Data Manipulation and Management

Data analysis has as its end point the use of forms of data summary that will convey, fairly and succinctly, the information that is in the data. The fitting of a model is itself a form of data summary.

Be warned of the opportunities that simple forms of data summary, which seem superficially harmless, can offer for misleading inferences. These issues affect, not just data summary per se, but all modeling. Data analysis is a task that should be undertaken with critical faculties fully engaged.

Data summaries that can lead to misleading inferences arise often, from a unbalance in the data and/or failure to account properly for important variables or factors.

## Alternative types of data objects

**Column objects:** These include (atomic) vectors, factors, and dates.

**Date and date-time objects:** The creation and manipulations of date objects will be described below.

**Data Frames:** These are rectangular structures. Columns may be "atomic" vectors, or factors, or other objects (such as dates) that are one-dimensional.

**Matrices and arrays:** Matrices<sup>1</sup> are rectangular arrays in which all elements have the same mode. An array is a generalization of a matrix to allow an arbitrary number of dimensions.

**Tables:** A table is a specialized form of array.

**Lists:** A list is a collection of objects that can be of arbitrary class. List elements are themselves lists. In more technical language, lists are *recursive* data structures.

**S3 model objects:** These are lists that have a defined structure.

**S4 objects:** These are specialized data structures with tight control on the structure. Unlike S3 objects, they cannot be manipulated as lists. Modeling functions in certain of the newer packages<sup>2</sup> return S4 objects.

# 6.1 Manipulations with Lists, Data Frames and Arrays

Recall that data frames are lists of columns that all have the same length. They are thus a specialised form of list. Matrices are two-dimensional arrays. Tables are in essence arrays that hold numeric values.

### 6.1.1 Tables and arrays

The dataset UCBAdmissions is stored as a 3-dimensional table. If we convert it to an array, very little changes:

A data frame is a list of column objects, all of the same length.

<sup>&</sup>lt;sup>1</sup> Internally, matrices are one long vector in which the columns follow one after the other.

<sup>&</sup>lt;sup>2</sup> These include *lme4*, the Bioconductor packages, and the spatial analysis packages.

It changes from a table object to a numeric object, which affects the way that it is handled by some functions. In either case, what we have is a numeric vector of length 24 (=  $2 \times 2 \times 6$ ) that is structured to have dimensions 2 by 2 by 6.

#### 6.1.2 Conversion between data frames and tables

The three-way table UCBAdmissions are admission frequencies, by Gender, for the six largest departments at the University of California at Berkeley in 1973. For a reference to a web page that has the details; see the belp page for UCBAdmissions. Type

```
help(UCBAdmissions)
                        # Get details of the data
example(UCBAdmissions)
```

Note the margins of the table:

```
str(UCBAdmissions)
```

```
'table' num [1:2, 1:2, 1:6] 512 313 89 19 353 207 17 8 120 205 ...
- attr(*, "dimnames")=List of 3
..$ Admit : chr [1:2] "Admitted" "Rejected"
 ..$ Gender: chr [1:2] "Male" "Female"
 ..$ Dept : chr [1:6] "A" "B" "C" "D"
```

In general, operations with a table or array are easiest to conceptualise if the table is first converted to a data frame in which the separate dimensions of the table become columns. Thus, the UCBAdmissions table will be converted to a data frame that has columns Admit. Gender and Dept. Either use the as.data.frame.table() command from base R, or use the adply() function from the plyr pack-

The following uses the function as.data.frame.table() to convert the 3-way table UCBAdmissions into a data frame in which the margins are columns:

```
UCBdf <- as.data.frame.table(UCBAdmissions)</pre>
head(UCBdf, 5)
```

```
Admit Gender Dept Freq
1 Admitted Male
                   A 512
2 Rejected
                    A 313
            Male
3 Admitted Female
                      89
4 Rejected Female
                    Α
                       19
5 Admitted
            Male
                       353
```

Alternatively, use the function adply() from the plyr package that is described in Section 6.2. Here the identity() function does the manipulation, working with all three dimensions of the array:

