

Models with Multiple Predictors

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```
library(tidyverse)
```

Horse hearts

We will use the *horses' hearts* dataset. There are seven variables represented as columns. They comprise six ultrasound measurements and the weights of 46 horses' hearts, specifically:

1. INNERSYS : Inner-wall ultrasound measurement in systole phase.
2. INNERDIA : Inner-wall ultrasound measurement in diastole phase.
3. OUTERSYS : Outer-wall ultrasound measurement in systole phase.
4. OUTERDIA : Outer-wall ultrasound measurement in diastole phase.
5. EXTSYS : Exterior ultrasound measurement in systole phase.
6. EXTDIA : Exterior ultrasound measurement in diastole phase.
7. WEIGHT : Weight in kilograms.

We will build a multiple regression model to predict the weights of hearts using the six ultrasound measurements.

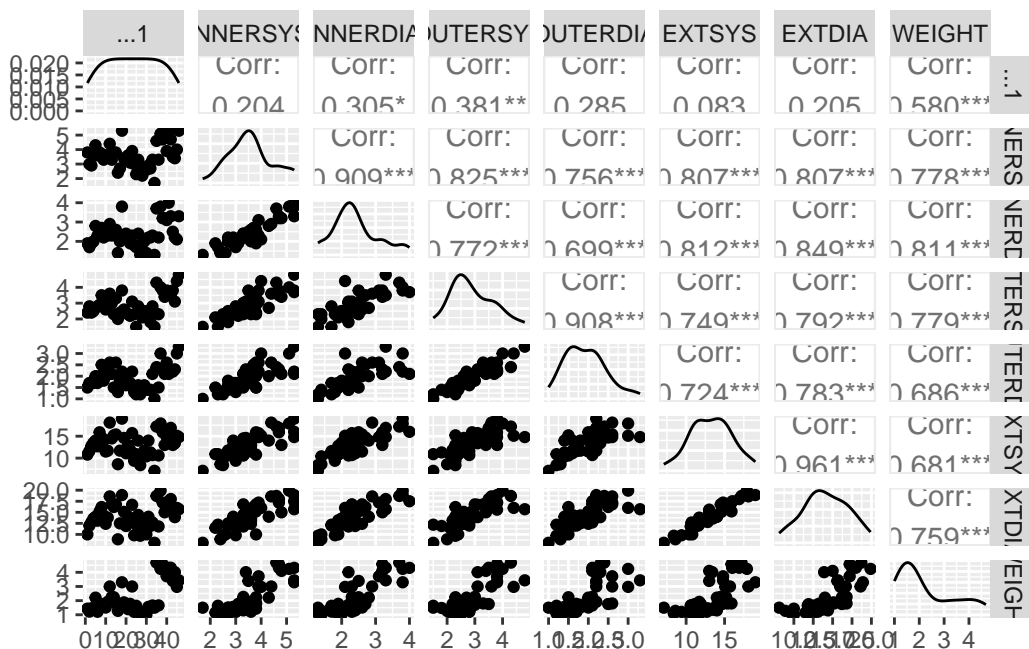
Load data

```
hh <- read_csv("../data/horsehearts.csv")
```

Pairs plot

```
library(GGally)

ggpairs(hh)
```



This plot reveals some very high correlation amongst predictors, particularly (not surprisingly) between the same measurements taken in the different phases (diastolic and systolic). Thus, multicollinearity is likely to be a problem when fitting a multiple regression model. The challenge will be choose the subset of variables that provides the best model fit.

lm output

Let's start by fitting the full model with all of the available predictor variables.

The formula `WEIGHT ~ .` fits a model with `WEIGHT` as the response variable and all other variables in the data frame as predictor variables.

```
mf <- lm(WEIGHT ~ ., data = hh)
```

```
summary(mf)
```

Call:

```
lm(formula = WEIGHT ~ ., data = hh)
```

Residuals:

Min	1Q	Median	3Q	Max
-0.92909	-0.30000	-0.00898	0.29517	1.38196

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-2.246014	0.427517	-5.254	6.00e-06 ***
...1	0.030946	0.007098	4.360	9.58e-05 ***
INNERSYS	0.487587	0.261681	1.863	0.0702 .
INNERDIA	0.145040	0.338119	0.429	0.6704
OUTERSYS	0.219805	0.294408	0.747	0.4599
OUTERDIA	-0.302799	0.377546	-0.802	0.4275
EXTSYS	-0.109803	0.119516	-0.919	0.3640
EXTDIA	0.217405	0.125150	1.737	0.0905 .

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.4968 on 38 degrees of freedom

Multiple R-squared: 0.835, Adjusted R-squared: 0.8047

F-statistic: 27.48 on 7 and 38 DF, p-value: 5.195e-13

💡 Interpreting `summary.lm` output

There is a lot of information in the above summary output to process. Let's break it down.

1. The **Call** part shows us the command we used to produce the model.
2. The **Residuals** part gives us a five-number summary of the residuals.
3. The **Coefficients** table provides the estimates of the model parameters. Specifically, the **Estimate** column gives us the estimates of the β -coefficients, which can be used to reconstruct the predictive formula. Here, that formula is:

$$\hat{y} = -1.6311 + 0.2321 \times \text{INNERSYS} + 0.5195 \times \text{INNERDIA} + \dots + 0.3387 \times \text{EXTDIA}$$

The **Std. Error** column gives the standard error for the estimates of the coefficients. That is, the expected average deviation of the estimator of the coefficient (b or $\hat{\beta}$) from the true population parameter (β). If we were to take many samples (of size n) from this population, a coefficient's standard error represents how much the estimate is expected to vary (due to sampling variation).

The **t value** is the estimate divided by its standard error, which can be used to test whether the effect of that variable is statistically different from zero. The p-value for this test is provided in the next column, headed **Pr(>|t|)**. If the p-value is

low, the observed coefficient estimate is unlikely to have resulted by chance due to sampling variation if the null hypothesis ($H_0 : \beta = 0$) is true. Asterisks indicate significant results, as coded by the `Signif. codes:` given below the table.

4. The final three lines give results for the entire model.

The final three lines give results for the entire model.

The **Residual standard error** is an estimate of the standard deviation of the residuals, i.e. the average absolute difference between the predicted values and the actual values. When estimating the weight of horse's hearts using this model, we would expect to, on average, be wrong by 0.6 kg. The **degrees of freedom** here are the residual degrees of freedom—the number of independent pieces of information with which the residual standard error was estimated.

Next, we have the **Multiple R-squared**, which is the proportion of the total variation in y that is explained by the model. Here, 75% of the variation is explained. The **Adjusted R-squared** is adjusted for the number of variables included in the model (see lecture slides). It cannot be interpreted in same way as the unadjusted R^2 can, but it can be used to compare models.

Finally, an **F-statistic**, associated degrees of freedom (DF) , and **p-value** are provided. This tests whether the model explains a significant proportion of the total variation in y . This can be thought of as testing whether any of the β coefficients in model are non-zero. Here, the p-value is very small so we reject the null hypothesis that all of the β coefficients in model are zero.

Variance Inflation Factor

We mentioned earlier that we were concerned with multicollinearity—correlation among the predictors. A consequence of multicollinearity is that it increases the uncertainty in the estimates of the coefficients—the standard errors of the coefficients are inflated. We can quantify this effect, for each coefficient, with the Variance Inflation Factor (VIF). This is given by the function `car::vif()`¹.

```
car::vif(mf)
```

```
...1  INNERSYS  INNERDIA  OUTERSYS  OUTERDIA  EXTSYS  EXTDIA
1.655390  9.236266  9.196188  9.031392  6.826111  18.501906  23.139222
```

¹The `car::vif()` notation calls the function `vif()` from within the package `car`. Alternatively, you can load the package into R with the command `library(car)`. After doing this, all functions in the `car` package become available, so you can call the function directly as `vif()`, omitting the `car::`. Either way, you must have the package installed, of course!

According to a rule of thumb, a $VIF > 5$ is cause for some concern. A $VIF > 10$ is definitely problematic. So, we have a problem here.

The above VIF values pertain to variances. I find it more intuitive to discuss the square root of the VIF because they relate to the standard errors.

```
sqrt(car::vif(mf))
```

```
...1 INNERSYS INNERDIA OUTERSYS OUTERDIA  EXTSYS  EXT DIA
1.286619 3.039123 3.032522 3.005227 2.612683 4.301384 4.810325
```

These \sqrt{VIF} values can be interpreted in the following way: the standard error for the effect of INNERSYS is around three times larger because of the presence of the other (correlated) variables in the model. The VIF is greatest for EXT DIA, which is consistent with this variable seeming to have the highest correlations with the other predictors.

Model selection

Statisticians use the term “parsimonious” to describe a model that contains no more predictors than necessary to adequately model the data—a model that has the right balance of complexity.

Let’s run a stepwise model selection process to try to find a more parsimonious model than the full model created above. The criterion we will use to assess the quality of the models is Akaike Information Criterion (AIC). Lower AIC values (i.e. closer to $-\infty$) are better.

We will undertake a stepwise process in individual steps, using the `drop1()` function.

```
drop1(mf)
```

Single term deletions

Model:

```
WEIGHT ~ ...1 + INNERSYS + INNERDIA + OUTERSYS + OUTERDIA + EXTSYS +
      EXT DIA
```

	Df	Sum of Sq	RSS	AIC
<none>			9.3771	-57.157
...1	1	4.6903	14.0675	-40.500
INNERSYS	1	0.8567	10.2339	-55.135
INNERDIA	1	0.0454	9.4226	-58.935
OUTERSYS	1	0.1376	9.5147	-58.487

OUTERDIA	1	0.1587	9.5359	-58.385
EXTSYS	1	0.2083	9.5854	-58.146
EXTDIA	1	0.7447	10.1218	-55.642

We have taken the full model (all predictors included) and asked what the AIC values² would be obtained if we dropped each one of the predictors (or none). The lowest AIC score is for the model with INNERSYS removed... so let's remove it and then use `drop1()` again.

