Statistical Modeling

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Goals

- Using data models
 - Types and purpose
- Common statistical models
 - Linear models
 - Logistic models
- The "formula interface" in R to express models

- Learning to extract and use the results of models
 - The broom package
 - Graphical representations
- What predictors/covariates are "important"
- Model building and selection
- Good practices

All models are wrong, but some are useful

G.E.P. Box

Models

Models are our way of understanding nature, usually using some sort of mathematical expression

Famous mathematical models include Newton's second law of motion, the laws of thermodynamics, the ideal gas law

All probability distributions, like Gaussian, Binomial, Poisson, Gamma, are models

Mendel's laws are models **that result in** particular mathematical models for inheritance and population prevalence

Models

We use models all the time to describe our understanding of different processes

- Cause-and-effect relationships
- Supply-demand curves
- Financial planning
- Optimizing travel plans (perhaps including traffic like Google Maps)
- Understanding the effects of change
 - Climate change
 - Rule changes via Congress or companies
 - Effect of a drug on disease outcomes
 - Effect of education and behavioral patterns on future earnings

Data-driven models

Can we use data collected on various aspects of a particular context to understand the relationships between the different aspects?

- How does increased smoking affect your risk of getting lung cancer? (causality/association)
 - o Does genetics matter?
 - Does the kind of smoking matter?
 - Does gender matter?

Data-driven models

Can we use data collected on various aspects of a particular context to understand the relationships between the different aspects?

- What is your lifetime risk of breast cancer? (prediction)
 - What if you have a sister with breast cancer?
 - What if you had early menarche?
 - What if you are of Ashkenazi Jewish heritage?

The Gail Model from NCI

Association models

These are more traditional, highly interpretative models that look at **how** different predictors affect outcome.

- Linear regression
- Logistic regression
- Cox proportional hazards regression
- Decision trees

Since these models have a particular known structure determined by the modeler, they can be used on relatively small datasets

You can easily understand which predictors have more "weight" in influencing the outcome

You can literally write down how a prediction would be made

Predictive models

These are more recent models that primarily look to provide good predictions of an outcome, and the way the predictions are made is left opaque (often called a *black box*)

- Deep Learning (or Neural Networks)
- Random Forests
- Support Vector Machines
- Gradient Boosting Machines

These models require data to both determine the structure of the model as well as make the predictions, so they require lots of data to *train* on

The relative "weight" of predictors in influencing the **predictions** can be obtained

The effect of individual predictors is not easily interpretable, though this is changing

They require a different **philosophic perspective** than traditional association models

Datasets

We will use the pbc data from the survival package, and the in-built mtcars dataset.

```
library(survival)
data(pbc)
str(pbc)
```

```
418 obs. of 20 variables:
'data.frame':
$ id
         : int 1 2 3 4 5 6 7 8 9 10 ...
         : int 400 4500 1012 1925 1504 2503 1832 2466 2400 51 ...
$ time
$ status : int 2 0 2 2 1 2 0 2 2 2 ...
         : int
               <u>58.8 5</u>6.4 70.1 54.7 38.1 ...
$ age
     : num
         : Factor w/ 2 levels "m", "f": 2 2 1 2 2 2 2 2 2 2 ...
$ ascites : int  1 0 0 0 0 0 0 0 0 1 ...
$ hepato : int 1101111000...
$ spiders : int 1 1 0 1 1 0 0 0 1
$ edema : num 1 0 0.5 0.5 0 0 0 0 0 1
$ bili
        : num 14.5 1.1 1.4 1.8 3.4 0.8 1 0.3 3.2 12.6 ...
         : int 261 302 176 244 279 248 322 280 562 200 ...
$ albumin : num 2.6 4.14 3.48 2.54 3.53 3.98 4.09 4 3.08 2.74 ...
$ copper : int 156 54 210 64 143 50 52 52 79 140 ...
$ ast
         : num 137.9 113.5 96.1 60.6 113.2 ...
$ trig
         : int 172 88 55 92 72 63 213 189 88 143 ...
$ platelet: int 190 221 151 183 136 NA 204 373 251 302 ...
$ protime : num 12.2 10.6 12 10.3 10.9 11 9.7 11 11 11.5 ...
$ stage
        : int 4344333324...
```

The formula interface

Representing model relationships

In R, there is a particularly convenient way to express models, where you have

- one dependent variable
- one or more independent variables, with possible transformations and interactions

```
y \sim x1 + x2 + x1:x2 + I(x3^2) + x4*x5
```

y depends on ...

