Data Aggregation

R provides a wide array of functions to aid in aggregating data. For simple tabulation and cross-tabulation, the table function is available. For more complex tasks, the available functions can be broken down into two groups: those that are designed to work effectively with arrays and/or lists, like apply, sweep, mapply, sapply, and lapply, and those that are oriented toward data frames (like aggregate and by). There is considerable overlap between the two tools, and the output of one can be converted to the equivalent of the output from another, so often the choice of an appropriate function is a matter of personal taste.

We'll start by looking at the table function, and then study the other functions which can be used to aggregate data from various sources.

8.1 table

The arguments to the table function can either be individual vectors representing the levels of interest, or a list or data frame composed of such vectors. The result from table will always be an array of as many dimensions as the number of vectors being tabulated, with dimnames extracted from the levels of the cross-tabulated variables. By default, table will not include missing values in its output; to override this, use the exclude=NULL argument. When passed a single vector of values, table returns an object of class table, which can be treated as a named vector. For simple queries regarding individual levels of a tabulated variable, this may be the most convenient form of displaying and storing the values:

```
> pets = c('dog','cat','duck','chicken','duck','cat','dog')
> tt = table(pets)
```

```
> tt
pets
    cat chicken dog duck
        2 1 2 2
> tt['duck']
duck
        2
> tt['dog']
dog
        2
```

Alternatively, the output from table can be converted to a data frame using as.data.frame:

```
> as.data.frame(tt)
        pets Freq
1        cat        2
2 chicken       1
3        dog        2
4        duck        2
```

When multiple vectors are passed to table, an array of as many dimensions as there are vectors is returned. For this example, the state.region and state.x77 datasets are used, creating a table that shows the number of states whose income is above and below the median income for all states, broken down by region:

```
> hiinc = state.x77[,'Income'] > median(state.x77[,'Income'])
> stateinc = table(state.region,hiinc)
> stateinc
               hiinc
                FALSE TRUE
state.region
  Northeast
                     4
                          5
  South
                    12
                          4
  North Central
                     5
                          7
                     4
                          9
  West
```

This result can be converted to a data frame using as.data.frame:

>	as.data.frame	(statei	inc)
	state.region	hiinc	Freq
1	Northeast	FALSE	4
2	South	FALSE	12
3	North Central	FALSE	5
4	West	FALSE	4
5	Northeast	TRUE	5
6	South	TRUE	4
7	North Central	TRUE	7
8	West	TRUE	9

When passed a data frame, table treats each column as a separate variable, resulting in a table that effectively counts how often each row appears in the data frame. This can be especially useful when the result of table is passed to as.data.frame, since its form will be similar to the input data frame. To illustrate, consider this small example:

```
> x = data.frame(a=c(1,2,2,1,2,2,1),b=c(1,2,2,1,1,2,1),
+
                 c=c(1,1,2,1,2,2,1))
> x
  a b c
1 1 1 1
2 2 2 1
3222
4 1 1 1
5212
6222
7 1 1 1
> as.data.frame(table(x))
  a b c Freq
1 1 1 1
           3
2 2 1 1
           0
3 1 2 1
           0
4 2 2 1
           1
5 1 1 2
           0
6212
           1
7 1 2 2
           0
8222
           2
```

Since the data frame was formed from a table, all possible combinations, including those with no observations, are included.

Sometimes it is helpful to display the margins of a table, that is, the sum of each row and/or column, in order to understand differences among the levels of the variables from which the table was formed. The addmargins function accepts a table and returns a similar table, with the requested margins added. To specify which dimensions should have margins added, the margin= argument accepts a vector of dimensions; a value of 1 in this vector means a new row with the margins for the columns will be added, and a value of 2 corresponds to a new column containing row margins. The default operation to create the margins is to use the sum function. If some other function is desired, it can be specified through the FUN= argument. When a margin is added, the dimnames for the table are adjusted to include a description of the margin. As an example of the use of addmargins, consider the infert dataset, which contains information about the education and parity of experimental subjects. First, we can generate a cross-tabulation in the usual way:

> tt = table(infert\$education,infert\$parity)