```
m2 <- update(mf, ~ . - INNERSYS)
drop1(m2)
```

Single term deletions

Model:

WEIGHT ~ ...1 + INNERDIA + OUTERSYS + OUTERDIA + EXTSYS + EXTDIA				
	Df	Sum of Sq	RSS	AIC
<none>			10.234	-55.135
...1	1	4.0379	14.272	-41.836
INNERDIA	1	1.7508	11.985	-49.871
OUTERSYS	1	0.4701	10.704	-55.069
OUTERDIA	1	0.0910	10.325	-56.728
EXTSYS	1	0.0442	10.278	-56.937
EXTDIA	1	0.3723	10.606	-55.491

Now we remove OUTERDIA and repeat.

```
m3 <- update(m2, ~ . - OUTERDIA)
drop1(m3)
```

Single term deletions

Model:

WEIGHT ~ ...1 + INNERDIA + OUTERSYS + EXTSYS + EXTDIA				
	Df	Sum of Sq	RSS	AIC
<none>			10.325	-56.728
...1	1	4.4141	14.739	-42.355
INNERDIA	1	1.9579	12.283	-50.740
OUTERSYS	1	0.5073	10.832	-56.522

²Negative values of AIC, as seen here, are uncommon but are nothing to worry about. This occurs when the values of the response variable are small.


```
EXTSYS    1    0.0208 10.346 -58.635
EXTDIA    1    0.2912 10.616 -57.448
```

This time, the best model is that with none removed, so the model selection process stops there. Note that this whole process could have been done in a single line of code.

```
mstep <- step(mf)
```

Start: AIC=-57.16

```
WEIGHT ~ ...1 + INNERSYS + INNERDIA + OUTERSYS + OUTERDIA + EXTSYS +
  EXTDIA
```

	Df	Sum of Sq	RSS	AIC
- INNERDIA	1	0.0454	9.4226	-58.935
- OUTERSYS	1	0.1376	9.5147	-58.487
- OUTERDIA	1	0.1587	9.5359	-58.385
- EXTSYS	1	0.2083	9.5854	-58.146
<none>			9.3771	-57.157
- EXTDIA	1	0.7447	10.1218	-55.642
- INNERSYS	1	0.8567	10.2339	-55.135
- ...1	1	4.6903	14.0675	-40.500

Step: AIC=-58.93

```
WEIGHT ~ ...1 + INNERSYS + OUTERSYS + OUTERDIA + EXTSYS + EXTDIA
```

	Df	Sum of Sq	RSS	AIC
- OUTERSYS	1	0.1311	9.5537	-60.299
- OUTERDIA	1	0.2021	9.6246	-59.959
- EXTSYS	1	0.2544	9.6769	-59.709
<none>			9.4226	-58.935
- EXTDIA	1	1.0850	10.5076	-55.921
- INNERSYS	1	2.5621	11.9847	-49.871
- ...1	1	5.2676	14.6902	-40.507

Step: AIC=-60.3

```
WEIGHT ~ ...1 + INNERSYS + OUTERDIA + EXTSYS + EXTDIA
```

	Df	Sum of Sq	RSS	AIC
- OUTERDIA	1	0.0739	9.6276	-61.945
- EXTSYS	1	0.2119	9.7655	-61.290
<none>			9.5537	-60.299
- EXTDIA	1	1.0287	10.5824	-57.595

```
- INNERSYS 1 3.6497 13.2034 -47.416
- ...1 1 6.9595 16.5132 -37.126
```

Step: AIC=-61.94

WEIGHT ~ ...1 + INNERSYS + EXTSYS + EXTDIA

	Df	Sum of Sq	RSS	AIC
- EXTSYS	1	0.1741	9.8017	-63.120
<none>			9.6276	-61.945
- EXTDIA	1	0.9636	10.5912	-59.557
- INNERSYS	1	3.7894	13.4170	-48.677
- ...1	1	6.8859	16.5134	-39.126

Step: AIC=-63.12

WEIGHT ~ ...1 + INNERSYS + EXTDIA

	Df	Sum of Sq	RSS	AIC
<none>			9.8017	-63.120
- EXTDIA	1	2.1043	11.9060	-56.174
- INNERSYS	1	3.6186	13.4203	-50.666
- ...1	1	9.8369	19.6386	-33.153

When you run this, the whole three-step process we executed above will print onscreen and the object `mstep` represents the stepwise-selected model.

Let's examine the stepwise model.

```
summary(mstep)
```

Call:

```
lm(formula = WEIGHT ~ ...1 + INNERSYS + EXTDIA, data = hh)
```

Residuals:

Min	1Q	Median	3Q	Max
-0.89894	-0.28511	-0.03404	0.30224	1.16660

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)	
(Intercept)	-2.418691	0.368870	-6.557	6.27e-08	***
...1	0.035665	0.005493	6.492	7.77e-08	***
INNERSYS	0.559216	0.142016	3.938	0.000304	***
EXTDIA	0.128883	0.042921	3.003	0.004492	**

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.4831 on 42 degrees of freedom

Multiple R-squared: 0.8276, Adjusted R-squared: 0.8153

F-statistic: 67.19 on 3 and 42 DF, p-value: 4.476e-16

We still have two variables that are very highly correlated: EXTSYS and EXT DIA. Let's see if this correlation is problematic, according to the VIF criterion.

