R-Adelaide 2016

Day 3: Linear and generalised linear models in R

Dr Steven Delean - Benham Rm 103 steven.delean@adelaide.edu.au

School of Biological Sciences - The University of Adelaide



COMMONWEALTH OF AUSTRALIA Copyright Regulations 1909 WARNING

This material has been reproduced and communicated to you by or an behalf of the University of Admisles under Part Villa of the Copyright And 1995 (fire Art). The resterial is this communication may be subject to copyright under the Art. Any Letter reproduction or communication of this material by you may be the subject of copyright protection under the Art.

Linear model design matrix

 Two R functions, formula and model.matrix are required to produce design matrices for a variety of models

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i, \quad i = 1, \dots, N$$

ullet Focus on the *observational unit* or *experimental unit* to N different entities from which we obtain a measurement

• For categorical variables often called dummy or indicator variables

• Simply indicate if experimental unit had a certain characteristic or not

Linear model design matrix

Using linear model algebra to represent model for design matrix X:

$$\mathbf{Y} = \left(\begin{array}{c} Y_1 \\ Y_2 \\ \vdots \\ Y_N \end{array} \right), \mathbf{X} = \left(\begin{array}{c} 1 & x_1 \\ 1 & x_2 \\ \vdots \\ 1 & x_N \end{array} \right), \beta = \left(\begin{array}{c} \beta_0 \\ \beta_1 \end{array} \right) \text{ and } \varepsilon = \left(\begin{array}{c} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_N \end{array} \right)$$

as

$$\begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_N \end{pmatrix} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots \\ 1 & x_N \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_N \end{pmatrix}$$

or simply

$$\mathbf{Y} = \mathbf{X}\beta + \varepsilon$$

Linear model design matrix

ullet Define a design matrix o find the least squares estimates by fitting the model

• In R, we directly provide a formula to the model fitting function (e.g., 1m)

 \bullet The formula statement in central to model fitting in R generally

• Generates a model.matrix, which is used internally by lm function



Specifying the design

- Design matrix is critical step in linear modeling
 - Encodes coefficients to be fit in model, and
 - Inter-relationship between samples
- Encodes assumptions about the relationships between the response and explanatory variables
- First component usually an intercept column (column of 1's)
- To compare differences between groups, second column specifies which samples are in second group



The basic formula - comparing groups

- Encode experimental design with:
 - Formula with the tilde symbol '~'
 - So model observations using variables to right of tilde
 - Then specify name of a variable that classifies samples into groups
- Two groups, control and high fat diet, with two samples each
- Tell R that these values should not be interpreted numerically, but as different levels of a **factor**

```
# Group is a factor
group <- factor( c(1,1,2,2) )
model.matrix(- group)
# Do not need to use formula function as '-' implies this
model.matrix(formula(- group))
```



The basic formula - comparing groups

- What happens if we don't tell R that 'group' should be interpreted as a factor?
 - Provided numeric variable so Formula with tilde symbol
 - Want second column to have only 0 and 1, indicating group membership
- Note: names of factor levels are irrelevant to model.matrix and lm
 - All that matters is order
- Tell R that these values should not be interpreted numerically, but as different levels of a factor

```
# Group is not a factor
group <- c(1,1,2,2)
model.matrix(- group)
# Using different names produces same model.matrix
group <- factor(c("control", "control", "highfat", "highfat"))
model.matrix(- group)
```



Formula extensions

```
# More groups
                                                                                    # Alternate formulation
group \leftarrow factor(c(1,1,2,2,3,3))
                                                                                    group <- factor(c(1,1,2,2,3,3))
model.matrix(~ group)
                                                                                    model.matrix(~ group + 0)
  (Intercept) group2 group3
                                                                                      group1 group2 group3
                          0
                                                                                                         0
                          0
attr(,"assign")
                                                                                    attr(,"assign")
Γ17 0 1 1
                                                                                    [1] 1 1 1
                                                                                    attr(,"contrasts")
attr(, "contrasts")
                                                                              10
                                                                                    attr(,"contrasts")$group
attr(, "contrasts") $group
[1] "contr.treatment"
                                                                                    [1] "contr.treatment"
```