> tt 2 3 0-5yrs 0 0 6-11yrs 42 42 21 12 12+ yrs 54 39 15

To add a row of margins, we can use the following call to addmargins:

```
> tt1 = addmargins(tt,1)
> tt1
               2
                  3
                     4
                         5
            1
                            6
           3
                     3
  0-5yrs
              0
                  0
                         0
                            6
  6-11yrs 42 42 21 12
                         3
                            0
  12+ yrs 54 39 15
                            2
                      3
                         3
  Sum
          99 81 36 18
                         6
                            8
```

To add margins to both rows and columns, use a margin= argument of c(1,2):

```
> tt12 = addmargins(tt,c(1,2))
> tt12
             1
                 2
                      3
                          4
                               5
                                   6 Sum
  0-5yrs
             3
                     0
                 0
                          3
                               0
                                   6
                                      12
                42
  6-11vrs
            42
                     21
                         12
                               3
                                   0 120
  12+ yrs
                          3
                               3
            54
                39
                     15
                                   2 116
  Sum
            99
                81
                     36
                         18
                               6
                                   8 248
> dimnames(tt12)
[[1]]
[1] "0-5yrs" "6-11yrs" "12+ yrs" "Sum"
[[2]]
[1] "1"
           "2"
                 "3"
                        "4"
                               "5"
                                     "6"
                                            "Sum"
```

Notice that the dimnames for the table have been updated.

When it's desired to have a table of proportions instead of counts, one strategy would be to use the sweep function (Section 8.4) dividing each row and column by its corresponding margin. The prop.table function provides a convenient wrapper around this operation. prop.table accepts a table, and a margin= argument, and returns a table of proportions. With no value specified for margin=, the sum of all the cells in the table will be 1; with margin=1, each row of the resulting table will add to 1, and with margin=2, each column will add to 1. Continuing with the previous example, we can convert our original table to one containing proportions, having each column add to 1, as follows:

> prop.table(tt,2)

1234560-5yrs0.030300.000000.000000.166670.000000.750006-11yrs0.424240.518520.583330.666670.500000.0000012+yrs0.545450.481480.416670.166670.500000.25000

For tables with more than two dimensions, it may be useful to present the table in a "flattened" form using the ftable function. To illustrate, consider the UCBAdmissions dataset, which is already a table with counts for admission to various departments based on gender. As a three-dimensional table, it would normally be displayed as a series of two-dimensional tables. Using ftable, the same information can be displayed in a more compact form:

> ftable(UCBAdmissions)								
		Dept	А	В	С	D	E	F
Admit	Gender							
Admitted	Male		512	353	120	138	53	22
	Female		89	17	202	131	94	24
Rejected	Male		313	207	205	279	138	351
	Female		19	8	391	244	299	317

The **xtabs** function can produce similar results to the **table** function, but uses the formula language interface. For example, the state income by region table could be reproduced using statements like these:

>	xtabs	(~state.1	region	+ hiin	c)
		ł	niinc		
st	tate.re	egion	FALSE	TRUE	
	Northe	east	4	5	
	${\tt South}$		12	4	
	North	Central	5	7	
	West		4	9	

If a variable is given on the left-hand side of the tilde ($\tilde{}$), it is interpreted as a vector of counts corresponding to the values of the variables on the right-hand side, making it very easy to convert already tabulated data into R's notion of a table:

```
> x = data.frame(a=c(1,2,2,1,2,2,1),b=c(1,2,2,1,1,2,1),
+ c=c(1,1,2,1,2,2,1))
> dfx = as.data.frame(table(x))
> xtabs(Freq ~ a + b + c,data=dfx)
, , c = 1
b
a 12
1 3 0
2 0 1
```

, , c = 2 b a 1 2 1 0 0 2 1 2

8.2 Road Map for Aggregation

When confronted with an aggregation problem, there are three main considerations:

- 1. How are the groups that divide the data defined?
- 2. What is the nature of the data to be operated on?
- 3. What is the desired end result?

Thinking about these issues will help to point you to the most effective solution for your needs. The following paragraphs should help you make the best choice.

Groups defined as list elements. If the groups you're interested in are already organized as elements of a list, then sapply or lapply (Section 8.3) are the appropriate functions; they differ in that lapply always returns a list, while sapply may simplify its output into a vector or array if appropriate. This is a very flexible approach, since the entire data frame for each group is available. Sometimes, if other methods are inappropriate, you can first use the split function to create a suitable list for use with sapply or lapply (Section 8.5).