- x1 and x2 linearly
- the interaction of x1 and x2 (represented as x1:x2)
- the square of x3 (the I() notation ensures that the ^ symbol is interpreted correctly)
- x4, x5 and their interaction (same as x4 + x5 + x4:x5)

Representing model relationships

```
y \sim x1 + x2 + x1:x2 + I(x3^2) + x4*x5
```

This interpretation holds for the vast majority of statistical models in R

• For decision trees and random forests and neural networks, don't add interactions or transformations, since the model will try to figure those out on their own

```
myLinearModel <- lm(chol ~ bili, data = pbc)</pre>
```

Note that everything in R is an **object**, so you can store a model in a variable name.

This statement runs the model and stored the fitted model in myLinearModel

R does not interpret the model, evaluate the adequacy or appropriateness of the model, or comment on whether looking at the relationship between cholesterol and bilirubin makes any kind of sense.

It just fits the model it is given

myLinearModel

```
Call:
lm(formula = chol ~ bili, data = pbc)

Coefficients:
(Intercept) bili
303.20 20.24
```

Not very informative, is it?

summary(myLinearModel)

```
Call:
lm(formula = chol ~ bili, data = pbc)
Residuals:
   Min 10 Median 30
                                Max
-565.39 -89.90 -35.36 44.92 1285.33
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 303.204 15.601 19.435 < 2e-16 ***
bili
      20.240
                   2.785 7.267 3.63e-12 ***
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
Residual standard error: 213.2 on 282 degrees of freedom
 (134 observations deleted due to missingness)
Multiple R-squared: 0.1577, Adjusted R-squared: 0.1547
F-statistic: 52.8 on 1 and 282 DF, p-value: 3.628e-12
```

A little better

broom::tidy(myLinearModel)

```
# A tibble: 2 x 5
term estimate std.error statistic p.value
<chr> <dbl> <dbl> <dbl> <dbl> <dbl> 1 (Intercept) 303. 15.6 19.4 5.65e-54
2 bili 20.2 2.79 7.27 3.63e-12
```

broom::glance(myLinearModel)

We do need some sense as to how well this model fit the data

```
# install.packages('ggfortify')
library(ggfortify)
autoplot(myLinearModel)
```

Let's see if we have some strangeness going on

```
ggplot(pbc, aes(x = bili))+geom_density()
```

We'd like this to be a bit more "Gaussian" for better behavior

Let's see if we have some strangeness going on

```
ggplot(pbc, aes(x = log(bili)))+geom_density()
```

```
myLinearModel2 <- lm(chol~log(bili), data = pbc)
summary(myLinearModel2)
```

```
Call:
lm(formula = chol ~ log(bili), data = pbc)
Residuals:
   Min 10 Median 30
                                Max
-440.07 -94.35 -21.07 42.67 1221.86
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 311.48 14.28 21.816 < 2e-16 ***
log(bili) 98.80 12.07 8.186 9.42e-15 ***
Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
Residual standard error: 208.9 on 282 degrees of freedom
 (134 observations deleted due to missingness)
Multiple R-squared: 0.192, Adjusted R-squared: 0.1891
F-statistic: 67.01 on 1 and 282 DF, p-value: 9.416e-15
```

autoplot(myLinearModel2)

Just the residual plot, please

autoplot(myLinearModel2, which=1)