Assume diet effect is same across sexes

```
Y_i = \beta_0 + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \varepsilon_i
```

```
# Effect of diet and difference in sexes
diet <- factor(c(1,1,1,1,2,2,2,2))
sex <- factor(c("f","f","m","m","f","f","m","m"))
table(diet,sex)
# To fit the additive model
diet <- factor(c(1,1,1,1,2,2,2,2))
sex <- factor(c("f","f","m","m","f","f","m","m"))
model.matrix(- diet + sex)</pre>
```

```
model.matrix(~ diet + sex + diet:sex)
model.matrix(~ diet*sex)
```



Reference level, data and continuous predictors

```
# Finding data
                                                                                     group <- 1:4
                                                                                     model.matrix(~ group, data=data.frame(group=5:8))
                                                                                     # Continuous variables
# Releveling
group <- factor(c(1,1,2,2))
                                                                                     tt <- seq(0,3.4,len=4)
group <- relevel(group, "2")
                                                                                     model.matrix(~ tt + I(tt^2))
model.matrix(~ group)
                                                                                     # Different contrasts
# Providing factor levels
                                                                                    d <- data.frame(time=factor(1:4))</pre>
group <- factor(group, levels=c("1","2"))</pre>
                                                                                    model.matrix(~time,data=d, contrasts.arg= list(time="contr.sum"))
model.matrix(~ group)
                                                                                       (Intercept) group
```

8

9

14

15

16

17

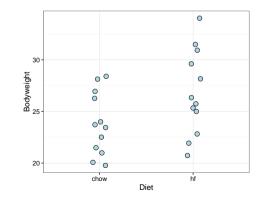
18

```
(Intercept) group1
      attr(,"assign")
      [1] 0 1
      attr(,"contrasts")
      attr(,"contrasts")$group
      [1] "contr.treatment"
        (Intercept) group2
16
      attr(, "assign")
19
      Γ17 0 1
20
      attr(, "contrasts")
21
      attr(, "contrasts") $group
      [1] "contr.treatment"
```

```
attr(."assign")
[1] 0 1
  (Intercept)
                               T(tt^2)
                       tt
            1 0.000000000 0.000000000
            1 1.133333333 1.284444444
            1 2.266666667 5.137777778
           1 3.400000000 11.560000000
attr(, "assign")
[1] 0 1 2
  (Intercept) time1 time2 time3
attr(."assign")
[1] 0 1 1 1
attr(, "contrasts")
```

Linear models - a first taste

- Does high fat diet lead to higher average body weight in mice?
 - Simple t-test problem but will demonstrate equivalence with 1m
- High fat diet group has higher weights, but with overlap
- Build design matrix X using formula ~Diet
 - Group with the 1's in second column is determined by second level of 'Diet'



The Mathematics Behind 1m()

- Quick look behind the scenes of function 1m
- ullet Form the design matrix ${f X}$ and calculate eta
 - Minimizes sum of squares
- Formula for solution is:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{Y}$$

- Calculate in R using:
 - Matrix multiplication operator %*%
 - Inverse function solve, and
 - Transpose function t

```
1 Y <- dat$Bodyweight
2 X <- model.matrix(- Diet, data=dat)
3 solve(t(X) %*% X) %*% t(X) %*% Y
```

```
1 [,1]
2 (Intercept) 23.813333333
3 Diethf 3.020833333
```

Coefficients are average of control group and difference of averages

```
1 s <- with(dat, split(Bodyweight, Diet))
2 mean(s[["chow"]])
3 mean(s[["ff"]]) - mean(s[["chow"]])</pre>
```

```
1 [1] 23.81333333
2 [1] 3.020833333
```



