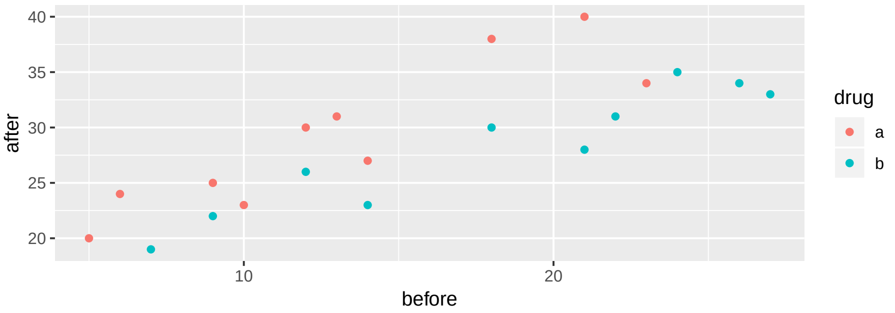


Figure 36: plot of chunk unnamed-chunk-213

- As before score goes up, after score goes up.
- Red points (drug A) generally above blue points (drug B), for

The means

```
prepost %>%
  group_by(drug) %>%
  summarize(
    before_mean = mean(before),
    after_mean = mean(after)
  )
```

```
## # A tibble: 2 x 3
##   drug  before_mean after_mean
##   <chr>       <dbl>      <dbl>
## 1 a            13.1       29.2
## 2 b            18         28.1
```

def

- Mean "after" score slightly higher for treatment A.
- Mean "before" score much higher for treatment B.

Testing for interaction

```
prepost.1 <- lm(after ~ before * drug, data = prepost)
anova(prepost.1)
```

```
## Analysis of Variance Table
##
## Response: after
##             Df Sum Sq Mean Sq F value    Pr(>F)
## before       1 430.92  430.92 62.6894  6.34e-07 ***
## drug         1 115.31  115.31 16.7743 0.0008442 ***
## before:drug  1  12.34   12.34  1.7948 0.1990662
## Residuals   16 109.98    6.87
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

def

- Interaction not significant. Will remove later.

Predictions, with interaction included

\begin{multicols}{2} Make combinations of before score and drug:

```
new <- crossing(
  before = c(5, 15, 25),
  drug = c("a", "b")
)
new
```

```
## # A tibble: 6 x 2
##   before drug
##    <dbl> <chr>
## 1      5 a
## 2      5 b
## 3     15 a
## 4     15 b
## 5     25 a
## 6     25 b
```

Making a plot with lines for each drug

```
g <- ggplot(
  prepost,
  aes(x = before, y = after, colour = drug)
) +
  geom_point() +
  geom_line(data = preds, aes(y = pred))
```

def

- Last line could (more easily) be

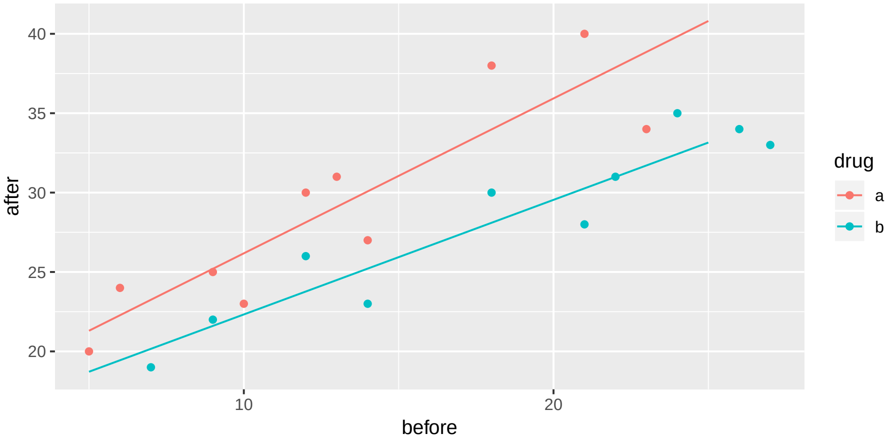
```
geom_smooth(method = "lm", se = F)
```

which would work here, but not for later plot.

- Here, final line:
- joins points by lines *for different data set* (`preds` rather than `prepost`)

The plot

```
g
```



def

- Lines almost parallel, but not quite.

Taking out interaction

{

```
prepost.2 <- update(prepost.1, . ~ . - before:drug)
anova(prepost.2)
```

```
## Analysis of Variance Table
##
## Response: after
##           Df Sum Sq Mean Sq F value    Pr(>F)
## before     1 430.92  430.92  59.890 5.718e-07 ***
## drug       1 115.31  115.31  16.025 0.0009209 ***
## Residuals 17 122.32    7.20
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

def }

- Take out non-significant interaction.
- before and drug strongly significant.

Predicted values again (no-interaction model)

```
pred <- predict(prepost.2, new)
preds <- bind_cols(new, pred = pred)
preds
```

```
## # A tibble: 6 x 3
##   before drug   pred
##    <dbl> <chr> <dbl>
## 1      5 a      22.5
## 2      5 b      17.3
## 3     15 a      30.8
## 4     15 b      25.6
## 5     25 a      39.0
## 6     25 b      33.9
```

Each increase of 10 in before score results in 8.3 in predicted after score, *the same for both drugs*.

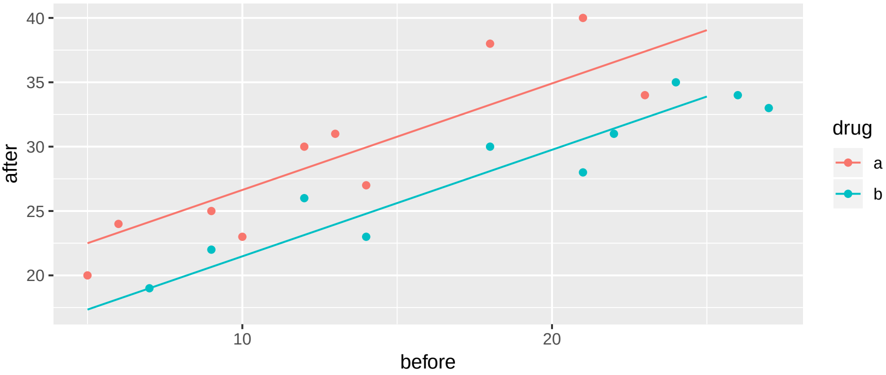
Making a plot, again

```
g <- ggplot(
  prepost,
  aes(x = before, y = after, colour = drug)
) +
  geom_point() +
  geom_line(data = preds, aes(y = pred))
```

def Exactly same as before, but using new predictions.

The no-interaction plot of predicted values

```
g
```



def Lines now *parallel*. No-interaction model forces them to have the same slope.

Different look at model output

- `anova(prepost.2)` tests for significant effect of before score and of drug, but doesn't help with interpretation.
- `summary(prepost.2)` views as regression with slopes: \begin{scriptsize}

```
summary(prepost.2)
```

```
##
## Call:
## lm(formula = after ~ before + drug, data = prepost)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.6348 -2.5099 -0.2038  1.8871  4.7453
##
## Coefficients:
```

Understanding those slopes

```
tidy(prepost.2)
```

```
## # A tibble: 3 x 5
##   term        estimate std.error statistic  p.value
##   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)   18.4      1.51       12.1  8.35e-10
## 2 before         0.827    0.0955      8.66 1.21e- 7
## 3 drugb         -5.15     1.29       -4.00 9.21e- 4
```

- `before` ordinary numerical variable; `drug` categorical.
- `lm` uses first category `druga` as baseline.
- Intercept is prediction of after score for before score 0 and *drug A*.
- `before` slope is predicted change in after score when before score increases by 1 (usual slope)
- Slope for `drugb` is *change* in predicted after score for being on drug B

Summary

- ANCOVA model: fits different regression line for each group, predicting response from covariate.
- ANCOVA model with interaction between factor and covariate allows different slopes for each line.
- Sometimes those lines can cross over!
- If interaction not significant, take out. Lines then parallel.
- With parallel lines, groups have consistent effect regardless of value of covariate.

Section 7

Multivariate ANOVA

Multivariate analysis of variance

- Standard ANOVA has just one response variable.
- What if you have more than one response?
- Try an ANOVA on each response separately.
- But might miss some kinds of interesting dependence between the responses that distinguish the groups.

Packages

```
library(car)
```

```
## Warning: package 'car' was built under R version 3.5.1

## Loading required package: carData

## Warning: package 'carData' was built under R version 3.5.1
```

```
library(tidyverse)
```

```
##  Attaching packages  tidyverse 1.2.1

##  ggplot2 3.1.1          purrr   0.3.2
##  tibble  2.1.1          dplyr   0.8.0.1
##  tidyr   0.8.3.9000     stringr 1.4.0
##  readr   1.3.1          forcats 0.3.0

## Warning: package 'ggplot2' was built under R version 3.5.3

## Warning: package 'tibble' was built under R version 3.5.3
```

Small example

- Measure yield and seed weight of plants grown under 2 conditions: low and high amounts of fertilizer.
- Data (fertilizer, yield, seed weight):

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/manova1.txt
hilo <- read_delim(my_url, " ")
```

```
## Parsed with column specification:
## cols(
##   fertilizer = col_character(),
##   yield = col_double(),
##   weight = col_double()
## )
```

def

- 2 responses, yield and seed weight.

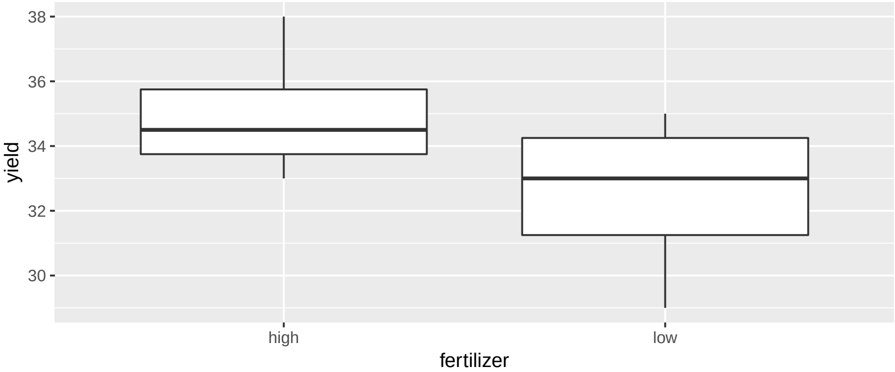
The data

```
hilo
```

```
## # A tibble: 8 x 3
##   fertilizer yield weight
##   <chr>      <dbl>  <dbl>
## 1 low           34     10
## 2 low           29     14
## 3 low           35     11
## 4 low           32     13
## 5 high          33     14
## 6 high          38     12
## 7 high          34     13
## 8 high          35     14
```

Boxplot for yield for each fertilizer group

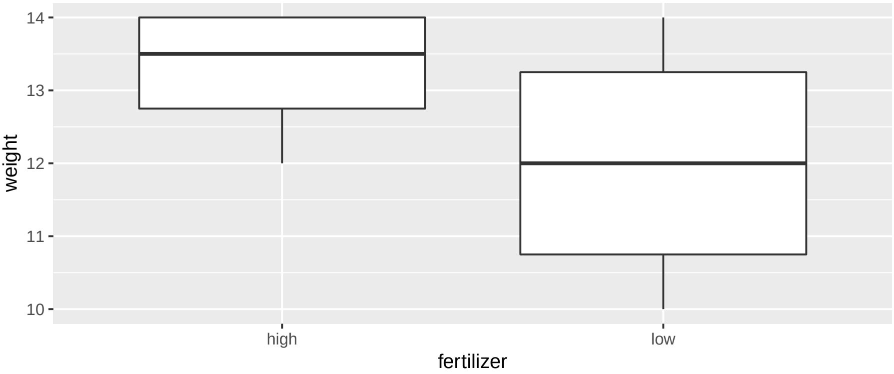
```
ggplot(hilo, aes(x = fertilizer, y = yield)) + geom_boxplot()
```



def Yields overlap for fertilizer groups.

Boxplot for weight for each fertilizer group

```
ggplot(hilo, aes(x = fertilizer, y = weight)) + geom_boxplot()
```



def

Weights overlap for fertilizer groups.

ANOVAs for yield and weight

{

```
hilo.y <- aov(yield ~ fertilizer, data = hilo)
summary(hilo.y)
```

```
##             Df Sum Sq Mean Sq F value Pr(>F)
## fertilizer   1   12.5  12.500   2.143  0.194
## Residuals    6   35.0   5.833
```

```
hilo.w <- aov(weight ~ fertilizer, data = hilo)
summary(hilo.w)
```

```
##             Df Sum Sq Mean Sq F value Pr(>F)
## fertilizer   1  3.125   3.125   1.471  0.271
## Residuals    6 12.750   2.125
```

def }

Neither response depends significantly on fertilizer. But...

Plotting both responses at once

Have two response variables (not more), so can plot the response variables against *each other*, labelling points by which fertilizer group they're from.

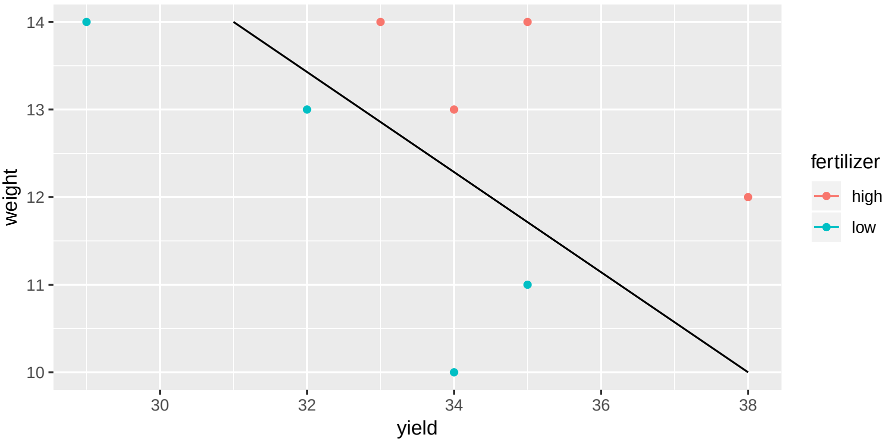
```
g <- ggplot(hilo, aes(
  x = yield, y = weight,
  colour = fertilizer
)) + geom_point()
```

Want line through points $(31, 14)$ and $(38, 10)$ (why? Later):

```
d <- tribble(
  ~line_x, ~line_y,
  31, 14,
  38, 10
)
g <- g + geom_line(data = d, aes(
  x = line_x, y = line_y,
  colour = NULL
```

The plot

```
g
```



def

MANOVA

```
g
```

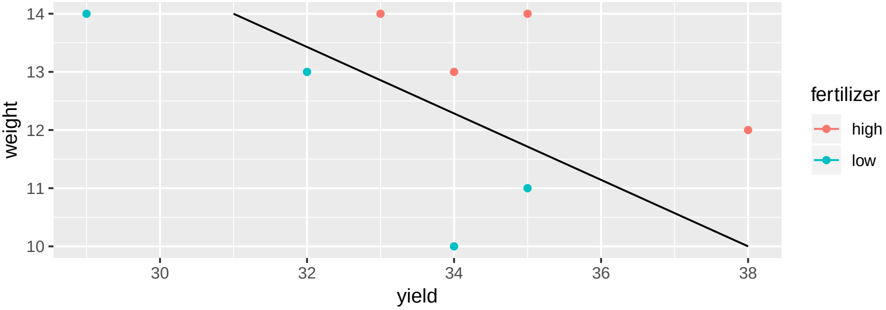


Figure 37: plot of chunk unnamed-chunk-231

* High-fertilizer plants have both yield and weight high.

* True even though no sig difference in yield or weight individually.

MANOVA finds multivariate differences

- Is difference found by diagonal line significant? MANOVA finds out.

```
response <- with(hilo, cbind(yield, weight))
hilo.1 <- manova(response ~ fertilizer, data = hilo)
summary(hilo.1)
```

```
##            Df  Pillai approx F num Df den Df  Pr(>F)
## fertilizer  1 0.80154   10.097      2      5 0.01755 *
## Residuals   6
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

def

- Yes! Difference between groups is *diagonally*, not just up/down (weight) or left-right (yield). The *yield-weight combination* matters.

Strategy

- Create new response variable by gluing together columns of responses, using `cbind`.
- Use `manova` with new response, looks like `lm` otherwise.
- With more than 2 responses, cannot draw graph. What then?
- If MANOVA test significant, cannot use Tukey. What then?
- Use {*discriminant analysis*} *(of which more later).*

Another way to do MANOVA

Install (once) and load package `car`:

```
library(car)
```

def

Another way...

```
hilo.2.lm <- lm(response ~ fertilizer, data = hilo)
hilo.2 <- Manova(hilo.2.lm)
hilo.2
```

```
##
## Type II MANOVA Tests: Pillai test statistic
##            Df test stat approx F num Df den Df  Pr(>F)
## fertilizer  1   0.80154   10.097      2      5 0.01755 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

- Same result as small-m `manova`.
- `Manova` will also do *repeated measures*, coming up later.

Another example: peanuts

- Three different varieties of peanuts (mysteriously, 5, 6 and 8) planted in two different locations.
- Three response variables: `y`, `smk` and `w`.

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/peanuts.txt
(peanuts.orig <- read_delim(my_url, " "))
```

```
## # A tibble: 12 x 6
##      obs location variety     y   smk     w
##    <dbl>    <dbl>   <dbl> <dbl> <dbl> <dbl>
##  1     1        1       5  195.  153.  51.4
##  2     2        1       5  194.  168.  53.7
##  3     3        2       5  190.  140.  55.5
##  4     4        2       5  180.  121.  44.4
##  5     5        1       6  203   157.  49.8
##  6     6        1       6  196.  166   45.8
```

Setup for analysis

```
peanuts <- peanuts.orig %>%
  mutate(
    location = factor(location),
    variety = factor(variety)
  )
response <- with(peanuts, cbind(y, smk, w))
head(response)
```

```
##              y   smk    w
## [1,] 195.3 153.1 51.4
## [2,] 194.3 167.7 53.7
## [3,] 189.7 139.5 55.5
## [4,] 180.4 121.1 44.4
## [5,] 203.0 156.8 49.8
## [6,] 195.9 166.0 45.8
```

def

Analysis (using Manova)

```
peanuts.1 <- lm(response ~ location * variety, data = peanuts)
peanuts.2 <- Manova(peanuts.1)
peanuts.2
```

```
##
## Type II MANOVA Tests: Pillai test statistic
##                   Df test stat approx F num Df den Df    Pr(>
## location           1   0.89348  11.1843      3      4 0.0205
## variety            2   1.70911   9.7924      6     10 0.0010
## location:variety   2   1.29086   3.0339      6     10 0.0587
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

def

- Interaction not quite significant, but main effects are.
- Combined response variable (`y,smk,w`) definitely depends on location

Section 8

Repeated measures by profile analysis

Repeated measures by profile analysis

- More than one response {*measurement*} *for each subject. Might be*
- *measurements of the same thing at different times*
- *measurements of different but related things*
- *Generalization of matched pairs ("matched triples", etc.).*
- *Variation: each subject does several different treatments at different times (called* {crossover design}).
- Expect measurements on same subject to be correlated, so assumptions of independence will fail.
- Called {*repeated measures*}*. Different approaches, but* {profile analysis} uses `Manova` (set up right way).
- Another approach uses *mixed models* (random effects).

Packages

```
library(car)
```

```
## Warning: package 'car' was built under R version 3.5.1

## Loading required package: carData

## Warning: package 'carData' was built under R version 3.5.1
```

```
library(tidyverse)
```

```
##  Attaching packages  tidyverse 1.2.1

##  ggplot2 3.1.1          purrr   0.3.2
##  tibble  2.1.1          dplyr   0.8.0.1
##  tidyr   0.8.3.9000     stringr 1.4.0
##  readr   1.3.1          forcats 0.3.0

## Warning: package 'ggplot2' was built under R version 3.5.3

## Warning: package 'tibble' was built under R version 3.5.3
```

Example: histamine in dogs

- 8 dogs take part in experiment.
- Dogs randomized to one of 2 different drugs.
- Response: log of blood concentration of histamine 0, 1, 3 and 5 minutes after taking drug. (Repeated measures.)
- Data in `dogs.txt`, column-aligned.

Read in data

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/dogs.txt"
dogs <- read_table(my_url)
```

```
## Parsed with column specification:
## cols(
##   dog = col_character(),
##   drug = col_character(),
##   x = col_character(),
##   lh0 = col_double(),
##   lh1 = col_double(),
##   lh3 = col_double(),
##   lh5 = col_double()
## )
```

Setting things up

```
dogs
```

```
## # A tibble: 8 x 7
##   dog   drug         x       lh0   lh1   lh3   lh5
##   <chr> <chr>        <chr> <dbl> <dbl> <dbl> <dbl>
## 1 A     Morphine     N     -3.22 -1.61 -2.3  -2.53
## 2 B     Morphine     N     -3.91 -2.81 -3.91 -3.91
## 3 C     Morphine     N     -2.66  0.34 -0.73 -1.43
## 4 D     Morphine     N     -1.77 -0.56 -1.05 -1.43
## 5 E     Trimethaphan N     -3.51 -0.48 -1.17 -1.51
## 6 F     Trimethaphan N     -3.51  0.05 -0.31 -0.51
## 7 G     Trimethaphan N     -2.66 -0.19  0.07 -0.22
## 8 H     Trimethaphan N     -2.41  1.14  0.72  0.21
```

```
response <- with(dogs, cbind(lh0, lh1, lh3, lh5))
dogs.lm <- lm(response ~ drug, data = dogs)
```

The repeated measures MANOVA

Get list of response variable names; we call them `times`. Save in data frame.

{

```
times <- colnames(response)
times.df <- data.frame(times)
dogs.manova <- Manova(dogs.lm,
  idata = times.df,
  idesign = ~times
)
dogs.manova
```

```
##
## Type II Repeated Measures MANOVA Tests: Pillai test statistic
##             Df test stat approx F num Df den Df   Pr(>F)
## (Intercept)  1   0.76347  19.3664      1      6 0.004565 **
## drug         1   0.34263   3.1272      1      6 0.127406
## times        1   0.94988  25.2690      3      4 0.004631 **
## drug:times   1   0.89476  11.3362      3      4 0.020023 *
## ---
```

Wide and long format

- Want to investigate interaction.
- But data frame has several observations per line ("wide format"):

```
dogs %>% print(n = 5)
```

```
## # A tibble: 8 x 7
##   dog   drug         x       lh0   lh1   lh3   lh5
##   <chr> <chr>        <chr> <dbl> <dbl> <dbl> <dbl>
## 1 A     Morphine     N     -3.22 -1.61 -2.3  -2.53
## 2 B     Morphine     N     -3.91 -2.81 -3.91 -3.91
## 3 C     Morphine     N     -2.66  0.34 -0.73 -1.43
## 4 D     Morphine     N     -1.77 -0.56 -1.05 -1.43
## 5 E     Trimethaphan N     -3.51 -0.48 -1.17 -1.51
## # … with 3 more rows
```

def

- Plotting works with data in "long format": one response per line

Running gather, try 1

```
dogs %>% gather(time, lh, lh0:lh5) %>% print(n = 12)
```

```
## # A tibble: 32 x 5
##    dog   drug         x     time     lh
##    <chr> <chr>        <chr> <chr> <dbl>
##  1 A     Morphine     N     lh0   -3.22
##  2 B     Morphine     N     lh0   -3.91
##  3 C     Morphine     N     lh0   -2.66
##  4 D     Morphine     N     lh0   -1.77
##  5 E     Trimethaphan N     lh0   -3.51
##  6 F     Trimethaphan N     lh0   -3.51
##  7 G     Trimethaphan N     lh0   -2.66
##  8 H     Trimethaphan N     lh0   -2.41
##  9 A     Morphine     N     lh1   -1.61
## 10 B     Morphine     N     lh1   -2.81
## 11 C     Morphine     N     lh1    0.34
```

Getting the times

Not quite right: for the times, we want just the numbers, not the letters `lh` every time. Want new variable containing just number in `time`: `parse_number`.

```
dogs %>%
  gather(timex, lh, lh0:lh5) %>%
  mutate(time = parse_number(timex)) %>%
  print(n = 10)
```

```
## # A tibble: 32 x 6
##    dog   drug         x     timex    lh  time
##    <chr> <chr>        <chr> <chr> <dbl> <dbl>
##  1 A     Morphine     N     lh0   -3.22     0
##  2 B     Morphine     N     lh0   -3.91     0
##  3 C     Morphine     N     lh0   -2.66     0
##  4 D     Morphine     N     lh0   -1.77     0
##  5 E     Trimethaphan N     lh0   -3.51     0
```

What I did differently

- I realized that `gather` was going to produce something like `lh1`, which I needed to do something further with, so this time I gave it a temporary name `timex`.
- This enabled me to use the name `time` for the actual numeric time.
- This works now, so next save into a new data frame `dogs.long`.

Saving the chained results

```
dogs.long <- dogs %>%
  gather(timex, lh, lh0:lh5) %>%
  mutate(time = parse_number(timex))
```

This says:

- Take data frame dogs, and then:
- Combine the columns `lh0` through `lh5` into one column called `lh`, with the column that each `lh` value originally came from labelled by `timex`, and then:
- Pull out numeric values in `timex`, saving in `time` and then:
- save the result in a data frame `dogs.long`.

reshape

- Converts between wide and long format.
- Need to tell R what our repeated-measures responses are.
- Convenient variable naming: all responses are `lh` followed by a number representing time.
- Like this:

«»= detach(dogs) d2=reshape(dogs,varying=3:6,sep="", direction="long")
@ %def

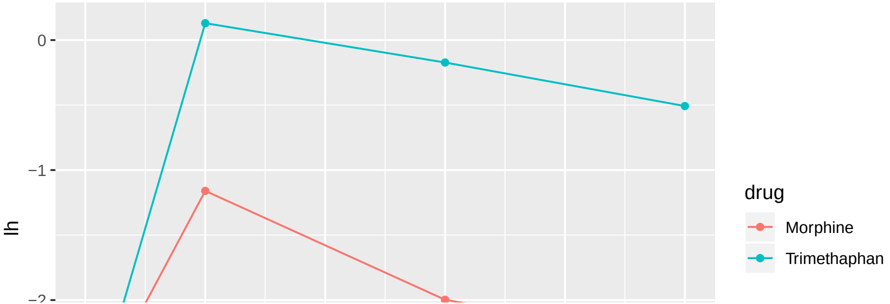
Long data frame, top 12 lines

«»= head(d2,n=12) @ %def

`id` labels dog, `time` labels time. Perfect for interaction plot.

Interaction plot

```
ggplot(dogs.long, aes(
  x = time, y = lh,
  colour = drug, group = drug
)) +
  stat_summary(fun.y = mean, geom = "point") +
  stat_summary(fun.y = mean, geom = "line")
```



Comments

- Plot mean `lh` value at each time, joining points on same drug by lines.
- drugs same at time 0
- after that, Trimethaphan higher than Morphine.
- Effect of drug not consistent over time: significant interaction.

Take out time zero

- Lines on interaction plot would then be parallel, and so interaction should no longer be significant.
- Go back to original "wide" dogs data frame.

```
response <- with(dogs, cbind(lh1, lh3, lh5)) # excluding time
dogs.lm <- lm(response ~ drug, data = dogs)
times <- colnames(response)
times.df <- data.frame(times)
dogs.manova <- Manova(dogs.lm,
  idata = times.df,
  idesign = ~times
)
```

def

Results and comments

```
dogs.manova
```

```
##
## Type II Repeated Measures MANOVA Tests: Pillai test statist
##                Df test stat approx F num Df den Df    Pr(>F)
## (Intercept)  1   0.54582   7.2106      1      6 0.036281 *
## drug         1   0.44551   4.8207      1      6 0.070527 .
## times        1   0.85429  14.6569      2      5 0.008105 **
## drug:times   1   0.43553   1.9289      2      5 0.239390
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '
```

def

- Correct: interaction no longer significant.
- Significant effect of time.
- Drug effect not quite significant (some variety among dogs within

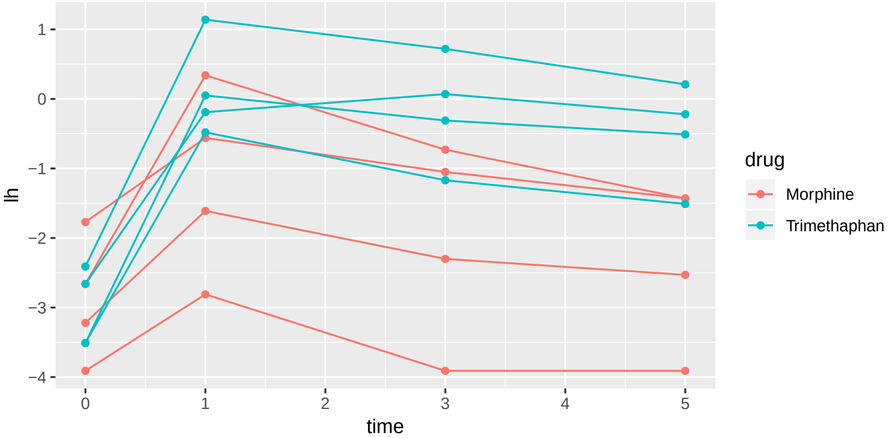
Is the non-significant drug effect reasonable?

- Plot *actual data*: `lh` against `days`, labelling observations by drug: "spaghetti plot".
- Uses long data frame (confusing, yes I know):
- Plot (time,lh) points coloured by drug
- and connecting measurements for each *dog* by lines.
- This time, we want `group=dog` (want the measurements for each *dog* joined by lines), but `colour=drug`:

```
g <- ggplot(dogs.long, aes(
  x = time, y = lh,
  colour = drug, group = dog
)) +
  geom_point() + geom_line()
```

The spaghetti plot

```
g
```



Comments

- For each dog over time, there is a strong increase and gradual decrease in log-histamine. This explains the significant time effect.
- The pattern is more or less the same for each dog, regardless of drug. This explains the non-significant interaction.
- Most of the trimethaphan dogs (blue) have higher log-histamine throughout (time 1 and after), and some of the morphine dogs have lower.
- *But* two of the morphine dogs have log-histamine profiles like the trimethaphan dogs. This ambiguity is probably why the `drug` effect is not quite significant.

The exercise data

- 30 people took part in an exercise study.
- Each subject was randomly assigned to one of two diets ("low fat" or "non-low fat") and to one of three exercise programs ("at rest", "walking", "running").
- There are $2 \times 3 = 6$ experimental treatments, and thus each one is replicated $30/6 = 5$ times.
- Nothing unusual so far.
- However, each subject had their pulse rate measured at three different times (1, 15 and 30 minutes after starting their exercise), so have repeated measures.