As UCBAdmissions is a table (not an array). as.data.frame(UCBAdmissions) will give the same result.

```
library(plyr)
UCBdf <- adply(.data=UCBAdmissions,</pre>
                 .margins=1:3,
                 .fun=identity)
names(UCBdf)[4] <- "Freq"</pre>
```

First, calculate overall admission percentages for females and males. The following calculates also the total accepted, and the total who applied:

```
library(dplyr)
gpUCBgender <- dplyr::group_by(UCBdf, Gender)</pre>
AdmitRate <- dplyr::summarise(gpUCBgender,
                               Accept=sum(Freq[Admit=="Admitted"]),
                               Total=sum(Freq),
                               pcAccept=100*Accept/Total)
AdmitRate
```

```
# A tibble: 2 x 4
  Gender Accept Total pcAccept
  <fct> <dbl> <dbl>
1 Male
         1198 2691
                         44.5
                         30.4
2 Female
          557 1835
```

Now calculate admission rates, total number of females applying, and total number of males applying, for each department:

```
gpUCBgd <- dplyr::group_by(UCBdf, Gender, Dept)</pre>
rateDept <- dplyr::summarise(gpUCBgd,</pre>
    Total=sum(Freq),
    pcAccept=100*sum(Freq[Admit=="Admitted"])/Total)
```

Results can conveniently be displayed as follows. First show admission rates, for females and males separately:

```
xtabs(pcAccept~Gender+Dept, data=rateDept)
```

```
Dept
Gender
                           C
                                   D
        62.061 63.036 36.923 33.094 27.749 5.898
 Male
 Female 82.407 68.000 34.064 34.933 23.919 7.038
```

Now show total numbers applying:

```
xtabs(Total~Gender+Dept, data=rateDept)
```

```
Dept
                 C D E
Gender
         Α
             В
        825 560 325 417 191 373
 Male
 Female 108 25 593 375 393 341
```

As a fraction of those who applied, females were strongly favored in department A, and males somewhat favored in departments C and

The overall bias arose because males favored departments where admission rates were relatively high.

E. Note however that relatively many males applied to A and B, where admission rates were high. This biased overall male rates upwards. Relatively many females applied to C, D and F, where rates were low. This biased the overall female rates downwards.

## 6.1.3 Table margins

For working directly on tables, note the function margin.table(). The following retains margin 1 (Admit) and margin 2 (Gender), adding over Dept (the remaining margin):

```
Admit
Gender Admitted Rejected
Male 1198 1493
Female 557 1278
```

Use the function margin.table() to turn this into a table that has the proportions in each row:

```
prop.table(margin21, margin=1)
```

```
Admit
Gender Admitted Rejected
Male 0.4452 0.5548
Female 0.3035 0.6965
```

## 6.1.4 Categorization of continuous data

The data frame bronchit, in the *DAAGviz* package, has observations on 212 men in a sample of Cardiff (Wales, UK) enumeration districts. Variables are r (1 if respondent suffered from chronic bronchitis and 0 otherwise), cig (number of cigarettes smoked per day) and pol1 (the smoke level in the locality).

It will be convenient to define a function props that calculates the proportion of the total in the first (or other nominated element) of a vector:

```
props <- function(x, elem=1)sum(x[elem])/sum(x)</pre>
```

Now use the function cut() to classify the data into four categories, and form tables:

Take margin 2, first, then margin 1, gving a table where rows correspond to levels of **Gender**.

The dataset **bronchit** may alternatively be found in the *SMIR* package.

```
library(DAAGviz)
include.lowest=TRUE))
tab <- with(bronchit, table(r, catcig))</pre>
round(apply(tab, 2, props, elem=2), 3)
```

```
[0,1]
        (1,10] (10,30]
0.072
        0.281
                 0.538
```

There is a clear increase in the risk of bronchitis with the number of cigarettes smoked.

This categorization was purely for purposes of preliminary analysis. Categorization for purposes of analysis is, with the methodology and software that are now available, usually undesirable. Tables that are based on categorization can nevertheless be useful in data exploration.