Linear model using lm()

9

14

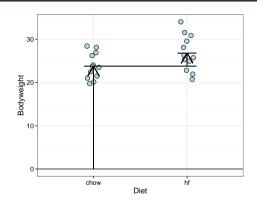
16

18

19 20

```
fit <- lm(Bodyweight - Diet, data=dat)
summary(fit)
(coefs <- coef(fit))</pre>
```

```
Ca11:
lm(formula = Bodyweight ~ Diet, data = dat)
Residuals:
       10 Median
                      30 Max
  Min
-6.104 -2.436 -0.414 2.834 7.186
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 23.81 1.04 22.91 <2e-16 ***
Diethf
       3.02 1.47 2.06 0.052
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ', 1
Residual standard error: 3.6 on 22 degrees of freedom
Multiple R-squared: 0.161, Adjusted R-squared: 0.123
F-statistic: 4.22 on 1 and 22 DF, p-value: 0.0519
(Intercept)
                Diethf
23.813333333 3.020833333
```



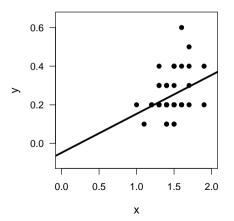
```
mytt <- t.test(s[["hf"]], s[["chow"]], var.equal=TRUE)
summary(fit)$coefficients[2, 3]
mytt$statistic</pre>
```

```
[1] 2.055173992
t
2.055173992
```

Overarching regression framework

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

$$\varepsilon_i \sim N\left(0, \sigma^2\right)$$
(1)



Data

y = response variablex = predictor

Parameters

 $\beta_0 = \text{intercept}$

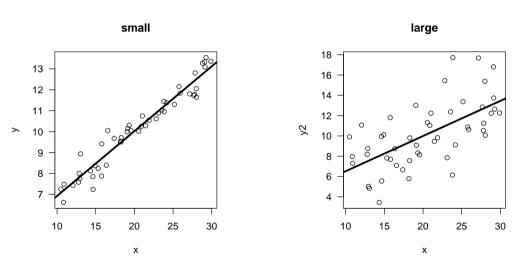
 $\beta_1 = \mathsf{slope}$

 $\sigma = {\rm residual} \ {\rm variation}$

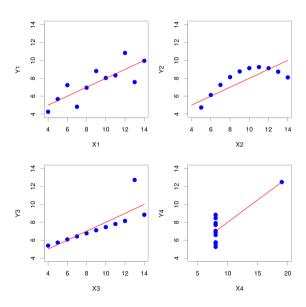
 $\varepsilon = \mathsf{residuals}$

Residual variation (error)

• Our model doesn't perfectly predict Y; residuals are used to estimate error of model



Always plot your data first!



Anscombe data - Linear models

$$\bullet$$
 $\bar{x}=9$ and $\bar{y}=7.5$ for each dataset

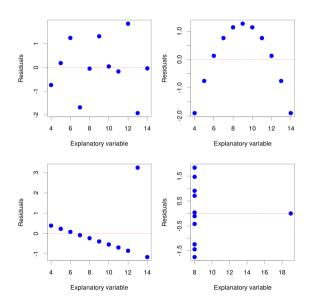
$$s_x^2 = 11, s_y^2 = 4.1$$

• For all data sets, fitted regression is same:

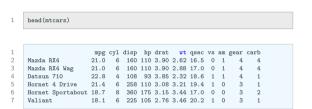
•
$$\hat{Y} = 3.0 + 0.5 * X$$

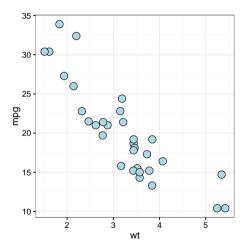
ullet All models have $R^2=0.67,\,\sigma^2=1.24$ and slope coefficients are significant at <1% level