Reading the data

Separated by *tabs*:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/exercise.tx
exercise.long <- read_tsv(my_url)
```

```
## Parsed with column specification:
## cols(
##   id = col_double(),
##   diet = col_character(),
##   exertype = col_character(),
##   pulse = col_double(),
##   time = col_character()
## )
```

The data

```
exercise.long %>% print(n = 8)
```

```
## # A tibble: 90 x 5
##      id diet      exertype pulse time
##   <dbl> <chr>     <chr>    <dbl> <chr>
## 1     1 nonlowfat atrest      85 min01
## 2     1 nonlowfat atrest      85 min15
## 3     1 nonlowfat atrest      88 min30
## 4     2 nonlowfat atrest      90 min01
## 5     2 nonlowfat atrest      92 min15
## 6     2 nonlowfat atrest      93 min30
## 7     3 nonlowfat atrest      97 min01
## 8     3 nonlowfat atrest      97 min15
## # … with 82 more rows
```

- This is “long format”, which is usually what we want.

Making wide format

- Spread needs three things: a data frame, a column that is going to be split, and the column to make the values out of:

```
exercise.wide <- spread(exercise.long, time, pulse)
exercise.wide %>% print(n = 6)
```

```
## # A tibble: 30 x 6
##      id diet      exertype min01 min15 min30
##   <dbl> <chr>     <chr>    <dbl> <dbl> <dbl>
## 1     1 nonlowfat atrest      85    85    88
## 2     2 nonlowfat atrest      90    92    93
## 3     3 nonlowfat atrest      97    97    94
## 4     4 nonlowfat atrest      80    82    83
## 5     5 nonlowfat atrest      91    92    91
## 6     6 lowfat    atrest      83    83    84
## # … with 24 more rows
```

Setting up the repeated-measures analysis

- Make a response variable consisting of min01, min15, min30:

```
response <- with(
  exercise.wide,
  cbind(min01, min15, min30)
)
```

- Predict that from diet and exertype and interaction using lm:

```
exercise.1 <- lm(response ~ diet * exertype,
  data = exercise.wide
)
```

- Run this through Manova:

```
times <- colnames(response)
times.df <- data.frame(times)
exercise.2 <- Manova(exercise.1,
  idata = times.df
```

Results

“‘r exercise.2 “‘

“‘ Type II Repeated Measures MANOVA Tests: Pillai test statistic Df test stat approx F num Df den Df Pr(>F) (Intercept) 1 0.99767 10296.7 1 24 < 2.2e-16 *** diet 1 0.37701 14.5 1 24 0.0008483 *** exertype 2 0.79972 47.9 2 24 4.166e-09 *** diet:exertype 2 0.28120 4.7 2 24 0.0190230 * times 1 0.78182 41.2 2 23 2.491e-08 *** diet:times 1 0.25153 3.9 2 23 0.0357258 * exertype:times 2 0.83557 8.6 4 48 2.538e-05 *** diet:exertype:times 2 0.51750 4.2 4 48 0.0054586 ** — Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1 “‘

- Three-way interaction significant, so cannot remove anything.
- Pulse rate depends on diet and exercise type *combination*, and *that* is different for each time.

Making some graphs

- Three-way interactions are difficult to understand. To make an attempt, look at some graphs.
- Plot time trace of pulse rates for each individual, joined by lines, and make *separate* plots for each `diet-exertype` combo.
- `ggplot` again. Using *long* data frame:

```
g <- ggplot(exercise.long, aes(
  x = time, y = pulse,
  group = id
)) + geom_point() + geom_line() +
  facet_grid(diet ~ exertype)
```

- `facet_grid(diet~exertype)`: do a separate plot for each combination of diet and exercise type, with diets going down the page and exercise types going across. (Graphs are usually landscape, so have the factor `exertype` with more levels going across.)

The graph(s)

```
g
```

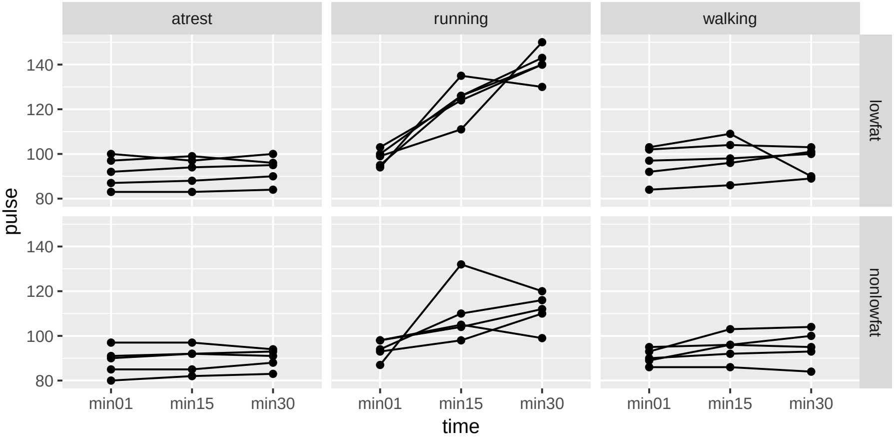


Figure 40: plot of chunk unnamed-chunk-258

Comments on graphs

- For subjects who were at rest, no change in pulse rate over time, for both diet groups.
- For walking subjects, not much change in pulse rates over time. Maybe a small increase on average between 1 and 15 minutes.
- For both running groups, an overall increase in pulse rate over time, but the increase is stronger for the `lowfat` group.
- No consistent effect of diet over all exercise groups.
- No consistent effect of exercise type over both diet groups.
- No consistent effect of time over all diet-exercise type combos.

"Simple effects" of diet for the subjects who ran

- Looks as if there is only any substantial time effect for the runners. For them, does diet have an effect?
- Pull out only the runners from the wide data:

```
runners.wide <- exercise.wide %>%
  filter(exertype == "running")
```

- Create response variable and do MANOVA. Some of this looks like before, but I have different data now:

```
response <- with(runners.wide, cbind(min01, min15, min30))
runners.1 <- lm(response ~ diet, data = runners.wide)
times <- colnames(response)
times.df <- data.frame(times)
runners.2 <- Manova(runners.1,
  idata = times.df,
  idesign = ~times
```

Results

{

```
runners.2
```

```
##
## Type II Repeated Measures MANOVA Tests: Pillai test statistic
##               Df test stat approx F num Df den Df    Pr(>F)
## (Intercept)  1   0.99912   9045.3      1      8 1.668e-13 ***
## diet         1   0.84986     45.3      1      8 0.0001482 ***
## times        1   0.92493     43.1      2      7 0.0001159 ***
## diet:times   1   0.68950      7.8      2      7 0.0166807 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

}

- The `diet` by `time` interaction is still significant (at $\alpha = 0.05$): the effect of time on pulse rates is different for the two diets.
- At $\alpha = 0.01$, the interaction is not significant, and then we have only two (very) significant main effects of `diet` and `time`.

How is the effect of diet different over time?

- Table of means. Only I need long data for this, so make it (in a pipe):

```
summ <- runners.wide %>%
  gather(time, pulse, min01:min30) %>%
  group_by(time, diet) %>%
  summarize(
    mean = mean(pulse),
    sd = sd(pulse)
  )
```

- Result of `summarize` is data frame, so can save it (and do more with it if needed).

Understanding diet-time interaction

- The summary:

```
summm
```

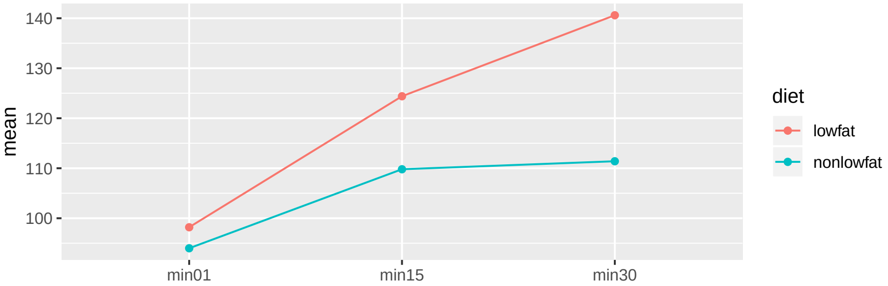
```
## # A tibble: 6 x 4
## # Groups:   time [3]
##   time  diet       mean    sd
##   <chr> <chr>     <dbl> <dbl>
## 1 min01 lowfat     98.2  3.70
## 2 min01 nonlowfat  94    4.53
## 3 min15 lowfat    124.   8.62
## 4 min15 nonlowfat 110.  13.1
## 5 min30 lowfat    141.   7.20
## 6 min30 nonlowfat 111.   7.92
```

- Pulse rates at any given time higher for `lowfat` (diet effect),
- Pulse rates increase over time of exercise (time effect),

Interaction plot

- We went to trouble of finding means by group, so making interaction plot is now mainly easy:

```
ggplot(summ, aes(
  x = time, y = mean, colour = diet,
  group = diet
)) + geom_point() + geom_line()
```



Section 9

Discriminant analysis

Discriminant analysis

- ANOVA and MANOVA: predict a (counted/measured) response from group membership.
- Discriminant analysis: predict group membership based on counted/measured variables.
- Covers same ground as logistic regression (and its variations), but emphasis on classifying observed data into correct groups.
- Does so by searching for linear combination of original variables that best separates data into groups (canonical variables).
- Assumption here that groups are known (for data we have). If trying to "best separate" data into unknown groups, see {*cluster analysis*}.
- *Examples: revisit seed yield and weight data, peanut data, professions/activities data; remote-sensing data.*

Packages

```
library(MASS)
library(tidyverse)
```

```
##  Attaching packages  tidyverse 1.2.1

##  ggplot2 3.1.1          purrr   0.3.2
##  tibble  2.1.1          dplyr   0.8.0.1
##  tidyr   0.8.3.9000     stringr 1.4.0
##  readr   1.3.1          forcats 0.3.0

## Warning: package 'ggplot2' was built under R version 3.5.3

## Warning: package 'tibble' was built under R version 3.5.3

## Warning: package 'tidyr' was built under R version 3.5.3

## Warning: package 'readr' was built under R version 3.5.2

## Warning: package 'purrr' was built under R version 3.5.3
```

About `select`

- Both `dplyr` (in `tidyverse`) and `MASS` have a function called `select`, and *they do different things*.
- How do you know which `select` is going to get called?
- With `library`, the one loaded *last* is visible, and others are not.
- Thus we can access the `select` in `dplyr` but not the one in `MASS`. If we wanted that one, we'd have to say `MASS::select`.
- This is why I loaded `MASS` before `tidyverse`. If I had done it the other way around, the `tidyverse` `select`, which I want to use, would have been the invisible one.

Example 1: seed yields and weights

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/manova1.txt
hilo <- read_delim(my_url, " ")
g <- ggplot(hilo, aes(
  x = yield, y = weight,
  colour = fertilizer
)) + geom_point(size = 4)
```

“‘r g “‘
`![plot of chunk berzani](figure/berzani-1.pdf)`

Recall data from MANOVA: needed a multivariate analysis to find difference in seed yield and weight based on whether they were high or low fertilizer.

Basic discriminant analysis

```
hilo.1 <- lda(fertilizer ~ yield + weight, data = hilo)
```

- Uses `lda` from package MASS.
- “Predicting” group membership from measured variables.

Output

```
hilo.1
```

```
## Call:
## lda(fertilizer ~ yield + weight, data = hilo)
##
## Prior probabilities of groups:
## high  low
##  0.5  0.5
##
## Group means:
##      yield weight
## high  35.0  13.25
## low   32.5  12.00
##
## Coefficients of linear discriminants:
##                LD1
## yield  -0.7666761
```

Things to take from output

- Group means: high-fertilizer plants have (slightly) higher mean yield and weight than low-fertilizer plants.
- "Coefficients of linear discriminants": `LD1, LD2,`…are scores constructed from observed variables that best separate the groups.
- For any plant, get LD1 score by taking -0.76 times yield plus -1.25 times weight, add up, standardize.
- Understand by pretending all variables standardized (mean 0, $+$ above mean, $-$ below mean). If yield and weight high (above average), contribute a $+$ to LD1 score, so LD1 *negative*. If yield and weight low (think $-$), LD1 score *positive*.
- High-fertilizer plants have higher yield and weight, thus negative LD1 score. Low-fertilizer plants have low yield and weight, thus positive LD1 score.
- One LD1 score for each observation. Plot with actual groups.

How many linear discriminants?

- Number of variables
- Number of groups *minus 1*
- Smaller of these
- Seed yield and weight: 2 variables, 2 groups, $\min(2, 2-1) = 1$.

Getting LD scores

Feed output from LDA into `predict`:

```
hilo.pred <- predict(hilo.1)
```

Component x contains LD score(s), here in descending order:

```
d <- cbind(hilo, hilo.pred$x) %>% arrange(desc(LD1))
d
```

```
##   fertilizer yield weight        LD1
## 1        low    34     10  3.0931414
## 2        low    29     14  1.9210963
## 3        low    35     11  1.0751090
## 4        low    32     13  0.8724245
## 5       high    34     13 -0.6609276
## 6       high    33     14 -1.1456079
## 7       high    38     12 -2.4762756
## 8       high    35     14 -2.6789600
```

Plotting LD1 scores

With one LD score, plot against (true) groups, eg. boxplot:

```
ggplot(d, aes(x = fertilizer, y = LD1)) + geom_boxplot()
```

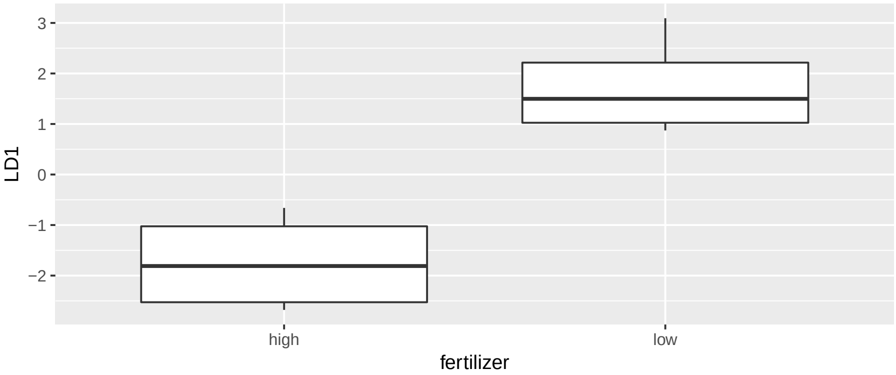


Figure 42: plot of chunk unnamed-chunk-272

Potentially misleading

- These are like regression slopes:

```
hilo.1$scaling
```

```
##                 LD1
## yield  -0.7666761
## weight -1.2513563
```

- Reflect change in LD1 score for 1-unit change in variables.
- But one-unit change in variables might not be comparable:

```
summary(hilo)
```

```
##  fertilizer            yield          weight
##  Length:8           Min.   :29.00   Min.   :10.00
##  Class :character   1st Qu.:32.75   1st Qu.:11.75
##  Mode  :character   Median :34.00   Median :13.00
##                     Mean   :33.75   Mean   :12.62
```

What else is in `hilo.pred`?

```
names(hilo.pred)
```

```
## [1] "class"     "posterior" "x"
```

- `class`: predicted fertilizer level (based on values of `yield` and `weight`).
- `posterior`: predicted probability of being low or high fertilizer given `yield` and `weight`.

Predictions and predicted groups

...based on `yield` and `weight`:

```
cbind(hilo, predicted = hilo.pred$class)
```

```
##   fertilizer yield weight predicted
## 1        low    34     10       low
## 2        low    29     14       low
## 3        low    35     11       low
## 4        low    32     13       low
## 5       high    33     14      high
## 6       high    38     12      high
## 7       high    34     13      high
## 8       high    35     14      high
```

```
table(obs = hilo$fertilizer, pred = hilo.pred$class)
```

```
##       pred
## obs     high low
```

Understanding the predicted groups

- Each predicted fertilizer level is exactly same as observed one (perfect prediction).
- Table shows no errors: all values on top-left to bottom-right diagonal.

Posterior probabilities

show how clear-cut the classification decisions were:

```
pp <- round(hilo.pred$posterior, 4)
d <- cbind(hilo, hilo.pred$x, pp)
d
```

```
##   fertilizer yield weight        LD1   high    low
## 1        low    34     10  3.0931414 0.0000 1.0000
## 2        low    29     14  1.9210963 0.0012 0.9988
## 3        low    35     11  1.0751090 0.0232 0.9768
## 4        low    32     13  0.8724245 0.0458 0.9542
## 5       high    33     14 -1.1456079 0.9818 0.0182
## 6       high    38     12 -2.4762756 0.9998 0.0002
## 7       high    34     13 -0.6609276 0.9089 0.0911
## 8       high    35     14 -2.6789600 0.9999 0.0001
```

$ Only obs. 7 has any doubt: `yield` low for a high-fertilizer, but high weight makes up for it.

Contour plot of LD1

First, get some new yield and weight values for prediction. Then predict LD1 for them:

«»= yy=seq(29,38,0.5) ww=seq(10,14,0.5)
hilo.new=expand.grid(yield=yy,weight=ww)
hilo.pred=predict(hilo.lda,hilo.new) @

Then: plot original data, and overlay contours showing value of LD1 for each `yield` and `weight` (over):

Contour plot

\begin{minipage}[t]{0.7}

«santini,fig.height=5»= plot(yield,weight,col=fno,pch=fno)
z=matrix(hilo.pred$x,length(yy), length(ww),byrow=F)
contour(yy,ww,z,add=T) @
\end{minipage}

*
'LD1'
$<$
0:
top
right
*
'LD1'
$>$
0:

Example 2: the peanuts

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/peanuts.txt
peanuts <- read_delim(my_url, " ")
peanuts
```

```
## # A tibble: 12 x 6
##       obs location variety     y   smk     w
##     <dbl>    <dbl>   <dbl> <dbl> <dbl> <dbl>
##  1      1        1       5  195.  153.  51.4
##  2      2        1       5  194.  168.  53.7
##  3      3        2       5  190.  140.  55.5
##  4      4        2       5  180.  121.  44.4
##  5      5        1       6  203   157.  49.8
##  6      6        1       6  196.  166   45.8
##  7      7        2       6  203.  166.  60.4
##  8      8        2       6  198.  162.  54.1
##  9      9        1       8  194.  164.  57.8
```

Location-variety combos

```
peanuts %>% unite(combo, c(variety, location)) ->
peanuts.combo
peanuts.combo
```

```
## # A tibble: 12 x 5
##       obs combo     y   smk     w
##     <dbl> <chr> <dbl> <dbl> <dbl>
##  1      1 5_1    195.  153.  51.4
##  2      2 5_1    194.  168.  53.7
##  3      3 5_2    190.  140.  55.5
##  4      4 5_2    180.  121.  44.4
##  5      5 6_1    203   157.  49.8
##  6      6 6_1    196.  166   45.8
##  7      7 6_2    203.  166.  60.4
##  8      8 6_2    198.  162.  54.1
##  9      9 8_1    194.  164.  57.8
```

Discriminant analysis

```
peanuts.1 <- lda(combo ~ y + smk + w, data = peanuts.combo)
peanuts.1$scaling
```

```
##            LD1         LD2         LD3
## y   -0.4027356 -0.02967881  0.18839237
## smk -0.1727459  0.06794271 -0.09386294
## w    0.5792456  0.16300221  0.07341123
```

```
peanuts.1$svd
```

```
## [1] 6.141323 2.428396 1.075589
```

- Now 3 LDs (3 variables, 6 groups, $\min(3, 6-1) = 3$).
- First: relationship of LDs to original variables. Look for coeffs far from zero: here,
- high `LD1` mainly high `w` or low `y`.

Group means by variable

```
peanuts.1$means
```

```
##            y    smk     w
## 5_1 194.80 160.40 52.55
## 5_2 185.05 130.30 49.95
## 6_1 199.45 161.40 47.80
## 6_2 200.15 163.95 57.25
## 8_1 190.25 164.80 58.20
## 8_2 200.75 170.30 66.10
```

$

- 5_2 clearly smallest on `y`, `smk`, near smallest on `w`
- 8_2 clearly biggest on `smk`, `w`, also largest on `y`
- 8_1 large on `w`, small on `y`.
- `scaling` links LDs with original variables, `means` links original

The predictions and misclassification

```
peanuts.pred <- predict(peanuts.1)
table(
  obs = peanuts.combo$combo,
  pred = peanuts.pred$class
)
```

```
##      pred
## obs   5_1 5_2 6_1 6_2 8_1 8_2
##   5_1   2   0   0   0   0   0
##   5_2   0   2   0   0   0   0
##   6_1   0   0   2   0   0   0
##   6_2   1   0   0   1   0   0
##   8_1   0   0   0   0   2   0
##   8_2   0   0   0   0   0   2
```

$ Actually classified very well. Only one 6_2 classified as a 5_1, rest all correct.

Posterior probabilities

```r
pp <- round(peanuts.pred$posterior, 2)
peanuts.combo %>%
  select(-c(y, smk, w)) %>%
  cbind(., pred = peanuts.pred$class, pp)
```

```
##    obs combo pred  5_1 5_2 6_1  6_2  8_1  8_2
## 1    1   5_1  5_1 0.69   0   0 0.31 0.00 0.00
## 2    2   5_1  5_1 0.73   0   0 0.27 0.00 0.00
## 3    3   5_2  5_2 0.00   1   0 0.00 0.00 0.00
## 4    4   5_2  5_2 0.00   1   0 0.00 0.00 0.00
## 5    5   6_1  6_1 0.00   0   1 0.00 0.00 0.00
## 6    6   6_1  6_1 0.00   0   1 0.00 0.00 0.00
## 7    7   6_2  6_2 0.13   0   0 0.87 0.00 0.00
## 8    8   6_2  5_1 0.53   0   0 0.47 0.00 0.00
## 9    9   8_1  8_1 0.02   0   0 0.02 0.75 0.21
## 10  10   8_1  8_1 0.00   0   0 0.00 0.99 0.01
```

Discriminant scores, again

- How are discriminant scores related to original variables?
- Construct data frame with original data and discriminant scores side by side:

```
peanuts.1$scaling
```

```
##            LD1         LD2         LD3
## y   -0.4027356 -0.02967881  0.18839237
## smk -0.1727459  0.06794271 -0.09386294
## w    0.5792456  0.16300221  0.07341123
```

```
lds <- round(peanuts.pred$x, 2)
mm <- with(
  peanuts.combo,
  data.frame(combo, y, smk, w, lds)
)
```

Discriminant scores for data

```
mm
```

```
##    combo     y   smk    w   LD1   LD2   LD3
## 1    5_1 195.3 153.1 51.4 -1.42 -1.01  0.26
## 2    5_1 194.3 167.7 53.7 -2.20  0.38 -1.13
## 3    5_2 189.7 139.5 55.5  5.56 -1.10  0.79
## 4    5_2 180.4 121.1 44.4  6.06 -3.89 -0.05
## 5    6_1 203.0 156.8 49.8 -6.08 -1.25  1.25
## 6    6_1 195.9 166.0 45.8 -7.13 -1.07 -1.24
## 7    6_2 202.7 166.1 60.4 -1.43  1.12  1.10
## 8    6_2 197.6 161.8 54.1 -2.28 -0.05  0.08
## 9    8_1 193.5 164.5 57.8  1.05  0.86 -0.67
## 10   8_1 187.0 165.1 58.6  4.02  1.22 -1.90
## 11   8_2 201.5 166.8 65.0  1.60  1.95  1.15
## 12   8_2 200.0 173.8 67.2  2.27  2.83  0.37
```

- Obs. 5 and 6 have most negative `LD1`: large `y`, small `w`.

Predict typical LD1 scores

First and third quartiles for three response variables (reading down):

```
quartiles <- peanuts %>%
  select(y:w) %>%
  map_df(quantile, c(0.25, 0.75))
quartiles
```

```
## # A tibble: 2 x 3
##         y   smk     w
##     <dbl> <dbl> <dbl>
## 1  193.  156.  51
## 2  200.  166.  59.0
```

```
new <- with(quartiles, crossing(y, smk, w))
```

The combinations

```
new
```

```
## # A tibble: 8 x 3
##         y   smk     w
##     <dbl> <dbl> <dbl>
## 1   193.  156.  51
## 2   193.  156.  59.0
## 3   193.  166.  51
## 4   193.  166.  59.0
## 5   200.  156.  51
## 6   200.  156.  59.0
## 7   200.  166.  51
## 8   200.  166.  59.0
```

```
pp <- predict(peanuts.1, new)
```

Predicted typical LD1 scores

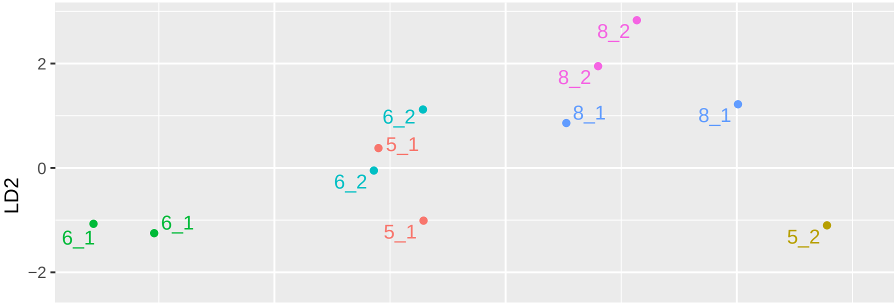
```
cbind(new, pp$x) %>% arrange(LD1)
```

```
##         y     smk     w        LD1        LD2         LD3
## 1 200.375 166.275 51.00 -5.9688625 -0.3330095 -0.04523828
## 2 200.375 155.875 51.00 -4.1723048 -1.0396138  0.93093630
## 3 192.550 166.275 51.00 -2.8174566 -0.1007728 -1.51940856
## 4 200.375 166.275 59.05 -1.3059358  0.9791583  0.54572212
## 5 192.550 155.875 51.00 -1.0208989 -0.8073770 -0.54323399
## 6 200.375 155.875 59.05  0.4906219  0.2725540  1.52189670
## 7 192.550 166.275 59.05  1.8454701  1.2113950 -0.92844817
## 8 192.550 155.875 59.05  3.6420278  0.5047907  0.04772641
```

- Very negative LD1 score with large `y` and small `w`
- `smk` doesn't contribute much to LD1
- Very positive LD1 score with small `y` and large `w`.
- Same as we saw from Coefficients of Linear Discriminants

Plot LD1 vs. LD2, labelling by combo

```
g <- ggplot(mm, aes(
  x = LD1, y = LD2, colour = combo,
  label = combo
)) + geom_point() +
  geom_text_repel() + guides(colour = F)
g
```

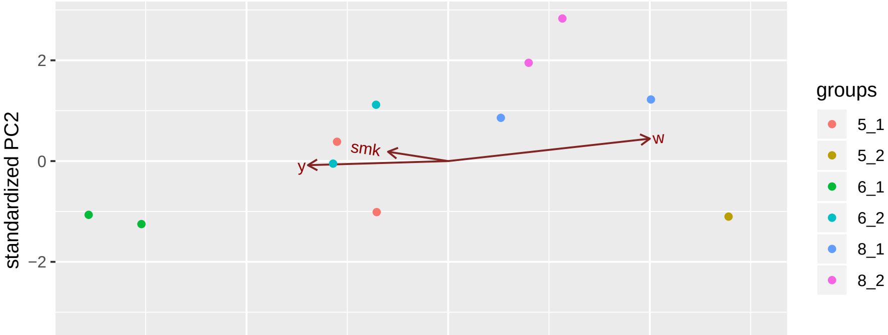


"Bi-plot" from ggbiplot

«echo=F,message=F»= library(plyr) library(tidyverse) library(ggbiplot) @

«eval=F»= library(ggbiplot) @

```
ggbiplot(peanuts.1,
  groups = factor(peanuts.combo$combo)
)
```



Installing ggbiplot

- ggbiplot not on CRAN, so usual install.packages will not work.
- Install package devtools first (once):

```
install.packages("devtools")
```

- Then install ggbiplot (once):

```
library(devtools)
install_github("vqv/ggbiplot")
```

Cross-validation

- So far, have predicted group membership from same data used to form the groups — dishonest!
- Better: *cross-validation*: form groups from all observations *except one*, then predict group membership for that left-out observation.
- No longer cheating!
- Illustrate with peanuts data again.

Misclassifications

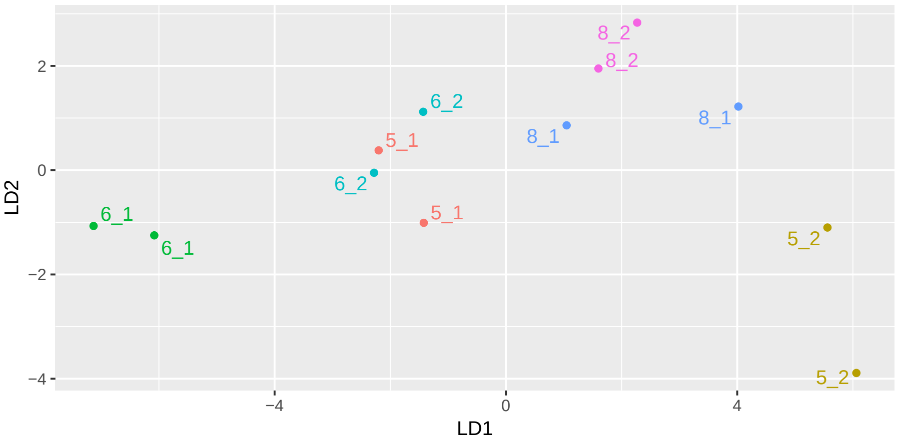
- Fitting and prediction all in one go:

```
peanuts.cv <- lda(combo ~ y + smk + w,
  data = peanuts.combo, CV = T
)
table(
  obs = peanuts.combo$combo,
  pred = peanuts.cv$class
)
```

```
##      pred
## obs   5_1 5_2 6_1 6_2 8_1 8_2
##   5_1   0   0   0   2   0   0
##   5_2   0   1   0   0   1   0
##   6_1   0   0   2   0   0   0
##   6_2   1   0   0   1   0   0
##   8_1   0   1   0   0   0   1
```

Repeat of LD plot

```
g
```



Posterior probabilities

```r
pp <- round(peanuts.cv$posterior, 3)
data.frame(
  obs = peanuts.combo$combo,
  pred = peanuts.cv$class, pp
)
```

```
##     obs pred  X5_1 X5_2  X6_1  X6_2  X8_1  X8_2
## 1   5_1  6_2 0.162 0.00 0.000 0.838 0.000 0.000
## 2   5_1  6_2 0.200 0.00 0.000 0.799 0.000 0.000
## 3   5_2  8_1 0.000 0.18 0.000 0.000 0.820 0.000
## 4   5_2  5_2 0.000 1.00 0.000 0.000 0.000 0.000
## 5   6_1  6_1 0.194 0.00 0.669 0.137 0.000 0.000
## 6   6_1  6_1 0.000 0.00 1.000 0.000 0.000 0.000
## 7   6_2  6_2 0.325 0.00 0.000 0.667 0.001 0.008
## 8   6_2  5_1 0.821 0.00 0.000 0.179 0.000 0.000
## 9   8_1  8_2 0.000 0.00 0.000 0.000 0.000 1.000
## 10  8_1  5_2 0.000 1.00 0.000 0.000 0.000 0.000
```

Why more misclassification?

- When predicting group membership for one observation, only uses the *other one* in that group.
- So if two in a pair are far apart, or if two groups overlap, great potential for misclassification.
- Groups 5_1 and 6_2 overlap.
- 5_2 closest to 8_1s looks more like an 8_1 than a 5_2 (other one far away).
- 8_1s relatively far apart and close to other things, so one appears to be a 5_2 and the other an 8_2.