#### 6.1.5 \*Matrix Computations

Let X(n by p), Y(n by p) and B(p by k) be numeric matrices. Some of the possibilities are:

```
X + Y
                  # Elementwise addition
X * Y
                  # Elementwise multiplication
X %*% B
                  # Matrix multiplication
                  # Solve X B = Y for B
solve(X, Y)
svd(X)
                  # Singular value decomposition
qr(X)
                  # QR decomposition
                  # Transpose of X
```

Calculations with data frames that are slow and time consuming will often be much faster if they can be formulated as matrix calculations. This is in general become an issue only for very large datasets, with perhaps millions of observations. Section 6.4 has examples. For small or modest-sized datasets, convenience in formulating the calculations is likely to be more important than calculation efficiency.

#### 6.2 plyr, dplyr & reshape2 Data Manipulation

The *plyr* package has functions that together:

- provide a systematic approach to computations that perform a desired operation across one or more dimensions of an array, or of a data frame, or of a list:
- allow the user to choose whether results will be returned as an array, or as a data frame, or as a list.

The argument breaks can be either the number of intervals, or it can be a vector of break points such that all data values lie within the range of the breaks. If the smallest of the break points equals the smallest data value, supply the argument include.lowest=TRUE.

It was at one time common practice to categorize continuous data, in order to allow analysis methods for multi-way tables. There is a loss of information. which can at worst be serious.

Note that if t() is used with a data frame, a matrix is returned. If necessary, all values are coerced to the same mode.

Section 4.3.7 will discuss the use of apply() for operations with matrices, arrays and tables.

The dplyr package has functions for performing various summary and other operations on data frames. For many purposes, it supersedes the *plyr* package.

The reshape2 package is, as its name suggests, designed for moving between alternative data layouts.

## *6.2.1* plyr

The *plyr* package has a separate function for each of the nine possible mappings. The first letter of the function name (one of a = array, d = data frame, 1 = list) denotes the class of the input object, while the second letter (the same choice of one of three letters) denotes the class of output object that is required. This pair of letters is then followed by ply.

Here is the choice of functions:

	Class of Output Object		
	a (array)	d (data frame)	1 (list)
Class of Input Object			
a (array)	aaply	adply	alply
d (data frame)	daply	ddply	dlply
l (list)	laply	ldply	llply

First observe how the function adply can be used to change from a tabular form of representation to a data frame. The dimension names will become columns in the data frame.

```
detach("package:dplyr")
library(plyr)
dreamMoves <-
   matrix(c(5,3,17,85), ncol=2,
          dimnames=list("Dreamer"=c("Yes","No"),
                         "Object"=c("Yes","No")))
(dfdream <- plyr::adply(dreamMoves, 1:2,</pre>
                        .fun=identity))
```

```
Dreamer Object V1
      Yes
             Yes
             Yes 3
2
       No
3
              No 17
      Yes
              No 85
       No
```

To get the table back, do:

```
plyr::daply(dfdream, 1:2, function(df)df[,3])
```

```
0bject
Dreamer Yes No
```

```
Yes 5 17
No 3 85
```

The following calculates sums over the first two dimensions of the table UCBAdmissions:

```
plyr::aaply(UCBAdmissions, 1:2, sum)
```

```
Gender
Admit Male Female
Admitted 1198 557
Rejected 1493 1278
```

The following calculates, for each level of the column trt in the data frame nswdemo, the number of values of re74 that are zero:

```
0 1
195 131
```

To calculate the proportion that are zero, for each of control and treatment and for each of non-black and black, do:

```
black
trt 0 1
0 0.353 0.435
1 0.254 0.403
```

The function colwise() takes as argument a function that operates on a column of data, returning a function that operates on all nominated columns of a data frame. To get information on the proportion of zeros for both of the columns re75 and re78, and for each of non-black and black, do:

```
trt black re75 re78
1 0 0 0.353 0.1529
2 0 1 0.435 0.3412
3 1 0 0.254 0.0847
4 1 1 0.403 0.2605
```

Here, aaply() behaves exactly like apply().

Notice the use of the syntax .(trt, black) to identify the columns trt and black. This is an alternative to c("trt", "black").

Here, colwise() operates on the objects that are returned by splitting up the data frame nswdemo according to levels of trt and black. Note the use of ddply(), not daply().