Checking assumptions graphically - Anscombe data residual plots



Exploratory Data Analysis (EDA)





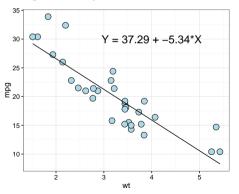
Fitting, saving and working with a linear model

```
# Example:
fit <= with(mtcars, lm(mpg - wt))
summary(fit)
confint(fit)</pre>
```

```
Call:
lm(formula = mpg ~ wt)
Residuals:
          10 Median
  Min
-4.543 -2.365 -0.125 1.410 6.873
Coefficients:
           Fetimate Std Error t value Pr(>|t|)
(Intercept) 37.285
                        1.878
                               19.86 < 2e-16 ***
             -5 344
                        0.559
                               -9.56 1.3e-10 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '. '0.1 ' 1
Residual standard error: 3.05 on 30 degrees of freedom
Multiple R-squared: 0.753. Adjusted R-squared: 0.745
F-statistic: 91.4 on 1 and 30 DF. p-value: 1.29e-10
           2.5 % 97.5 %
(Intercept) 33.45 41.1
           -6.49 -4.2
```

19

- Results of linear saved as:
 - fit.lm <- lm(Y ~ X1 + X2, mydata)
- fit.lm is a linear model object
- Use extractor functions to view
- e.g., 'summary', 'coef', 'residuals', and 'fitted'



Model diagnostics

Estimation and inference from a linear model depend on several assumptions We check these assumptions using *regression diagnostics*; Assume. . .

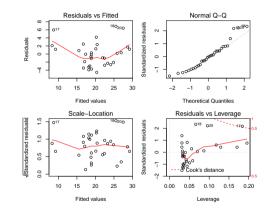
- errors are independent
- errors have constant variance
- errors are normally distributed
- all observations "fit" the model and none have large influence on the model

Violations of these assumptions can invalidate our model

Model diagnostics

- Residuals vs Fitted (check constant variance assumption)
- Normal Q-Q (check normality assumption)
- Scale-Location (check constant variance assumption)
- Residuals vs Leverage (check for influential observations)

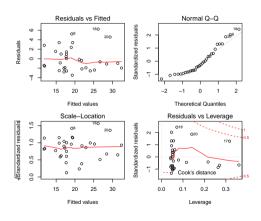
```
# Call the plot function on model object
plot(fit)
```



```
9
14
16
18
19
20
21
```

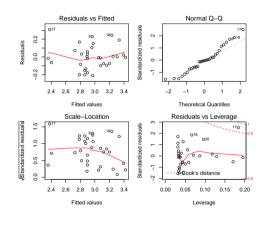
```
# Example:
fit.poly2 <- update(fit, . - poly(wt, degree=2))
summary(fit.poly2)
confint(fit.poly2)
```

```
Call:
lm(formula = mpg ~ poly(wt, degree = 2))
Residuals:
   Min
          10 Median
                              Max
-3.483 -1.997 -0.773 1.462 6.238
Coefficients:
                     Estimate Std. Error t value Pr(>|t|)
(Intercept)
                       20.091
                                   0.469
poly(wt, degree = 2)1 -29.116
                                  2.651
                                        -10.98 7.5e-12 ***
poly(wt, degree = 2)2
                        8.636
                                  2.651
                                           3.26
                                                0.0029 **
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '. ' 0.1 ' 1
Residual standard error: 2.65 on 29 degrees of freedom
Multiple R-squared: 0.819. Adjusted R-squared: 0.807
F-statistic: 65.6 on 2 and 29 DF, p-value: 1.71e-11
                      2.5 % 97.5 %
(Intercept)
                      19.13 21.0
polv(wt. degree = 2)1 -34.54 -23.7
poly(wt. degree = 2)2 3.21 14.1
```



```
# Example:
fit.log <- update(fit, log(mpg) - .)
summary(fit.log)
confint(fit.log)</pre>
```