Example 3: professions and leisure activities

- 15 individuals from three different professions (politicians, administrators and belly dancers) each participate in four different leisure activities: reading, dancing, TV watching and skiing. After each activity they rate it on a 0–10 scale.
- Some of the data:

```
bellydancer 7 10 6 5
bellydancer 8 9 5 7
bellydancer 5 10 5 8
politician 5 5 5 6
politician 4 5 6 5
admin 4 2 2 5
admin 7 1 2 4
admin 6 3 3 3
```

- How can we best use the scores on the activities to predict a person's

Discriminant analysis

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/profile.txt
active <- read_delim(my_url, " ")
active.1 <- lda(job ~ reading + dance + tv + ski, data = activ
active.1$svd
```

```
## [1] 9.856638 3.434555
```

```
active.1$scaling
```

```
##                 LD1        LD2
## reading -0.01297465  0.4748081
## dance   -0.95212396  0.4614976
## tv      -0.47417264 -1.2446327
## ski      0.04153684  0.2033122
```

- Two discriminants, first fair bit more important than second.
- LD1 depends (negatively) most on dance, a bit on tv.

Misclassification

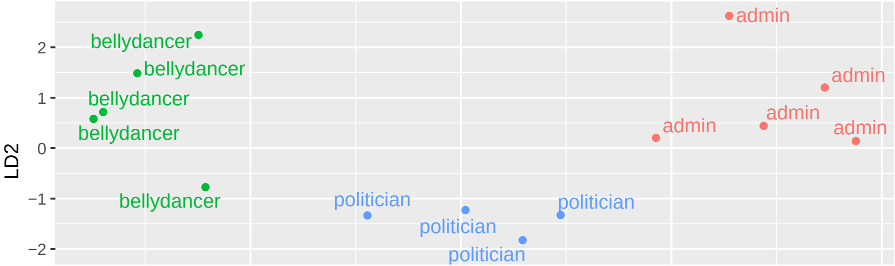
```
active.pred <- predict(active.1)
table(obs = active$job, pred = active.pred$class)
```

```
##              pred
## obs           admin bellydancer politician
##   admin           5           0          0
##   bellydancer     0           5          0
##   politician      0           0          5
```

Everyone correctly classified.

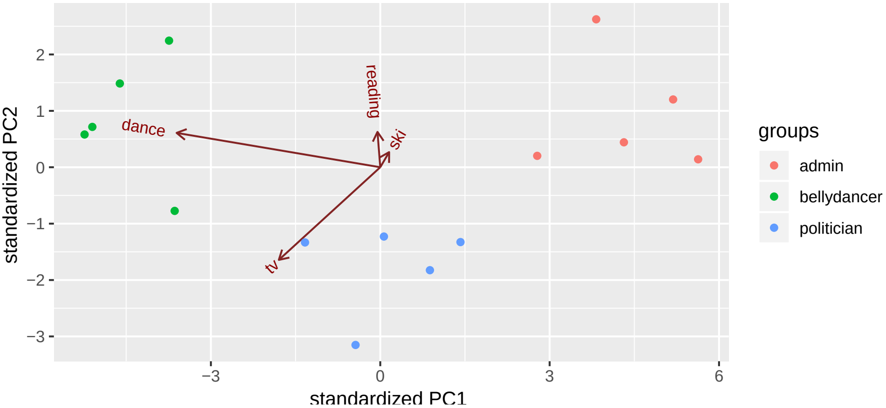
Plotting LDs

```
mm <- data.frame(job = active$job, active.pred$x, person = 1:1
g <- ggplot(mm, aes(
  x = LD1, y = LD2,
  colour = job, label = job
)) + geom_point() +
  geom_text_repel() + guides(colour = F)
g
```



Biplot

```
ggbiplot(active.1, groups = active$job)
```



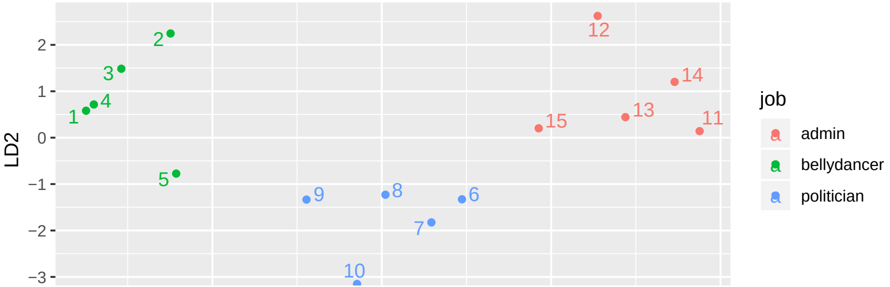
Comments on plot

- Groups well separated: bellydancers top left, administrators top right, politicians lower middle.
- Bellydancers most negative on `LD1`: like dancing most.
- Administrators most positive on `LD1`: like dancing least.
- Politicians most negative on `LD2`: like TV-watching most.

Plotting individual persons

Make `label` be identifier of person. Now need legend:

```
ggplot(mm, aes(
  x = LD1, y = LD2,
  colour = job, label = person
)) + geom_point() +
  geom_text_repel()
```



Posterior probabilities

```
pp <- round(active.pred$posterior, 3)
data.frame(obs = active$job, pred = active.pred$class, pp)
```

```
##            obs        pred admin bellydancer politician
## 1  bellydancer bellydancer 0.000       1.000      0.000
## 2  bellydancer bellydancer 0.000       1.000      0.000
## 3  bellydancer bellydancer 0.000       1.000      0.000
## 4  bellydancer bellydancer 0.000       1.000      0.000
## 5  bellydancer bellydancer 0.000       0.997      0.003
## 6   politician  politician 0.003       0.000      0.997
## 7   politician  politician 0.000       0.000      1.000
## 8   politician  politician 0.000       0.000      1.000
## 9   politician  politician 0.000       0.002      0.998
## 10  politician  politician 0.000       0.000      1.000
## 11       admin       admin 1.000       0.000      0.000
## 12       admin       admin 1.000       0.000      0.000
```

Cross-validating the jobs-activities data

Recall: no need for `predict`. Just pull out `class` and make a table:

```
active.cv <- lda(job ~ reading + dance + tv + ski,
  data = active, CV = T
)
table(obs = active$job, pred = active.cv$class)
```

```
##                pred
## obs             admin bellydancer politician
##   admin             5           0          0
##   bellydancer       0           4          1
##   politician        0           0          5
```

This time one of the bellydancers was classified as a politician.

and look at the posterior probabilities

picking out the ones where things are not certain:

```
pp <- round(active.cv$posterior, 3)
data.frame(obs = active$job, pred = active.cv$class, pp) %>%
  mutate(max = pmax(admin, bellydancer, politician)) %>%
  filter(max < 0.9995)
```

```
##             obs        pred admin bellydancer politician   max
## 1 bellydancer politician 0.000       0.001      0.999 0.99
## 2  politician politician 0.006       0.000      0.994 0.99
## 3  politician politician 0.001       0.000      0.999 0.99
## 4  politician politician 0.000       0.009      0.991 0.99
## 5       admin      admin 0.819       0.000      0.181 0.81
```

$

- Bellydancer was “definitely” a politician!
- One of the administrators might have been a politician too

Why did things get misclassified?

`![plot of chunk nesta](figure/nesta-1.pdf)`

* Go back to plot of discriminant scores:
* one bellydancer much closer to the politicians,
* one administrator a bit closer to the politicians.

Example 4: remote-sensing data

- View 38 crops from air, measure 4 variables `x1`–`x4`.
- Go back and record what each crop was.
- Can we use the 4 variables to distinguish crops?

Reading in

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/remote-sens
crops <- read_table(my_url)
```

```
## Parsed with column specification:
## cols(
##   crop = col_character(),
##   x1 = col_double(),
##   x2 = col_double(),
##   x3 = col_double(),
##   x4 = col_double(),
##   cr = col_character()
## )
```

Starting off: number of LDs

```
crops.lda <- lda(crop ~ x1 + x2 + x3 + x4, data = crops)
crops.lda$svd
```

```
## [1] 2.2858251 1.1866352 0.6394041 0.2303634
```

- 4 LDs (four variables, six groups).
- 1st one important, maybe 2nd as well.

Connecting original variables and LDs

```
crops.lda$means
```

```
##                  x1       x2       x3       x4
## Clover     46.36364 32.63636 34.18182 36.63636
## Corn       15.28571 22.71429 27.42857 33.14286
## Cotton     34.50000 32.66667 35.00000 39.16667
## Soybeans   21.00000 27.00000 23.50000 29.66667
## Sugarbeets 31.00000 32.16667 20.00000 40.50000
```

```
round(crops.lda$scaling, 3)
```

```
##       LD1    LD2    LD3    LD4
## x1 -0.061  0.009 -0.030 -0.015
## x2 -0.025  0.043  0.046  0.055
## x3  0.016 -0.079  0.020  0.009
## x4  0.000 -0.014  0.054 -0.026
```

- Links groups to original variables to LDs.

LD1 and texttt{LD2}

```r
round(crops.lda$scaling, 3)
```

```
##       LD1    LD2    LD3    LD4
## x1 -0.061  0.009 -0.030 -0.015
## x2 -0.025  0.043  0.046  0.055
## x3  0.016 -0.079  0.020  0.009
## x4  0.000 -0.014  0.054 -0.026
```

$

- LD1 mostly x1 (minus), so clover low on LD1, corn high.
- LD2 x3 (minus), x2 (plus), so sugarbeets should be high on LD2.

Predictions

- Thus:

```
crops.pred <- predict(crops.lda)
table(obs = crops$crop, pred = crops.pred$class)
```

```
##             pred
## obs          Clover Corn Cotton Soybeans Sugarbeets
##   Clover          6    0      3        0          2
##   Corn            0    6      0        1          0
##   Cotton          3    0      1        2          0
##   Soybeans        0    1      1        3          1
##   Sugarbeets      1    1      0        2          2
```

- Not very good, eg. only 6 of 11 `Clover` classified correctly.
- Set up for plot:

```
mm <- data.frame(crop = crops$crop, crops.pred$x)
```

Plotting the LDs

```
ggplot(mm, aes(x = LD1, y = LD2, colour = crop)) +
  geom_point()
```

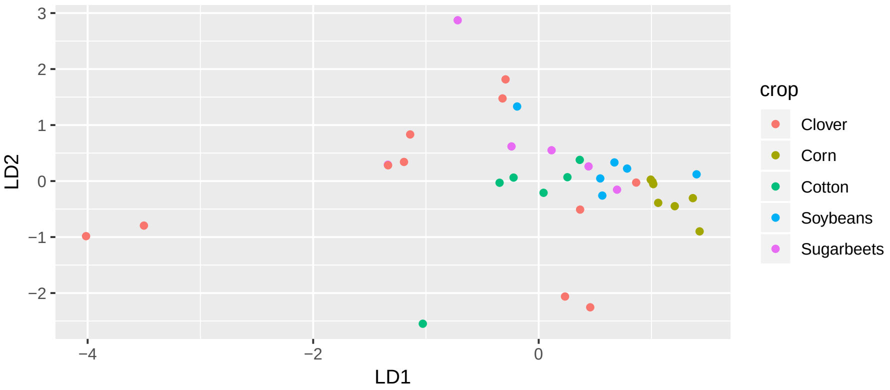
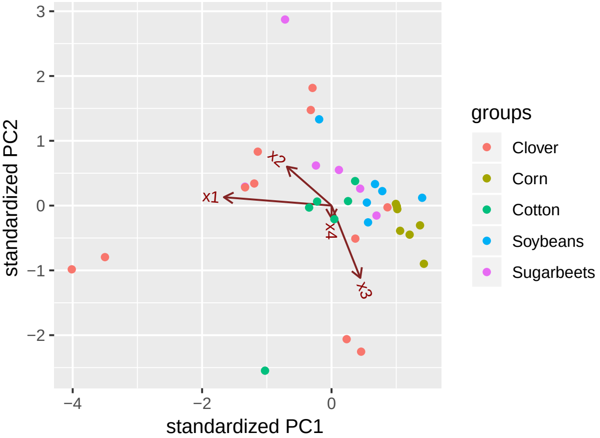


Figure 48: plot of chunk piacentini

Biplot

```
ggbiplot(crops.lda, groups = crops$crop)
```



Try removing Clover

- the `dplyr` way:

```
crops %>% filter(crop != "Clover") -> crops2
crops2.lda <- lda(crop ~ x1 + x2 + x3 + x4, data = crops2)
```

- LDs for `crops2` will be different from before.
- Concentrate on plot and posterior probs.

```
crops2.pred <- predict(crops2.lda)
mm <- data.frame(crop = crops2$crop, crops2.pred$x)
```

lda output

Different from before:

```
crops2.lda$means
```

```
##                  x1       x2       x3       x4
## Corn       15.28571 22.71429 27.42857 33.14286
## Cotton     34.50000 32.66667 35.00000 39.16667
## Soybeans   21.00000 27.00000 23.50000 29.66667
## Sugarbeets 31.00000 32.16667 20.00000 40.50000
```

```
crops2.lda$svd
```

```
## [1] 3.3639389 1.6054750 0.4180292
```

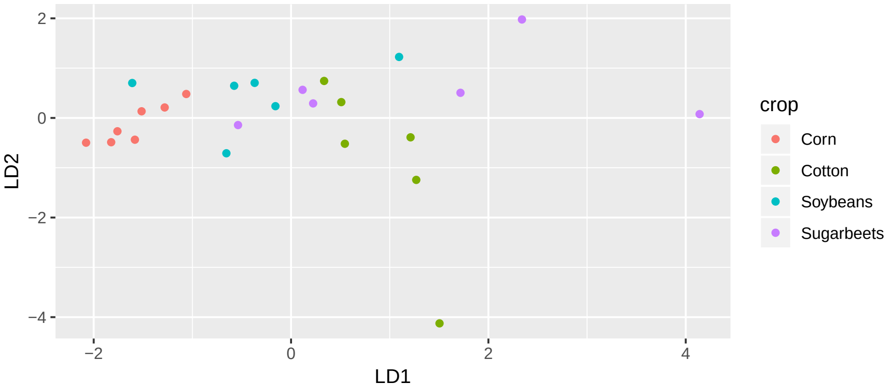
```
crops2.lda$scaling
```

```
##           LD1          LD2          LD3
## x1 0.14077479  0.007780184 -0.0312610362
```

Plot

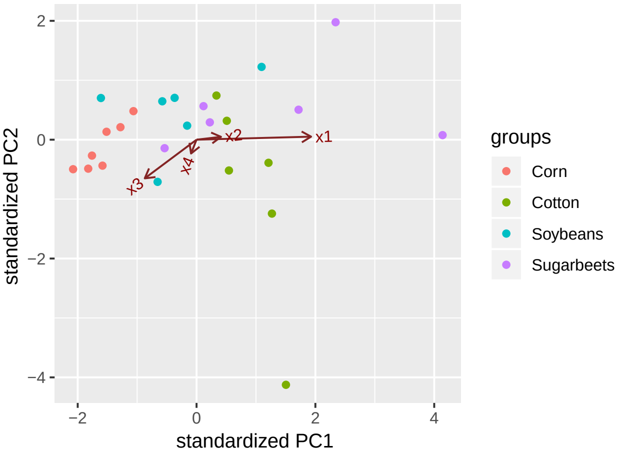
A bit more clustered:

```
ggplot(mm, aes(x = LD1, y = LD2, colour = crop)) +
  geom_point()
```



Biplot

```
ggbiplot(crops2.lda, groups = crops2$crop)
```



Quality of classification

```
table(obs = crops2$crop, pred = crops2.pred$class)
```

```
##             pred
## obs          Corn Cotton Soybeans Sugarbeets
##   Corn          6      0        1          0
##   Cotton        0      4        2          0
##   Soybeans      2      0        3          1
##   Sugarbeets    0      0        3          3
```

Better.

Posterior probs, the wrong ones

def {

```
post <- round(crops2.pred$posterior, 3)
data.frame(obs = crops2$crop, pred = crops2.pred$class, post) %>%
  filter(obs != pred)
```

```
##          obs       pred  Corn Cotton Soybeans Sugarbeets
## 1       Corn   Soybeans 0.443  0.034    0.494      0.029
## 2   Soybeans Sugarbeets 0.010  0.107    0.299      0.584
## 3   Soybeans       Corn 0.684  0.009    0.296      0.011
## 4   Soybeans       Corn 0.467  0.199    0.287      0.047
## 5     Cotton   Soybeans 0.056  0.241    0.379      0.324
## 6     Cotton   Soybeans 0.066  0.138    0.489      0.306
## 7 Sugarbeets   Soybeans 0.381  0.146    0.395      0.078
## 8 Sugarbeets   Soybeans 0.106  0.144    0.518      0.232
## 9 Sugarbeets   Soybeans 0.088  0.207    0.489      0.216
```

}

- These were the misclassified ones, but the posterior probability of being correct was not usually too low.

MANOVA

Began discriminant analysis as a followup to MANOVA. Do our variables significantly separate the crops (excluding Clover)?

```
response <- with(crops2, cbind(x1, x2, x3, x4))
crops2.manova <- manova(response ~ crop, data = crops2)
summary(crops2.manova)
```

```
##           Df Pillai approx F num Df den Df  Pr(>F)
## crop       3 0.9113   2.1815     12     60 0.02416 *
## Residuals 21
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Yes, at least one of the crops differs (in means) from the others. So it is worth doing this analysis.

We did this the wrong way around, though!

The right way around

- *First*, do a MANOVA to see whether any of the groups differ significantly on any of the variables.
- *If the MANOVA is significant*, do a discriminant analysis in the hopes of understanding how the groups are different.
- For remote-sensing data (without Clover):
- LD1 a fair bit more important than LD2 (definitely ignore LD3).
- LD1 depends mostly on `x1`, on which Cotton was high and Corn was low.
- Discriminant analysis in MANOVA plays the same kind of role that Tukey does in ANOVA.

Section 10

Cluster analysis

Cluster Analysis

- One side-effect of discriminant analysis: could draw picture of data (if 1st 2s `LD`s told most of story) and see which individuals "close" to each other.
- Discriminant analysis requires knowledge of groups.
- Without knowledge of groups, use {*cluster analysis*}*: see which individuals close, which groups suggested by data.*
- *Idea: see how individuals group into "clusters" of nearby individuals.*
- *Base on "dissimilarities" between individuals.*
- *Or base on standard deviations and correlations between variables (assesses dissimilarity behind scenes).*

Packages

```
library(MASS) # for lda later
library(tidyverse)
```

```
##  Attaching packages  tidyverse 1.2.1

##  ggplot2 3.1.1           purrr   0.3.2
##  tibble  2.1.1           dplyr   0.8.0.1
##  tidyr   0.8.3.9000      stringr 1.4.0
##  readr   1.3.1           forcats 0.3.0

## Warning: package 'ggplot2' was built under R version 3.5.3

## Warning: package 'tibble' was built under R version 3.5.3

## Warning: package 'tidyr' was built under R version 3.5.3

## Warning: package 'readr' was built under R version 3.5.2

## Warning: package 'purrr' was built under R version 3.5.3
```

One to ten in 11 languages

	English	Norwegian	Danish	Dutch	German
1	one	en	en	een	eins
2	two	to	to	twee	zwei
3	three	tre	tre	drie	drei
4	four	fire	fire	vier	vier
5	five	fem	fem	vijf	funf
6	six	seks	seks	zes	sechs
7	seven	sju	syv	zeven	sieben
8	eight	atte	otte	acht	acht
9	nine	ni	ni	negen	neun
10	ten	ti	ti	tien	zehn

One to ten

	French	Spanish	Italian	Polish	Hungarian	Finnish
1	un	uno	uno	jeden	egy	yksi
2	deux	dos	due	dwa	ketto	kaksi
3	trois	tres	tre	trzy	harom	kolme
4	quatre	cuatro	quattro	cztery	negy	nelja
5	cinq	cinco	cinque	piec	ot	viisi
6	six	seis	sei	szesc	hat	kuusi
7	sept	siete	sette	siedem	het	seitseman
8	huit	ocho	otto	osiem	nyolc	kahdeksan
9	neuf	nueve	nove	dziewiec	kilenc	yhdeksan
10	dix	diez	dieci	dziesiec	tiz	kymmenen

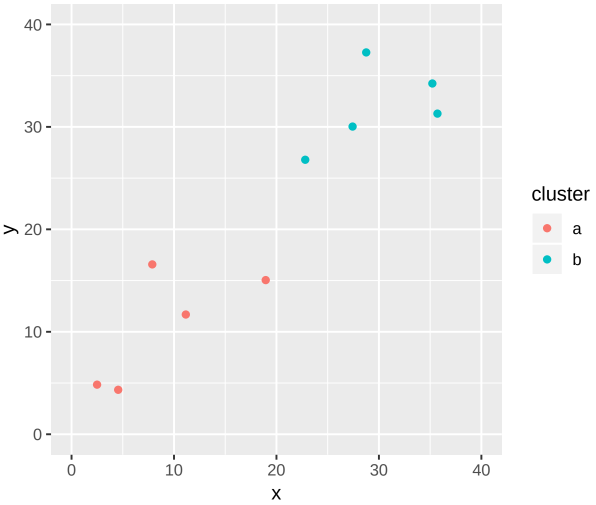
Dissimilarities and languages example

- Can define dissimilarities how you like (whatever makes sense in application).
- Sometimes defining "similarity" makes more sense; can turn this into dissimilarity by subtracting from some maximum.
- Example: numbers 1–10 in various European languages. Define similarity between two languages by counting how often the same number has a name starting with the same letter (and dissimilarity by how often number has names starting with different letter).
- Crude (doesn't even look at most of the words), but see how effective.

Two kinds of cluster analysis

- Looking at process of forming clusters (of similar languages): **hierarchical cluster analysis** (`hclust`).
- Start with each individual in cluster by itself.
- Join "closest" clusters one by one until all individuals in one cluster.
- How to define closeness of two *clusters*? Not obvious, investigate in a moment.
- Know how many clusters: which division into that many clusters is "best" for individuals? **K-means clustering** (`kmeans`).

Two made-up clusters



Single-linkage distance

Find the red point and the blue point that are closest together:

```
## Error in loadNamespace(j <- i[[1L]], c(lib.loc, .libPaths()
## Error in apply(distances, 1, min): object 'distances' not f
## Error in apply(distances, 2, min): object 'distances' not f
## Error in `[.data.frame`(a, wm1, ): object 'wm1' not found
## Error in fortify(data): object 'closest' not found
```

Single-linkage distance between 2 clusters is distance between their closest points.

Complete linkage

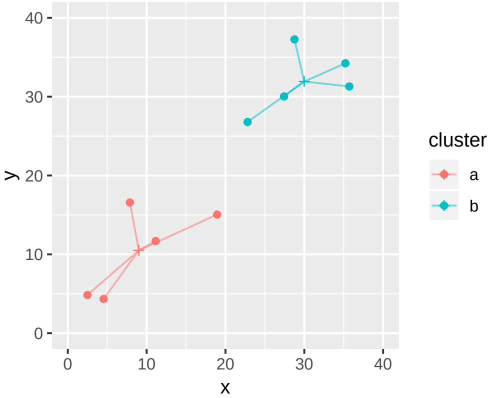
Find the red and blue points that are farthest apart:

```
## Error in apply(distances, 1, max): object 'distances' not f

## Error in apply(distances, 2, max): object 'distances' not f

## Error in `[.data.frame`(a, wm1, ): object 'wm1' not found

## Error in fortify(data): object 'closest' not found
```

Complete-linkage distance is distance between farthest points.

Ward's method

Work out mean of each cluster and join point to its mean:



- Work out sum of squared distances of points from means.

Ward's method part 2

Now imagine combining the two clusters and working out overall mean. Join each point to this mean:

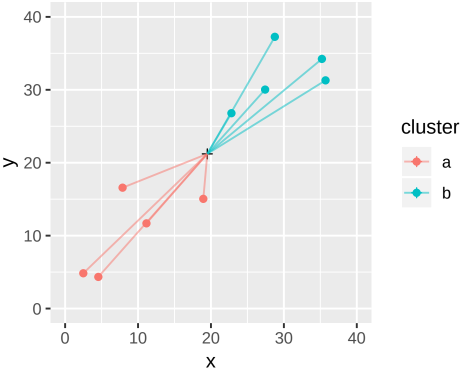


Figure 53: plot of chunk unnamed-chunk-323

Ward's method part 3

- (ii) will be bigger than (i) (points closer to own cluster mean than combined mean).
- Ward's distance is (ii) minus (i).
- Think of as "cost" of combining clusters:
- if clusters close together, (ii) only a little larger than

(i)

- if clusters far apart, (ii) a lot larger than (i) (as in example).

Hierarchical clustering revisited

- Single linkage, complete linkage, Ward are ways of measuring closeness of clusters.
- Use them, starting with each observation in own cluster, to repeatedly combine two closest clusters until all points in one cluster.
- They will give different answers (clustering stories).
- Single linkage tends to make "stringy" clusters because clusters can be very different apart from two closest points.
- Complete linkage insists on whole clusters being similar.
- Ward tends to form many small clusters first.

Dissimilarity data in R

Dissimilarities for language data *were how many number names had* different* first letter:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/languages.t
number.d <- read_table(my_url)
number.d
```

```
## # A tibble: 11 x 12
##      la       en    no    dk    nl    de    fr    es    it
##      <chr> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
##    1 en        0     2     2     7     6     6     6     6
##    2 no        2     0     1     5     4     6     6     6
##    3 dk        2     1     0     6     5     6     5     5
##    4 nl        7     5     6     0     5     9     9     9
##    5 de        6     4     5     5     0     7     7     7
##    6 fr        6     6     6     9     7     0     2     1
##    7 es        6     6     5     9     7     2     0     1
```

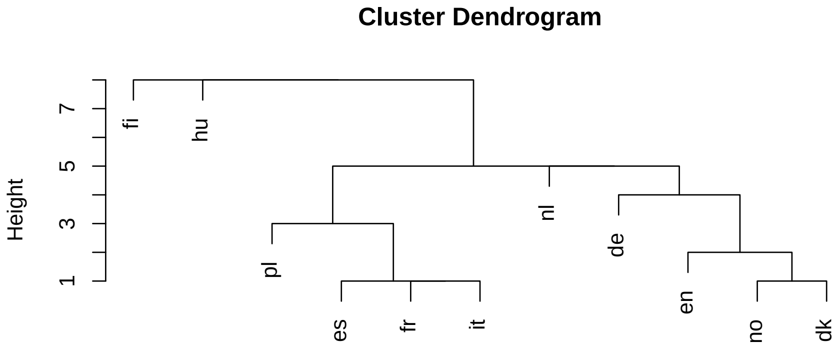
Making a distance object

```
d <- number.d %>%
  select(-la) %>%
  as.dist()
d
```

```
##    en no dk nl de fr es it pl hu
## no  2
## dk  2  1
## nl  7  5  6
## de  6  4  5  5
## fr  6  6  6  9  7
## es  6  6  5  9  7  2
## it  6  6  5  9  7  1  1
## pl  7  7  6 10  8  5  3  4
## hu  9  8  8  8  9 10 10 10 10
## fi  9  9  9  9  9  9  9  8  9  8
```

Cluster analysis and dendrogram

```
d.hc <- hclust(d, method = "single")
plot(d.hc)
```



Comments

- Tree shows how languages combined into clusters.
- First (bottom), Spanish, French, Italian joined into one cluster, Norwegian and Danish into another.
- Later, English joined to Norse languages, Polish to Romance group.
- Then German, Dutch make a Germanic group.
- Finally, Hungarian and Finnish joined to each other and everything else.

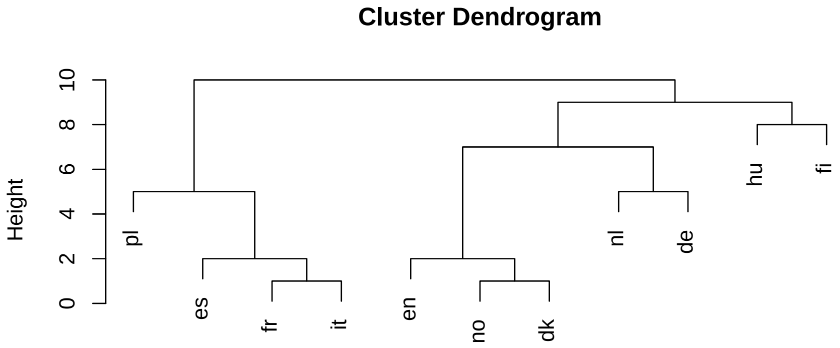
Clustering process

def
“‘r d.hc$labels$“‘
“‘ [1] ”en” ”no” ”dk” ”nl” [5] ”de” ”fr” ”es” ”it” [9] ”pl” ”hu” ”fi” “‘
“‘r d.hc$merge$“‘
“‘ [,1] [,2] [1,] -2 -3 [2,] -6 -8 [3,] -7 2 [4,] -1 1 [5,] -9 3 [6,] -5 4 [7,] -4 6 [8,] 5 7 [9,] -10 8 [10,] -11 9 “‘

* Lines of ‘merge‘ show what was combined
* First, languages 2 and 3 (‘no‘ and ‘dk‘)
* Then languages 6 and 8 (‘fr‘ and ‘it‘)
* Then #7 combined with cluster formed at step 2 (‘es‘ joined to ‘fr‘ and ‘it‘).
* Then ‘en‘ joined to ‘no‘ and ‘dk‘ ...
* Finally ‘fi‘ joined to all others.

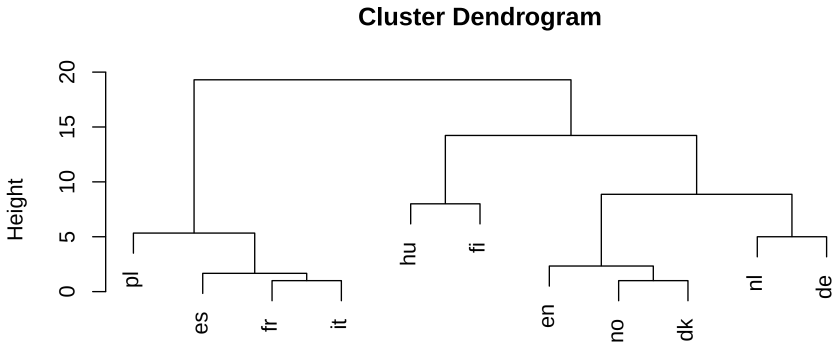
Complete linkage

```
d.hc <- hclust(d, method = "complete")
plot(d.hc)
```



Ward

```
d.hc <- hclust(d, method = "ward.D")
plot(d.hc)
```



Chopping the tree

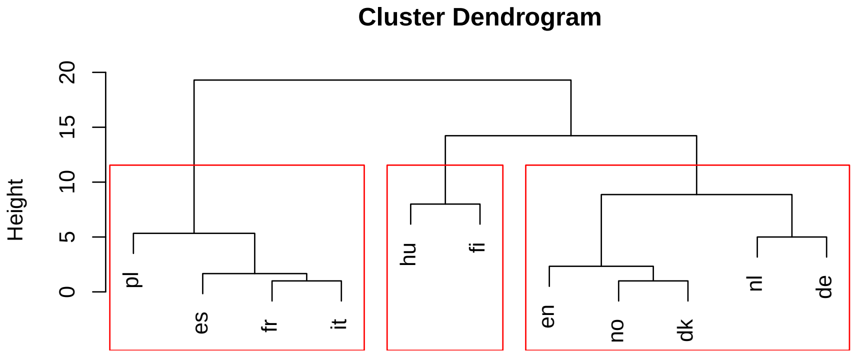
- Three clusters (from Ward) looks good:

```
cutree(d.hc, 3)
```

```
## en no dk nl de fr es it
##  1  1  1  1  1  2  2  2
## pl hu fi
##  2  3  3
```

Drawing those clusters on the tree

```
plot(d.hc)
rect.hclust(d.hc, 3)
```



Comparing single-linkage and Ward

- In Ward, Dutch and German get joined earlier (before joining to Germanic cluster).
- Also Hungarian and Finnish get combined earlier.