Groups defined by rows or columns of a matrix. When the goal is to operate on each column or row of a matrix, the apply function (Section 8.4) is the logical choice. apply will usually return its results as a vector or array, but will return a list if the results of operating on the rows or columns are of different dimensions.

Groups based on one or more grouping variables. A wide array of choices is available for the very common task of operating on subsets of data based on the value of a grouping variable. If the computations you desire each involve only a single vector and produce a single scalar as a result (like calculating a scalar-valued statistic for a variable or set of variables), the **aggregate** function (Section 8.5) is the most likely choice. Since aggregate always returns a data frame, it is especially useful if the desired result is to create a plot or fit a statistical model to the aggregated data.

If your computations involve a single vector, but the result is a vector (for example, a set of quantiles or a vector of different statistics), tapply (Section 8.5) is one available option. Unlike aggregate, tapply returns its results in a vector or array for which individual elements are easy to access,

but may produce a difficult-to-interpret display for complex problems. Another approach to the problem is provided by the **reshape** package, available through CRAN, and documented in Section 8.6. It uses a formula interface, and can produce output in a variety of forms.

When the desired result requires access to more than one variable at a time (for example, calculating a correlation matrix, or creating a scatter plot), row indices can be passed to tapply to extract the appropriate rows corresponding to each group. Alternatively, the by function can be used. Unlike tapply, the special list returned by by has a print method which will always produce an easily-readable display of the aggregation, but accessing individual elements of the returned list may be inconvenient. Naturally, for tasks like plotting, there is no clear reason to choose one approach over the other.

As mentioned previously, using split and sapply/lapply is a good solution if you find that other methods don't provide the flexibility you need. Finally, if nothing else seems to work, you can write a loop to iterate over the values returned by unique or intersection, and perform whatever operations you desire. If you take this route, make sure to consider the issues about memory management in loops found in Section 8.7.

8.3 Mapping a Function to a Vector or List

Although most functions in R will automatically operate on each element of a vector, the same is not true for lists. Since many R functions return lists, it's often useful to process each list element in the same way that R naturally does for vectors. To handle situations like this, R provides two functions: lapply and sapply. Each of these functions takes a list or vector as its first argument, and a function to be applied to each element as its second argument. The difference between the two functions is that lapply will always return its result as a list, while sapply will simplify its output to a vector or matrix if possible. For example, suppose we have a vector of character strings, and we want to find out how many words are in each vector. Like most functions in R, the strsplit function will operate on each element of a vector, returning for each element a new vector containing the individual pieces of that element:

```
> text = c('R is a free environment for statistical analysis',
+ 'It compiles and runs on a variety of platforms',
+ 'Visit the R home page for more information')
> result = strsplit(text,' ')
> result
[[1]]
[1] "R" "is" "a"
[4] "free" "environment" "for"
[7] "statistical" "analysis"
```

[[2]]		
[1] "It"	"compiles"	"and"
[4] "runs"	"on"	"a"
[7] "variety"	"of"	"platforms"
[[3]]		
[1] "Visit"	"the"	"R"
[4] "home"	"page"	"for"
[7] "more"	"informat	ion"

Since each vector could potentially contain different numbers of words, strsplit puts its result into a list. The length function will not automatically operate on each list element; instead, it properly reports the number of elements in the returned list:

```
> length(result)
[1] 3
```

To find the length of the individual elements, we can use either sapply or lapply; since the length of each element will be a scalar, sapply would be most appropriate:

```
> nwords = sapply(result,length)
> nwords
[1] 8 9 8
```

Another important use of sapply relates to data frames. When treated as a list, each column of a data frame retains its mode and class. Suppose we're working with the built-in ChickWeight data frame, and we wish to learn more about the nature of each column. Simply using the class function on the data frame will give information about the data frame, not the individual columns:

```
> class(ChickWeight)
[1] "nfnGroupedData" "nfGroupedData"
[3] "groupedData" "data.frame"
```

To get the same information for each variable, use sapply:

```
> sapply(ChickWeight,class)
$weight
[1] "numeric"
$Time
[1] "numeric"
$Chick
[1] "ordered" "factor"
$Diet
[1] "factor"
```

Notice that in this case, since the class for Chick was of length 2, sapply returned its result as a list. This will always be the case when the structure of the data would be lost if sapply tried to simplify it into a vector or array.