#### 6.2.2 Use of dplyr with Word War 1 cricketer data

Data in the data frame cricketer, extracted by John Aggleton (now at Univ of Cardiff), are from records of UK first class cricketers born 1840 – 1960. Variables are

- Year of birth
- Years of life (as of 1990)
- 1990 status (dead or alive)
- Cause of death: killed in action / accident / in bed
- Bowling hand right or left

The following creates a data frame in which the first column has the year, the second the number of right-handers born in that year, and the third the number of left-handers born in that year. .

```
library(DAAG)
detach("package:plyr")
library(dplyr)
names(cricketer)[1] <- "hand"
gpByYear <- group_by(cricketer, year)</pre>
lefrt <- dplyr::summarise(gpByYear,</pre>
                            left=sum(hand=='left'),
                            right=sum(hand=='right'))
## Check first few rows
lefrt[1:4, ]
```

Both plyr and dplyr have functions summarise(). As in the code shown, detach plyr before proceeding. Alternatively, or additionally, specify dplyr::summarise() rather than summarise()

```
# A tibble: 4 x 3
  year left right
  <int> <int> <int>
  1840
           1
                 6
2 1841
            4
                 16
3
  1842
            5
                 16
  1843
            3
                 25
```

The data frame is split by values of year. Numbers of left and right handers are then tabulated.

From the data frame cricketer, we determine the range of birth years for players who died in World War 1. We then extract data for all cricketers, whether dying or surviving until at least the final year of Workd War 1, whose birth year was within this range of years. The following code extracts the relevant range of birth years.

```
## Use subset() from base R
ww1kia <- subset(cricketer,
                 kia==1 & (year+life)%in% 1914:1918)
range(ww1kia$year)
```

```
[1] 1869 1896
```

Note that a cricketer who was born in 1869 would be 45 in 1914, while a cricketer who was born in 1896 would be 18 in 1914.

Alternatively, use filter() from *dplyr*:

For each year of birth between 1869 and 1896, the following expresses the number of cricketers killed in action as a fraction of the total number of cricketers (in action or not) who were born in that year:

```
# A tibble: 4 x 4
  year
         kia all
                      prop
 <int> <int> <int> <dbl>
                 37 0.0270
  1869
           1
  1870
            2
                 36 0.0556
                 45 0.0222
  1871
            1
                 39 0
            0
  1872
```

For an introduction to *dplyr*, enter:

```
vignette("introduction", package="dplyr")
```

## 6.2.3 reshape2: melt(), acast() & dcast()

The *reshape2* package has functions that move between a dataframe layout where selected columns are unstacked, and a layout where they are stacked. In moving from an unstacked to a stacked layout, column names become levels of a factor. In the move back from stacked to unstacked, factor levels become column names.

Here is an example of the use of melt():

The dataset is now in a suitable form for creating a Florence Nightingale style wedge plot, in Figure C.2.

The dataset Crimean has been included in the *DAAGviz* package.

## Reshaping data for Motion Chart display – an example

The following inputs and displays World Bank Development Indicator data that has been included with the package DAAGviz:

```
## DAAGviz must be installed, need not be loaded
path2file <- system.file("datasets/wdiEx.csv", package="DAAGviz")</pre>
wdiEx <- read.csv(path2file)</pre>
print(wdiEx, row.names=FALSE)
```

```
Country.Name Country.Code
                             Indicator.Name Indicator.Code
                                                              X2010
                                                                       X2000
                     AUS Labor force, total SL.TLF.TOTL.IN 1.17e+07 9.62e+06
   Australia
   Australia
                     AUS Population, total
                                               SP.POP.TOTL 2.21e+07 1.92e+07
                     CHN Labor force, total SL.TLF.TOTL.IN 8.12e+08 7.23e+08
      China
      China
                     CHN Population, total SP.POP.TOTL 1.34e+09 1.26e+09
```

A googleVis Motion Chart does not make much sense for this dataset as it stands, with data for just two countries and two years. Motion charts are designed for showing how scatterplot relationships, here between forest area and population, have changed over a number of years. The dataset will however serve for demonstrating the reshaping that is needed.