Making those dissimilarities

Original data:

def

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/one-ten.txt
lang <- read_delim(my_url, " ")
lang
```

```
## # A tibble: 10 x 11
##    en    no    dk    nl    de    fr     es     it     pl
##    <chr> <chr> <chr> <chr> <chr> <chr>  <chr>  <chr>  <chr>
##  1 one   en    en    een   eins  un     uno    uno    jeden
##  2 two   to    to    twee  zwei  deux   dos    due    dwa
##  3 three tre   tre   drie  drei  trois  tres   tre    trzy
##  4 four  fire  fire  vier  vier  quatre cuat… quatt… czter
##  5 five  fem   fem   vijf  funf  cinq   cinco  cinque piec
##  6 six   seks  seks  zes   sechs six    seis   sei    szesc
```

Tidy, and extract first letter

```
lang.long <- lang %>%
  mutate(number = row_number()) %>%
  gather(language, name, -number) %>%
  mutate(first = str_sub(name, 1, 1))
lang.long %>% print(n = 12)
```

```
## # A tibble: 110 x 4
##    number language name  first
##     <int> <chr>    <chr> <chr>
##  1      1 en       one   o
##  2      2 en       two   t
##  3      3 en       three t
##  4      4 en       four  f
##  5      5 en       five  f
##  6      6 en       six   s
##  7      7 en       seven s
```

Calculating dissimilarity

- Suppose we wanted dissimilarity between English and Norwegian. It's the number of first letters that are different.
- First get the lines for English:

```
english <- lang.long %>% filter(language == "en")
english
```

```
## # A tibble: 10 x 4
##    number language name  first
##     <int> <chr>    <chr> <chr>
##  1      1 en       one   o
##  2      2 en       two   t
##  3      3 en       three t
##  4      4 en       four  f
##  5      5 en       five  f
##  6      6 en       six   s
```

And then the lines for Norwegian

```
norwegian <- lang.long %>% filter(language == "no")
norwegian
```

```
## # A tibble: 10 x 4
##    number language name  first
##     <int> <chr>    <chr> <chr>
##  1      1 no       en    e
##  2      2 no       to    t
##  3      3 no       tre   t
##  4      4 no       fire  f
##  5      5 no       fem   f
##  6      6 no       seks  s
##  7      7 no       sju   s
##  8      8 no       atte  a
##  9      9 no       ni    n
## 10     10 no       ti    t
```

The join

```
english %>% left_join(norwegian, by = "number")
```

```
## # A tibble: 10 x 7
##    number language.x name.x first.x language.y name.y first
##     <int> <chr>      <chr>  <chr>   <chr>      <chr>  <chr>
## 1       1 en         one    o       no         en     e
## 2       2 en         two    t       no         to     t
## 3       3 en         three  t       no         tre    t
## 4       4 en         four   f       no         fire   f
## 5       5 en         five   f       no         fem    f
## 6       6 en         six    s       no         seks   s
## 7       7 en         seven  s       no         sju    s
## 8       8 en         eight  e       no         atte   a
## 9       9 en         nine   n       no         ni     n
## 10     10 en         ten    t       no         ti     t
```

`first.x` is 1st letter of English word, `first.y` 1st letter of Norwegian

Counting the different ones

```
english %>%
  left_join(norwegian, by = "number") %>%
  mutate(different = (first.x != first.y)) %>%
  summarize(diff = sum(different))
```

```
## # A tibble: 1 x 1
##    diff
##   <int>
## 1     2
```

Words for 1 and 8 start with different letter; rest are same.

Function to do this for any two languages

```
countdiff <- function(lang.1, lang.2, d) {
  lang1d <- d %>% filter(language == lang.1)
  lang2d <- d %>% filter(language == lang.2)
  lang1d %>%
    left_join(lang2d, by = "number") %>%
    mutate(different = (first.x != first.y)) %>%
    summarize(diff = sum(different)) %>%
    pull(diff)
}
```

Test:

```
countdiff("en", "no", lang.long)
```

```
## [1] 2
```

For all pairs of languages?

- First need all the languages:

```
languages <- names(lang)
languages
```

```
##  [1] "en" "no" "dk" "nl" "de" "fr" "es" "it" "pl"
## [10] "hu" "fi"
```

- and then all *pairs* of languages:

```
pairs <- crossing(lang = languages, lang2 = languages) %>% pri
```

```
## # A tibble: 121 x 2
##    lang  lang2
##    <chr> <chr>
##  1 de    de
##  2 de    dk
##  3 de    en
```

Run countdiff for all those language pairs

```
thediffs <- pairs %>%
  mutate(diff = map2_int(lang, lang2, countdiff, lang.long)) %
  print(n = 12)
```

```
## # A tibble: 121 x 3
##    lang  lang2  diff
##    <chr> <chr> <int>
##  1 de    de        0
##  2 de    dk        5
##  3 de    en        6
##  4 de    es        7
##  5 de    fi        9
##  6 de    fr        7
##  7 de    hu        9
##  8 de    it        7
##  9 de    nl        5
```

Make square table of these

def

```
thediffs %>% spread(lang2, diff)
```

```
## # A tibble: 11 x 12
##    lang     de    dk    en    es    fi    fr    hu    it
##    <chr> <int> <int> <int> <int> <int> <int> <int> <int>
##  1 de        0     5     6     7     9     7     9     7
##  2 dk        5     0     2     5     9     6     8     5
##  3 en        6     2     0     6     9     6     9     6
##  4 es        7     5     6     0     9     2    10     1
##  5 fi        9     9     9     9     0     9     8     9
##  6 fr        7     6     6     2     9     0    10     1
##  7 hu        9     8     9    10     8    10     0    10
##  8 it        7     5     6     1     9     1    10     0
##  9 nl        5     6     7     9     9     9     8     9
## 10 no        4     1     2     6     9     6     8     6
```

Another example

Birth, death and infant mortality rates for 97 countries (variables not dissimilarities):

{

```
24.7  5.7  30.8 Albania         12.5 11.9  14.4 Bulgaria
13.4 11.7  11.3 Czechoslovakia  12   12.4   7.6 Former_E._Germany
11.6 13.4  14.8 Hungary         14.3 10.2    16 Poland
13.6 10.7  26.9 Romania           14    9  20.2 Yugoslavia
17.7   10    23 USSR            15.2  9.5  13.1 Byelorussia_SSR
13.4 11.6    13 Ukrainian_SSR   20.7  8.4  25.7 Argentina
46.6   18   111 Bolivia         28.6  7.9    63 Brazil
23.4  5.8  17.1 Chile           27.4  6.1    40 Columbia
32.9  7.4    63 Ecuador         28.3  7.3    56 Guyana
...
```

}

- Want to find groups of similar countries (and how many groups, which countries in each group).
- Tree would be unwieldy with 97 countries.

Reading in

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/birthrate.t
vital <- read_table(my_url)
```

```
## Parsed with column specification:
## cols(
##   birth = col_double(),
##   death = col_double(),
##   infant = col_double(),
##   country = col_character()
## )
```

The data

```
vital
```

```
## # A tibble: 97 x 4
##    birth death infant country
##    <dbl> <dbl>  <dbl> <chr>
##  1  24.7   5.7   30.8 Albania
##  2  13.4  11.7   11.3 Czechoslovakia
##  3  11.6  13.4   14.8 Hungary
##  4  13.6  10.7   26.9 Romania
##  5  17.7  10     23   USSR
##  6  13.4  11.6   13   Ukrainian_SSR
##  7  46.6  18    111   Bolivia
##  8  23.4   5.8   17.1 Chile
##  9  32.9   7.4   63   Ecuador
## 10  34.8   6.6   42   Paraguay
## # … with 87 more rows
```

Standardizing

- Infant mortality rate numbers bigger than others, consequence of measurement scale (arbitrary).
- Standardize (numerical) columns of data frame to have mean 0, SD 1, done by `scale`.

```
vital.s <- vital %>% mutate_if(is.numeric, scale)
```

Three clusters

Pretend we know 3 clusters is good. Take off the 4th column (of countries) and run `kmeans` on the resulting data frame, asking for 3 clusters:

```
vital.km3 <- vital.s %>% select(-4) %>% kmeans(3)
names(vital.km3)
```

```
## [1] "cluster"      "centers"      "totss"
## [4] "withinss"     "tot.withinss" "betweenss"
## [7] "size"         "iter"         "ifault"
```

A lot of output, so look at these individually.

What's in the output?

- Cluster sizes:

```
vital.km3$size
```

```
## [1] 29 44 24
```

def

- Cluster centres:

```
vital.km3$centers
```

```
##        birth      death     infant
## 1  0.4737967 -0.4878149  0.2466440
## 2 -0.9593341 -0.4322350 -0.8904328
## 3  1.1862748  1.3818738  1.3344318
```

def

- Cluster 2 has lower than average rates on everything; cluster 3 has

Cluster sums of squares and membership

```
vital.km3$withinss
```

```
## [1] 14.96356 25.13922 26.78049
```

def

Cluster 1 compact relative to others (countries in cluster 1 more similar).

```
vital.km3$cluster
```

```
##  [1] 2 2 2 2 2 2 3 2 1 1 2 3 2 2 2 2 2 2 2 2 2 3 1 2 2 1 1
## [29] 2 1 2 1 1 2 2 1 1 1 3 3 1 1 3 3 1 3 3 3 1 2 2 2 2 2 2
## [57] 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 1 1 1 1 2 3 2 1 1 3 1 2
## [85] 3 3 3 3 1 3 3 3 3 3 1 3 3
```

def

The cluster membership for each of the 97 countries.

Store countries and clusters to which they belong

```
vital.3 <- tibble(
  country = vital.s$country,
  cluster = vital.km3$cluster
)
```

Next, which countries in which cluster?

Write function to extract them:

```
get_countries <- function(i, d) {
  d %>% filter(cluster == i) %>% pull(country)
}
```

Cluster membership: cluster 2

```
get_countries(2, vital.3)
```

```
##  [1] "Albania"               "Czechoslovakia"
##  [3] "Hungary"               "Romania"
##  [5] "USSR"                  "Ukrainian_SSR"
##  [7] "Chile"                 "Uruguay"
##  [9] "Finland"               "France"
## [11] "Greece"                "Italy"
## [13] "Norway"                "Spain"
## [15] "Switzerland"           "Austria"
## [17] "Canada"                "Israel"
## [19] "Kuwait"                "China"
## [21] "Korea"                 "Singapore"
## [23] "Thailand"              "Bulgaria"
## [25] "Former_E._Germany"     "Poland"
## [27] "Yugoslavia"            "Byelorussia_SSR"
```

Cluster 3

```r
get_countries(3, vital.3)
```

```
##  [1] "Bolivia"      "Mexico"       "Afghanistan"
##  [4] "Bangladesh"   "Gabon"        "Ghana"
##  [7] "Namibia"      "Sierra_Leone" "Swaziland"
## [10] "Uganda"       "Zaire"        "Cambodia"
## [13] "Nepal"        "Angola"       "Congo"
## [16] "Ethiopia"     "Gambia"       "Malawi"
## [19] "Mozambique"   "Nigeria"      "Somalia"
## [22] "Sudan"        "Tanzania"     "Zambia"
```

Cluster 1

```
get_countries(1, vital.3)
```

```
##  [1] "Ecuador"      "Paraguay"     "Iran"
##  [4] "Oman"         "Turkey"       "India"
##  [7] "Mongolia"     "Pakistan"     "Algeria"
## [10] "Botswana"     "Egypt"        "Libya"
## [13] "Morocco"      "South_Africa" "Zimbabwe"
## [16] "Brazil"       "Columbia"     "Guyana"
## [19] "Peru"         "Iraq"         "Jordan"
## [22] "Lebanon"      "Saudi_Arabia" "Indonesia"
## [25] "Malaysia"     "Philippines"  "Vietnam"
## [28] "Kenya"        "Tunisia"
```

Problem!

- `kmeans` uses randomization. So result of one run might be different from another run.
- Example: just run again on 3 clusters, `table` of results:

```
vital.km3a <- vital.s %>% select(-4) %>% kmeans(3)
table(
  first = vital.km3$cluster,
  second = vital.km3a$cluster
)
```

```
##        second
## first  1  2  3
##     1  1  0 28
##     2  0 40  4
##     3 24  0  0
```

- Clusters are similar but *not same*.

How many clusters?

- Three was just a guess.
- Idea: try a whole bunch of #clusters (say 2–20), obtain measure of goodness of fit for each, make plot.
- Appropriate measure is `tot.withinss`.
- Use loop to run `kmeans` for each #clusters, keep track of `tot.withinss`.

Function to get `tot.withinss`

…for an input number of clusters, taking only numeric columns of input data frame:

```
ss <- function(i, d) {
  km <- d %>%
    select_if(is.numeric) %>%
    kmeans(i, nstart = 20)
  km$tot.withinss
}
```

Note: writing function to be as general as possible, so that we can re-use it later.

Constructing within-cluster SS

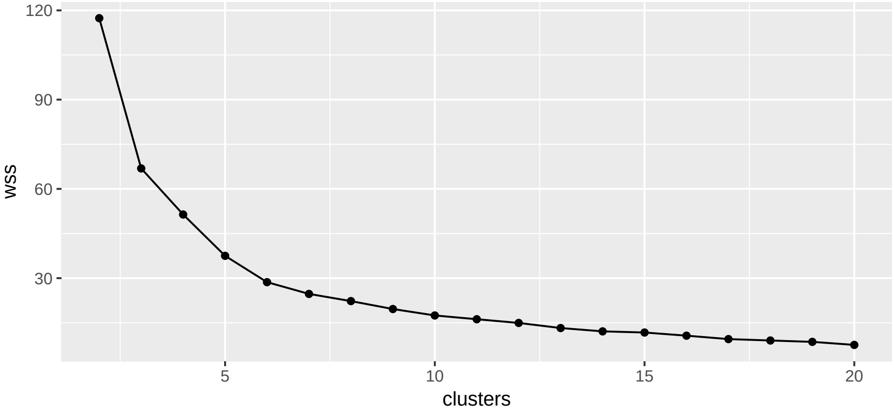
Make a data frame with desired numbers of clusters, and fill it with the total within-group sums of squares. ‘`For each number of clusters, runss''`, somap_dbl‘.

```
ssd <- tibble(clusters = 2:20) %>%
  mutate(wss = map_dbl(clusters, ss, vital.s)) %>%
  print(n = 10)
```

```
## # A tibble: 19 x 2
##    clusters   wss
##       <int> <dbl>
##  1        2 117.
##  2        3  66.9
##  3        4  51.4
##  4        5  37.5
##  5        6  28.7
##  6        7  24.7
```

Scree plot

```
ggplot(ssd, aes(x = clusters, y = wss)) + geom_point() +
  geom_line()
```



Interpreting scree plot

- Lower `wss` better.
- But lower for larger #clusters, harder to explain.
- Compromise: low-ish `wss` and low-ish #clusters.
- Look for "elbow" in plot.
- Idea: this is where `wss` decreases fast then slow.
- On our plot, small elbow at 6 clusters. Try this many clusters.

Six clusters, using nstart

```
vital.km6 <- vital.s %>%
  select(-4) %>%
  kmeans(6, nstart = 20)
vital.km6$size
```

```
## [1] 24  8 30 15 18  2
```

```
vital.km6$centers
```

```
##        birth      death     infant
## 1  0.4160993 -0.5169988  0.2648754
## 2  1.3043848  2.1896567  1.9470306
## 3 -1.1737104 -0.1856375 -0.9534370
## 4 -0.4357690 -1.1438599 -0.7281108
## 5  1.2092406  0.7441347  1.0278003
## 6 -0.2199722  2.1116577 -0.4544435
```

```
vital.6 <- tibble(
```

Cluster 1

Below-average death rate, though other rates a little higher than average:

```
get_countries(1, vital.6)
```

```
##  [1] "Ecuador"      "Paraguay"     "Oman"
##  [4] "Turkey"       "India"        "Mongolia"
##  [7] "Pakistan"     "Algeria"      "Egypt"
## [10] "Libya"        "Morocco"      "South_Africa"
## [13] "Zimbabwe"     "Brazil"       "Guyana"
## [16] "Peru"         "Iraq"         "Jordan"
## [19] "Lebanon"      "Saudi_Arabia" "Indonesia"
## [22] "Philippines"  "Vietnam"      "Tunisia"
```

Cluster 2

High on everything:

```
get_countries(2, vital.6)
```

```
## [1] "Afghanistan"  "Sierra_Leone" "Angola"
## [4] "Ethiopia"     "Gambia"       "Malawi"
## [7] "Mozambique"   "Somalia"
```

Cluster 3

Low on everything, though death rate close to average:

```
get_countries(3, vital.6)
```

```
##  [1] "Czechoslovakia"    "Hungary"
##  [3] "Romania"           "USSR"
##  [5] "Ukrainian_SSR"     "Uruguay"
##  [7] "Finland"           "France"
##  [9] "Greece"            "Italy"
## [11] "Norway"            "Spain"
## [13] "Switzerland"       "Austria"
## [15] "Canada"            "Bulgaria"
## [17] "Former_E._Germany" "Poland"
## [19] "Yugoslavia"        "Byelorussia_SSR"
## [21] "Belgium"           "Denmark"
## [23] "Germany"           "Ireland"
## [25] "Netherlands"       "Portugal"
```

Cluster 4

Low on everything, especially death rate:

```
get_countries(4, vital.6)
```

```
##  [1] "Albania"                "Chile"
##  [3] "Israel"                 "Kuwait"
##  [5] "China"                  "Singapore"
##  [7] "Thailand"               "Argentina"
##  [9] "Columbia"               "Venezuela"
## [11] "Bahrain"                "United_Arab_Emirates"
## [13] "Hong_Kong"              "Malaysia"
## [15] "Sri_Lanka"
```

Cluster 5

Higher than average on everything, though not the highest:

```
get_countries(5, vital.6)
```

```
##  [1] "Bolivia"     "Iran"        "Bangladesh"
##  [4] "Botswana"    "Gabon"       "Ghana"
##  [7] "Namibia"     "Swaziland"   "Uganda"
## [10] "Zaire"       "Cambodia"    "Nepal"
## [13] "Congo"       "Kenya"       "Nigeria"
## [16] "Sudan"       "Tanzania"    "Zambia"
```

Cluster 6

Very high death rate, just below average on all else:

```
get_countries(6, vital.6)
```

```
## [1] "Mexico" "Korea"
```

Comparing our 3 and 6-cluster solutions

```
table(three = vital.km3$cluster, six = vital.km6$cluster)
```

```
##       six
## three  1  2  3  4  5  6
##     1 24  0  0  2  3  0
##     2  0  0 30 13  0  1
##     3  0  8  0  0 15  1
```

Compared to 3-cluster solution:

- most of cluster 1 gone to (new) cluster 1
- cluster 2 split into clusters 3 and 4 (two types of “richer” countries)
- cluster 3 split into clusters 2 and 5 (two types of “poor” countries, divided by death rate).
- cluster 6 (Mexico and Korea) was split before.

Getting a picture from `kmeans`

- Use multidimensional scaling (later)
- Use discriminant analysis on clusters found, treating them as "known" groups.

MANOVA and discriminant analysis

- Go back to 1st 3 columns of `vital.s` (variables, standardized), plus `cf` (cluster as factor). `clus` (6 clusters).
- First, do they actually differ by group? (MANOVA):

```
v <- vital.s %>% select(-4) %>% as.matrix()
cf <- as.factor(vital.km6$cluster)
vital.manova <- manova(v ~ cf)
summary(vital.manova)
```

```
##           Df Pillai approx F num Df den Df
## cf         5 1.9215   32.427     15    273
## Residuals 91
##              Pr(>F)
## cf        < 2.2e-16 ***
## Residuals
## ---
```

Discriminant analysis

- So what makes the groups different?
- Uses package MASS (loaded):

```
vital.lda <- lda(cf ~ birth + death + infant, data = vital.s)
vital.lda$svd
```

```
## [1] 21.687195  8.851811  1.773006
```

```
vital.lda$scaling
```

```
##              LD1        LD2        LD3
## birth  2.6879695  1.1224202  1.9483853
## death  0.6652712 -2.7213044  0.6049358
## infant 2.1111801  0.7650912 -2.3542296
```

def

- LD1 is some of everything, but not so much death rate (high=poor,

To make a plot

- Get predictions first:

```
vital.pred <- predict(vital.lda)
d <- data.frame(
  country = vital.s$country,
  cluster = vital.km6$cluster, vital.pred$x
)
glimpse(d)
```

```
## Observations: 97
## Variables: 5
## $ country <fct> Albania, Czechoslovakia, Hungar…
## $ cluster <int> 4, 3, 3, 3, 3, 3, 5, 4, 1, 1, 3…
## $ LD1     <dbl> -2.74034473, -5.01874312, -4.97…
## $ LD2     <dbl> 2.2311427, -2.5427640, -3.62910…
## $ LD3     <dbl> -0.086392118, 0.067491502, -0.1…
```

$ %$ %$

The plot

```
g
```

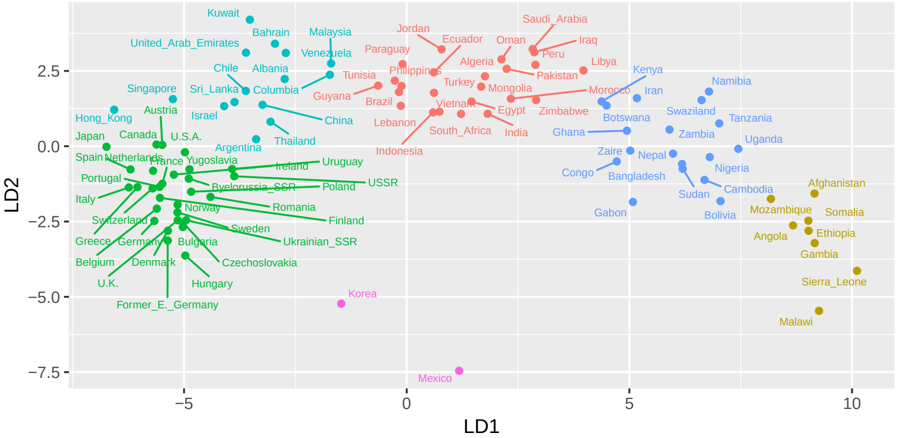
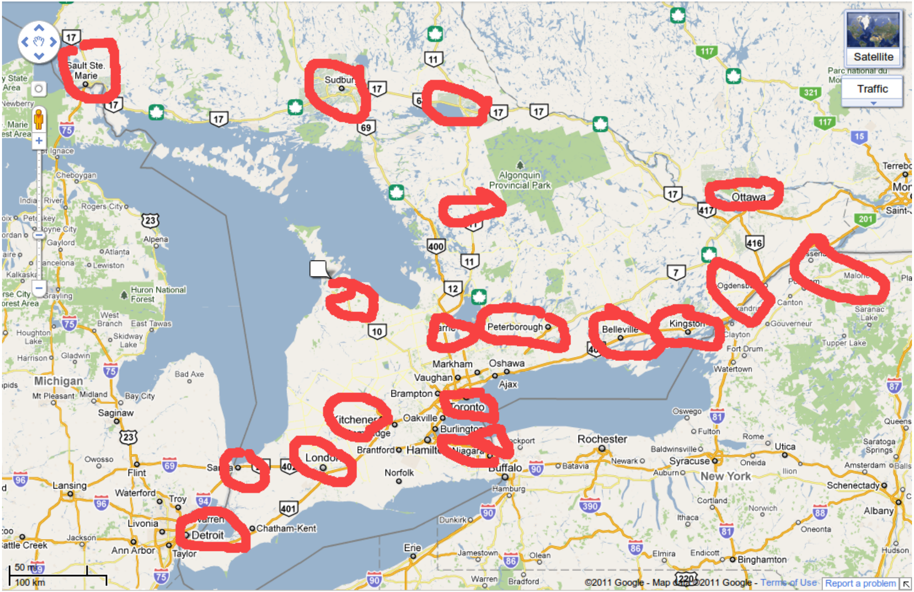


Figure 50: plot of chunk unnamed-chunk-270

Final example: a hockey league

- An Ontario hockey league has teams in 21 cities. How can we arrange those teams into 4 geographical divisions?
- Distance data in spreadsheet.
- Take out spaces in team names.
- Save as "text/csv".
- Distances, so back to `hclust`.

A map

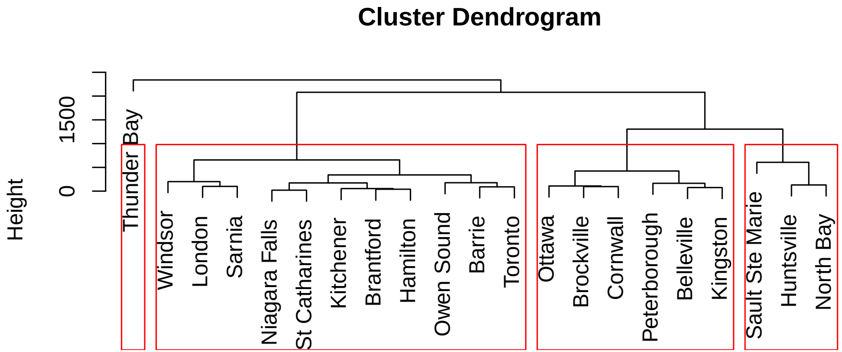


Attempt 1

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/ontario-roa
ontario <- read_csv(my_url)
ontario.d <- ontario %>% select(-1) %>% as.dist()
ontario.hc <- hclust(ontario.d, method = "ward.D")
```

Plot, with 4 clusters

```
plot(ontario.hc)
rect.hclust(ontario.hc, 4)
```

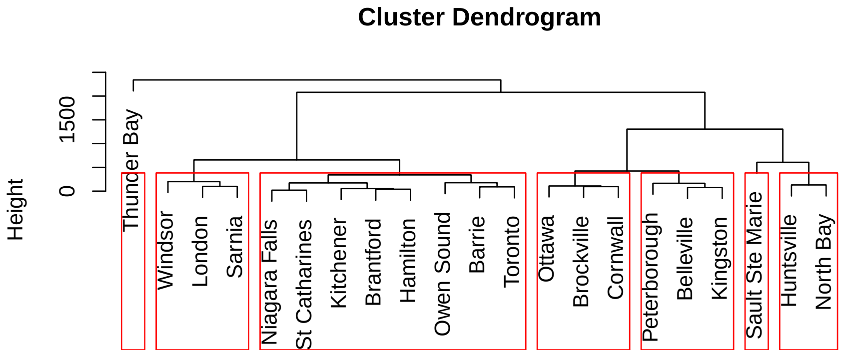


Comments

- Can't have divisions of 1 team!
- "Southern" divisions way too big!
- Try splitting into more. I found 7 to be good:

Seven clusters

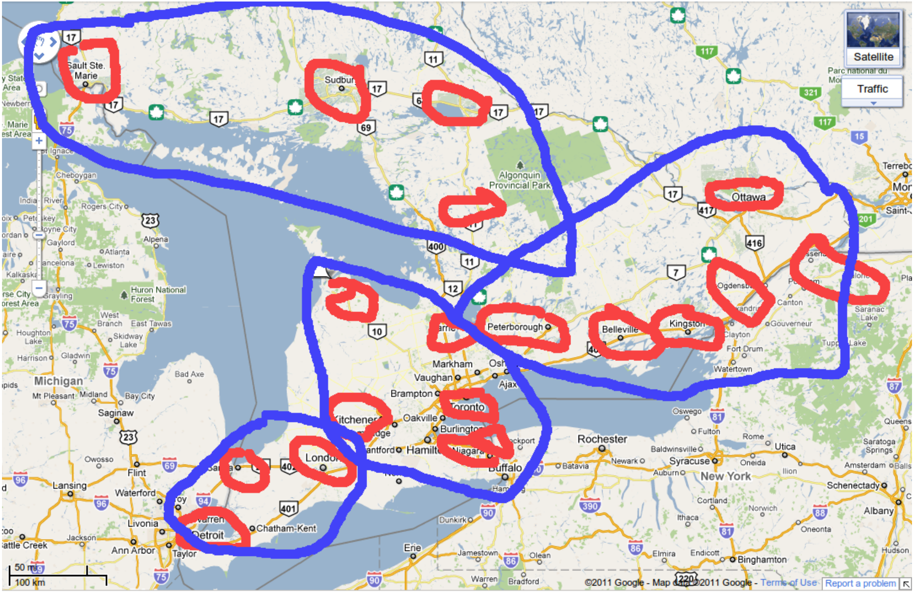
```
plot(ontario.hc)
rect.hclust(ontario.hc, 7)
```



Divisions now

- I want to put Huntsville and North Bay together with northern teams.
- I'll put the Eastern teams together. Gives:
- North: Sault Ste Marie, Sudbury, Huntsville, North Bay
- East: Brockville, Cornwall, Ottawa, Peterborough, Belleville, Kingston
- West: Windsor, London, Sarnia
- Central: Owen Sound, Barrie, Toronto, Niagara Falls, St Catharines, Brantford, Hamilton, Kitchener
- Getting them same size beyond us!

Another map


Sault Ste. Marie
Sudbury
Algonquin Provincial Park
Ottawa
Peterborough
Belleville
Kingston
Markham
Vaughan
Brampton
Toronto
Oakville
Burlington
Hamilton
Kitchener
London
Chatham-Kent
Detroit
Buffalo
Rochester
Syracuse
New York
Watertown
Oswego
Utica
Schenectady
Albany
Binghamton
Michigan
Saginaw
Flint
Lansing
Ann Arbor
Livonia
Taylor
Erie
Satellite
Traffic
50 mi
100 km
©2011 Google - Map data ©2011 Google - Terms of Use
Report a problem

Section 11

Multidimensional scaling

Multidimensional Scaling

- Have distances between individuals.
- Want to draw a picture (map) in 2 dimensions showing individuals so that distances (or order of distances) as close together as possible. (Or maybe 3 with `rgl`.)
- If want to preserve actual distances, called {*metric multidimensional scaling} (in R, `cmdscale`).*
- *If only want to preserve order of distances, called {*non-metric multidimensional scaling} (in R, `isoMDS` in package `MASS`).
- Metric scaling has solution that can be worked out exactly.
- Non-metric only has iterative solution.
- Assess quality of fit, see whether use of resulting map is reasonable. (Try something obviously 3-dimensional and assess its failure.)

Packages

The usual, plus a new one:

```
library(MASS)
library(tidyverse)
```

```
## Warning: package 'ggplot2' was built under R
## version 3.5.3

## Warning: package 'tibble' was built under R
## version 3.5.3

## Warning: package 'tidyr' was built under R version
## 3.5.3

## Warning: package 'readr' was built under R version
## 3.5.2

## Warning: package 'purrr' was built under R version
## 3.5.3
```

Metric scaling: European cities

CSV file europe.csv contains road distances (in km) between 16 European cities. Can we reproduce a map of Europe from these distances?

Read in data:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/europe.csv"
europe <- read_csv(my_url)
```

```
## Warning: Missing column names filled in: 'X1' [1]
```

```
## Parsed with column specification:
## cols(
##   X1 = col_character(),
##   Amsterdam = col_double(),
##   Athens = col_double(),
##   Barcelona = col_double(),
##   Berlin = col_double(),
##   Cologne = col_double(),
```

The data

```
europe
```

```
## # A tibble: 16 x 17
##    X1     Amsterdam Athens Barcelona Berlin Cologne Copenhag
##    <chr>      <dbl>  <dbl>     <dbl>  <dbl>   <dbl>       <db
##  1 Amst…          0   3082      1639    649     280          9
##  2 Athe…       3082      0      3312   2552    2562         34
##  3 Barc…       1639   3312         0   1899    1539         22
##  4 Berl…        649   2552      1899      0     575          7
##  5 Colo…        280   2562      1539    575       0          7
##  6 Cope…        904   3414      2230    743     730
##  7 Edin…       1180   3768      2181   1727    1206         18
##  8 Gene…       1014   2692       758   1141     765         15
##  9 Lond…        494   3099      1512   1059     538         11
## 10 Madr…       1782   3940       628   2527    1776         25
## 11 Mars…       1323   2997       515   1584    1208         19
## 12 Muni…        875   2210      1349    604     592          1
```

Multidimensional scaling

- Create distance object first using all but first column of `europe`. `europe` has distances in it already, so make into `dist` with `as.dist`.
- Then run multidimensional scaling and look at result:

```
europe.d <- europe %>% select(-1) %>% as.dist()
europe.scale <- cmdscale(europe.d)
head(europe.scale)
```

```
##                  [,1]      [,2]
## Amsterdam  -348.162277  528.2657
## Athens     2528.610410 -509.5208
## Barcelona  -695.970779 -984.6093
## Berlin      384.178025  634.5239
## Cologne       5.153446  356.7230
## Copenhagen -187.104072 1142.5926
```

- This is a `matrix` of x and y coordinates.