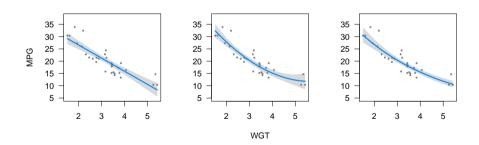
```
Ca11 -
lm(formula = log(mpg) ~ wt)
Residuals:
     Min
               10 Median
                                        Max
-0.21035 -0.08593 -0.00614 0.06133 0.30862
Coefficients:
           Estimate Std. Error t value Pr(>|t|)
(Intercept)
              3.832
                         0.084
                                  45.6 < 2e-16 ***
wt:
             -0.272
                         0.025
                                 -10.9 6.3e-12 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 0.136 on 30 degrees of freedom
Multiple R-squared: 0.798. Adjusted R-squared: 0.791
F-statistic: 118 on 1 and 30 DF, p-value: 6.31e-12
            2.5 % 97.5 %
(Intercept) 3.660 4.003
           -0.323 -0.221
wt
```



Visualising linear models - visreg

• Comparison of fitted models

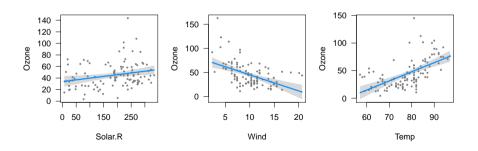
```
library(visreg)
visreg(fit, ylim = c(5, 38), ylab = "MPG", xlab = "")
visreg(fit.log, "ylim = c(5, 38), ylab = "", xlab = "WGT")
visreg(fit.log, "wt", trans = exp, ylim = c(5, 38), partial = TRUE, rug = FALSE, ylab = "", xlab = "")
```



Visualising linear models - visreg

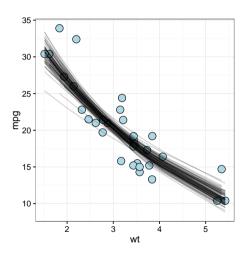
 Particularly useful when you have multiple predictors, combinations of continuous and categorical predictors, interactions

```
1 fitShow <- lm(Ozone - Solar.R + Wind + Temp, data = airquality)
2 visreg(fitShow)
```



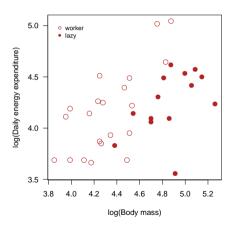
The extra mile - augment and bootstrap

```
.rownames mpg wt .fitted .se.fit .resid
         Mazda RX4 21.0 2.62
                               23.3
                                     0.634 -2.283
     Mazda RX4 Wag 21.0 2.88
                               21.9
                                     0.571 -0.920
        Datsun 710 22.8 2.32
                               24.9 0.736 -2.086
    Hornet 4 Drive 21.4 3.21
                                     0.538 1.297
                               20.1
5 Hornet Sportabout 18.7 3.44
                               18.9
                                     0.553 -0.200
           Valiant 18.1 3.46
                                     0.555 -0.693
                               18.8
```



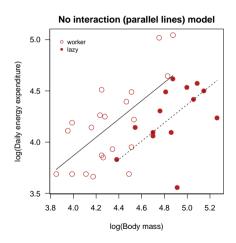
Continuous and categorical explanatory variables

- Mole rats have distinct social castes
- Single queen and small number males reproducing, remaining are workers
- Damaraland mole rats have two worker castes (worker and lazy)
- Do the groups have physiological differences?



Energy-body mass relationships for mole rats

- Energy expenditure appears to vary with body mass
- But lazy workers are heavier than frequent workers
- How different is mean daily energy expenditure between caste groups when adjusted for differences in body mass?