This same idea can be used to extract columns of a data frame that meet a particular condition. For example, to create a data frame containing only numeric variables, we could use

```
df[,sapply(df,class) == 'numeric']
```

sapply or lapply can be used as an alternative to loops for performing repetitive tasks. When you use these functions, they take care of the details of deciding on the appropriate form of the output, and eliminate the need to incrementally build up a vector or matrix to store the result. To illustrate, suppose that we wish to generate matrices of random numbers and determine the highest correlation coefficient between any of the variables in the matrix. The first step is to create a function that will generate a single matrix and calculate the maximum correlation coefficient:

```
maxcor = function(i,n=10,m=5){
    mat = matrix(rnorm(n*m),n,m)
    corr = cor(mat)
    diag(corr) = NA
    max(corr,na.rm=TRUE)
}
```

Since sapply will always pass an argument to the applied function, a dummy argument (i) is added to the function. Since the diagonal of a correlation matrix will always be 1, the diagonal elements of the correlation matrix were masked by assigning them values of NA. Suppose we want to generate 1000 100×5 matrices, and find the average value of the maximum correlation:

```
> maxcors = sapply(1:1000,maxcor,n=100)
> mean(maxcors)
[1] 0.1548143
```

Notice that additional arguments to the function being applied (like n=100 in this case) are passed to the function by including them in the argument list after the function name or definition.

For simpler simulations of this type, the **replicate** function can be used. This function takes as its first argument the number of replications desired, and as its second argument an expression (not a function!) that calculates the desired statistic for the simulation. For example, we can generate a single t-statistic from two groups of normally distributed observations with the following expression:

Using replicate, we can generate as many of these statistics as we want:

8.4 Mapping a function to a matrix or array

When your data has the added organization of an array, R provides a convenient way to operate on each dimension of the data through the apply function. This function requires three arguments: the array on which to perform the operation, an index telling apply which dimension to operate on, and the function to use. Like sapply, additional arguments to the function can be placed at the end of the argument list. For matrices, a second argument of 1 means "operate on the rows", and 2 means "operate on the columns".

One common use of apply is in conjunction with functions like scale, which require summary statistics calculated for each column of a matrix. Without additional arguments, the scale function will subtract the mean of each column and divide by the standard deviation, resulting in a matrix of zscores. To use other statistics, appropriate vectors of values can be calculated using apply and provided to scale using the center= and scale= arguments. For example, by providing a vector of medians for centering, and a vector of mean average deviations for scaling, an alternative standardization to z-scores can be performed. Using the built-in state.x77 dataset, we could perform such a transformation as follows:

Similar to sapply, apply will try to return its results in a vector or matrix when appropriate, making it useful in cases where several quantities need to be calculated for each row or column of a matrix. Suppose we wish to produce a matrix containing the number of nonmissing observations, the mean and the standard deviation for each column of a matrix. The first step is writing a function which will return what we want for a single column:

```
summfn = function(x)c(n=sum(!is.na(x)),mean=mean(x),sd=sd(x))
```

Now we can apply the function to a data frame with all numeric columns, or a numeric matrix like state.x77:

```
> x = apply(state.x77,2,sumfun)
```

> t(x)			
	n	mean	sd
Population	50	4246.4200	4.464491e+03
Income	50	4435.8000	6.144699e+02
Illiteracy	50	1.1700	6.095331e-01
Life Exp	50	70.8786	1.342394e+00
Murder	50	7.3780	3.691540e+00
HS Grad	50	53.1080	8.076998e+00
Frost	50	104.4600	5.198085e+01
Area	50	70735.8800	8.532730e+04

This example illustrates another advantage of using apply instead of a loop, namely, that apply will use names that are present in the input matrix or data frame to properly label the result that it returns.