As a data frame; make picture

We know how to plot data frames, so make one first.

```
europe_coord <- europe.scale %>%
  as_tibble() %>%
  mutate(city = europe$City) %>%
  print(n = 12)
```

```
## Warning: `as_tibble.matrix()` requires a matrix with column
## This warning is displayed once per session.

## Warning: Unknown or uninitialised column: 'City'.

## # A tibble: 16 x 2
##          V1     V2
##       <dbl>  <dbl>
##  1  -348.    528.
##  2  2529.   -510.
##  3  -696.   -985.
```

The map

```
g
```

```
## Error in FUN(X[[i]], ...): object 'city' not found
```

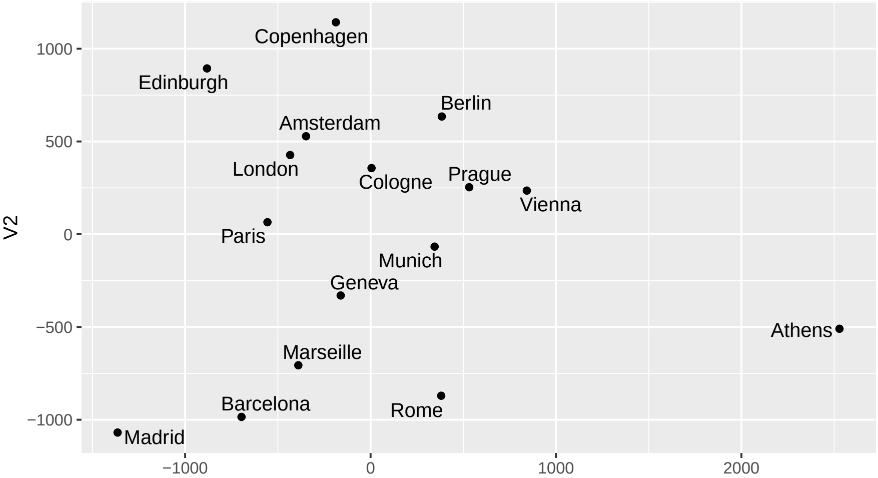
Making a function

- Idea: given input distance matrix (as stored in a CSV file), output a map (like the one on the previous page).

```
mds_map <- function(filename) {
  x <- read_csv(filename)
  dist <- x %>%
    select_if(is.numeric) %>%
    as.dist()
  x.scale <- cmdscale(dist) # this is a matrix
  x_coord <- x.scale %>%
    as_tibble() %>%
    mutate(place = row.names(x.scale))
  ggplot(x_coord, aes(x = V1, y = V2, label = place)) +
    geom_point() + geom_text_repel() +
    coord_fixed()
}
```

Does it work?

```
mds_map("europe.csv")
```



A square

\begin{multicols}{2}

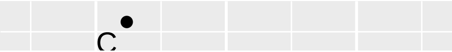
- The data, in `square.csv`: \begin{small}

```
x,A  ,B  ,C  ,D
A,0  ,1  ,1  ,1.4
B,1  ,0  ,1.4,1
C,1  ,1.4,0  ,1
D,1.4,1  ,1  ,0
```

\end{small}

- The map (on right):

```
mds_map("square.csv")
```



Drawing a map of the real Europe

- Works with package ggmap.
- First find latitudes and longitudes of our cities, called *geocoding*:

```
latlong <- geocode(europe$City)
latlong <- bind_cols(city = europe$City, latlong)
latlong %>% print(n = 6)
```

$ %$ %$

```
## # A tibble: 16 x 3
##   city         lon   lat
##   <chr>      <dbl> <dbl>
## 1 Amsterdam   4.90  52.4
## 2 Athens     23.7   38.0
## 3 Barcelona   2.17  41.4
## 4 Berlin     13.4   52.5
## 5 Cologne     6.96  50.9
```

Making the map

- Get a map of Europe from Google Maps (specify what you want a map of any way you can in Google Maps). This one centres the map on the city shown and zooms it so all the cities appear (I had to experiment):

```
map <- get_map("Memmingen DE", zoom = 5)
```

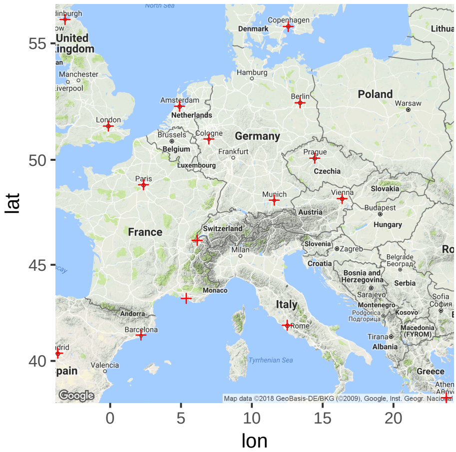
- Plot the map with ggmap. This is ggplot, so add anything to it that you would add to a ggplot, such as cities we want to show:

```
g2 <- ggmap(map) +
  geom_point(
    data = latlong, aes(x = lon, y = lat),
    shape = 3, colour = "red"
  )
```

- We don't have a default data frame or aes for our geom_point, so have to specify one.

The real Europe with our cities

```
g2
```



Compare our scaling map

```
## Error in FUN(X[[i]], ...): object 'city' not found
```

Comments

- North-south not quite right: Edinburgh and Copenhagen on same latitude, also Amsterdam and Berlin; Athens should be south of Rome.
- Rotating clockwise by about 45 degrees should fix that.
- General point: MDS only uses distances, so answer can be "off" by rotation (as here) or reflection (flipping over, say exchanging west and east while leaving north and south same).

Exploring the map by plotting in 3 dimensions

- Package rgl makes 3D plots.
- We have to fake up a 3rd dimension (by setting all its values to 1).
- Try this code:

```
library(rgl)
es.2 <- cbind(europe.scale, 1)
plot3d(es.2, zlim = c(-1000, 1000))
text3d(es.2, text = d$city)
```

- Opens a graphics window with the cities plotted and named.
- Click and hold left mouse button to rotate plot. “Rotate away” 3rd dimension to get a possible map (that preserves distances).

Ontario, the same way

…using our function:

```
g <- mds_map("ontario-road-distances.csv")
g
```

Removing points

- Messy: have to find which rows and columns contain those cities, then remove just those rows and columns.
- Better:
- "tidy" the distance matrix
- then remove rows we don't need
- then "untidy" it again
- save into .csv file
- Illustrate with square data first (easier to see).

Square data

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/square.csv"
square <- read_csv(my_url)
square
```

```
## # A tibble: 4 x 5
##   x         A     B     C     D
##   <chr> <dbl> <dbl> <dbl> <dbl>
## 1 A       0     1     1     1.4
## 2 B       1     0     1.4   1
## 3 C       1     1.4   0     1
## 4 D       1.4   1     1     0
```

Make tidy

```
square %>% gather(point, distance, -1)
```

```
## # A tibble: 16 x 3
##    x     point distance
##    <chr> <chr>    <dbl>
##  1 A     A          0
##  2 B     A          1
##  3 C     A          1
##  4 D     A          1.4
##  5 A     B          1
##  6 B     B          0
##  7 C     B          1.4
##  8 D     B          1
##  9 A     C          1
## 10 B     C          1.4
## 11 C     C          0
```

Remove all references to point C

In column x or point:

```
square %>%
  gather(point, distance, -1) %>%
  filter(x != "C", point != "C")
```

```
## # A tibble: 9 x 3
##   x     point distance
##   <chr> <chr>    <dbl>
## 1 A     A          0
## 2 B     A          1
## 3 D     A          1.4
## 4 A     B          1
## 5 B     B          0
## 6 D     B          1
## 7 A     D          1.4
## 8 B     D          1
```

Put back as distance matrix

and save as .csv when we are happy:

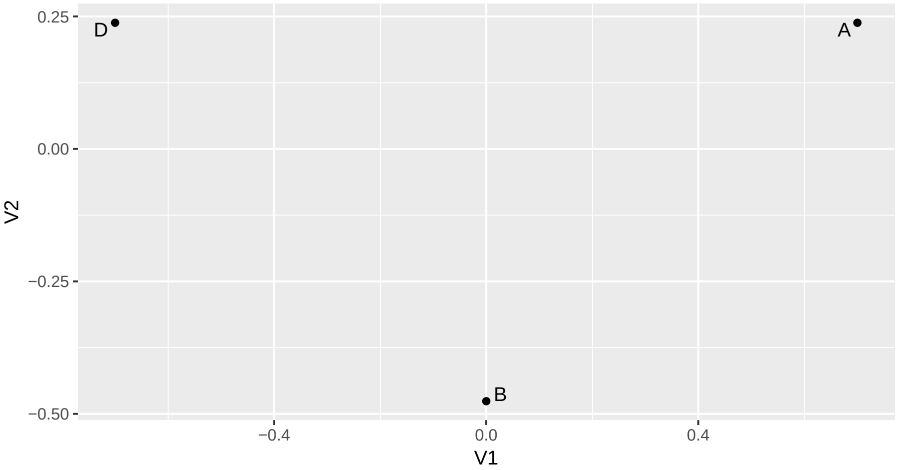
```
noc <- square %>%
  gather(point, distance, -1) %>%
  filter(x != "C", point != "C") %>%
  spread(point, distance)
noc
```

```
## # A tibble: 3 x 4
##   x         A     B     D
##   <chr> <dbl> <dbl> <dbl>
## 1 A       0       1   1.4
## 2 B       1       0   1
## 3 D       1.4     1   0
```

```
noc %>% write_csv("no-c.csv")
```

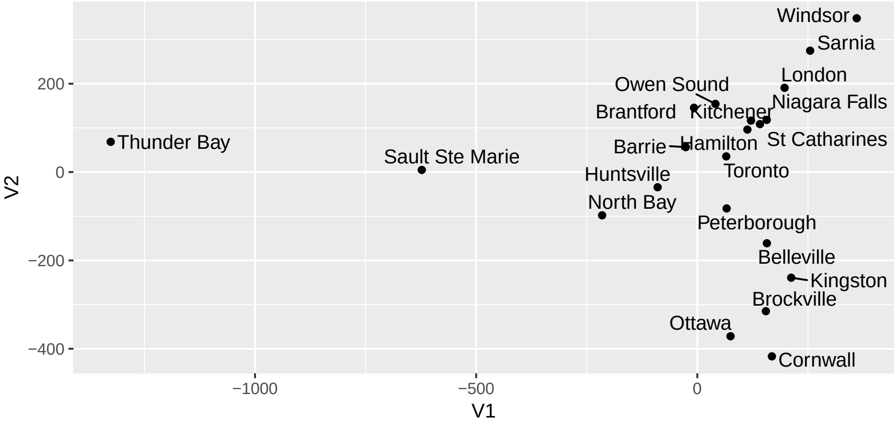
Make map of square-without-C

```
mds_map("no-c.csv")
```



Back to Ontario

```
g
```



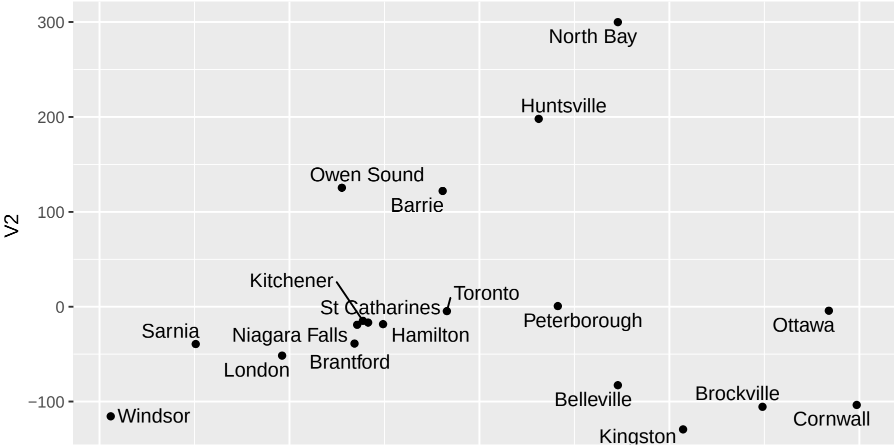
Tidy, remove, untidy

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/ontario-roa
ontario2 <- read_csv(my_url) %>%
  gather(place, distance, -1) %>%
  filter(
    x != "Thunder Bay",
    place != "Thunder Bay",
    x != "Sault Ste Marie",
    place != "Sault Ste Marie"
  ) %>%
  spread(place, distance) %>%
  write_csv("southern-ontario.csv")
```

```
## Warning in (~x != "Thunder Bay") & ~place != "Thunder Bay":
## longer object length is not a multiple of shorter object le

## Warning in (~x != "Thunder Bay") & ~place != "Thunder Bay"
## = "Sault Ste Marie": longer object length is not a multiple
```

Map of Southern Ontario

```r
g <- mds_map("southern-ontario.csv")
g
```



What about that cluster of points?

- Plot looks generally good, but what about that cluster of points?
- "Zoom in" on area between -150 and -100 on x axis, -50 to 0 on y axis.
- Code below overrides the `coord_fixed` we had before.

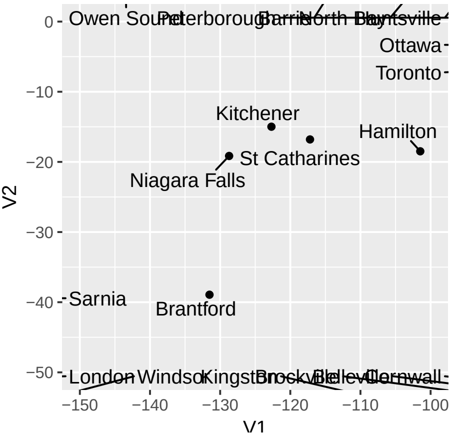
```
g2 <- g + coord_fixed(xlim = c(-150, -100), ylim = c(-50, 0))
```

```
## Coordinate system already present. Adding new coordinate sy
```

Zoomed-in plot

Ignore the arrows to points off the map:

```
g2
```



Does that make sense?

- Get a Google map of the area, with the points labelled.
- First geocode the cities of interest:

```
cities <- c(
  "Kitchener ON", "Hamilton ON", "Niagara Falls ON",
  "St Catharines ON", "Brantford ON"
)
latlong <- geocode(cities)
latlong <- bind_cols(city = cities, latlong) %>% print()
```

```
## # A tibble: 5 x 3
##   city                 lon   lat
##   <chr>              <dbl> <dbl>
## 1 Kitchener ON       -80.5  43.5
## 2 Hamilton ON        -79.9  43.3
## 3 Niagara Falls ON   -79.1  43.1
```

Making the Google map

Plot the map, plus the cities, plus labels for the cities:

```
gmap <- ggmap(map) +
  geom_point(
    data = latlong,
    aes(x = lon, y = lat),
    shape = 3, colour = "red"
  ) +
  geom_text_repel(
    data = latlong,
    aes(label = city)
  )
```

\begin{frame}[frame]{The `mds` map and Google map}

"'r g2 "'

"'r gmap "'

![plot of chunk

![plot of chunk

Quality of fit

- Read in "southern Ontario" data set from file:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/southern-or
ontario2 <- read_csv(my_url)
```

- Calling cmdscale with eig=T gives more info:

```
ontario2.2 <- ontario2 %>%
  select_if(is.numeric) %>%
  cmdscale(eig = T)
names(ontario2.2)
```

```
## [1] "points" "eig"    "x"      "ac"     "GOF"
```

```
ontario2.2$GOF
```

```
## [1] 0.8381590 0.8914059
```

```
ontario2.3 <- ontario2 %>%
```

Comments

- Coordinates now in `points`.
- `GOF` is R-squared-like measure saying how well map distances match real ones. Higher is better.
- For Ontario road distances, `GOF` better for 3 dimensions than 2, presumably to accommodate St Catharines and Niagara Falls?

3-dimensional coordinates, cities attached

```
ontario2.3$points %>%
  as_tibble() %>%
  mutate(city = ontario2$x)
```

```
## # A tibble: 19 x 4
##         V1      V2     V3 city
##      <dbl>   <dbl>  <dbl> <chr>
##  1  -38.7  122.      4.17 Barrie
##  2  146.   -82.8     1.53 Belleville
##  3 -132.   -38.9    14.1  Brantford
##  4  298.  -106.     -7.74 Brockville
##  5  397.  -104.    -22.0  Cornwall
##  6 -101.   -18.5    30.0  Hamilton
##  7   62.4  198.    -14.0  Huntsville
##  8  214.  -129.     10.8  Kingston
##  9 -123.   -15.0    -6.44 Kitchener
```

RGL code for 3 dimensions

```
library(rgl)
plot3d(ontario.3)
text3d(ontario.3, text = d2$city)
```

\begin{frame}[fragile]{Comparing MDS solution with "reality": Procrustes rotation}

- How to tell that an MDS map makes a good correspondence with "what should be"?
- Problem: MDS map might be rotated/scaled/reflected from reality.
- How to find rotation/scaling/reflection that best matches reality?
- Answer: **Procrustes rotation**.
- In R: `procOPA` in package `shapes`.

"True" coordinates

- Get latitudes and longitudes of cities by geocoding, as before. Glue "ON" onto city names to make sure we get right ones:

```
lookup <- str_c(ontario2$x, " ON")
latlong <- geocode(lookup)
latlong <- bind_cols(city = ontario2$x, latlong) %>% print(n =
```

```
## # A tibble: 19 x 3
##   city          lon   lat
##   <chr>       <dbl> <dbl>
## 1 Barrie      -79.7  44.4
## 2 Belleville  -77.4  44.2
## 3 Brantford   -80.3  43.1
## 4 Brockville  -75.7  44.6
## # … with 15 more rows
```

- Not (x, y) coordinates: one degree of latitude is always 110.25 km, but

"True" coordinates part 2

- Make coordinates by multiplying by cosine of "typical" latitude.
- Find mean latitude:

```
m <- mean(latlong$lat)
m
```

```
## [1] 44.01851
```

- Turn into radians and find its cosine:

```
mult <- cos(m * pi / 180)
mult
```

```
## [1] 0.7191153
```

- Create "true" coords by multiplying the longitudes by that. This needs to be R `matrix`, not data frame:

```
truecoord <- with(latlong, cbind(V1 = lon * mult, V2 = lat))
```

Using procOPA

- Feed 2 things into procOPA: first, “true” coordinates, second MDS coordinates.
- Get out:
- `(centred and scaled) first set of coordinates `Ahat``
- (centred and scaled) second set of coordinates Bhat
- sum of squared differences between two sets of coordinates OSS
- Rotation matrix R
- Ahat and Bhat coordinates supposed to match as well as possible.

```
ontario.pro <- procOPA(
  truecoord,
  ontario2.2$points
)
names(ontario.pro)
```

Make data frames of output, glue together

- Two sets of coordinates, `Ahat` are actual, `Bhat` are from MDS.

```
A <- ontario.pro$Ahat %>%
  as_tibble() %>%
  mutate(which = "actual", city = ontario2$x)
B <- ontario.pro$Bhat %>%
  as_tibble() %>%
  mutate(which = "MDS", city = ontario2$x)
dp <- bind_rows(A, B)
dp %>% sample_n(6)
```

```
## # A tibble: 6 x 4
##          V1     V2 which  city
##       <dbl>  <dbl> <chr>  <chr>
## 1  2.39      0.348 MDS    Brockville
## 2  0.000652 -0.929 actual Niagara Falls
## 3 -1.00     -0.568 actual Kitchener
```

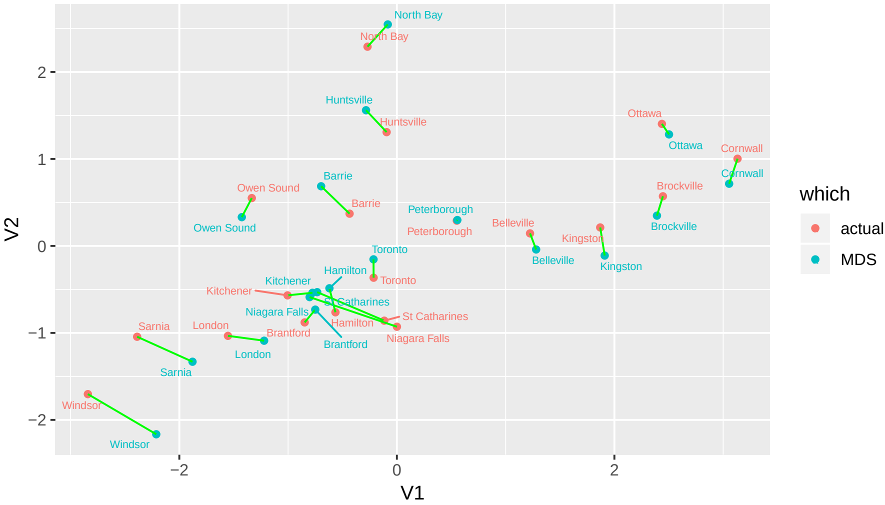
Procrustes rotation plot

- Strategy: plot all the locations, and colour them by whether they were the true location (red) or the MDS one (blue), which is in `which`. Label each location with the city name in the appropriate colour.
- I realized it was actually easy to join the two instances of a city by a line (in green, here, 3rd line) by setting `group=city`:

```
g_opa <- ggplot(dp, aes(
  x = V1, y = V2, colour = which,
  label = city
)) + geom_point() +
  geom_line(aes(group = city), colour = "green") +
  geom_text_repel(size = 2)
```

- On plot, look to see whether points that are same city are joined by a short green line (good) or a long one (bad).

The maps


North Bay
North Bay
Huntsville
Huntsville
Ottawa
Ottawa
Cornwall
Cornwall
Barrie
Owen Sound
Barrie
Owen Sound
Peterborough
Peterborough
Belleville
Brockville
Brockville
Kingston
Kingston
Belleville
Toronto
Toronto
Hamilton
Kitchener
Kitchener
St Catharines
Niagara Falls
St Catharines
Hamilton
Brantford
Brantford
Niagara Falls
Sarnia
London
London
Sarnia
Windsor
Windsor
V1
V2
which
actual
MDS

Comments

- True locations red, MDS locations blue
- Most things in roughly right place (esp. relative to other things)
- Extreme cities off by a bit, but OK relative to neighbours.
- St Catharines, Niagara Falls off by most.
- Sarnia, Windsor also off noticeably.
- These four cities had largest “third dimension” in 3D representation `ontario2.3`.

Rotation matrix

Shows how MDS map needs to be rotated to get best match with actual coordinates:

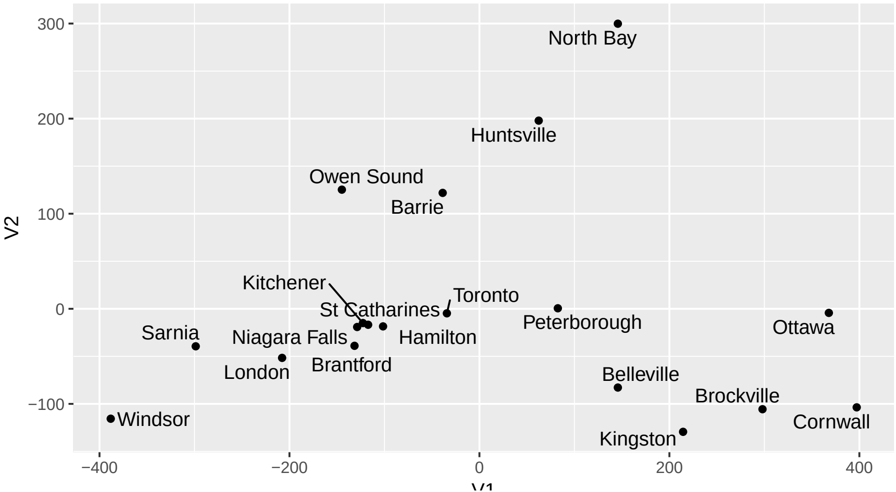
```
ontario.pro$R
```

```
##               [,1]      [,2]
## [1,]  0.8845749 0.4663981
## [2,] -0.4663981 0.8845749
```

Rotation angle θ such that $\cos\theta = 0.885$, $\sin\theta = 0.466$: $\theta = 23$ degrees (counterclockwise). $ %$ %$

Is that right? Look at MDS map again

```
g
```



A cube

```
a-----b
|\    |\
| c---- d
| |   | |
e-|---f |
\|    \|
g-----h
```

Cube has side length 1, so distance across diagonal on same face is $\sqrt{2} \simeq 1.4$ and "long" diagonal of cube is $\sqrt{3} \simeq 1.7$.

Try MDS on this obviously 3-dimensional data.

Cube data as distances

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/cube.txt"
cube <- read_delim(my_url, " ")
cube
```

```
## # A tibble: 8 x 9
##   x     `  a` `  b` `  c` `  d` `  e` `   f` `g`   `  h`
##   <chr> <chr> <chr> <chr> <chr> <chr> <chr>  <chr> <chr>
## 1 a     "  0" " NA" " NA" " NA" " NA" "  NA" <NA>  " NA"
## 2 b     "  1" "  0" " NA" " NA" " NA" "  NA" <NA>  " NA"
## 3 c     "  1" "  1" "  0" " NA" " NA" "  NA" <NA>  " NA"
## 4 d     1.4   "  1" "  1" "  0" " NA" "  NA" <NA>  " NA"
## 5 e     "  1" 1.4   1.4   1.7   "  0" "  NA" <NA>  " NA"
## 6 f     1.4   "  1" 1.7   1.4   "  1" "   0" <NA>  " NA"
## 7 g     1.4   1.7   "  1" 1.4   "  1" " 1.4" " 0"  " NA"
## 8 h     1.7   1.4   1.4   "  1" 1.4   "   1" " 1"  "  0"
```

Making dist object

```
cube.d <- cube %>% select(-1) %>% as.dist()
```

```
## Warning in storage.mode(m) <- "numeric": NAs introduced by
## coercion
```

```
cube.d
```

```
##          a   b   c   d   e    f   g
##    b  1.0
##    c  1.0 1.0
##    d  1.4 1.0 1.0
##    e  1.0 1.4 1.4 1.7
##     f 1.4 1.0 1.7 1.4 1.0
##   g   1.4 1.7 1.0 1.4 1.0  1.4
##    h  1.7 1.4 1.4 1.0 1.4  1.0 1.0
```

MDS and plotting commands

- By default in 2 dimensions; save the extra stuff for later:

```
cube.2 <- cube.d %>% cmdscale(eig = T)
```

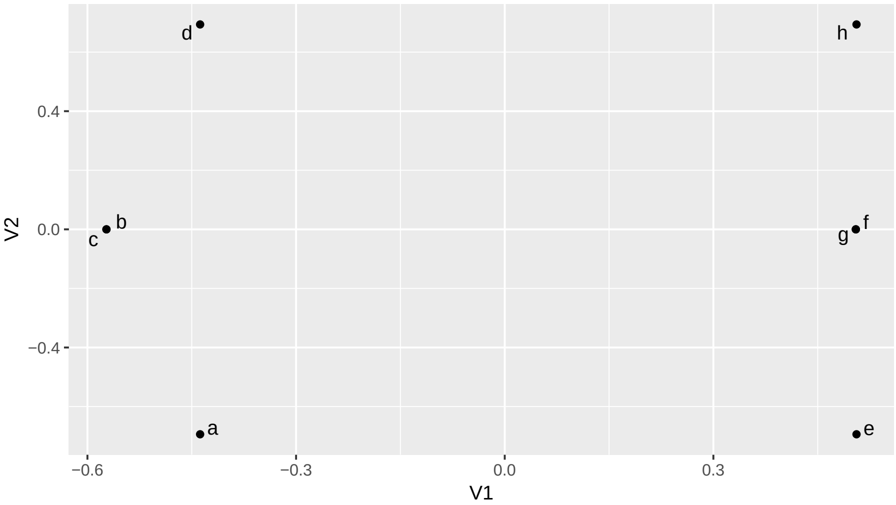
- Make data frame to plot, remembering the points to plot are in `points` now:

```
d <- cube.2$points %>%
  as_tibble() %>%
  mutate(corners = cube$x)
```

- Plot points labelled by our names for the corners:

```
g <- ggplot(d, aes(x = V1, y = V2, label = corners)) +
  geom_point() + geom_text_repel()
```

The "cube"



2 and 3 dimensions

```
cube.3 <- cube.d %>% cmdscale(3, eig = T)
cube.2$GOF
```

```
## [1] 0.639293 0.664332
```

```
cube.3$GOF
```

```
## [1] 0.9143532 0.9501654
```

- Really need 3rd dimension to represent cube.

Non-metric scaling

- Sometimes distances not meaningful *as distances*
- Only order matters: closest should be closest, farthest farthest on map, but how much further doesn't matter.
- Non-metric scaling, aims to minimize **stress**, measure of lack of fit.
- Example: languages. Make map based on "similarity" of number names, without requiring that 1 is "eight times better" than 8.

The languages

- Recall language data (from cluster analysis): 1–10, measure dissimilarity between two languages by how many number names {*differ*} *in first letter:*

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/languages.t
number.d <- read_table(my_url)
number.d
```

```
## # A tibble: 11 x 12
##    la       en    no    dk    nl    de    fr    es
##    <chr> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
##  1 en        0     2     2     7     6     6     6
##  2 no        2     0     1     5     4     6     6
##  3 dk        2     1     0     6     5     6     5
##  4 nl        7     5     6     0     5     9     9
##  5 de        6     4     5     5     0     7     7
##  6 fr        6     6     6     9     7     0     2
```

Non-metric scaling

- Turn language dissimilarities into `dist` object
- Run through `isoMDS` from `MASS` package; works like `cmdscale`.
- Map only reproduces {*relative*} *closeness of languages.*

```
d <- number.d %>%
  select_if(is.numeric) %>%
  as.dist()
number.nm <- d %>% isoMDS()
```

```
## initial  value 12.404671
## iter   5 value 5.933653
## iter  10 value 5.300747
## final  value 5.265236
## converged
```

```
names(number.nm)
```

Results

- Stress is very low (5%, good):

```
number.nm$stress
```

```
## [1] 5.265236
```

$ %$ %$

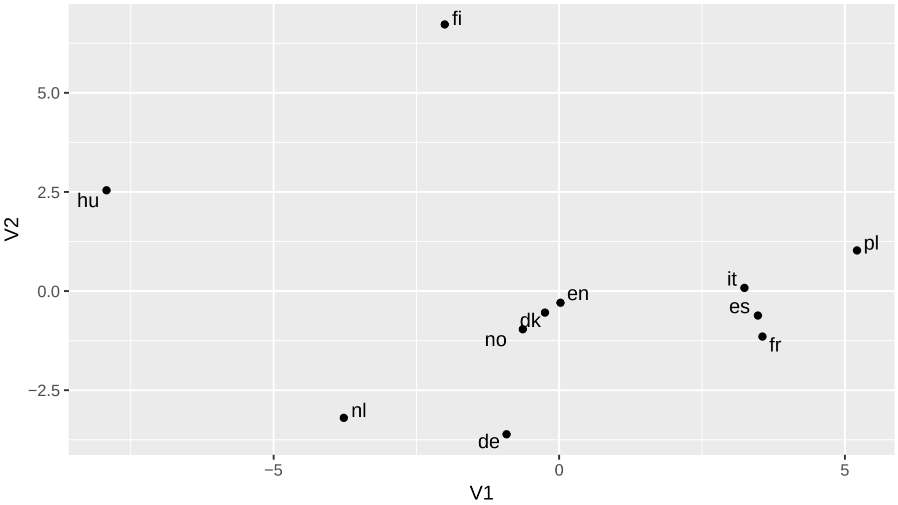
- Familiar process: make a data frame to plot. Use name `dd` for data frame this time since used `d` for distance object:

```
dd <- number.nm$points %>%
  as_tibble() %>%
  mutate(lang = number.d$la)
```

- Make plot:

```
g <- ggplot(dd, aes(x = V1, y = V2, label = lang)) +
  geom_point() + geom_text_repel()
```

The languages map



Comments

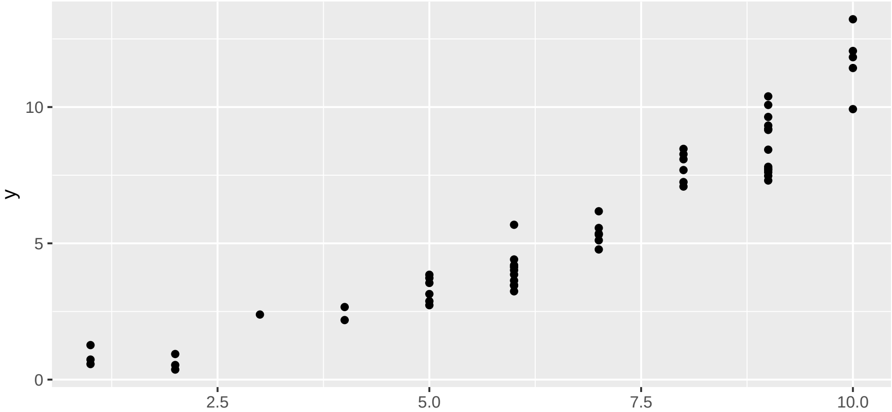
- Tight clusters: Italian-Spanish-French, English-Danish-Norwegian.
- Dutch and German close to English group.
- Polish close to French group.
- Hungarian, Finnish distant from everything else and each other!
- Similar conclusions as from the cluster analysis.

Shepard diagram

- Stress for languages data was 5.3%, very low.
- How do observed dissimilarities and map distances correspond?
- For low stress, expect larger dissimilarity to go with larger map distance, almost all the time.
- Not necessarily a linear trend since non-metric MDS works with *order* of values.
- Actual dissimilarity on x-axis; map distances on y-axis.

Shepard diagram for languages

```
Shepard(d, number.nm$points) %>%
  as_tibble() %>%
  ggplot(aes(x = x, y = y)) + geom_point()
```



Cube, revisited

```
cube.d <- cube %>% select(-x) %>% as.dist(cube)
```

```
## Warning in storage.mode(m) <- "numeric": NAs introduced
## by coercion
```

```
cube.2 <- isoMDS(cube.d, trace = F)
cube.2$stress
```

```
## [1] 17.97392
```

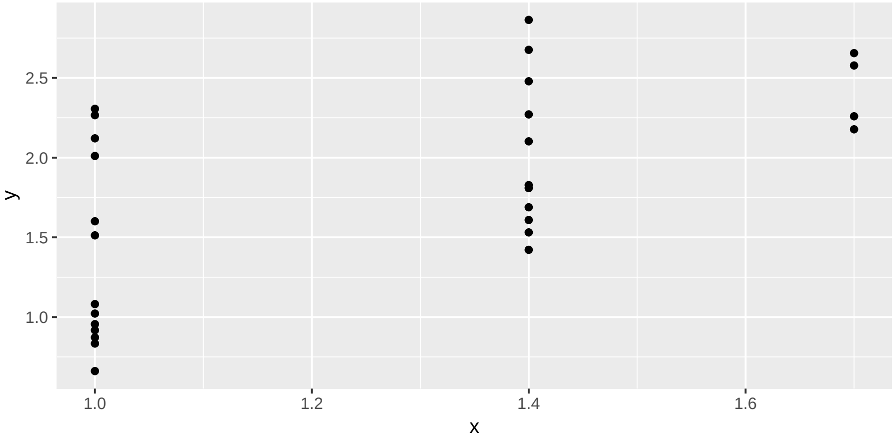
```
cube.3 <- isoMDS(cube.d, k = 3, trace = F)
cube.3$stress
```

```
## [1] 0.007819523
```

- Stress is 18% for 2 dimensions, basically 0% for 3.
- Three dimensions correct, two dimensions bad.
- Shepard diagrams for these:

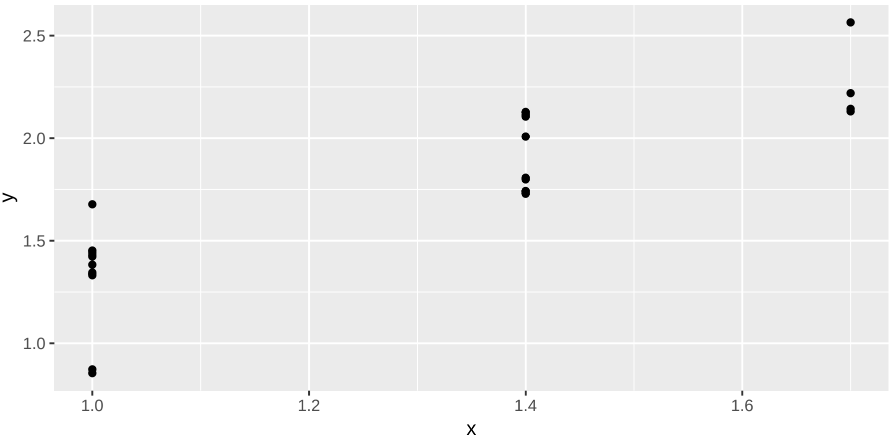
Shepard diagram for 2-dimensional cube

```
g2
```



Shepard diagram for 3-dimensional cube

```
g3
```



Guidelines for stress values, in %

Smaller is better:

Stress value	Interpretation
Less than 5	Excellent: no prospect of misinterpretation (rarely achieved)
5–10	Good: most distances reproduced well, small prospect of false inferences
10–20	Fair: usable, but some distances misleading.
More than 20	Poor: may be dangerous to interpret

- Languages: stress in "good" range.
- Cube:
- 2 dimensions "fair", almost "poor";
- 3 dimensions, "excellent". «echo=F, warning=F»= pkgs = names(sessionInfo()$otherPkgs) pkgs=paste('package:', pkgs, sep = "") x=lapply(pkgs, detach, character.only = TRUE, unload = TRUE)

Section 12

Principal components

Principal Components

- Have measurements on (possibly large) number of variables on some individuals.
- Question: can we describe data using fewer variables (because original variables correlated in some way)?
- Look for direction (linear combination of original variables) in which values {*most spread out*}. *This is* {first principal component}.
- Second principal component then direction uncorrelated with this in which values then most spread out. And so on.

Principal components

- See whether small number of principal components captures most of variation in data.
- Might try to interpret principal components.
- If 2 components good, can make plot of data.
- (Like discriminant analysis, but no groups.)
- "What are important ways that these data vary?"

Packages

```
## Warning: package 'plyr' was built under R version 3.5.1
## Warning: package 'ggbiplot' was built under R version
## 3.5.1
## Warning: package 'scales' was built under R version
## 3.5.1
```

You might not have installed the first of these. See over for instructions.