Energy-body mass relationships for mole rats

InMass

caste

Residuals

0.64

0.09

2.72

0.64

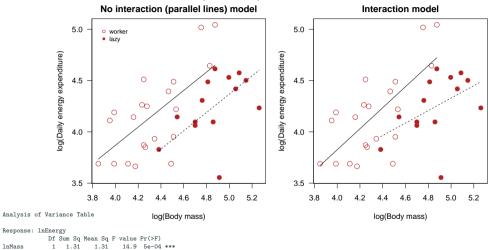
0.09

0.09

0.01 *

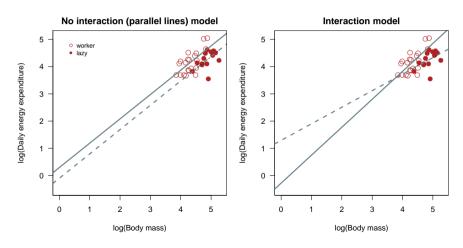
1.0 0.32

• Need to test for interaction - non-parallel slopes

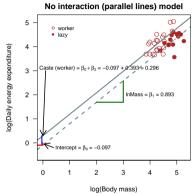


Visualising the parameter space

• Extend plotting limits to 'see' intercepts



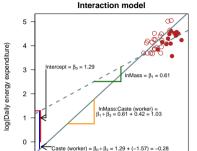
Interpretation of parameters



lm(lnEnergy ~ lnMass + caste)

	Estimate	Std.	Error	t	value	Pr(> t)		
(Intercept)	-0.097		0.942		-0.1	0.92		
lnMass	0.893		0.193		4.6	6e-05	***	
casteworker	0.393		0.146		2.7	0.01	*	

Residual standard error: 0.3 on 32 degrees of freedom Multiple R-squared: 0.41, Adjusted R-squared: 0.37 F-statistic: 11 on 2 and 32 DF, p-value: 0.00022



log(Body mass)
lm(lnEnergy ~ lnMass + caste + lnMass*caste)

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	1.29	1.67	0.8	0.44	
lnMass	0.61	0.34	1.8	0.09	
casteworker	-1.57	1.95	-0.8	0.43	
lnMass:casteworker	0.42	0.41	1.0	0.32	

Residual standard error: 0.3 on 31 degrees of freedom Multiple R-squared: 0.43,Adjusted R-squared: 0.37 F-statistic: 7.7 on 3 and 31 DF, p-value: 0.00054

• Describe relationship between mean of response and linear predictor using a link function

 \bullet Describe relationship between variance and mean using a variance function

Logistic Regression

ullet Sometimes our response is binary: yes/no, success/failure, diseased/non-diseased, etc. Usually coded as 1 and 0

• We use logistic regression to model the log odds of binary response

ullet Let p be the probability that response is 1. Then linear model is:

$$log(\frac{p}{1-p}) = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k$$

Converting log odds to probability

• We usually transform log odds to probability when making predictions

• Say $log(\frac{p}{1-p}) = x$. We transform to probability as follows:

$$p = \frac{e^x}{1 + e^x}$$

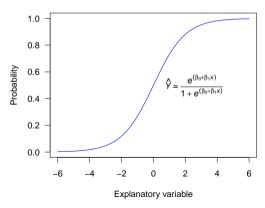
• R can easily do this for us (plogis)

Doing Logistic Regression in R

- Logistic regression is a type of generalized linear model (glm)
- We fit GLM models in R using the glm() function. It works like the lm() function except we specify which glm to fit using the family argument
- Logistic regression requires family=binomial
 - Default link is logit, but should be specified for transparency
 - Alternatives are probit and cloglog

Generalised linear model for binary data - inverse link

- The logistic function has the advantage that it:
 - Yields probabilities between 0 and 1
 - ullet Can incorporate relationships with explanatory variables through the eta parameters



Generalised linear model for binary data - link function

ullet So our model for the probability that Y=1 is the logistic function:

$$\hat{Y} = \frac{e^{\beta_0 + \beta_1 * X_1 + \dots + \beta_p * X_p}}{1 + e^{\beta_0 + \beta_1 * X_1 + \dots + \beta_p * X_p}}$$