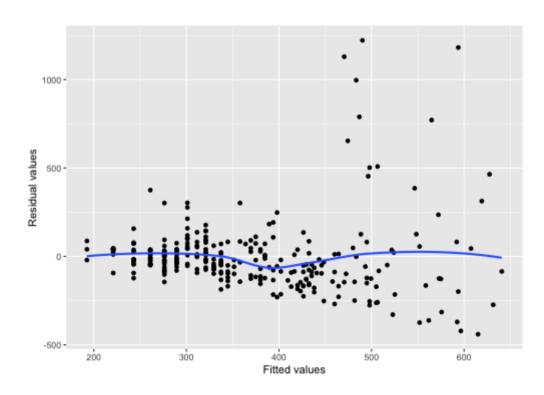
Just the residual plot, please

```
d <- broom::augment(myLinearModel2)
d</pre>
```

```
# A tibble: 284 x 10
   .rownames chol log.bili. .fitted .se.fit .resid
                                                       .hat .sigma .cooksd
             <int>
                       <dbl>
                               <dbl>
                                       <dbl> <dbl>
                                                      <dbl> <dbl>
                                                                      <dbl>
   <chr>
                      2.67
                                                    0.0181
               261
                                576.
                                        28.1 -315.
                                                               208. 2.13e-2
               302
                      0.0953
                                321.
                                        13.7 -18.9 0.00433
                                                               209. 1.79e-5
               176
                      0.336
                                345.
                                        12.8 -169.
                                                    0.00373
                                                               209. 1.23e-3
               244
                      0.588
                                370.
                                        12.4 -126.
                                                    0.00352
                                                               209. 6.41e-4
               279
                     1.22
                                432.
                                        14.6 -153.
                                                    0.00487
                                                               209. 1.33e-3
 6 6
               248
                     -0.223
                                289.
                                        15.8 -41.4 0.00571
                                                               209. 1.14e-4
               322
                     0
                                311.
                                        14.3
                                              10.5 0.00467
                                                              209. 5.98e-6
 8 8
               280
                     -1.20
                                193.
                                        24.9
                                               87.5 0.0142
                                                               209. 1.28e-3
9 9
               562
                     1.16
                                426.
                                        14.2 136. 0.00463
                                                              209. 9.84e-4
10 10
               200
                      2.53
                                562.
                                        26.6 -362. 0.0162
                                                               208. 2.51e-2
# ... with 274 more rows, and 1 more variable: .std.resid <dbl>
```

Just the residual plot, please

```
ggplot(d, aes(x = .fitted, y = .resid))+geom_point()+ geom_smooth(se=F)+
  labs(x = 'Fitted values', y = 'Residual values')
```



Predictions

```
head(predict(myLinearModel2, newdata = pbc))
```

```
1 2 3 4 5 6
575.6925 320.9006 344.7277 369.5578 432.3941 289.4371
```

The newdata has to have the same format and components as the original data the model was trained on

Categorical predictors

```
myLM3 <- lm(chol ~ log(bili) + sex, data = pbc)
broom::tidy(myLM3)</pre>
```

```
# A tibble: 3 x 5
             estimate std.error statistic p.value
 term
 <chr>
               <dbl>
                         <dbl>
                                  <dbl>
                                           <dbl>
               283.
                                7.71 2.14e-13
1 (Intercept)
                          36.6
2 log(bili)
                99.6
                         12.1 8.22 7.37e-15
3 sexf
                32.5
                          37.8
                                  0.858 3.92e- 1
```

R has a somewhat unfortunate notation for categorical variables here, as {variable name}{level}

Logistic regression

The logistic transformation

For an outcome which is binary (0/1), what is really modeled is the **probability** that the outcome is 1, usually denoted by p.

However, we know $0 \le p \le 1$, so what if the model gives a prediction outside this range!!