For input to Motion Charts, we want indicators to be columns, and years to be rows. The melt() and dcast()<sup>3</sup> functions from the reshape2 package can be used to achieve the desired result. First, create a single column of data, indexed by classifying factors:

```
<sup>3</sup> Note also acast(), which outputs an
array or a matrix.
```

```
library(reshape2)
wdiLong <- melt(wdiEx, id.vars=c("Country.Code",</pre>
                 "Indicator.Name"),
                 measure.vars=c("X2000", "X2010"))
## More simply: wdiLong <- melt(wdiEx[, -c(2,4)])</pre>
wdiLong
```

```
Country.Code
                Indicator.Name variable
        AUS Labor force, total X2000 9.62e+06
                                 X2000 1.92e+07
         AUS Population, total
2
         CHN Labor force, total
3
                                  X2000 7.23e+08
         CHN Population, total
                                  X2000 1.26e+09
         AUS Labor force, total
                                 X2010 1.17e+07
5
6
         AUS Population, total
                                 X2010 2.21e+07
          CHN Labor force, total
                                 X2010 8.12e+08
8
          CHN Population, total
                                 X2010 1.34e+09
```

Now use dcast() to "cast" the data frame into a form where the indicator variables are columns:

If a matrix or array is required, use acast() in place of dcast().

```
names(wdiLong)[3] <- "Year"</pre>
wdiData <- dcast(wdiLong,</pre>
                   Country.Code+Year ~ Indicator.Name,
                   value.var="value")
wdiData
```

```
Country.Code
                 Year Labor force, total Population, total
            AUS X2000
                                  9.62e + 06
                                                      1.92e + 07
2
                                  1.17e + 07
                                                      2.21e+07
            AUS X2010
3
            CHN X2000
                                  7.23e+08
                                                      1.26e+09
            CHN X2010
                                  8.12e + 08
                                                      1.34e + 09
```

A final step is to replace the factor Year by a variable that has the values 2000 and 2010.

```
wdiData <- within(wdiData, {
    levels(Year) <- substring(levels(Year),2)
    Year <- as.numeric(as.character(Year))
})
wdiData</pre>
```

```
Country.Code Year Labor force, total Population, total
           AUS 2000
                               9.62e + 06
                                                   1.92e+07
2
           AUS 2010
                                1.17e + 07
                                                    2.21e+07
3
           CHN 2000
                                7.23e + 08
                                                    1.26e+09
4
            CHN 2010
                                8.12e + 08
                                                    1.34e + 09
```

## 6.3 Session and Workspace Management

## 6.3.1 Keep a record of your work

A recommended procedure is to type commands into an editor window, then sending them across to the command line. This makes it possible to recover work on those hopefully rare occasions when the session aborts.

Be sure to save the script file from time to time during the session, and upon quitting the session.

## 6.3.2 Workspace management

For tasks that make heavy memory demands, it may be important to ensure that large data objects do not remain in memory once they are no longer needed. There are two complementary strategies:

- Objects that cannot easily be reconstructed or copied from elsewhere, but are not for the time being required, are conveniently saved to an image file, using the save() function.
- Use a separate working directory for each major project.

Note the utility function dir() (get the names of files, by default in the current working directory).

Several image files ("workspaces") that have distinct names can live in the one working directory. The image file, if any, that is called **.RData** is the file whose contents will be loaded at the beginning of a new session in the directory.

Use getwd() to check the name and path of the current working directory. Use setwd() to change to a new working directory, while leaving the workspace contents unchanged.

The removal of clutter: Use a command of the form rm(x, y,tmp) to remove objects (here x, y, tmp) that are no longer required.

Movement of files between computers: Files that are saved in the default binary save file format, as above, can be moved between different computer systems.

Further possibilities – saving objects in text form: An alternative to saving objects<sup>4</sup> in an image file is to dump them, in a text format, as dump files, e.g.

```
volume <- c(351, 955, 662, 1203, 557, 460)
weight <- c(250, 840, 550, 1360, 640, 420)
dump(c("volume", "weight"), file="books.R")
```

The objects can be recreated <sup>5</sup> from this "dump" file by inputting the lines of books.R one by one at the command line. This is what, effectively, the command source() does.

```
source("books.R")
```

For long-term archival storage, dump (.R) files may be preferable to image files. For added security, retain a printed version. If a problem arises (from a system change, or because the file has been corrupted), it is then possible to check through the file line by line to find what is wrong.