```
car::vif(mstep)
```

```
...1 INNERSYS EXT DIA
1.048398 2.876504 2.877824
```

With VIF scores for these two variables still well above 5, this is certainly a problem. This illustrates an important point: you must not naively accept a model which results from a stepwise selection process. Always scrutinise a model before accepting it.

We will force a step where we drop either EXTSYS or EXT DIA.

```
drop1(mstep)
```

Single term deletions

Model:

WEIGHT ~ ...1 + INNERSYS + EXT DIA

	Df	Sum of Sq	RSS	AIC
<none>			9.8017	-63.120
...1	1	9.8369	19.6386	-33.153
INNERSYS	1	3.6186	13.4203	-50.666
EXT DIA	1	2.1043	11.9060	-56.174

```
mstep2 <- update(mstep, ~ . - EXT DIA)
```

Now, let's try another step.

```
drop1(mstep2)
```

Single term deletions

Model:

```
WEIGHT ~ ...1 + INNERSYS
```

	Df	Sum of Sq	RSS	AIC
<none>			11.906	-56.174
...1	1	10.535	22.441	-29.017
INNERSYS	1	25.822	37.728	-5.119

It seems that the model with EXTSYS removed, leaving only INNERDIA and OUTERSYS, is actually preferable. Once the latter two variables are included, EXTSYS does not add any strength to the model. Let's make this model and check for further removals, and our VIFs.

```
mstep3 <- update(mstep2, ~ . - EXTSYS)
drop1(mstep3)
```

Single term deletions

Model:

```
WEIGHT ~ ...1 + INNERSYS
```

	Df	Sum of Sq	RSS	AIC
<none>			11.906	-56.174
...1	1	10.535	22.441	-29.017
INNERSYS	1	25.822	37.728	-5.119

```
car::vif(mstep3)
```

```
...1 INNERSYS
1.043276 1.043276
```

It seems that this model cannot be improved by dropping any further variables. The variables INNERDIA and OUTERSYS, though correlated ($r = 0.77$), do not exert undue influence on each other in the model.

To summarise, let's see the AIC scores for all the models we've made so far.

```
AIC(mf, m2, m3, mstep, mstep2, mstep3)
```

	df	AIC
mf	9	75.38552
m2	8	77.40723
m3	7	75.81462
mstep	5	69.42241
mstep2	4	76.36871
mstep3	4	76.36871

All of these models have very similar AIC. Statisticians say that AIC scores within, say, 3 points can be considered equivalent, and so often we take the approach of choosing the simplest model (i.e. that with the fewest predictors) of all those within 3 AIC points of the lowest score. In some fields it is common to report all models within 10 AIC points or produce an ensemble model bases on AIC weight (not covered in this course). So, while the `mstep3` model isn't the absolute lowest, it is the simplest model from a bunch of models with roughly equivalent AIC scores. Also, it is a good choice because it doesn't have the problems with severe multicollinearity found in the other models.

Don't worry about the fact that the two functions `drop1()` and `AIC()` give different scores. Remember the AIC is a tool for comparing models—the actual scores don't matter. If you look at the difference in AIC scores between two models from the two functions, they are the same. It also should not be compared on models that have different data sources because it is unit less and only acts to compare the models in a specific set.

Difference between AIC scores for `mstep2` and `mstep3` from the `drop1(mstep2)` output:

```
-40.395 - (-42.083)
```

```
[1] 1.688
```

And from the `AIC(mf, m2, m3, mstep, mstep2, mstep3)` output:

```
92.14759 - 90.45888
```

```
[1] 1.68871
```

So now we can choose `mstep3` and clean up.

```
rm(mf, m2, m3, mstep, mstep2) # this code removes these variables
```

Let's examine the summary for our chosen model.

```
summary(mstep3)
```

Call:

```
lm(formula = WEIGHT ~ ...1 + INNERSYS, data = hh)
```

Residuals:

	Min	1Q	Median	3Q	Max
	-1.19304	-0.32850	-0.02243	0.37865	1.16895

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-1.837792	0.342098	-5.372	2.97e-06 ***
...1	0.036819	0.005969	6.168	2.08e-07 ***
INNERSYS	0.899656	0.093160	9.657	2.46e-12 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.5262 on 43 degrees of freedom

Multiple R-squared: 0.7906, Adjusted R-squared: 0.7808

F-statistic: 81.15 on 2 and 43 DF, p-value: 2.529e-15

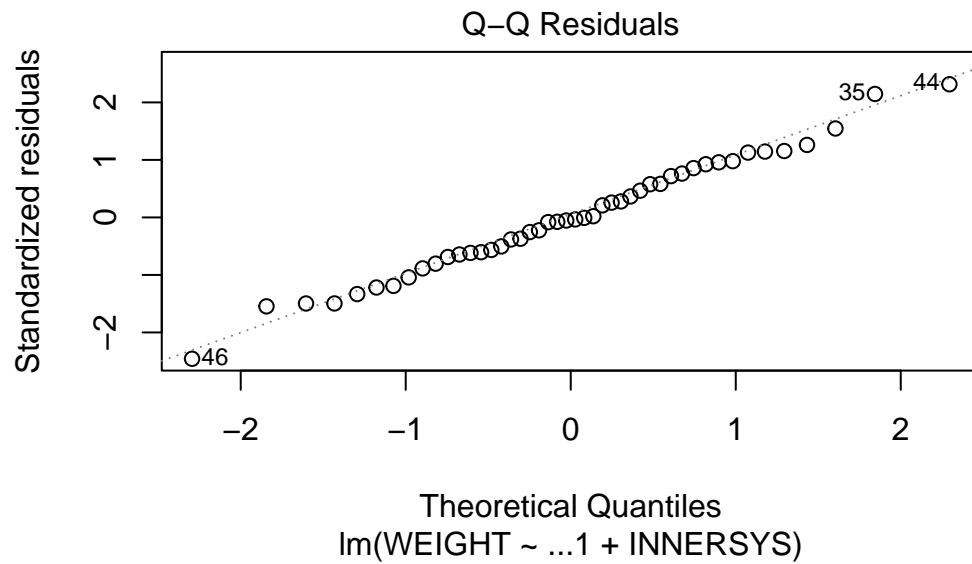
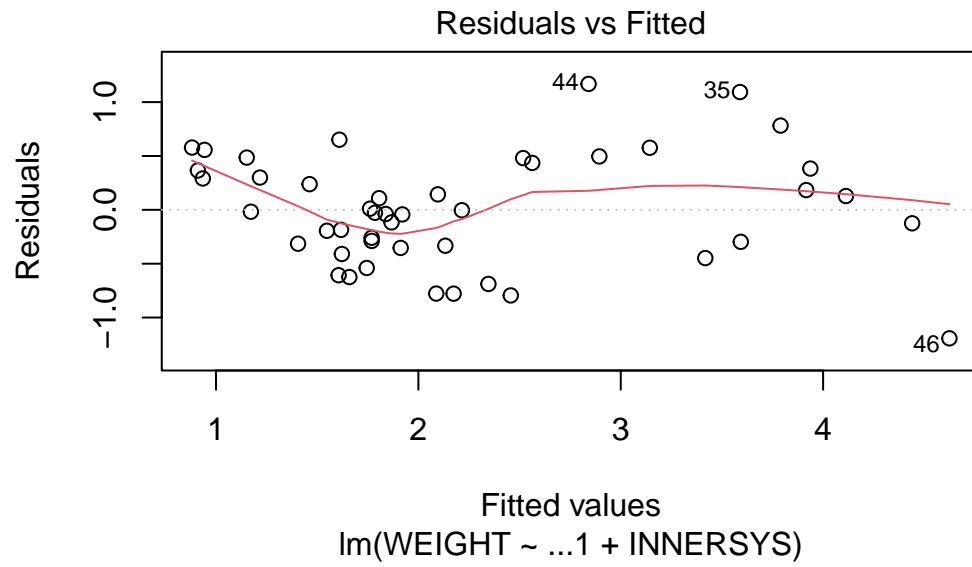
We are now explaining 72% of the variation in heart weights with two variables, as opposed to 75% of the variation with six variables in the original full model. Note also that, in the full model, INNERDIA was not significant and OUTER SYS was only weakly significant. In the smaller model, both these predictors were highly significant. Personally, I would definitely prefer the more parsimonious two-variable model, especially if it meant that I had only to take two, rather than six, ultrasound measurements on a thousand horses!

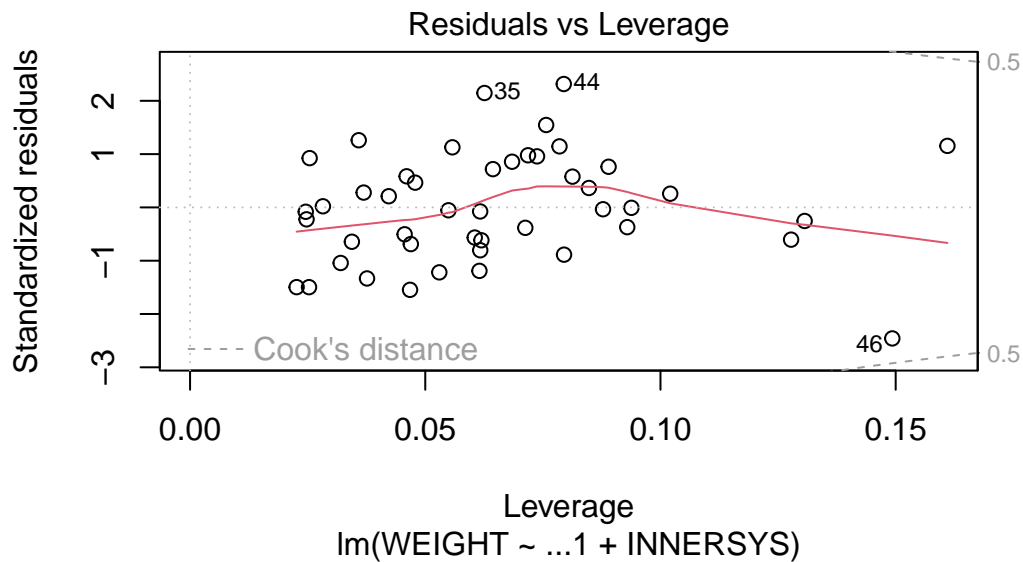
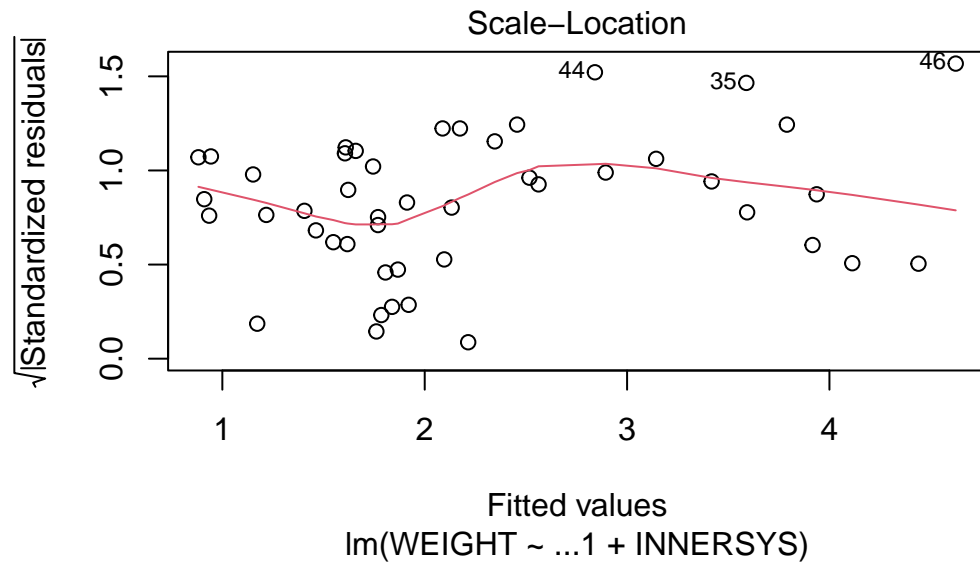
But we're not done yet. We must use some diagnostic tools to examine whether our model meets the assumptions of linear regression before we can accept it.

Model diagnostics

Examine the usual four diagnostic plots.