The logistic transform takes p to

$$logit(p) = log\left(\frac{p}{1-p}\right)$$

and we model logit(p), which has a range from $-\infty$ to ∞

Logistic regression

Logistic regression is a special case of a **generalized linear model**, so the function we use to run a logistic regression is glm

```
myLR <- glm(spiders ~ albumin + bili + chol, data = pbc, family = binomial)
myLR
```

```
Call: glm(formula = spiders ~ albumin + bili + chol, family = binomial, data = pbc)

Coefficients:
(Intercept) albumin bili chol
2.3326484 -0.9954927 0.0995915 -0.0003176

Degrees of Freedom: 283 Total (i.e. Null); 280 Residual
(134 observations deleted due to missingness)
Null Deviance: 341.4
Residual Deviance: 315.2 AIC: 323.2
```

- We have to add the family = binomial as an argument, since this is a special kind of GLM
- All these models only use complete data; they kick out rows with missing data

Logistic regression

broom::tidy(myLR)

```
# A tibble: 4 x 5
                 estimate std.error statistic p.value
  term
                                <dbl>
  <chr>
                     <dbl>
                                            <dbl> <dbl>
1 (Intercept) 2.33 1.30
                                           1.80 0.0717
                -0.995 0.362

      0.362
      -2.75
      0.00595

      0.0344
      2.89
      0.00381

2 albumin
               0.0996
3 bili
                -0.000318 0.000615 -0.517 0.605
4 chol
```

broom::glance(myLR)

Predictions from logistic regression

```
head(predict(myLR))

1 2 3 4 5 6
1.10554163 -1.77506554 -1.04814132 -0.09414055 -0.93144911 -1.62851203
```

These are on the "wrong" scale. We would expect probabilities

```
head(predict(myLR, type='response'))

1 2 3 4 5 6
0.7512970 0.1449135 0.2595822 0.4764822 0.2826308 0.1640343
```

or you can use plogis(predict(myLR)) for the inverse logistic transform

Model selection

How to get the "best" model

Generally getting to the best model involves

- looking at a lot of graphs
- Fitting lots of models
- Comparing the model fits to see what seems good

Sometimes if you have two models that fit about the same, you take the smaller, less complex model (Occam's Razor)

Generally it is not recommended that you use automated model selection methods. It screws up your error rates and may not be the right end result for your objectives

Model building and selection is an art

Clues to follow

You can look at the relative weights (size of coefficient and its p-value) of different predictors

• These weights will change once you change the model, so be aware of that

You can trim the number of variables based on collinearities

• If several variables are essentially measuring the same thing, use one of them

You can look at residuals for clues about transformations

You can look at graphs, as well as science, for clues about interactions (synergies and antagonisms)

Automated model selection

```
# install.packages('leaps')
library(leaps)
mtcars1 <- mtcars %>% mutate_at(vars(cyl, vs:carb), as.factor)
all_subsets <- regsubsets(mpg~., data = mtcars1)
all_subsets</pre>
```

```
Subset selection object
Call: regsubsets.formula(mpg ~ ., data = mtcars1)
16 Variables (and intercept)
      Forced in Forced out
         FALSE
cyl6
                    FALSE
         FALSE
                    FALSE
cyl8
         FALSE
                    FALSE
disp
         FALSE
                     FALSE
hp
         FALSE
                     FALSE
drat
         FALSE
                     FALSE
wt
         FALSE
                     FALSE
gsec
         FALSE
                     FALSE
vs1
am1
         FALSE
                     FALSE
         FALSE
                     FALSE
gear4
         FALSE
                     FALSE
gear5
         FALSE
                     FALSE
carb2
carb3
         FALSE
                     FALSE
carb4
         FALSE
                    FALSE
         FALSE
                     FALSE
carb6
carb8
         FALSE
                     FALSE
1 subsets of each size up to 8
Selection Algorithm: exhaustive
```