#### 6.4 Computer Intensive Computations

Computations may be computer intensive because of the size of datasets. Or the computations may themselves be time-consuming, even for data sets that are of modest size.

Note that using all of the data for an analysis or for a plot is not always the optimal strategy. Running calculations separately on different subsets may afford insights that are not otherwise available. The subsets may be randomly chosen, or they may be chosen to reflect, e.g., differences in time or place.

Where it is necessary to look for ways to speed up computations, it is important to profile computations to find which parts of the code are taking the major time. Really big improvements will come from implementing key parts of the calculation in C or Fortran rather than in an application oriented language such as R or Python. Python may do somewhat better than R.

There can be big differences between the alternatives that may be available in R for handling a calculation. Some broad guidelines will As noted in Section 2.2.2, a good precaution can be to make an archive of the workspace before such removal.

The relatively new Julia language appears to offer spectacular improvements on both R and Python, with times that are within a factor of 2 of the Fortran or C times. See http://julialang.org/.

<sup>&</sup>lt;sup>4</sup> Dumps of S4 objects and environments, amongs others, cannot currently be retrieved using source(). See help(dump).

<sup>&</sup>lt;sup>5</sup> The same checks are performed on dump files as if the text had been entered at the command line. These can slow down entry of the data or other object. Checks on dependencies can be a problem. These can usually be resolved by editing the R source file to change or remove offending code.

now be provided, with examples of how differences in the handling of calculations can affect timings.

## 6.4.1 Considerations for computations with large datasets

Consider supplying, matrices in preference to data frames: Most of R's modeling functions (regression, smoothing, discriminant analysis, etc.) are designed to accept data frames as input. The computational and associated memory requirements of the steps needed to form the matrices used for the numerical computations can. for large datasets, generate large overheads. The matrix computations that follow use highly optimized compiled code, and are much more efficient than if directly implemented in R code. Where it is possible to directly input the matrices that will be required for the calculations, this can greatly reduce the time and memory requirements.

Matrix arithmetic can be faster than the equivalent computations that use apply(). Here are timings for alternatives that find the sums of rows of the matrix xy that was generated thus:

```
xy <- matrix(rnorm(5*10^7), ncol=100)
dim(xy)

system.time(xy+1)

user system elapsed
0.155  0.242  0.396

xy.df <- data.frame(xy)
system.time(xy.df+1)

user system elapsed
0.151  0.117  0.268</pre>
```

*Use efficient coding:* Matrix arithmetic can be faster than the equivalent computations that use apply(). Here are timings for some alternatives that find the sums of rows of the matrix xy above:

	user	system	elapsed
apply(xy,1,sum)	0.528	0.087	0.617
xy %*% rep(1,100)	0.019	0.001	0.019
rowSums(xy)	0.034	0.001	0.035

The bigmemory project: For details, go to http://www.bigmemory.org/. The bigmemory package for R "supports the creation, storage, access, and manipulation of massive matrices". Note also the associated packages biganalytics, bigtabulate, synchronicity, and bigalgebra.

Biological expression array applications are among those that are commonly designed to work with data that is in a matrix format. The matrix or matrices may be components of a more complex data structure.

Timings are on a mid 2012 1.8 Ghz Intel i5 Macbook Air laptop with 8 gigabytes of random access memory. *The data.table package:* This allows the creation of data.table objects from which information can be quickly extracted, often in a fraction of the time required for extracting the same information from a data frame. The package has an accompanying vignette. To display it (assuming that the package has been installed), type

vignette("datatable-intro", package="data.table")

On 64-bit systems, massive data sets, e.g., with tens or hundreds of millions of rows, are possible. For such large data objects, the time saving can be huge.

#### 6.5 Summary

apply(), and sapply() can be useful for manipulations with data frames and matrices. Note also the functions melt(), dcast() and acast() from the reshape2 package.

Careful workspace management is important when files are large. It pays to use separate working directories for each different project, and to save important data objects as image files when they are, for the time being, no longer required.

In computations with large datasets, operations that are formally equivalent can differ greatly in their use of computational resources.