- ullet But, the logistic is a nonlinear function, so we cannot estimate the eta parameters using a (generalised) linear model
- Remember that we have used the inverse link $g^{-1}(\hat{Y})$
- So we have to specify this in terms of the *link function* itself, not its inverse
 - This is the *logit link* (*logit* is the *log* of the *odds*)

$$\quad \bullet \ g(\hat{Y}) = \mathit{logit}(\hat{Y}) = \log(\frac{\hat{Y}}{1 - \hat{Y}})$$

- Nesting horseshoe crabs; female with male in nest
- Do female characteristics dictate satellite males?
- \bullet $\,H_A\colon$ Big females have more satellites

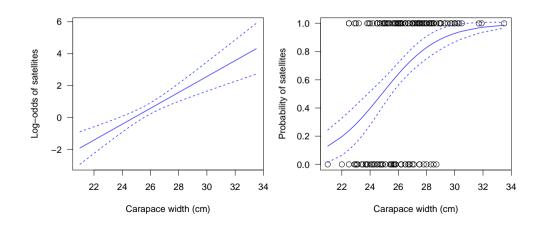


- Binary response; female with satellite male or not
- Carapace width is measure of female fitness

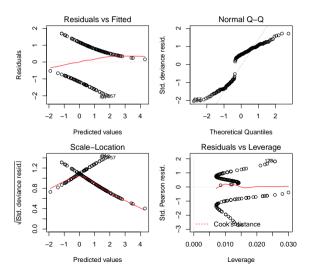
```
spine width.cm nsatellites mass.kg satPresent
        color
        medium both had
                            28 3
                                               3 05
                           22.5
2 dark-medium both had
                                               1 55
3 light-medium
                  good
                           26.0
                                               2.30
4 dark-medium both had
                           24 8
                                               2 10
5 dark-medium both had
                           26 0
                                               2 60
                                                             1
       medium both bad
                           23.8
                                               2.10
                                                             0
```

```
Call:
glm(formula = satPresent ~ width.cm, family = binomial("logit"),
   data = satt)
Deviance Residuals:
           10 Median
-2.028 -1.046 0.548
                      0.907 1.694
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) -12.351
                         2.629
                                -4.70 2.6e-06 ***
width.cm
              0.497
                         0.102
                                4.89 1.0e=06 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 225.76 on 172 degrees of freedom
Residual deviance: 194.45 on 171 degrees of freedom
ATC: 198 5
Number of Fisher Scoring iterations: 4
             2.5 % 97.5 %
(Intercept) -17.810 -7.457
width cm
             0.308 0.709
Single term deletions
Model.
estPresent ~ width cm
        Df Deviance AIC
                           LRT Pr(>Chi)
<none>
              194.4 198.4
width cm 1 225 8 227 8 31 31 2 20=08 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '. '0.1 ' 1
```

- Binary response; female with satellite male or not
- Carapace width is measure of female fitness



• Standard residual diagnostic plots are not informative



Challenge: Survival of passengers on the Titanic

- Sinking of the RMS Titanic is one of most infamous shipwrecks in history
- One of reasons that shipwreck led to such loss of life was that there were not enough lifeboats for passengers and crew
- Although there was some element of luck involved in surviving the sinking, some groups of people were more likely to survive than others, such as women, children, and the upper-class

Challenge question

What sorts of people were likely to survive?

This is actually part of a kaggle competition

Challenge: Survival of passengers on the Titanic

```
titanic <- read.csv("data-raw/titanic_long.csv")
head(titanic)

class age sex survived

1 first adult male 1

3 2 first adult male 1

4 first adult male 1

5 4 first adult male 1

6 5 first adult male 1

6 6 first adult male 1

6 6 first adult male 1
```