Automated model selection

Which has the best R²?

```
ind <- which.max(summary(all_subsets)$adjr2)
summary(all_subsets)$which[ind,]</pre>
```

```
(Intercept)
                    cyl6
                                 cyl8
                                             disp
                                                                       drat
                                                            hp
                    TRUE
                               FALSE
                                            FALSE
                                                                      FALSE
       TRUE
                                                          TRUE
         wt
                    gsec
                                 vs1
                                              am1
                                                         gear4
                                                                      gear5
       TRUE
                   FALSE
                                TRUE
                                             TRUE
                                                         FALSE
                                                                      FALSE
      carb2
                   carb3
                               carb4
                                            carb6
                                                         carb8
      FALSE
                   FALSE
                               FALSE
                                            FALSE
                                                         FALSE
```

Using the tidyverse to run multiple univariate models

Suppose I want to run a series of univariate regressions on the mtcars dataset, seeing how mpg is related to each of the continuous variables.

Let's build this

```
mtcars <- as_tibble(mtcars)
mtcars %>% select(mpg, disp:qsec)
```

```
# A tibble: 32 x 6
    mpg disp
                 hp drat
                          wt asec
  <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <
   21
         160
                110 3.9
                          2.62
                               16.5
   21
         160
                          2.88
                               17.0
   22.8
         108
               93 3.85
                          2.32
                               18.6
   21.4
         258
               110 3.08
                               19.4
        360
   18.7
               175 3.15
                          3.44
                               17.0
   18.1
         225
                105 2.76
                          3.46
                               20.2
        360
   14.3
                245 3.21
                          3.57
                               15.8
   24.4 147.
                62 3.69
                                20
   22.8 141.
                95 3.92
                         3.15
                               22.9
   19.2 168.
                123 3.92 3.44 18.3
# ... with 22 more rows
```

```
mtcars %>% select(mpg, disp:qsec) %>%
gather(variable, value, -mpg)
```

```
# A tibble: 160 x 3
    mpg variable value
  <dbl> <chr>
                <dbl>
       disp
                160
   21
  21 disp
                160
  22.8 disp
                 108
4 21.4 disp
                 258
5 18.7 disp
                 360
6 18.1 disp
                 225
7 14.3 disp
                 360
                147.
8 24.4 disp
9 22.8 disp
                141.
10 19.2 disp
                168.
# ... with 150 more rows
```

```
mtcars %>% select(mpg, disp:qsec) %>%
  gather(variable, value, -mpg) %>%
  group_by(variable) %>%
  lm(mpg~value, data=.)
```

```
Call:
lm(formula = mpg ~ value, data = .)

Coefficients:
(Intercept) value
21.28328 -0.01483
```

```
mtcars %>% select(mpg, disp:qsec) %>%
  gather(variable, value, -mpg) %>%
  nest(-variable)
```

```
bl <- mtcars %>% select(mpg, disp:qsec) %>%
  gather(variable, value, -mpg) %>%
  nest(-variable)
bl$data[[1]]
```

```
# A tibble: 32 x 2
    mpg value
  <dbl> <dbl>
  21 160
        160
2 21
  22.8 108
  21.4 258
  18.7 360
  18.1
        225
7 14.3 360
  24.4 147.
  22.8 141.
  19.2 168.
# ... with 22 more rows
```

```
mtcars %>% select(mpg, disp:qsec) %>%
  gather(variable, value, -mpg) %>%
  nest(-variable) %>%
  mutate(models = map(data, ~lm(mpg~value, data=.)))
```

```
mtcars %>% select(mpg, disp:qsec) %>%
  gather(variable, value, -mpg) %>%
  nest(-variable) %>%
  mutate(models = map(data, ~lm(mpg~value, data=.)),
      outputs = map(models, ~tidy(.)))
```

```
# A tibble: 10 x 6
  variable term
                       estimate std.error statistic p.value
                         <dbl>
                                   <dbl>
                                             <dbl> <dbl>
  <chr>
           <chr>
 1 disp
                       29.6
                                 1.23
                                                   3.58e-21
          (Intercept)
                                            24.1
           value
2 disp
                        -0.0412
                                 0.00471
                                            -8.75 9.38e-10
3 hp
           (Intercept)
                       30.1
                                 1.63
                                            18.4
                                                   6.64e-18
                        -0.0682
                                 0.0101
4 hp
           value
                                            -6.74 1.79e- 7
           (Intercept) -7.52
                                 5.48
                                            -1.37 1.80e- 1
5 drat
6 drat
           value
                        7.68
                                 1.51
                                            5.10 1.78e- 5
7 wt
           (Intercept) 37.3
                                 1.88
                                            19.9
                                                   8.24e-19
                        -5.34
                                 0.559
                                            -9.56 1.29e-10
8 wt
           value
          (Intercept)
                       -5.11
                                10.0
                                            -0.510 6.14e- 1
9 qsec
           value
                        1.41
                                 0.559
                                             2.53 1.71e- 2
10 qsec
```

```
# A tibble: 5 x 6
 variable term estimate std.error statistic p.value
        <chr> <dbl> <dbl>
                                <dbl> <dbl>
 <chr>
 disp
        value -0.0412
                      0.00471
                             -8.75 9.38e-10
2 hp
        value -0.0682
                      0.0101 -6.74 1.79e- 7
                      1.51 5.10 1.78e- 5
3 drat
       value 7.68
                            -9.56 1.29e-10
4 wt
       value -5.34
                      0.559
5 qsec
        value 1.41
                      0.559
                                 2.53 1.71e- 2
```

```
# A tibble: 5 x 6
 variable term estimate std.error statistic p.value
                                 <dbl> <dbl>
                        <dbl>
 <chr>
         <chr> <dbl>
 disp
        value -0.041
                       0.005
                                 -8.75 0
2 hp
        value -0.068
                      0.01 -6.74 0
        value 7.68
                       1.51 5.1<u>0</u> 0
3 drat
4 wt
        value -5.34
                        0.559
                             -9.56 0
5 qsec
        value
              1.41
                        0.559
                                 2.52 0.017
```