```
plot(mstep3)
```





The Residuals-vs-Fitted plot shows a slight decreasing trend in the residuals at low fitted values, but it is only a few points. It might pay, though, to bear in mind that the model is likely to overestimate lower heart weights.

The normal Q-Q plot is not too worrying, although there are a few higher-than-expected residuals.

The Scale-Location plot shows no strong evidence of heteroscedasticity—the variance appears fairly constant across fitted values.

And, finally, there are no very large values of Cook's distance or leverage.

There are many other diagnostic tools and graphs available, many in the `car` library, which we do not have time to go into here. If you're interested, this website is a good place to start: <http://www.statmethods.net/stats/riagnostics.html>.

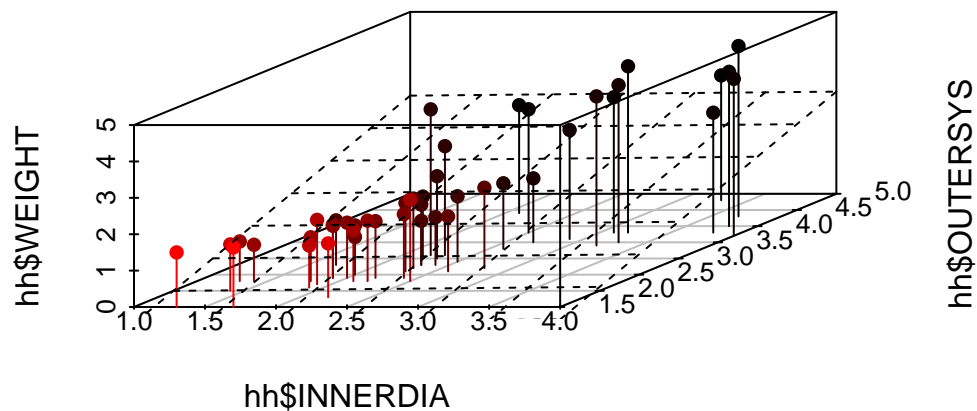
3D plots

Since there are three variables involved in this model, it might be useful to examine their relationship using 3D plots. We can include the 2D plane that represents our regression model on the plot, using the following code.