```
library(ggbiplot) # see over
library(tidyverse)
library(ggrepel)
```

Installing ggbiplot

- `ggbiplot` not on CRAN, so usual `install.packages` will not work.
- Install package `devtools` first (once):

```
install.packages("devtools")
```

- Then install `ggbiplot` (once):

```
library(devtools)
install_github("vqv/ggbiplot")
```

Small example: 2 test scores for 8 people

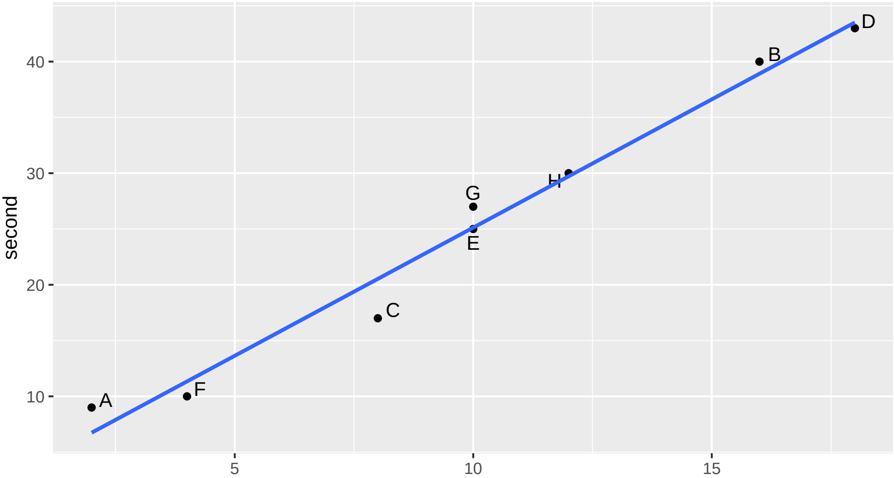
```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/test12.txt'
test12 <- read_table2(my_url)
test12
```

```
## # A tibble: 8 x 3
##   first second id
##   <dbl>  <dbl> <chr>
## 1     2      9 A
## 2    16     40 B
## 3     8     17 C
## 4    18     43 D
## 5    10     25 E
## 6     4     10 F
## 7    10     27 G
## 8    12     30 H
```

```
g <- ggplot(test12, aes(x = first, y = second, label = id)) +
```

The plot

```r
g + geom_smooth(method = "lm", se = F)
```



Principal component analysis

- Grab just the numeric columns:

```
test12_numbers <- test12 %>% select_if(is.numeric)
```

- Strongly correlated, so data nearly 1-dimensional:

```
cor(test12_numbers)
```

```
##             first   second
## first  1.000000 0.989078
## second 0.989078 1.000000
```

- Make a score summarizing this one dimension. Like this:

```
test12.pc <- test12_numbers %>% princomp(cor = T)
summary(test12.pc)
```

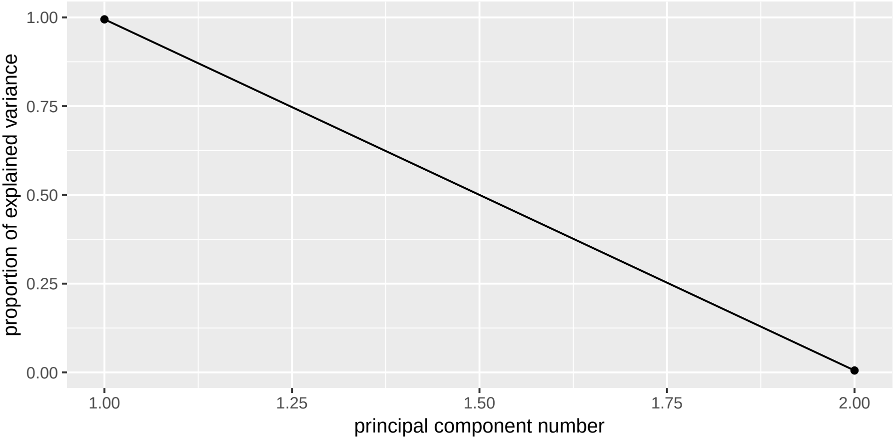
```
## Importance of components:
##                            Comp.1     Comp.2
```

Comments

- "Standard deviation" shows relative importance of components (as for LDs in discriminant analysis)
- Here, first one explains almost all (99.4%) of variability.
- That is, look only at first component and ignore second.
- `cor=T` standardizes all variables first. Usually wanted, because variables measured on different scales. (Only omit if variables measured on same scale and expect similar variability.)

Scree plot

```
ggscreeplot(test12.pc)
```



Component loadings

explain how each principal component depends on (standardized) original variables (test scores):

```
test12.pc$loadings
```

```
##
## Loadings:
##        Comp.1 Comp.2
## first   0.707  0.707
## second  0.707 -0.707
##
##                Comp.1 Comp.2
## SS loadings       1.0    1.0
## Proportion Var    0.5    0.5
## Cumulative Var    0.5    1.0
```

First component basically negative sum of (standardized) test scores. That

Component scores

```
d <- data.frame(test12, test12.pc$scores)
d
```

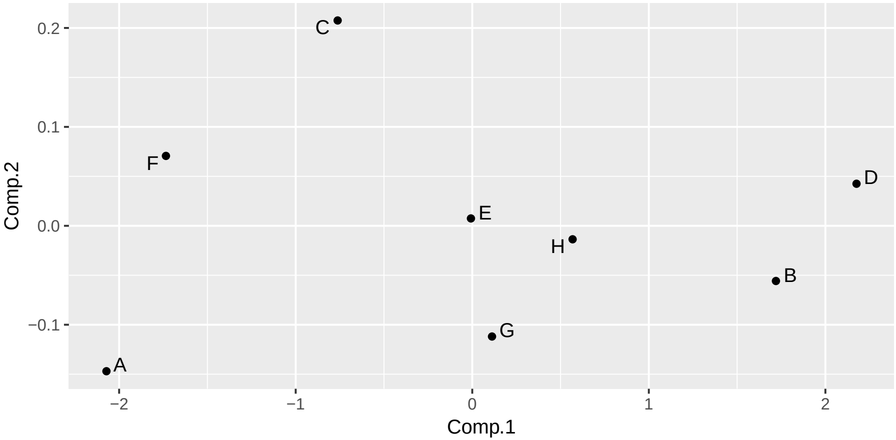
```
##   first second id       Comp.1       Comp.2
## 1     2      9  A -2.071819003 -0.146981782
## 2    16     40  B  1.719862811 -0.055762223
## 3     8     17  C -0.762289708  0.207589512
## 4    18     43  D  2.176267535  0.042533250
## 5    10     25  E -0.007460609  0.007460609
## 6     4     10  F -1.734784030  0.070683441
## 7    10     27  G  0.111909141 -0.111909141
## 8    12     30  H  0.568313864 -0.013613668
```

$

- Person A is a low scorer, high positive `comp.1` score.
- Person D is high scorer, high negative `comp.1` score.

Plot of scores

```
ggplot(d, aes(x = Comp.1, y = Comp.2, label = id)) +
  geom_point() + geom_text_repel()
```



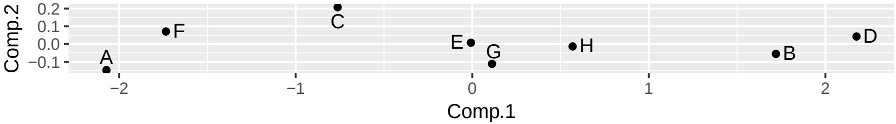
Comments

- Vertical scale exaggerates importance of comp.2.
- Fix up to get axes on same scale:

```
g <- ggplot(d, aes(x = Comp.1, y = Comp.2, label = id)) +
  geom_point() + geom_text_repel() +
  coord_fixed()
```

- Shows how exam scores really spread out along one dimension:

```
g
```

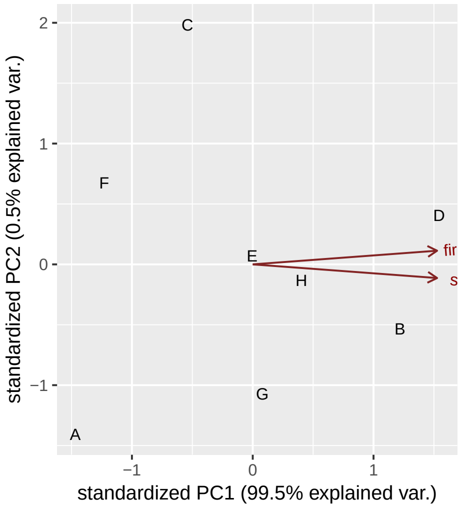


The biplot

- Plotting variables and individuals on one plot.
- Shows how components and original variables related.
- Shows how individuals score on each component, and therefore suggests how they score on each variable.
- Add `labels` option to identify individuals:

```
g <- ggbiplot(test12.pc, labels = test12$id)
```

The biplot


C
F
D
E
fir
H
s
B
G
A
2
1
0
−1
−1
0
1
standardized PC2 (0.5% explained var.)
standardized PC1 (99.5% explained var.)

Comments

- Variables point almost same direction (left). Thus very negative value on `comp.1` goes with high scores on both tests, and test scores highly correlated.
- Position of individuals on plot according to scores on principal components, implies values on original variables. Eg.:
- D very negative on `comp.1`, high scorer on both tests.
- A and F very positive on `comp.1`, poor scorers on both tests.
- C positive on `comp.2`, high score on first test relative to second.
- A negative on `comp.2`, high score on second test relative to first.

Track running data

(1984) track running records for distances 100m to marathon, arranged by country. Countries labelled by (mostly) Internet domain names (ISO 2-letter codes):

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/men_track_f
track <- read_table(my_url)
track %>% sample_n(12)
```

```
## # A tibble: 12 x 9
##      m100  m200  m400  m800 m1500 m5000 m10000 marathon coun
##     <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>  <dbl>    <dbl> <chr
## 1   10.4  20.8  46.8  1.79  3.6   13.3   27.7     136. at
## 2   10.0  19.7  45.3  1.73  3.6   13.2   27.5     131. it
## 3   10.3  20.6  46.0  1.77  3.62  13.5   28.4     133. hu
## 4   10.2  20.2  45.7  1.76  3.63  13.6   28.1     130. ca
## 5   10.4  21.0  45.9  1.76  3.64  13.2   27.7     132. ro
## 6   10.2  20.2  45.4  1.76  3.6   13.3   27.9     132. pl
```

Country names

Also read in a table to look country names up in later:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/isocodes.cs
iso <- read_csv(my_url)
iso
```

```
## # A tibble: 251 x 4
##    Country        ISO2  ISO3    M49
##    <chr>          <chr> <chr> <dbl>
##  1 <NA>           <NA>  <NA>     NA
##  2 Afghanistan    af    afg       4
##  3 Aland Islands  ax    ala     248
##  4 Albania        al    alb       8
##  5 Algeria        dz    dza      12
##  6 American Samoa as    asm      16
##  7 Andorra        ad    and      20
##  8 Angola         ao    ago      24
```

Data and aims

- Times in seconds 100m–400m, in minutes for rest (800m up).
- This taken care of by standardization.
- 8 variables; can we summarize by fewer and gain some insight?
- In particular, if 2 components tell most of story, what do we see in a plot?

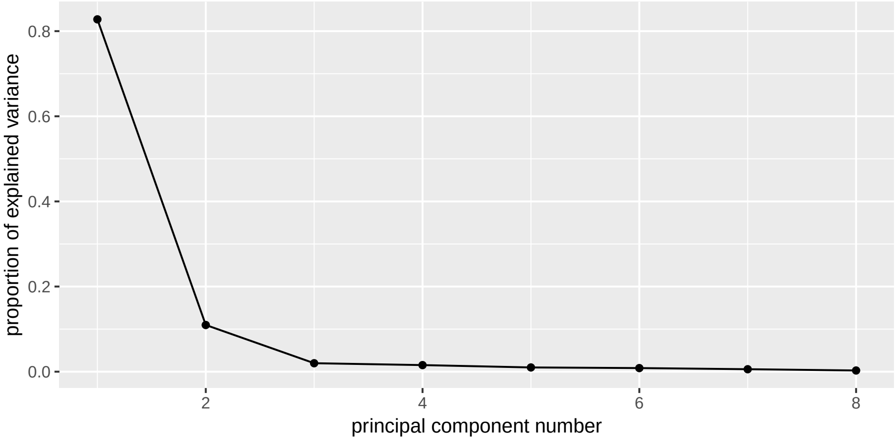
Fit and examine principal components

```
track_num <- track %>% select_if(is.numeric)
track.pc <- princomp(track_num, cor = T)
summary(track.pc)
```

```
## Importance of components:
##                           Comp.1    Comp.2
## Standard deviation     2.5733531 0.9368128
## Proportion of Variance 0.8277683 0.1097023
## Cumulative Proportion  0.8277683 0.9374706
##                            Comp.3     Comp.4
## Standard deviation     0.39915052 0.35220645
## Proportion of Variance 0.01991514 0.01550617
## Cumulative Proportion  0.95738570 0.97289187
##                             Comp.5      Comp.6
## Standard deviation     0.282630981 0.260701267
## Proportion of Variance 0.009985034 0.008495644
## Cumulative Proportion  0.982876903 0.991372547
```

Scree plot

```
ggscreeplot(track.pc)
```



How many components?

- As for discriminant analysis, look for “elbow” in scree plot.
- See one here at 3 components; everything 3 and beyond is “scree”.
- So take 2 components.
- Note difference from discriminant analysis: want “large” rather than “small”, so go 1 step left of elbow.
- Another criterion: any component with eigenvalue bigger than about 1 is worth including. 2nd one here has eigenvalue just less than 1.
- Refer back to `summary`: cumulative proportion of variance explained for 2 components is 93.7%, pleasantly high. 2 components tell almost whole story.

How do components depend on original variables?

Loadings:

```
track.pc$loadings
```

```
##
## Loadings:
##          Comp.1 Comp.2 Comp.3 Comp.4 Comp.5 Comp.6 Comp.7
## m100      0.318  0.567  0.332  0.128  0.263  0.594  0.136
## m200      0.337  0.462  0.361 -0.259 -0.154 -0.656 -
0.113
## m400      0.356  0.248 -0.560  0.652 -0.218 -0.157
## m800      0.369        -0.532 -0.480  0.540        -
0.238
## m1500     0.373 -0.140 -0.153 -0.405 -0.488  0.158  0.610
## m5000     0.364 -0.312  0.190        -0.254  0.141 -
0.591
## m10000    0.367 -0.307  0.182        -0.133  0.219 -
```

Comments

- `comp.1` loads about equally (has equal weight) on times over all distances.
- `comp.2` has large positive loading for long distances, large negative for short ones.
- `comp.3`: large negative for middle distance, large positive especially for short distances.
- Country overall good at running will have lower than average record times at all distances, so `comp.1` *large*. Conversely, for countries bad at running, `comp.1` very negative.
- Countries relatively better at sprinting (low times) will be *positive* on `comp.2`; countries relatively better at distance running *negative* on `comp.2`.

Commands for plots

- Principal component scores (first two). Also need country names.

```
d <- data.frame(track.pc$scores,
  country = track$country
)
names(d)
```

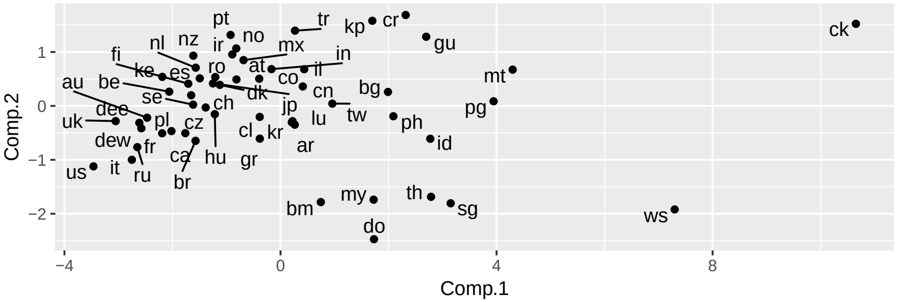
```
## [1] "Comp.1"  "Comp.2"  "Comp.3"  "Comp.4"  "Comp.5"
## [6] "Comp.6"  "Comp.7"  "Comp.8"  "country"
```

```
g1 <- ggplot(d, aes(
  x = Comp.1, y = Comp.2,
  label = country
)) +
  geom_point() + geom_text_repel() +
  coord_fixed()
```

- Biplot:

Principal components plot

```
g1
```

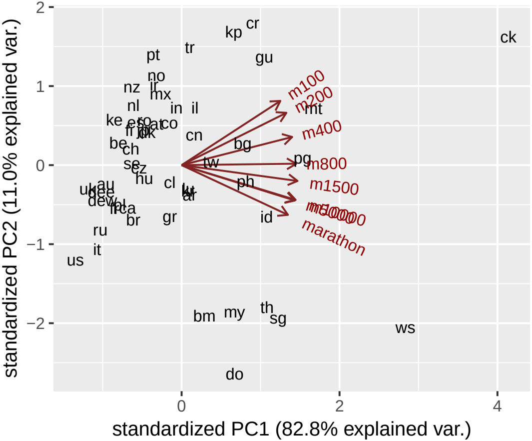


Comments on principal components plot

- Good running countries at right of plot: US, UK, Italy, Russia, East and West Germany.
- Bad running countries at left: Western Samoa, Cook Islands.
- Better sprinting countries at bottom: US, Italy, Russia, Brazil, Greece. `do` is Dominican Republic, where sprinting records relatively good, distance records very bad.
- Better distance-running countries at top: Portugal, Norway, Turkey, Ireland, New Zealand, Mexico. `ke` is Kenya.

Biplot

g2


standardized PC2 (11.0% explained var.)
standardized PC1 (82.8% explained var.)
2
1
0
−1
−2
0
2
4
m100
m200
m400
m800
m1500
marathon
ck
kp
cr
tr
pt
gu
no
nz
ir
mx
nl
in
il
mt
ke
co
cn
be
ch
bg
pg
se
cz
tw
hu
cl
ph
au
ru
it
us
br
gr
id
bm
my
th
sg
ws
do

Comments on biplot

- Had to do some pre-work to interpret PC plot. Biplot more self-contained.
- All variable arrows point left; countries on left have large (bad) record times overall, countries on right good overall.
- Variable arrows extend negatively as well. Top left = bad at distance running, bottom right = good at distance running.
- Bottom left = bad at sprinting, top right = good at sprinting.
- Doesn't require so much pre-interpretation of components.

How do I know which country is which?

Need to look up two-letter abbreviations in ISO table, eg. for best 8 running countries:

```
d %>%
  arrange(desc(Comp.1)) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.1, country, Country) %>%
  slice(1:8)
```

```
##      Comp.1 country          Country
## 1 10.652914      ck     Cook Islands
## 2  7.297865      ws            Samoa
## 3  4.297909      mt            Malta
## 4  3.945224      pg Papua New Guinea
## 5  3.150886      sg        Singapore
## 6  2.787273      th         Thailand
## 7  2.773125      id        Indonesia
```

Best 8 running countries

```
d %>%
  arrange(Comp.1) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.1, country, Country) %>%
  slice(1:8)
```

```
##      Comp.1 country                  Country
## 1 -3.462175      us United States of America
## 2 -3.052104      uk           United Kingdom
## 3 -2.752084      it                    Italy
## 4 -2.651062      ru       Russian Federation
## 5 -2.613964     dee             East Germany
## 6 -2.576272     dew             West Germany
## 7 -2.468919      au                Australia
## 8 -2.191917      fr                   France
```

Worst 8 running countries

```
d %>%
  arrange(desc(Comp.1)) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.1, country, Country) %>%
  slice(1:8)
```

```
##      Comp.1 country          Country
## 1 10.652914      ck     Cook Islands
## 2  7.297865      ws            Samoa
## 3  4.297909      mt            Malta
## 4  3.945224      pg Papua New Guinea
## 5  3.150886      sg        Singapore
## 6  2.787273      th         Thailand
## 7  2.773125      id        Indonesia
## 8  2.697066      gu             Guam
```

Better at distance running

```
d %>%
  arrange(desc(Comp.2)) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.2, country, Country) %>%
  slice(1:8)
```

```
##      Comp.2 country                      Country
## 1 1.6860391      cr                   Costa Rica
## 2 1.5791490      kp                Korea (North)
## 3 1.5226742      ck                 Cook Islands
## 4 1.3957839      tr                       Turkey
## 5 1.3167578      pt                     Portugal
## 6 1.2829272      gu                         Guam
## 7 1.0663756      no                       Norway
## 8 0.9547437      ir Iran, Islamic Republic of
```

Better at sprinting

```
d %>%
  arrange(Comp.2) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.2, country, Country) %>%
  slice(1:10)
```

```
##        Comp.2 country                  Country
## 1  -2.4715736      do       Dominican Republic
## 2  -1.9196130      ws                    Samoa
## 3  -1.8055052      sg                Singapore
## 4  -1.7832229      bm                  Bermuda
## 5  -1.7386063      my                 Malaysia
## 6  -1.6851772      th                 Thailand
## 7  -1.1204235      us United States of America
## 8  -0.9989821      it                    Italy
## 9  -0.7639385      ru       Russian Federation
## 10 -0.6470634      br                   Brazil
```

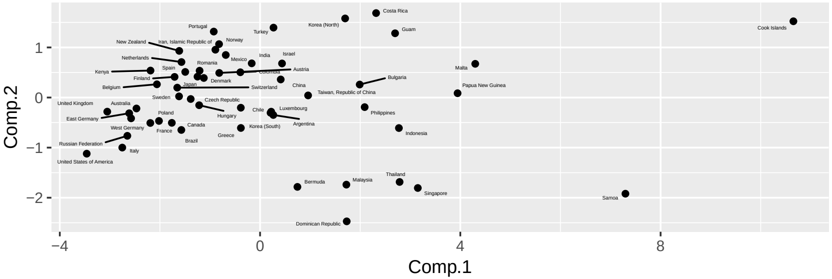
Plot with country names

```
g <- d %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Comp.1, Comp.2, Country) %>%
  ggplot(aes(x = Comp.1, y = Comp.2, label = Country)) +
  geom_point() + geom_text_repel(size = 1) +
  coord_fixed()
```

```
## Warning: Column `country`/`ISO2` joining factor and
## character vector, coercing into character vector
```

The plot

```
g
```


Costa Rica
Korea (North)
Cook Islands
Portugal
Turkey
Guam
New Zealand
Iran, Islamic Republic of
Norway
Netherlands
India
Israel
Mexico
Romania
Kenya
Spain
Colombia
Austria
Malta
Finland
Denmark
Bulgaria
Belgium
Japan
Switzerland
China
Papua New Guinea
Taiwan, Republic of China
Sweden
Czech Republic
United Kingdom
Australia
Chile
Luxembourg
Poland
Hungary
Philippines
East Germany
Canada
Argentina
West Germany
France
Korea (South)
Greece
Indonesia
Brazil
Russian Federation
Italy
United States of America
Thailand
Bermuda
Malaysia
Singapore
Samoa
Dominican Republic
Comp.2
Comp.1
1
0
−1
−2
−4
0
4
8

Principal components from correlation matrix

Create data file like this: cov.txt and read in like this:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/cov.txt"
mat <- read_table(my_url, col_names = F)
mat
```

```
## # A tibble: 3 x 3
##       X1     X2     X3
##    <dbl>  <dbl>  <dbl>
## 1  1      0.970 -0.96
## 2  0.970  1     -0.998
## 3 -0.96  -0.998  1
```

Pre-processing

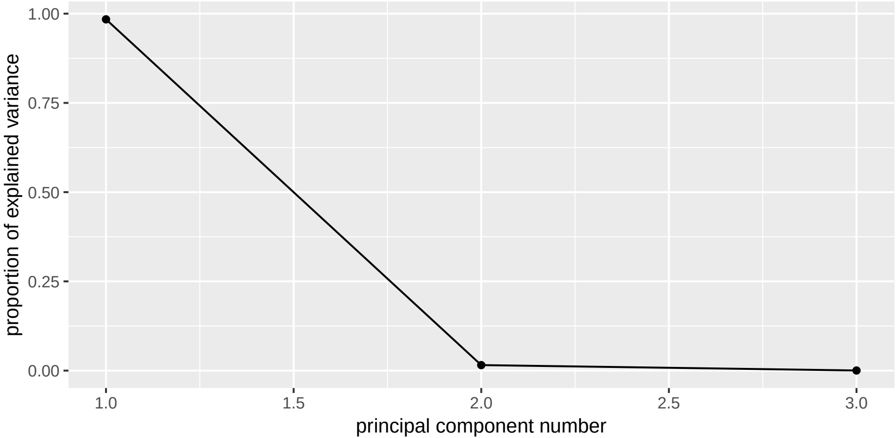
A little pre-processing required:

- Turn into matrix (from data frame)
- Feed into `princomp` as `covmat=`

```
mat.pc <- mat %>%
  as.matrix() %>%
  princomp(covmat = .)
```

Scree plot: one component fine

```
ggscreeplot(mat.pc)
```



Component loadings

Compare correlation matrix:
“‘r mat “‘
“‘ A tibble: 3 x 3 X1 X2 X3 <dbl> <dbl> <dbl> 1 1 0.970 -0.96 2 0.970 1 -0.998 3 -0.96 -0.998 1 “‘
with component loadings
“‘r mat.pc$loadings$“‘
“‘ Loadings: Comp.1 Comp.2 Comp.3 X1 0.573 0.812 0.112 X2 0.581 -0.306 -0.755 X3 -0.578 0.498 -0.646 Comp.1 Comp.2 Comp.3 SS loadings 1.000 1.000 1.000 Proportion Var 0.333 0.333 0.333 Cumulative Var 0.333 0.667 1.000 “‘

* When X1 large, X2 also large, X3 small.
* Then ‘comp.1‘ *negative*.
* When X1 small, X2 small, X3 large.
* Then ‘comp.1‘ *positive*.

No scores

- With correlation matrix rather than data, no component scores
- So no principal component plot
- and no biplot.

Section 13

Exploratory factor analysis

Principal components and factor analysis

- Principal components:
- Purely mathematical.
- Find eigenvalues, eigenvectors of correlation matrix.
- No testing whether observed components reproducible, or even probability model behind it.
- Factor analysis:
- some way towards fixing this (get test of appropriateness)
- In factor analysis, each variable modelled as: "common factor" (eg. verbal ability) and "specific factor" (left over).
- Choose the common factors to "best" reproduce pattern seen in correlation matrix.
- Iterative procedure, different answer from principal components.

Packages

```
library(lavaan) # for confirmatory, later
library(ggbiplot)
library(tidyverse)
```

Example

- 145 children given 5 tests, called PARA, SENT, WORD, ADD and DOTS. 3 linguistic tasks (paragraph comprehension, sentence completion and word meaning), 2 mathematical ones (addition and counting dots).
- Correlation matrix of scores on the tests:

```
para 1     0.722 0.714 0.203 0.095
sent 0.722 1     0.685 0.246 0.181
word 0.714 0.685 1     0.170 0.113
add  0.203 0.246 0.170 1     0.585
dots 0.095 0.181 0.113 0.585 1
```

- Is there small number of underlying “constructs” (unobservable) that explains this pattern of correlations?