Predictive modeling

```
library(tidyverse)
library(caret)
diamonds <- as_tibble(diamonds)
diamonds <- diamonds %>% sample_frac(size=0.1)
set.seed(12356)
index_train <- sample(1:nrow(diamonds), 0.8 * nrow(diamonds))
diamonds_train <- diamonds[index_train,]
diamonds_test <- diamonds[-index_train,]
(nrow(diamonds) == (nrow(diamonds_train) + nrow(diamonds_test)))</pre>
```

[1] TRUE

diamonds

```
# A tibble: 5,394 x 10
  carat cut
                 color clarity depth table price
                               <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
  <dbl> <ord>
                 <ord> <ord>
1 0.71 Very Good G
                       VS2
                                61.8
                                        56 2647
                                                5.69
                                                      5.74 3.53
2 1.03 Ideal
                       SI1
                                59.7
                                       55 4585 6.6
                                                       6.64 3.95
   1.35 Premium
                                           5758
                       SI2
                                61.5
                                                7.11
                                                      7.06 4.36
                                       58
                                58.2
  1.52 Good
                       SI2
                                           9028
                                                7.52
                                                      7.63
                                       60
                                                            4.41
                                                6.92 6.83
  1.2 Premium
                       SI2
                                59.8
                                       58
                                           4032
6 0.53 Ideal
                                                5.23
                       VS1
                                61.6
                                       56
                                           2340
                                                      5.19
                                                            3.21
   0.54 Ideal
                       VS2
                                61
                                           1754
                                                5.25 5.28
                                        56
                                                            3.21
   0.9
        Good
                       I1
                                63.6
                                           2344
                                                 6.07 6.03
                                       61
                                                            3.85
                       VS1
                                61.4
                                           675 4.33 4.3
   0.3 Premium
                                       59
                                                            2.65
10
        Good
                       VVS2
                                56.5
                                       63
                                          7016 6.65 6.62 3.75
```

Let's fit a random forest to this data

```
rf_fit <- train(price ~ ., data=diamonds_train, method = 'rf')
rf_fit

diamonds_predict <- predict(rf_fit, diamonds_test)</pre>
```

I'm not showing results because it was taking too long