```
library(scatterplot3d)

hh3d <- scatterplot3d(
  hh$INNERDIA,
  hh$OUTERSYS,
  hh$WEIGHT,
  type="h",
  highlight.3d=T,
  pch=16
)

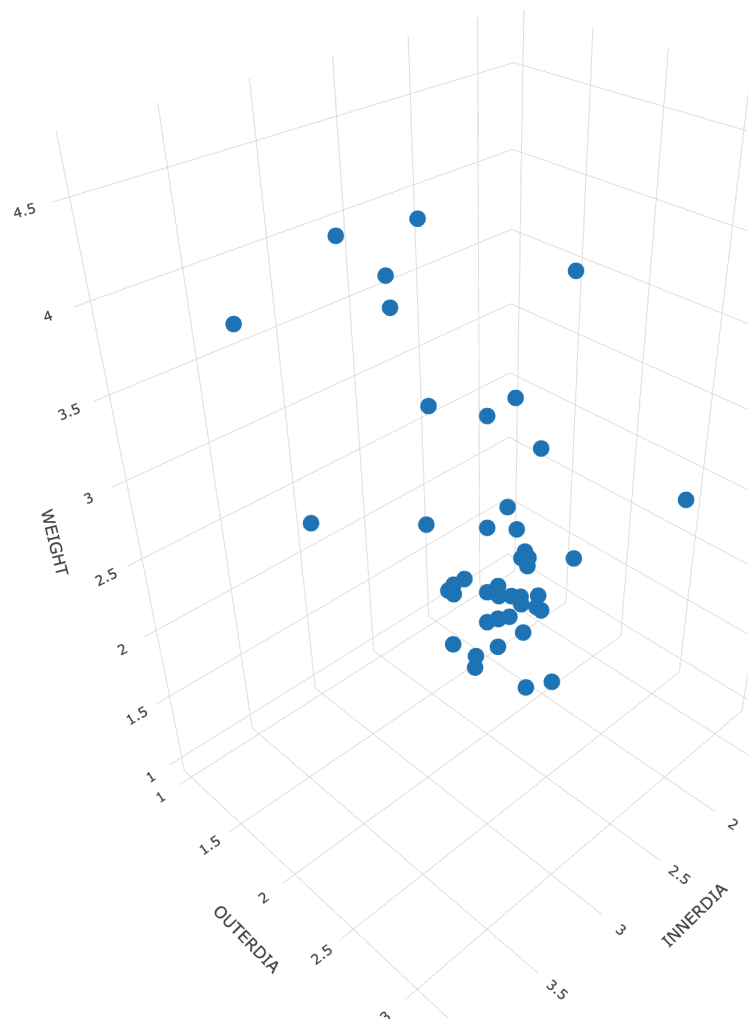
hh3d$plane3d(mstep3)
```



Finally, use `plotly` to create a dynamic 3D plot which you can rotate using your mouse. Don't say I never treat you!

```
library(plotly)

plot_ly(
  hh,
  x = ~INNERDIA,
  y = ~OUTERDIA,
  z = ~WEIGHT
) |>
  add_markers()
```

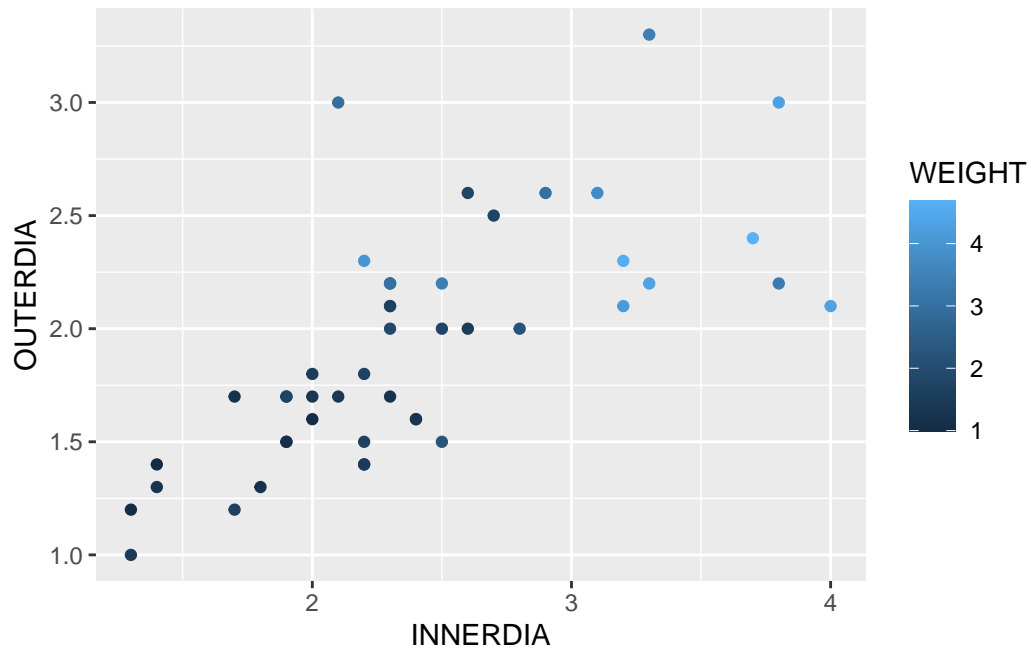


I do not recommend 3-D plots for print reports/publications. They are often best viewed

interactively. Instead try using colors or bubbles for continuous third variables and shapes or facets for discrete third variables.

For example:

```
hh |> ggplot(aes(y=OUTERDIA, x=INNERDIA, color=WEIGHT))+  
  geom_point()
```



Dataset Prestige

We will continue to use dataset `Prestige` from the `car` R package.

Exercise 7.1

Obtain the matrix plot of the numerical variables `education`, `income`, `women`, and `prestige`.

```
library(car)
library(GGally)
library(tidyverse)
```

```
Prestige |>
  select(prestige, education, income, women) |>
  ggpairs(aes(colour=Prestige$type))
```

Obtain their correlation matrix.

```
# Old style pairs plot
Prestige |>
  select(prestige, education, income, women) |>
  pairs()
```

```
Prestige |>
  select(prestige, education, income, women) |>
  cor()
```

Fit a (full) multiple regression of `prestige` on `education`, `income`, & `women`.

```
full.reg <- lm(prestige ~ education + income + women,
               data = Prestige)
```

Obtain the plots for residual diagnostics. Residual plots

```

library(ggfortify)

autoplot(full.reg, 1:6)

# Old style plots
plot(full.reg, 1) # the argument 1 can be changed up to 6

# or just use
par(mfrow=c(2,2))
plot(full.reg)

```

Regression outputs

```
summary(full.reg)
```

Call:

```
lm(formula = prestige ~ education + income + women, data = Prestige)
```

Residuals:

Min	1Q	Median	3Q	Max
-19.8246	-5.3332	-0.1364	5.1587	17.5045

Coefficients:

	Estimate	Std. Error	t value	Pr(> t)
(Intercept)	-6.7943342	3.2390886	-2.098	0.0385 *
education	4.1866373	0.3887013	10.771	< 2e-16 ***
income	0.0013136	0.0002778	4.729	7.58e-06 ***
women	-0.0089052	0.0304071	-0.293	0.7702

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 7.846 on 98 degrees of freedom

Multiple R-squared: 0.7982, Adjusted R-squared: 0.792

F-statistic: 129.2 on 3 and 98 DF, p-value: < 2.2e-16

```
anova(full.reg)
```

Analysis of Variance Table

Response: prestige

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
education	1	21608.4	21608.4	350.9741	< 2.2e-16 ***
income	1	2248.1	2248.1	36.5153	2.739e-08 ***
women	1	5.3	5.3	0.0858	0.7702
Residuals	98	6033.6	61.6		

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```
extractAIC(full.reg)
```

```
[1] 4.0000 424.1724
```

Exercise 7.2

Perform stepwise regression analysis of prestige on education, income, & women.

```
full.reg = lm(prestige ~ education + income + women,  
              data = Prestige)
```

```
step(full.reg)
```

```
step(full.reg, direction="backward")
```

```
step(full.reg, direction="both")
```

The function `update()` is handy for making adjustments to a model. For example, see try the following codes:

```
m1 = update(full.reg, . ~ . - women)
```

```
summary(m1)
```

Note that `. ~ . - women` means that the model is fitted without the `women` variable.

Further options are available in `leaps` and `HH` packages (installation commands are given below).

```
install.packages("leaps", repos = "https://cran.r-project.org")  
install.packages("HH",  
  repos = "https://cran.r-project.org")
```

```

library(leaps)

model = regsubsets(prestige ~ education + income + women,
                  data = Prestige)

library(HH)

summaryHH(model)

plot(summaryHH(model))

```

Exercise 7.3

Perform a polynomial regression of `prestige` on `income`.

```

# Cubic fit
p.model <- lm(prestige ~ poly(income,3),
             data = Prestige)

summary(p.model)

extractAIC(p.model)

plot(p.model)

autoplot(p.model)

```

Try it yourself

Use the river data from Assignment 1:

```

riv <- read_csv("riverdat.csv")

```

Exercise 7.4

Make a scatterplot of all the raw values of **Temperature** (x-axis) and **CHLA Mean** (y-axis) for the Canterbury region only, with the points coloured by **Catchment name**. Fit a linear regression to the plot using `geom_smooth`.

```
# your code goes here
```

Exercise 7.5

Fit a multiple linear regression for the Canterbury region only with the raw values of **CHLA Mean** as the response variable, **Temperature** and **Dissolved oxygen** as predictor variables. Produce a summary table and ANOVA table of your results.

```
# your code goes here
```

Exercise 7.6

Make an indicator variable for the **Waimakariri River** catchment in Canterbury (0 = not in that catchment, 1 = in that catchment). Add this to your regression from exercise 7.5. Produce new tables and discuss your results.

```
# your code goes here
```

- More R code examples are [here](#)