To start: principal components

Using correlation matrix:

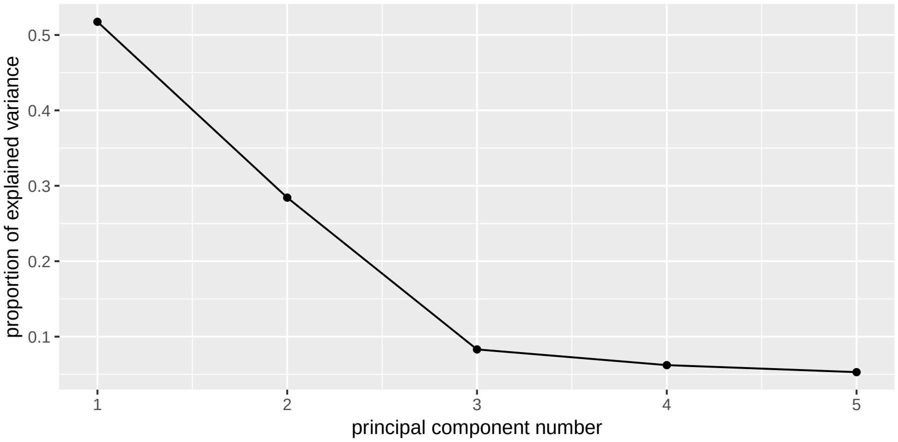
```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/rex2.txt"
kids <- read_delim(my_url, " ")
kids
```

```
## # A tibble: 5 x 6
##   test   para  sent  word   add  dots
##   <chr> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 para  1     0.722 0.714 0.203 0.095
## 2 sent  0.722 1     0.685 0.246 0.181
## 3 word  0.714 0.685 1     0.17  0.113
## 4 add   0.203 0.246 0.17  1     0.585
## 5 dots  0.095 0.181 0.113 0.585 1
```

```
kids.pc <- kids %>%
  select_if(is.numeric) %>%
  as.matrix() %>%
```

Scree plot

```
ggscreeplot(kids.pc)
```



Principal component results

- Need 2 components. Loadings:

```
kids.pc$loadings
```

```
##
## Loadings:
##      Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## para  0.534  0.245  0.114         0.795
## sent  0.542  0.164         0.660 -0.489
## word  0.523  0.247 -0.144 -0.738 -0.316
## add   0.297 -0.627  0.707
## dots  0.241 -0.678 -0.680         0.143
##
##                Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## SS loadings       1.0    1.0    1.0    1.0    1.0
## Proportion Var    0.2    0.2    0.2    0.2    0.2
## Cumulative Var    0.2    0.4    0.6    0.8    1.0
```

Factor analysis

- Specify number of factors first, get solution with exactly that many factors.
- Includes hypothesis test, need to specify how many children wrote the tests.
- Works from correlation matrix via `covmat` or actual data, like `princomp`.
- Introduces extra feature, *rotation*, to make interpretation of loadings (factor-variable relation) easier.

Factor analysis for the kids data

- Create "covariance list" to include number of children who wrote the tests.
- Feed this into `factanal`, specifying how many factors (2).

```
km <- kids %>%
  select_if(is.numeric) %>%
  as.matrix()
km2 <- list(cov = km, n.obs = 145)
kids.f2 <- factanal(factors = 2, covmat = km2)
```

Uniquenesses

```
kids.f2$uniquenesses
```

```
##      para      sent      word       add      dots
## 0.2424457 0.2997349 0.3272312 0.5743568 0.1554076
```

$

- Uniquenesses say how "unique" a variable is (size of specific factor). Small uniqueness means that the variable is summarized by a factor (good).
- Mildly worried by how large `add`'s uniqueness is.
- Also see "communality" for this, where *large* is good.

Loadings

"'r kids.f2$loadings$"'

"' Loadings: Factor1 Factor2 [1,] 0.867 [2,] 0.820 0.166 [3,] 0.816 [4,] 0.167 0.631 [5,] 0.918 Factor1 Factor2 SS loadings 2.119 1.282 Proportion Var 0.424 0.256 Cumulative Var 0.424 0.680 "'

* Loadings show how each factor depends on variables. Blanks indicate "small", less than 0.1.
* Factor 1 clearly the "linguistic" tasks, factor 2 clearly the "mathematical" ones.
* Two factors together explain 68% of variability (like regression R-squared).

Are 2 factors enough?

```
kids.f2$STATISTIC
```

```
## objective
## 0.5810578
```

```
kids.f2$dof
```

```
## [1] 1
```

```
kids.f2$PVAL
```

```
## objective
##  0.445898
```

P-value not small, so 2 factors OK.

1 factor

```
kids.f1 <- factanal(factors = 1, covmat = km2)
kids.f1$STATISTIC
```

```
## objective
##  58.16534
```

```
kids.f1$dof
```

```
## [1] 5
```

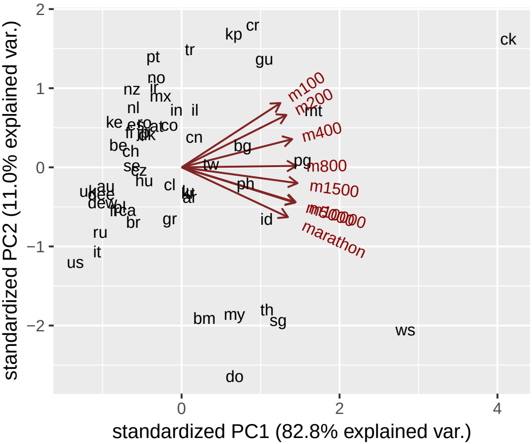
```
kids.f1$PVAL
```

```
##    objective
## 2.907856e-11
```

1 factor rejected (P-value small). Definitely need more than 1.

Track running records revisited

```
g2
```



Benefit of rotation

- 100m and marathon arrows almost perpendicular, but components don't match anything much:
- sprinting: top left and bottom right
- distance running: bottom left and top right.
- Can we arrange things so that components (factors) correspond to something meaningful?

Track records by factor analysis

Obtain factor scores (have actual data):

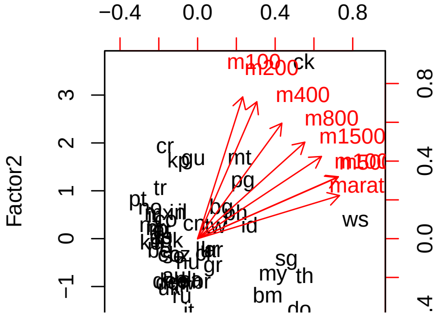
```
track
```

```
## # A tibble: 55 x 9
##     m100  m200  m400  m800 m1500 m5000 m10000 marathon
##    <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>  <dbl>    <dbl>
##  1  10.4  20.8  46.8  1.81  3.7   14.0   29.4     138.
##  2  10.3  20.1  44.8  1.74  3.57  13.3   27.7     128.
##  3  10.4  20.8  46.8  1.79  3.6   13.3   27.7     136.
##  4  10.3  20.7  45.0  1.73  3.6   13.2   27.4     130.
##  5  10.3  20.6  45.9  1.8   3.75  14.7   30.6     147.
##  6  10.2  20.4  45.2  1.73  3.66  13.6   28.6     133.
##  7  10.6  21.5  48.3  1.8   3.85  14.4   30.3     140.
##  8  10.2  20.2  45.7  1.76  3.63  13.6   28.1     130.
##  9  10.3  20.8  46.2  1.79  3.71  13.6   29.3     134.
## 10  10.5  21.0  47.3  1.81  3.73  13.9   29.1     134.
```

Track data biplot

Not so nice-looking:

```
biplot(track.f$scores, track.f$loadings,
  xlabs = track$country
)
```



Comments

- This time 100m "up" (factor 2), marathon "right" (factor 1).
- Countries most negative on factor 2 good at sprinting.
- Countries most negative on factor 1 good at distance running.

Rotated factor loadings

{

```
track.f$loadings
```

```
##
## Loadings:
##          Factor1 Factor2
## m100     0.291   0.914
## m200     0.382   0.882
## m400     0.543   0.744
## m800     0.691   0.622
## m1500    0.799   0.530
## m5000    0.901   0.394
## m10000   0.907   0.399
## marathon 0.915   0.278
##
##                Factor1 Factor2
## SS loadings      4.112   3.225
## Proportion Var   0.514   0.403
```

The best sprinting countries

Most negative on factor 2:

```
scores %>%
  arrange(Factor2) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Country, Factor1, Factor2) %>%
  slice(1:10)
```

```
##                     Country     Factor1    Factor2
## 1  United States of America -0.21942697 -1.7251036
## 2                     Italy -0.18436705 -1.4990521
## 3        Dominican Republic  2.12906546 -1.4666402
## 4        Russian Federation -0.32473110 -1.2236590
## 5                   Bermuda  1.46541593 -1.1704466
## 6            United Kingdom -0.58969058 -1.0139983
## 7                    France -0.25301846 -0.9519162
## 8              West Germany -0.46748876 -0.9079005
```

The best distance-running countries

Most negative on factor 1:

```
scores %>%
  arrange(Factor1) %>%
  left_join(iso, by = c("country" = "ISO2")) %>%
  select(Country, Factor1, Factor2) %>%
  slice(1:10)
```

```
##                       Country    Factor1     Factor2
## 1                    Portugal -1.2509805  0.78366889
## 2                      Norway -0.9920727  0.62299560
## 3                 New Zealand -0.9813348  0.26603491
## 4                       Kenya -0.9749696 -0.07099477
## 5   Iran, Islamic Republic of -0.9231505  0.50271208
## 6                 Netherlands -0.9078661  0.23948200
## 7                     Romania -0.8178386  0.18555001
## 8                      Mexico -0.8096291  0.51446762
```

A bigger example: BEM sex role inventory

- 369 women asked to rate themselves on 60 traits, like "self-reliant" or "shy".
- Rating 1 "never or almost never true of me" to 7 "always or almost always true of me".
- 60 personality traits is a lot. Can we find a smaller number of factors that capture aspects of personality?
- The whole BEM sex role inventory on next page.

The whole inventory

1. self reliant
2. yielding
3. helpful
4. defends own beliefs
5. cheerful
6. moody
7. independent
8. shy
9. conscientious
10. athletic
11. affectionate
12. theatrical
13. assertive
14. flatterable
15. happy
16. strong personality
17. loyal
18. unpredictable
19. forceful
20. feminine
21. reliable
22. analytical
23. sympathetic
24. jealous
25. leadership ability
26. sensitive to other's needs
27. truthful
28. willing to take risks
29. understanding
30. secretive
31. makes decisions easily
32. compassionate
33. sincere
34. self-sufficient
35. eager to soothe hurt feelings
36. conceited
37. dominant
38. soft spoken
39. likable
40. masculine
41. warm
42. solemn
43. willing to take a stand
44. tender
45. friendly
46. aggressive
47. gullible
48. inefficient
49. acts as a leader
50. childlike
51. adaptable
52. individualistic
53. does not use harsh language
54. unsystematic
55. competitive
56. loves children
57. tactful
58. ambitious
59. gentle
60. conventional

Some of the data

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/factor.txt'
bem <- read_tsv(my_url)
bem
```

```
## # A tibble: 369 x 45
##    subno helpful reliant defbel yielding cheerful indpt
##    <dbl>   <dbl>   <dbl>  <dbl>    <dbl>    <dbl> <dbl>
##  1     1       7       7      5        5        7     7
##  2     2       5       6      6        6        2     3
##  3     3       7       6      4        4        5     5
##  4     4       6       6      7        4        6     6
##  5     5       6       6      7        4        7     7
##  6     7       5       6      7        4        6     6
##  7     8       6       4      6        6        6     3
##  8     9       7       6      7        5        6     7
##  9    10       7       6      6        4        4     5
## 10    11       7       4      7        4        7     5
```

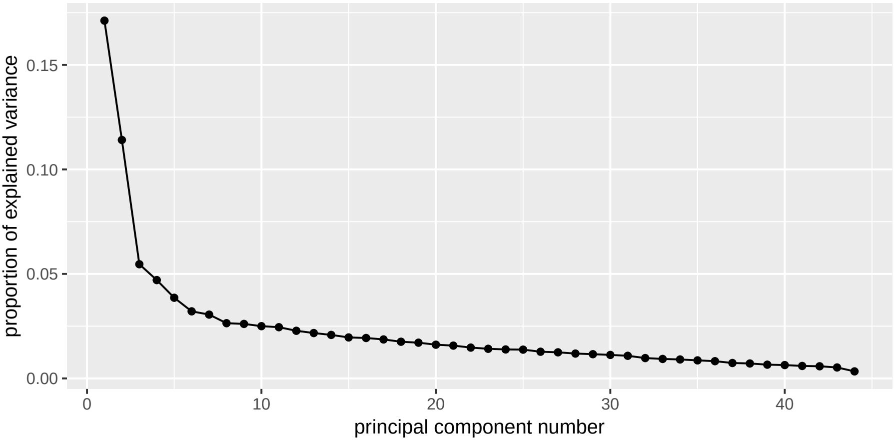
Principal components first

…to decide on number of factors:

```
bem.pc <- bem %>%
  select(-subno) %>%
  princomp(cor = T)
```

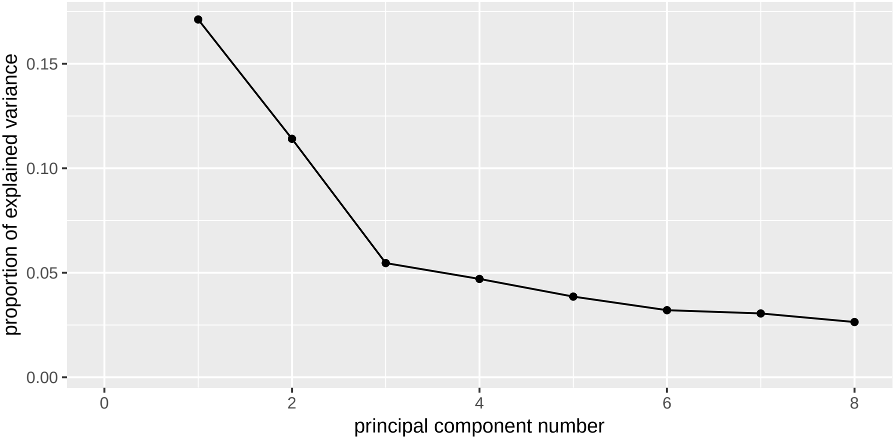
The scree plot

```
g <- ggscreeplot(bem.pc)
g
```



Zoom in to search for elbow

```
g + scale_x_continuous(limits = c(0, 8))
```



but is 2 really good?

{

```
summary(bem.pc)
```

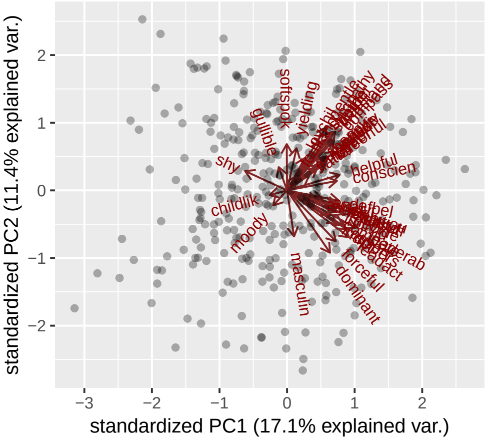
```
## Importance of components:
##                           Comp.1    Comp.2     Comp.3
## Standard deviation     2.7444993 2.2405789 1.55049106
## Proportion of Variance 0.1711881 0.1140953 0.05463688
## Cumulative Proportion  0.1711881 0.2852834 0.33992029
##                            Comp.4     Comp.5     Comp.6
## Standard deviation     1.43886350 1.30318840 1.18837867
## Proportion of Variance 0.04705291 0.03859773 0.03209645
## Cumulative Proportion  0.38697320 0.42557093 0.45766738
##                            Comp.7     Comp.8     Comp.9
## Standard deviation     1.15919129 1.07838912 1.07120568
## Proportion of Variance 0.03053919 0.02643007 0.02607913
## Cumulative Proportion  0.48820657 0.51463664 0.54071577
##                           Comp.10    Comp.11    Comp.12
## Standard deviation     1.04901318 1.03848656 1.00152287
## Proportion of Variance 0.02500974 0.02451033 0.02279655
## Cumulative Proportion  0.56572551 0.59023584 0.61303238
##                           Comp.13    Comp.14   Comp.15
## Standard deviation     0.97753974 0.95697572 0.9287543
## Proportion of Variance 0.02171782 0.02081369 0.0196042
```

Comments

- Want overall fraction of variance explained ("cumulative proportion") to be reasonably high.
- 2 factors, 28.5%. Terrible!
- Even 56% (10 factors) not that good!
- Have to live with that.

Biplot

```
ggbiplot(bem.pc, alpha = 0.3)
```



Comments

- Ignore individuals for now.
- Most variables point to 10 o'clock or 7 o'clock.
- Suggests factor analysis with rotation will get interpretable factors (rotate to 6 o'clock and 9 o'clock, for example).
- Try for 2-factor solution (rough interpretation, will be bad):

```
bem.2 <- bem %>%
  select(-subno) %>%
  factanal(factors = 2)
```

- Show output in pieces (just print `bem.2` to see all of it).

Uniquenesses

```
bem.2$uniquenesses
```

```
##   helpful  reliant   defbel yielding cheerful    indpt
## 0.7598223 0.7808058 0.7748448 0.8688473 0.8394916 0.7282742
##    athlet      shy   assert  strpers forceful   affect
## 0.9229702 0.8239496 0.6329347 0.5679398 0.5631857 0.6616625
##   flatter    loyal   analyt feminine sympathy    moody
## 0.9409500 0.8035264 0.8968744 0.8829927 0.7231450 0.9730607
##  sensitiv undstand  compass leaderab   soothe     risk
## 0.8018851 0.6194392 0.5937073 0.4091894 0.6596103 0.7789761
##    decide selfsuff conscien dominant masculin    stand
## 0.6938578 0.7210246 0.7974820 0.4942909 0.8453368 0.6024001
##     happy softspok     warm truthful   tender gullible
## 0.8008966 0.8339058 0.4764762 0.8889983 0.4928919 0.9583435
##   leadact childlik  individ foullang  lovchil  compete
## 0.4166153 0.9800360 0.7941998 0.9821662 0.8924392 0.7942910
```

Factor loadings, some

```
bem.2$loadings
```

```
##
## Loadings:
##          Factor1 Factor2
## helpful   0.314   0.376
## reliant   0.453   0.117
## defbel    0.434   0.193
## yielding -0.131   0.338
## cheerful  0.152   0.371
## indpt     0.521
## athlet    0.267
## shy      -0.414
## assert    0.605
## strpers   0.657
## forceful  0.649  -0.126
```

Making a data frame

There are too many to read easily, so make a data frame. This is a bit tricky:

```
loadings <- as.data.frame(unclass(bem.2$loadings)) %>%
  mutate(trait = rownames(bem.2$loadings))
loadings %>% slice(1:10)
```

```
##       Factor1      Factor2    trait
## 1   0.3137466  0.376484908  helpful
## 2   0.4532904  0.117140647  reliant
## 3   0.4336574  0.192602996   defbel
## 4  -0.1309965  0.337629288 yielding
## 5   0.1523718  0.370530549 cheerful
## 6   0.5212403  0.005870336    indpt
## 7   0.2670788  0.075542858   athlet
## 8  -0.4144579 -0.065372760      shy
## 9   0.6049588  0.033004846   assert
```

Pick out the big ones on factor 1

Arbitrarily defining > 0.4 or < -0.4 as "big":

```
loadings %>% filter(abs(Factor1) > 0.4)
```

```
##       Factor1      Factor2    trait
## 1   0.4532904  0.117140647  reliant
## 2   0.4336574  0.192602996   defbel
## 3   0.5212403  0.005870336    indpt
## 4  -0.4144579 -0.065372760      shy
## 5   0.6049588  0.033004846   assert
## 6   0.6569855  0.020777649  strpers
## 7   0.6487190 -0.126405816 forceful
## 8   0.7654924  0.069513572 leaderab
## 9   0.4416176  0.161238425     risk
## 10  0.5416796  0.112807957   decide
## 11  0.5109964  0.133626767 selfsuff
## 12  0.6676490 -0.244855780 dominant
```

Factor 2, the big ones

```
loadings %>% filter(abs(Factor2) > 0.4)
```

```
##         Factor1   Factor2    trait
## 1   0.17789112 0.5537994   affect
## 2   0.15121266 0.4166622    loyal
## 3   0.02301456 0.5256654 sympathy
## 4   0.13476970 0.4242037 sensitiv
## 5   0.09111299 0.6101294 undstand
## 6   0.11350643 0.6272223  compass
## 7   0.06061755 0.5802714   soothe
## 8   0.11893011 0.4300698    happy
## 9   0.07956978 0.7191610     warm
## 10  0.05113807 0.7102763   tender
## 11 -0.01873224 0.7022768   gentle
```

Plotting the two factors

A bi-plot, this time with the variables reduced in size. Looking for unusual individuals.

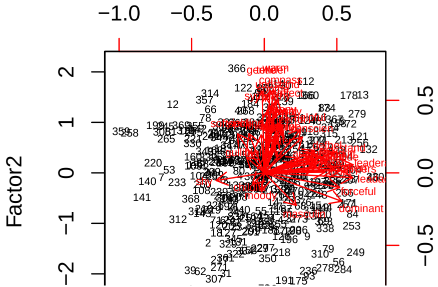
Have to run `factanal` again to get factor scores for plotting.

```
bem.2a <- factanal(bem[, -1], factors = 2, scores = "r")
biplot(bem.2a$scores, bem.2a$loadings, cex = c(0.5, 0.5))
```

Numbers on plot are row numbers of `bem` data frame.

The (awful) biplot

bFactor-biplot-two-again.png



Comments

- Variables mostly up ("feminine") and right ("masculine"), accomplished by rotation.
- Some unusual individuals: 311, 214 (low on factor 2), 366 (high on factor 2), 359, 258 (low on factor 1), 230 (high on factor 1).

Individual 366

\begin{multicols}{2}

```
bem %>% slice(366) %>% glimpse()
```

```
## Observations: 1
## Variables: 45
## $ subno    <dbl> 755
## $ helpful  <dbl> 7
## $ reliant  <dbl> 7
## $ defbel   <dbl> 5
## $ yielding <dbl> 7
## $ cheerful <dbl> 7
## $ indpt    <dbl> 7
## $ athlet   <dbl> 7
## $ shy      <dbl> 2
## $ assert   <dbl> 1
## $ strpers  <dbl> 3
```

Tidying original data

```
bem_tidy <- bem %>%
  mutate(row = row_number()) %>%
  gather(trait, score, c(-subno, -row))
bem_tidy
```

```
## # A tibble: 16,236 x 4
##     subno   row trait   score
##     <dbl> <int> <chr>   <dbl>
##  1      1     1 helpful     7
##  2      2     2 helpful     5
##  3      3     3 helpful     7
##  4      4     4 helpful     6
##  5      5     5 helpful     6
##  6      7     6 helpful     5
##  7      8     7 helpful     6
##  8      9     8 helpful     7
```

Recall data frame of loadings

```
loadings %>% slice(1:10)
```

```
##       Factor1      Factor2    trait
## 1   0.3137466  0.376484908  helpful
## 2   0.4532904  0.117140647  reliant
## 3   0.4336574  0.192602996   defbel
## 4  -0.1309965  0.337629288 yielding
## 5   0.1523718  0.370530549 cheerful
## 6   0.5212403  0.005870336    indpt
## 7   0.2670788  0.075542858   athlet
## 8  -0.4144579 -0.065372760      shy
## 9   0.6049588  0.033004846   assert
## 10  0.6569855  0.020777649  strpers
```

Want to add the factor scores for each trait to our tidy data frame `bem_tidy`. This is a left-join (over), matching on the column `trait` that is in both data frames (thus, the default):

Looking up loadings

```
bem_tidy <- bem_tidy %>% left_join(loadings)
```

```
## Joining, by = "trait"
```

```
bem_tidy %>% sample_n(12)
```

```
## # A tibble: 12 x 6
##    subno   row trait    score Factor1 Factor2
##    <dbl> <int> <chr>    <dbl>   <dbl>   <dbl>
##  1    32    22 compass      6  0.114    0.627
##  2   358   209 conscien     7  0.328    0.308
##  3   154   102 helpful      7  0.314    0.376
##  4    15    13 loyal        7  0.151    0.417
##  5     3     3 truthful     7  0.109    0.315
##  6   336   197 happy        7  0.119    0.430
##  7   485   274 sympathy     7  0.0230   0.526
##  8    89    55 stand        6  0.607    0.172
```

Individual 366, high on Factor 2

So now pick out the rows of the tidy data frame that belong to individual 366 (`row=366`) and for which the `Factor2` score exceeds 0.4 in absolute value (our "big" from before):

```
bem_tidy %>% filter(row == 366, abs(Factor2) > 0.4)
```

```
## # A tibble: 11 x 6
##     subno   row trait     score Factor1 Factor2
##     <dbl> <int> <chr>     <dbl>   <dbl>   <dbl>
##  1   755   366 affect        7  0.178    0.554
##  2   755   366 loyal         7  0.151    0.417
##  3   755   366 sympathy      7  0.0230   0.526
##  4   755   366 sensitiv      7  0.135    0.424
##  5   755   366 undstand      7  0.0911   0.610
##  6   755   366 compass       6  0.114    0.627
##  7   755   366 soothe        7  0.0606   0.580
##  8   755   366 happy         7  0.119    0.430
```

Several individuals

Rows 311 and 214 were *low* on Factor 2, so their scores should be low. Can we do them all at once?

```
bem_tidy %>% filter(
  row %in% c(366, 311, 214),
  abs(Factor2) > 0.4
)
```

```
## # A tibble: 33 x 6
##    subno   row trait    score Factor1 Factor2
##    <dbl> <int> <chr>    <dbl>   <dbl>   <dbl>
##  1   369   214 affect       1   0.178   0.554
##  2   534   311 affect       5   0.178   0.554
##  3   755   366 affect       7   0.178   0.554
##  4   369   214 loyal        7   0.151   0.417
##  5   534   311 loyal        4   0.151   0.417
##  6   755   366 loyal        7   0.151   0.417
```

Individual by column

Un-tidy, that is, spread:

```
bem_tidy %>%
  filter(
    row %in% c(366, 311, 214),
    abs(Factor2) > 0.4
  ) %>%
  select(-subno, -Factor1, -Factor2) %>%
  spread(row, score)
```

```
## # A tibble: 11 x 4
##    trait    `214` `311` `366`
##    <chr>    <dbl> <dbl> <dbl>
##  1 affect       1     5     7
##  2 compass      5     4     6
##  3 gentle       2     3     7
##  4 happy        4     3     7
```

Individuals 230, 258, 359

These were high, low, low on factor 1. Adapt code:

```
bem_tidy %>%
  filter(row %in% c(359, 258, 230), abs(Factor1) > 0.4) %>%
  select(-subno, -Factor1, -Factor2) %>%
  spread(row, score)
```

```
## # A tibble: 17 x 4
##    trait    `230` `258` `359`
##    <chr>    <dbl> <dbl> <dbl>
##  1 ambitiou     7     2     4
##  2 assert       7     3     1
##  3 compete      6     2     1
##  4 decide       7     1     2
##  5 defbel       7     1     1
##  6 dominant     7     1     1
##  7 forceful     7     1     1
```

Is 2 factors enough?

Suspect not:

```
bem.2$PVAL
```

```
##     objective
## 1.458183e-150
```

2 factors resoundingly rejected. Need more. Have to go all the way to 15 factors to not reject:

```
bem.15 <- bem %>%
  select(-subno) %>%
  factanal(factors = 15)
bem.15$PVAL
```

```
## objective
##  0.132617
```

Even then, only just over 50% of variability explained.

Get factor loadings

into a data frame, as before:

```
loadings <- as.data.frame(unclass(bem.15$loadings)) %>%
  mutate(trait = rownames(bem.15$loadings))
```

then show the highest few loadings on each factor.

Factor 1

```
loadings %>%
  arrange(desc(abs(Factor1))) %>%
  select(Factor1, trait) %>%
  slice(1:10)
```

```
##      Factor1    trait
## 1  0.8127595  compass
## 2  0.6756043 undstand
## 3  0.6611293 sympathy
## 4  0.6408327 sensitiv
## 5  0.5971006   soothe
## 6  0.3481290     warm
## 7  0.2797159   gentle
## 8  0.2788627   tender
## 9  0.2501505  helpful
## 10 0.2340594 conscien
```

Factor 2

```
loadings %>%
  arrange(desc(abs(Factor2))) %>%
  select(Factor2, trait) %>%
  slice(1:10)
```

```
##       Factor2    trait
## 1   0.7615492  strpers
## 2   0.7160312 forceful
## 3   0.6981500   assert
## 4   0.5041921 dominant
## 5   0.3929344 leaderab
## 6   0.3669560    stand
## 7   0.3507080  leadact
## 8  -0.3131682 softspok
## 9  -0.2866862      shy
## 10  0.2602525   analyt
```

Factor 3

```
loadings %>%
  arrange(desc(abs(Factor3))) %>%
  select(Factor3, trait) %>%
  slice(1:10)
```

```
##       Factor3    trait
## 1   0.6697542  reliant
## 2   0.6475496 selfsuff
## 3   0.6204018    indpt
## 4   0.3899607  helpful
## 5  -0.3393605 gullible
## 6   0.3333813  individ
## 7   0.3319003   decide
## 8   0.3294806 conscien
## 9   0.2877396 leaderab
## 10  0.2804170   defbel
```

Factor 4

```
loadings %>%
  arrange(desc(abs(Factor4))) %>%
  select(Factor4, trait) %>%
  slice(1:10)
```

```
##      Factor4    trait
## 1  0.6956206   gentle
## 2  0.6920303   tender
## 3  0.5992467     warm
## 4  0.4465546   affect
## 5  0.3942568 softspok
## 6  0.2779793  lovchil
## 7  0.2444249 undstand
## 8  0.2442119    happy
## 9  0.2125905    loyal
## 10 0.2022861   soothe
```

Factor 5

```
loadings %>%
  arrange(desc(abs(Factor5))) %>%
  select(Factor5, trait) %>%
  slice(1:10)
```

```
##      Factor5    trait
## 1  0.6956846  compete
## 2  0.6743459 ambitiou
## 3  0.3453425     risk
## 4  0.3423456  individ
## 5  0.2808623   athlet
## 6  0.2695570 leaderab
## 7  0.2449656   decide
## 8  0.2064415 dominant
## 9  0.1928159  leadact
## 10 0.1854989  strpers
```

Factor 6

```
loadings %>%
  arrange(desc(abs(Factor6))) %>%
  select(Factor6, trait) %>%
  slice(1:10)
```

```
##       Factor6    trait
## 1   0.8675651  leadact
## 2   0.6078869 leaderab
## 3   0.3378645 dominant
## 4   0.2014835 forceful
## 5  -0.1915632      shy
## 6   0.1789256     risk
## 7   0.1703440 masculin
## 8   0.1639190   decide
## 9   0.1594585  compete
## 10  0.1466037   athlet
```

Factor 7

```
loadings %>%
  arrange(desc(abs(Factor7))) %>%
  select(Factor7, trait) %>%
  slice(1:10)
```

```
##        Factor7    trait
## 1   0.6698996    happy
## 2   0.6667105 cheerful
## 3  -0.5219125    moody
## 4   0.2191425   athlet
## 5   0.2126626     warm
## 6   0.1719953   gentle
## 7  -0.1640302 masculin
## 8   0.1601472  reliant
## 9   0.1472926 yielding
## 10  0.1410481  lovchil
```

Factor 8

```
loadings %>%
  arrange(desc(abs(Factor8))) %>%
  select(Factor8, trait) %>%
  slice(1:10)
```

```
##       Factor8    trait
## 1   0.6296764   affect
## 2   0.5158355  flatter
## 3  -0.2512066 softspok
## 4   0.2214623     warm
## 5   0.1878549   tender
## 6   0.1846225  strpers
## 7  -0.1804838      shy
## 8   0.1801992  compete
## 9   0.1658105    loyal
## 10  0.1548617  helpful
```

Factor 9

```
loadings %>%
  arrange(desc(abs(Factor9))) %>%
  select(Factor9, trait) %>%
  slice(1:10)
```

```
##       Factor9    trait
## 1   0.8633171    stand
## 2   0.3403294   defbel
## 3   0.2446971  individ
## 4   0.1941110     risk
## 5  -0.1715481      shy
## 6   0.1710978   decide
## 7   0.1197126   assert
## 8   0.1157729 conscien
## 9   0.1120308   analyt
## 10 -0.1115140 gullible
```

Factor 10