One further use of apply is worth mentioning. If a vector needs to be processed in non-overlapping groups, it is sometimes easiest to temporarily treat the vector as a matrix, and use apply to operate on the groups. For example, suppose we wish to take the sum of every three adjacent values in a vector. By first forming a three-column matrix, we can process the groups conveniently using apply:

> x = 1:12
> apply(matrix(x,ncol=3,byrow=TRUE),1,sum)
[1] 6 15 24 33

The apply function is very general, and for certain applications, there may be more efficient methods available to perform the necessary computations. For example, if the statistic to be calculated is the sum or the mean, matrix computations will be more efficient than calling apply with the appropriate function. In cases like this, the rowSums, colSums, rowMeans, or functions can be used. Each of these functions accepts a matrix (or a data frame which will be coerced to a matrix), and an optional na.rm= argument to specify the handling of missing values. Since these functions will accept logical values as input as well as numeric values, they can be very useful for counting operations.

For example, consider the dataset USJudgeRatings, which has ratings for 43 judges in twelve categories. To get the mean rating for each category, the colMeans function could be used as follows:

```
> mns = colMeans(USJudgeRatings)
> mns
    CONT
              INTG
                       DMNR.
                                 DILG
                                          CFMG
7.437209 8.020930 7.516279 7.693023 7.479070
    DECI
             PREP
                       FAMI
                                 ORAL
                                          WRIT
7.565116 7.467442 7.488372 7.293023 7.383721
    PHYS
             RTEN
7.934884 7.602326
```

To count the number of categories for which each judge received a score of 8 or greater, the **rowSums** function can be used by providing the appropriate logical matrix:

A common situation when processing a matrix by rows or columns is that each row or column needs to be processed differently, based on the values of an auxiliary vector which already exists. In cases like this, the sweep function can be used. Like apply, the first two arguments to sweep are the matrix to be operated on and the index of the dimension to be used for repetitive processing. In addition, sweep takes a third argument representing the vector to be used when processing each column, and finally a fourth argument providing the function to be used. sweep operates by building matrices which can be operated on in a single call, so, unlike apply, only functions which can operate on arrays of values can be passed to sweep. All of the built-in binary operators, such as addition ("+"), subtraction ("-"), multiplication ("*"), and division ("/") can be used, but, in general, it will be necessary to make sure an arbitrary function will work properly with sweep. For example, suppose we have a vector representing the maximum value found in each column of a matrix, and we wish to divide each column of the matrix by its corresponding maximum. Using the state.x77 data frame, we could use sweep as follows:

```
> maxes = apply(state.x77,2,max)
> swept = sweep(state.x77,2,maxes,"/")
> head(swept)
           Population
                         Income Illiteracy Life Exp
                                                         Murder
Alabama
           0.17053496 0.5738717
                                 0.7500000 0.9381793 1.0000000
Alaska
           0.01721861 1.0000000 0.5357143 0.9417120 0.7483444
           0.10434947 0.7173397
                                 0.6428571 0.9585598 0.5165563
Arizona
Arkansas
           0.09953769 0.5349169
                                0.6785714 0.9600543 0.6688742
California 1.00000000 0.8098179
                                 0.3928571 0.9743207 0.6821192
Colorado
           0.11986980 0.7733967
                                 0.2500000 0.9790761 0.4503311
             HS Grad
                          Frost
                                      Area
           0.6136701 0.10638298 0.08952178
Alabama
Alaska
           0.9910847 0.80851064 1.00000000
           0.8632987 0.07978723 0.20023057
Arizona
Arkansas
           0.5928678 0.34574468 0.09170562
California 0.9301634 0.10638298 0.27604549
Colorado
           0.9494799 0.88297872 0.18319233
```

Now suppose that we wish to calculate the mean value for each variable using only those values which are greater than the median for that variable. We can calculate the medians using apply and then write a simple function to find the mean of the values we're interested in.

```
> meds = apply(state.x77,2,median)
> meanmed = function(var,med)mean(var[var>med])
> meanmed(state.x77[,1],meds[1])
[1] 7136.16
> meanmed(state.x77[,2],meds[2])
[1] 4917.92
```

Although the function works properly for individual columns, it returns only a single value when used in conjunction with sweep:

```
> sweep(state.x77,2,meds,meanmed)
[1] 15569.75
```