```r
loadings %>%
  arrange(desc(abs(Factor10))) %>%
  select(Factor10, trait) %>%
  slice(1:10)
```

```
##       Factor10    trait
## 1   0.80751267 feminine
## 2  -0.26378513 masculin
## 3   0.24507184 softspok
## 4   0.23175597 conscien
## 5   0.20192035 selfsuff
## 6   0.17584233 yielding
## 7   0.14127067   gentle
## 8   0.11282028  flatter
## 9   0.10934531   decide
## 10 -0.09407978  lovchil
```

Factor 11

```
loadings %>%
  arrange(desc(abs(Factor11))) %>%
  select(Factor11, trait) %>%
  slice(1:10)
```

```
##      Factor11    trait
## 1  0.91622589    loyal
## 2  0.18949077   affect
## 3  0.15883857 truthful
## 4  0.12464529  helpful
## 5  0.10440664   analyt
## 6  0.10076794   tender
## 7  0.09720457  lovchil
## 8  0.09635223 gullible
## 9  0.09350623 cheerful
## 10 0.08207596 conscien
```

Factor 12

```
loadings %>%
  arrange(desc(abs(Factor12))) %>%
  select(Factor12, trait) %>%
  slice(1:10)
```

```
##      Factor12    trait
## 1   0.6106933 childlik
## 2  -0.2845004 selfsuff
## 3  -0.2786751 conscien
## 4   0.2588843    moody
## 5   0.2013245      shy
## 6  -0.1669301   decide
## 7   0.1542031 masculin
## 8   0.1455526 dominant
## 9   0.1379163  compass
## 10 -0.1297408 leaderab
```

Factor 13

```
loadings %>%
  arrange(desc(abs(Factor13))) %>%
  select(Factor13, trait) %>%
  slice(1:10)
```

```
##      Factor13    trait
## 1   0.5729242 truthful
## 2  -0.2776490 gullible
## 3   0.2631046    happy
## 4   0.1885152     warm
## 5  -0.1671924      shy
## 6   0.1646031    loyal
## 7  -0.1438127 yielding
## 8  -0.1302900   assert
## 9   0.1137074   defbel
## 10 -0.1105583  lovchil
```

Factor 14

```
loadings %>%
  arrange(desc(abs(Factor14))) %>%
  select(Factor14, trait) %>%
  slice(1:10)
```

```
##      Factor14    trait
## 1   0.4429926   decide
## 2   0.2369714 selfsuff
## 3   0.1945034 forceful
## 4  -0.1862756 softspok
## 5   0.1604175     risk
## 6  -0.1484606  strpers
## 7   0.1461972 dominant
## 8   0.1279456    happy
## 9   0.1154479  compass
## 10  0.1054078 masculin
```

Factor 15

```
loadings %>%
  arrange(desc(abs(Factor15))) %>%
  select(Factor15, trait) %>%
  slice(1:10)
```

```
##      Factor15    trait
## 1  -0.3244092  compass
## 2   0.2471884   athlet
## 3   0.2292980 sensitiv
## 4   0.1986878     risk
## 5  -0.1638296   affect
## 6   0.1632164    moody
## 7  -0.1118135  individ
## 8   0.1100678     warm
## 9   0.1047347 cheerful
## 10  0.1012342  reliant
```

Anything left out? Uniquenesses

```r
data.frame(uniq = bem.15$uniquenesses) %>%
  rownames_to_column() %>%
  arrange(desc(uniq)) %>%
  slice(1:10)
```

```
##     rowname      uniq
## 1  foullang 0.9136126
## 2   lovchil 0.8242992
## 3    analyt 0.8120934
## 4  yielding 0.7911748
## 5  masculin 0.7228739
## 6    athlet 0.7217327
## 7       shy 0.7033071
## 8  gullible 0.7000779
## 9   flatter 0.6625008
## 10  helpful 0.6516863
```

Section 14

Confirmatory factor analysis}

Confirmatory factor analysis

- Exploratory: what do data suggest as hidden underlying factors (in terms of variables observed)?
- Confirmatory: have {*theory*} *about how underlying factors depend on observed variables; test whether theory supported by data:*
- *does theory provide* {some} explanation (better than nothing)
- can we do better?
- Also can compare two theories about factors: is more complicated one significantly better than simpler one?

Children and tests again

- Previously had this correlation matrix of test scores (based on 145 children):

```
km
```

```
##       para  sent  word   add  dots
## [1,] 1.000 0.722 0.714 0.203 0.095
## [2,] 0.722 1.000 0.685 0.246 0.181
## [3,] 0.714 0.685 1.000 0.170 0.113
## [4,] 0.203 0.246 0.170 1.000 0.585
## [5,] 0.095 0.181 0.113 0.585 1.000
```

def

- Will use package `lavaan` for confirmatory analysis.
- Can use actual data or correlation matrix.
- Latter (a bit) more work, as we see.

Two or three steps

- Make sure correlation matrix (if needed) is handy.
- Specify factor model (from theory)
- Fit factor model: does it fit acceptably?

Specifying a factor model

- Jargon: thing you cannot observe called **latent variable**.
- Thing you *can* observe called **manifest variable**.
- Model predicts latent variables from manifest variables.
- Model with one factor including all the tests:

```
test.model.1 <- "ability=~para+sent+word+add+dots"
```

def

- and a model that we really believe, that there are two factors, a verbal and a mathematical:

```
test.model.2 <- "\nverbal=~para+sent+word\nmath=~add+dots"
```

def

- Note the format: really all one line between single quotes, but putting

Fitting a 1-factor model

- Need to specify model, correlation matrix, n like this:

```
fit1 <- cfa(test.model.1,
  sample.cov = km,
  sample.nobs = 145
)
```

def

- Has summary, or briefer version like this:

```
fit1
```

```
## lavaan 0.6-3 ended normally after 16 iterations
##
##   Optimization method                           NLMINB
##   Number of free parameters                         10
##
##   Number of observations                           145
```

Two-factor model

```
fit2 <- cfa(test.model.2, sample.cov = km, sample.nobs = 145)
fit2
```

```
## lavaan 0.6-3 ended normally after 25 iterations
##
##   Optimization method                           NLMINB
##   Number of free parameters                         11
##
##   Number of observations                           145
##
##   Estimator                                         ML
##   Model Fit Test Statistic                       2.951
##   Degrees of freedom                                 4
##   P-value (Chi-square)                           0.566
```

def

- This fits OK: 2-factor model supported by the data

Comparing models

- Use anova as if this were a regression:

```
anova(fit1, fit2)
```

```
## Chi Square Difference Test
##
##      Df    AIC    BIC   Chisq Chisq diff Df diff Pr(>Chisq)
## fit2  4 1776.7 1809.4  2.9509
## fit1  5 1831.6 1861.4 59.8862     56.935       1  4.504e-
14
##
## fit2
## fit1 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Track and field data, yet again

- cfa works easier on actual data, such as the running records: {

```
track %>% print(n = 6)
```

```
## # A tibble: 55 x 9
##    m100  m200  m400  m800 m1500 m5000 m10000 marathon
##   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>  <dbl>    <dbl>
## 1  10.4  20.8  46.8  1.81  3.7   14.0   29.4     138.
## 2  10.3  20.1  44.8  1.74  3.57  13.3   27.7     128.
## 3  10.4  20.8  46.8  1.79  3.6   13.3   27.7     136.
## 4  10.3  20.7  45.0  1.73  3.6   13.2   27.4     130.
## 5  10.3  20.6  45.9  1.8   3.75  14.7   30.6     147.
## 6  10.2  20.4  45.2  1.73  3.66  13.6   28.6     133.
## # … with 49 more rows, and 1 more variable: country <chr>
```

def }

- Specify factor model. Factors seemed to be "sprinting" (up to 800m)

Fit and examine the model

- Fit the model. The observed variables are on different scales, so we should standardize them first via `std.ov`:

```
track.1 <- track %>%
  select(-country) %>%
  cfa(track.model, data = ., std.ov = T)
track.1
```

```
## lavaan 0.6-3 ended normally after 59 iterations
##
##   Optimization method                           NLMINB
##   Number of free parameters                         17
##
##   Number of observations                            55
##
##   Estimator                                         ML
##   Model Fit Test Statistic                      87.608
```

Factor model 2

- Define factor model:

```
track.model.2 <- "\nsprint=~m100+m200+m400\nmiddle=~m800+m150
```

def

- Fit and examine:

```
track.2 <- track %>%
  select(-country) %>%
  cfa(track.model.2, data = ., std.ov = T)
track.2
```

```
## lavaan 0.6-3 ended normally after 72 iterations
##
##   Optimization method                           NLMINB
##   Number of free parameters                         19
##
```

Comparing the two models

- Second model doesn't fit well, but is it better than first? {

```
anova(track.1, track.2)
```

```
## Chi Square Difference Test
##
##          Df    AIC    BIC  Chisq Chisq diff Df diff
## track.2 17 535.49 573.63 40.089
## track.1 19 579.01 613.13 87.608     47.519       2
##         Pr(>Chisq)
## track.2
## track.1  4.802e-11 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

def }

Section 15

Time Series

Packages

You might need to install these:

```
install.packages("ggfortify")
install.packages("forecast")
install.packages("devtools")
devtools::install_github("nxskok/mkac")
```

```
library(tidyverse)
```

```
##  Attaching packages  tidyverse 1.2.1

##  ggplot2 3.1.1          purrr   0.3.2
##  tibble  2.1.1          dplyr   0.8.0.1
##  tidyr   0.8.3.9000     stringr 1.4.0
##  readr   1.3.1          forcats 0.3.0

## Warning: package 'ggplot2' was built under R version 3.5.3

## Warning: package 'tibble' was built under R version 3.5.3
```

Time trends

```
## Error in eval(expr, envir, enclos): object 'opts_chunk' not
```

- Assess existence or nature of time trends with:
    - correlation
    - regression ideas.

World mean temperatures

Global mean temperature every year since 1880:

```
temp=read_csv("temperature.csv")
```

```
## Warning: Missing column names filled in: 'X1' [1]
## Parsed with column specification:
## cols(
##   X1 = col_double(),
##   Year = col_date(format = ""),
##   temperature = col_double(),
##   year = col_double()
## )
```

Actual time series

The Kings of England

- Age at death of Kings and Queens of England since William the Conqueror (1066):

```
kings=read_table("kings.txt", col_names=F)
```

```
## Parsed with column specification:
## cols(
##   X1 = col_double()
## )
```

```
kings.ts=ts(kings)
```

Data in one long column `X1`, so `kings` is data frame with one column. Turn into `ts` time series object.

```
kings.ts
```

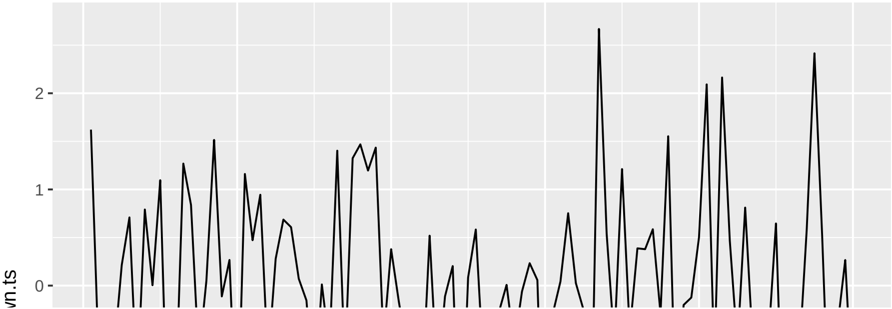
```
## Time Series:
## Start = 1
```

Time series basics

White noise

Independent random normal. Knowing one value tells you nothing about the next. “Random” process.

```
wn=rnorm(100)
wn.ts=ts(wn)
autoplot(wn.ts)
```



Section 16

Multiway frequency tables

Packages

```r
library(tidyverse)
```

Multi-way frequency analysis

- A study of gender and eyewear-wearing finds the following frequencies:

Gender	Contacts	Glasses	None
Female	121	32	129
Male	42	37	85

- Is there association between eyewear and gender?
- Normally answer this with chisquare test (based on observed and expected frequencies from null hypothesis of no association).
- Two categorical variables and a frequency.
- We assess in way that generalizes to more categorical variables.

The data file

```
gender contacts glasses none
female 121      32      129
male   42       37      85
```

- This is *not tidy!*
- Two variables are gender and *eyewear*, and those numbers all frequencies.

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/eyewear.txt
eyewear <- read_delim(my_url, " ")
eyewear
```

```
## # A tibble: 2 x 4
##   gender contacts glasses  none
##   <chr>     <dbl>   <dbl> <dbl>
## 1 female      121      32   129
```

Tidying the data

```
eyes <- eyewear %>%
  gather(eyewear, frequency, contacts:none)
eyes
```

```
## # A tibble: 6 x 3
##   gender eyewear  frequency
##   <chr>  <chr>        <dbl>
## 1 female contacts       121
## 2 male   contacts        42
## 3 female glasses         32
## 4 male   glasses         37
## 5 female none           129
## 6 male   none            85
```

```
xt <- xtabs(frequency ~ gender + eyewear, data = eyes)
xt
```

...

Modelling

- Last table on previous page is "reconstituted" contingency table, for checking.
- Predict frequency from other factors and combos. `glm` with `poisson` family.

```
eyes.1 <- glm(frequency ~ gender * eyewear,
  data = eyes,
  family = "poisson"
)
```

def

- Called **log-linear model**.

What can we get rid of?

{

```
drop1(eyes.1, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## frequency ~ gender * eyewear
##                Df Deviance    AIC    LRT  Pr(>Chi)
## <none>               0.000 47.958
## gender:eyewear  2   17.829 61.787 17.829 0.0001345 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

def }

Conclusions

- `drop1` says what we can remove at this step. Significant = must stay.
- Cannot remove anything.
- Frequency depends on `gender-wear` *combination*, cannot be simplified further.
- Gender and eyewear are *associated*.
- Stop here.

prop.table

Original table:

{

```
xt
```

```
##          eyewear
## gender   contacts glasses none
##   female      121      32  129
##   male         42      37   85
```

} Calculate eg. row proportions like this:

{

```
prop.table(xt, margin = 1)
```

```
##          eyewear
## gender     contacts   glasses      none
##   female 0.4290780 0.1134752 0.4574468
##   male   0.2560976 0.2256098 0.5182927
```

No association

- Suppose table had been as shown below:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/eyewear2.tx
eyewear2 <- read_table(my_url)
eyes2 <- eyewear2 %>% gather(eyewear, frequency, contacts:none
xt2 <- xtabs(frequency ~ gender + eyewear, data = eyes2)
xt2
```

```
##          eyewear
## gender    contacts glasses none
##   female       150      30  120
##   male          75      16   62
```

```
prop.table(xt2, margin = 1)
```

```
##          eyewear
## gender     contacts   glasses      none
##   female 0.5000000 0.1000000 0.4000000
```

Analysis for revised data

```
eyes.2 <- glm(frequency ~ gender * eyewear,
  data = eyes2,
  family = "poisson"
)
drop1(eyes.2, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## frequency ~ gender * eyewear
##                Df Deviance    AIC      LRT Pr(>Chi)
## <none>            0.000000 47.467
## gender:eyewear  2 0.047323 43.515 0.047323   0.9766
```

No longer any association. Take out interaction.

No interaction

{

```
eyes.3 <- update(eyes.2, . ~ . - gender:eyewear)
drop1(eyes.3, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## frequency ~ gender + eyewear
##          Df Deviance     AIC     LRT  Pr(>Chi)
## <none>         0.047  43.515
## gender   1    48.624  90.091  48.577 3.176e-12 ***
## eyewear  2   138.130 177.598 138.083 < 2.2e-16 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

}

- More females (gender effect)

Chest pain, being overweight and being a smoker

- In a hospital emergency department, 176 subjects who attended for acute chest pain took part in a study.
- Each subject had a normal or abnormal electrocardiogram reading (ECG), were overweight (as judged by BMI) or not, and were a smoker or not.
- How are these three variables related, or not?

The data

In modelling-friendly format:

```
ecg bmi smoke count
abnormal overweight yes 47
abnormal overweight no 10
abnormal normalweight yes 8
abnormal normalweight no 6
normal overweight yes 25
normal overweight no 15
normal normalweight yes 35
normal normalweight no 30
```

First step

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/ecg.txt"
chest <- read_delim(my_url, " ")
chest.1 <- glm(count ~ ecg * bmi * smoke,
  data = chest,
  family = "poisson"
)
drop1(chest.1, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## count ~ ecg * bmi * smoke
##               Df Deviance    AIC    LRT Pr(>Chi)
## <none>             0.0000 53.707
## ecg:bmi:smoke  1   1.3885 53.096 1.3885   0.2387
```

That 3-way interaction comes out.

Removing the 3-way interaction

```
chest.2 <- update(chest.1, . ~ . - ecg:bmi:smoke)
drop1(chest.2, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## count ~ ecg + bmi + smoke + ecg:bmi + ecg:smoke + bmi:smoke
##           Df Deviance    AIC     LRT  Pr(>Chi)
## <none>          1.3885 53.096
## ecg:bmi    1   29.0195 78.727 27.6310 1.468e-07 ***
## ecg:smoke  1    4.8935 54.601  3.5050   0.06119 .
## bmi:smoke  1    4.4689 54.176  3.0803   0.07924 .
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

At $\alpha = 0.05$, `bmi:smoke` comes out.

Removing bmi:smoke

```
chest.3 <- update(chest.2, . ~ . - bmi:smoke)
drop1(chest.3, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## count ~ ecg + bmi + smoke + ecg:bmi + ecg:smoke
##           Df Deviance    AIC    LRT  Pr(>Chi)
## <none>          4.469 54.176
## ecg:bmi    1   36.562 84.270 32.094 1.469e-08 ***
## ecg:smoke  1   12.436 60.144  7.968  0.004762 **
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

`ecg:smoke` has become significant. So we have to stop.

Understanding the final model

- Thinking of `ecg` as “response” that might depend on anything else.
- What is associated with `ecg`? Both `bmi` on its own and `smoke` on its own, but *not* the combination of both.
- `ecg:bmi` table:

```
xtabs(count ~ ecg + bmi, data = chest)
```

```
##             bmi
## ecg          normalweight overweight
##   abnormal             14         57
##   normal               65         40
```

- Most normal weight people have a normal ECG, but a majority of overweight people have an *abnormal* ECG. That is, knowing about BMI says something about likely ECG.

ecg:smoke

- ecg:smoke table:

```
xtabs(count ~ ecg + smoke, data = chest)
```

```
##           smoke
## ecg        no yes
##   abnormal 16  55
##   normal   45  60
```

- Most nonsmokers have a normal ECG, but smokers are about 50–50 normal and abnormal ECG.
- Don't look at smoke:bmi table since not significant.

Simpson's paradox: the airlines example

Airport	Alaska Airlines On time	Alaska Airlines Delayed	America West On time	America West Delayed
Los Angeles	497	62	694	117
Phoenix	221	12	4840	415
San Diego	212	20	383	65
San Francisco	503	102	320	129
Seattle	1841	305	201	61
Total	3274	501	6438	787

Use `status` as variable name for "on time/delayed".

- Alaska: 13.3% flights delayed $(501/(3274 + 501))$.
- America West: 10.9% $(787/(6438 + 787))$.
- America West more punctual, right?

Arranging the data

- Can only have single thing in columns, so we have to construct column names like this: \begin{small}

```
airport     aa_ontime aa_delayed aw_ontime aw_delayed
LosAngeles    497          62       694       117
Phoenix       221          12      4840       415
SanDiego      212          20       383        65
SanFrancisco 503          102       320       129
Seattle      1841         305       201        61
```

\end{small}

- Some tidying gets us the right layout, with frequencies all in one column and the airline and delayed/on time status separated out:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/airlines.tx
airlines <- read_table2(my_url)
```

The data frame punctual

```
## # A tibble: 20 x 4
##    airport       airline status   freq
##    <chr>         <chr>   <chr>   <dbl>
##  1 LosAngeles    aa      ontime    497
##  2 Phoenix       aa      ontime    221
##  3 SanDiego      aa      ontime    212
##  4 SanFrancisco  aa      ontime    503
##  5 Seattle       aa      ontime   1841
##  6 LosAngeles    aa      delayed    62
##  7 Phoenix       aa      delayed    12
##  8 SanDiego      aa      delayed    20
##  9 SanFrancisco  aa      delayed   102
## 10 Seattle       aa      delayed   305
## 11 LosAngeles    aw      ontime    694
## 12 Phoenix       aw      ontime   4840
## 13 SanDiego      aw      ontime    383
```

Proportions delayed by airline

- Two-step process: get appropriate subtable:

```
xt <- xtabs(freq ~ airline + status, data = punctual)
xt
```

```
##          status
## airline delayed ontime
##      aa     501   3274
##      aw     787   6438
```

- and then calculate appropriate proportions:

```
prop.table(xt, margin = 1)
```

```
##          status
## airline   delayed    ontime
##      aa 0.1327152 0.8672848
##      aw 0.1089273 0.8910727
```

Proportion delayed by airport, for each airline

```
xt <- xtabs(freq ~ airline + status + airport, data = punctual
xp <- prop.table(xt, margin = c(1, 3))
ftable(xp,
  row.vars = c("airport", "airline"),
  col.vars = "status"
)
```

```
##                          status    delayed     ontime
## airport       airline
## LosAngeles    aa                0.11091234 0.88908766
##               aw                0.14426634 0.85573366
## Phoenix       aa                0.05150215 0.94849785
##               aw                0.07897241 0.92102759
## SanDiego      aa                0.08620690 0.91379310
##               aw                0.14508929 0.85491071
## SanFrancisco  aa                0.16859504 0.83140496
##               aw                0.28730512 0.71269488
```

Simpson's Paradox

Airport	Alaska	America West
Los Angeles	11.4	14.4
Phoenix	5.2	7.9
San Diego	8.6	14.5
San Francisco	16.9	28.7
Seattle	14.2	23.2
Total	13.3	10.9

- America West more punctual overall,
- but worse at *every single* airport!
- How is that possible?
- Log-linear analysis sheds some light.

Model 1 and output

```
punctual.1 <- glm(freq ~ airport * airline * status,
  data = punctual, family = "poisson"
)
drop1(punctual.1, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ airport * airline * status
##                         Df Deviance    AIC    LRT Pr(>Chi)
## <none>                       0.0000 183.44
## airport:airline:status   4   3.2166 178.65 3.2166   0.5223
```

def

Remove 3-way interaction

```
punctual.2 <- update(punctual.1, ~ . - airport:airline:status)
drop1(punctual.2, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ airport + airline + status + airport:airline + airpo
##     airline:status
##                 Df Deviance    AIC    LRT  Pr(>Chi)
## <none>                  3.2  178.7
## airport:airline  4   6432.5 6599.9 6429.2 < 2.2e-16 ***
## airport:status   4    240.1  407.5  236.9 < 2.2e-16 ***
## airline:status   1     45.5  218.9   42.2 8.038e-11 ***
## ---
## Signif. codes:
## 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Understanding the significance

- airline:status:

```
xt <- xtabs(freq ~ airline + status, data = punctual)
prop.table(xt, margin = 1)
```

```
##          status
## airline     delayed    ontime
##       aa 0.1327152 0.8672848
##       aw 0.1089273 0.8910727
```

- More of Alaska Airlines' flights delayed overall.
- Saw this before.

Understanding the significance (2)

- `airport:status`:

```
xt <- xtabs(freq ~ airport + status, data = punctual)
prop.table(xt, margin = 1)
```

```
##                status
## airport            delayed     ontime
##   LosAngeles    0.13065693 0.86934307
##   Phoenix       0.07780612 0.92219388
##   SanDiego      0.12500000 0.87500000
##   SanFrancisco 0.21916509 0.78083491
##   Seattle       0.15199336 0.84800664
```

- Flights into San Francisco (and maybe Seattle) are often late, and flights into Phoenix are usually on time.
- Considerable variation among airports.

Understanding the significance (3)

- airport:airline:

```
xt <- xtabs(freq ~ airport + airline, data = punctual)
prop.table(xt, margin = 2)
```

```
##                airline
## airport                 aa         aw
##   LosAngeles    0.14807947 0.11224913
##   Phoenix       0.06172185 0.72733564
##   SanDiego      0.06145695 0.06200692
##   SanFrancisco  0.16026490 0.06214533
##   Seattle       0.56847682 0.03626298
```

- What fraction of each airline's flights are to each airport.
- Most of Alaska Airlines' flights to Seattle and San Francisco.
- Most of America West's flights to Phoenix.

The resolution

- Most of America West's flights to Phoenix, where it is easy to be on time.
- Most of Alaska Airlines' flights to San Francisco and Seattle, where it is difficult to be on time.
- Overall comparison looks bad for Alaska because of this.
- But, *comparing like with like*, if you compare each airline's performance *to the same airport*, Alaska does better.
- Aggregating over the very different airports was a (big) mistake: that was the cause of the Simpson's paradox.
- Alaska Airlines is *more* punctual when you do the proper comparison.

Ovarian cancer: a four-way table

- Retrospective study of ovarian cancer done in 1973.
- Information about 299 women operated on for ovarian cancer 10 years previously.
- Recorded:
- stage of cancer (early or advanced)
- type of operation (radical or limited)
- X-ray treatment received (yes or no)
- 10-year survival (yes or no)
- Survival looks like response (suggests logistic regression).
- Log-linear model finds any associations at all.

The data

after tidying:

{

```
stage operation xray survival freq
early radical no no 10
early radical no yes 41
early radical yes no 17
early radical yes yes 64
early limited no no 1
early limited no yes 13
early limited yes no 3
early limited yes yes 9
advanced radical no no 38
advanced radical no yes 6
advanced radical yes no 64
advanced radical yes yes 11
advanced limited no no 3
advanced limited no yes 1
advanced limited yes no 13
advanced limited yes yes 5
```

Stage 1

hopefully looking familiar by now:

```
my_url <- "http://www.utsc.utoronto.ca/~butler/d29/cancer.txt'
cancer <- read_delim(my_url, " ")
cancer %>% print(n = 6)
```

```
## # A tibble: 16 x 5
##   stage operation xray  survival  freq
##   <chr> <chr>     <chr> <chr>    <dbl>
## 1 early radical   no    no          10
## 2 early radical   no    yes         41
## 3 early radical   yes   no          17
## 4 early radical   yes   yes         64
## 5 early limited   no    no           1
## 6 early limited   no    yes         13
## # … with 10 more rows
```

```
cancer.1 <- glm(freq ~ stage * operation * xray * survival
```

Output 1

See what we can remove:

```
drop1(cancer.1, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ stage * operation * xray * survival
##                              Df Deviance    AIC     LRT
## <none>                            0.00000 98.130
## stage:operation:xray:survival  1  0.60266 96.732 0.60266
##                              Pr(>Chi)
## <none>
## stage:operation:xray:survival   0.4376
```

def

Non-significant interaction can come out.

Stage 2

```r
cancer.2 <- update(cancer.1, ~ .
- stage:operation:xray:survival)
drop1(cancer.2, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ stage + operation + xray + survival + stage:operatio
##     stage:xray + operation:xray + stage:survival + operatio
##     xray:survival + stage:operation:xray + stage:operation:
##     stage:xray:survival + operation:xray:survival
##                           Df Deviance    AIC     LRT
## <none>                       0.60266 96.732
## stage:operation:xray       1  2.35759 96.487 1.75493
## stage:operation:survival   1  1.17730 95.307 0.57465
## stage:xray:survival        1  0.95577 95.085 0.35311
```

Take out stage:xray:survival

```
cancer.3 <- update(cancer.2, . ~ . - stage:xray:survival)
drop1(cancer.3, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ stage + operation + xray + survival + stage:operatio
##     stage:xray + operation:xray + stage:survival + operatio
##     xray:survival + stage:operation:xray + stage:operation:
##     operation:xray:survival
##                          Df Deviance    AIC     LRT
## <none>                      0.95577 95.085
## stage:operation:xray      1  3.08666 95.216 2.13089
## stage:operation:survival  1  1.56605 93.696 0.61029
## operation:xray:survival   1  1.55124 93.681 0.59547
##                          Pr(>Chi)
```

Remove operation:xray:survival

```
cancer.4 <- update(cancer.3, . ~ . - operation:xray:survival)
drop1(cancer.4, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ stage + operation + xray + survival + stage:operatio
##     stage:xray + operation:xray + stage:survival + operatio
##     xray:survival + stage:operation:xray + stage:operation:
##                        Df Deviance    AIC    LRT Pr(>Chi)
## <none>                      1.5512 93.681
## xray:survival           1   1.6977 91.827 0.1464  0.70196
## stage:operation:xray    1   6.8420 96.972 5.2907  0.02144
## stage:operation:survival 1  1.9311 92.061 0.3799  0.53768
##
## <none>
```

Comments

- `stage:operation:xray` has now become significant, so won't remove that.
- Shows value of removing terms one at a time.
- There are no higher-order interactions containing both `xray` and `survival`, so now we get to test (and remove) `xray:survival`.

Remove xray:survival

```
cancer.5 <- update(cancer.4, . ~ . - xray:survival)
drop1(cancer.5, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ stage + operation + xray + survival + stage:operatio
##     stage:xray + operation:xray + stage:survival + operatio
##     stage:operation:xray + stage:operation:survival
##                           Df Deviance    AIC    LRT Pr(>Chi
## <none>                         1.6977 91.827
## stage:operation:xray       1   6.9277 95.057 5.2300   0.022
## stage:operation:survival   1   2.0242 90.154 0.3265   0.567
##
## <none>
## stage:operation:xray      *
```

Remove stage:operation:survival

```
cancer.6 <- update(cancer.5, . ~ . - stage:operation:survival)
drop1(cancer.6, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ stage + operation + xray + survival + stage:operatio
##     stage:xray + operation:xray + stage:survival + operatio
##     stage:operation:xray
##                      Df Deviance     AIC     LRT Pr(>Chi)
## <none>                   2.024   90.154
## stage:survival        1  135.198 221.327 133.173   <2e-
16
## operation:survival    1    4.116  90.245   2.092   0.1481
## stage:operation:xray  1    7.254  93.384   5.230   0.0222
##
```

Last step?

Remove `operation:survival`.

```
cancer.7 <- update(cancer.6, . ~ . - operation:survival)
drop1(cancer.7, test = "Chisq")
```

```
## Single term deletions
##
## Model:
## freq ~ stage + operation + xray + survival + stage:operatio
##     stage:xray + operation:xray + stage:survival + stage:op
##                      Df Deviance     AIC    LRT Pr(>Chi)
## <none>                     4.116  90.245
## stage:survival        1  136.729 220.859 132.61   <2e-16
## stage:operation:xray  1    9.346  93.475   5.23   0.0222
##
## <none>
## stage:survival        ***
```

Conclusions

- What matters is things associated with survival (survival is "response").
- Only significant such term is `stage:survival`:

```
xt <- xtabs(freq ~ stage + survival, data = cancer)
prop.table(xt, margin = 1)
```

```
##           survival
## stage             no       yes
##   advanced 0.8368794 0.1631206
##   early    0.1962025 0.8037975
```

- Most people in early stage of cancer survived, and most people in advanced stage did not survive.
- This true *regardless* of type of operation or whether or not X-ray treatment was received. These things have no impact on survival.

What about that other interaction?

```
xt <- xtabs(freq ~ operation + xray + stage, data = cancer)
ftable(prop.table(xt, margin = 3))
```

```
##                    stage   advanced      early
## operation xray
## limited   no             0.02836879 0.08860759
##           yes            0.12765957 0.07594937
## radical   no             0.31205674 0.32278481
##           yes            0.53191489 0.51265823
```

- Out of the people at each stage of cancer (since `margin=3` and `stage` was listed 3rd).
- The association is between `stage` and `xray` *only for those who had the limited operation*.
- For those who had the radical operation, there was no association between `stage` and `xray`.

General procedure

- Start with "complete model" including all possible interactions.
- `drop1` gives highest-order interaction(s) remaining, remove least non-significant.
- Repeat as necessary until everything significant.
- Look at subtables of significant interactions.
- Main effects not usually very interesting.
- Interactions with "response" usually of most interest: show association with response.

make DONE slide