The source of the problem is the inequality used to subset the variable values, since it will not properly operate on the array that **sweep** produces to calculate its results. In cases like this, the **mapply** function can be used. By converting the input matrix to a data frame, each variable in the input will be processed in parallel to the vector of medians, providing the desired result:

```
> mapply(meanmed,as.data.frame(state.x77),meds)
[1] 7136.160 4917.920 1.660 71.950 10.544
[6] 59.524 146.840 112213.400
```

By default, mapply will always simplify its results, as in the previous case where it consolidated the results in a vector. To override this behavior, and return a list with the results of applying the supplied function, use the SIMPLIFY=FALSE argument.

8.5 Mapping a Function Based on Groups

To calculate scalar data summaries of one or more columns of a data frame or matrix, the aggregate function can be used. Although this function is limited to returning scalar values, it can operate on multiple columns of its input argument, making it a natural choice for data summaries for multiple variables. The first argument to aggregate is a data frame or matrix containing the variables to be summarized, the second argument is a list containing the variables to be used for grouping, and the third argument is the function to be used to summarize the data. For example, the iris dataset contains the values of four variables measured on a variety of samples from three species of irises. To find the means of all four variables broken down by species, aggregate can be called as follows:

>	aggregate(iris[-5],iris[5],mean)				
	Species	Sepal.Length	Sepal.Width	Petal.Length	Petal.Width
1	setosa	5.006	3.428	1.462	0.246
2	versicolor	5.936	2.770	4.260	1.326
3	virginica	6.588	2.974	5.552	2.026

Since the second argument must be a list, when a data frame is being processed it is often convenient to refer to the grouping columns using single bracket subscripts, since columns accessed this way will naturally be in the form of a list. In addition, with more than one grouping variable, specifying the columns this way will insure that the grouping variables' names will be automatically transfered to the output data frame. If the columns are passed as manually constructed list, **aggregate** will use names like **Group.1** to identify the grouping variables, unless names are provided for the list elements.

As an example, suppose we wish to calculate the mean weight for observations in the ChickWeight data frame, broken down by the variables Time and Diet. Specifying the grouping variables as ChickWeight[c('Time', 'Diet')] will result in the grouping columns being properly labeled:

```
> cweights = > aggregate(ChickWeight$weight,
                          ChickWeight[c('Time','Diet')],mean)
+
> head(cweights)
  Time Diet
                    x
1
     0
          1 41.40000
2
     2
          1 47.25000
3
     4
          1 56.47368
4
     6
          1 66.78947
5
     8
          1 79.68421
6
          1 93.05263
    10
```

Alternatively, a constructed list like

```
list(Time=ChickWeight$Time,Diet=ChickWeight$Diet)
```

could be used to achieve the same result.

To process a single vector based on the values of one or more grouping vectors, the tapply function can also be used. The returned value from tapply will be an array with as many dimensions as there were vectors that defined the groups. For example, the PlantGrowth dataset contains information about the weight of plants receiving one of three different treatments. To find the maximum weight for plants exposed to each of the treatments, we could use tapply as follows:

```
> maxweight = tapply(PlantGrowth$weight,PlantGrowth$group,max)
> maxweight
ctrl trt1 trt2
6.11 6.03 6.31
```

Since there was only one grouping factor, the results were returned in the form of a named vector. To convert this vector into a data frame, it can temporarily be converted into a table using as.table, and then passed to as.data.frame, since there is a special method for converting tables into data frames:

```
> as.data.frame(as.table(maxweight))
Var1 Freq
1 ctrl 6.11
2 trt1 6.03
3 trt2 6.31
```

To use a name other than Freq in the data frame, as.data.frame.table can be called directly, using the responseName= argument:

Unlike aggregate, tapply is not limited to returning scalars. For example, if we wanted the range of weights for each group in the PlantGrowth dataset, we could use

```
> ranges = tapply(PlantGrowth$weight,PlantGrowth$group,range)
> ranges
$ctrl
[1] 4.17 6.11
$trt1
[1] 3.59 6.03
$trt2
[1] 4.92 6.31
```

In this case. tapply returns a named array of vectors. Individual elements can be accessed in the usual way:

> ranges[[1]]
[1] 4.17 6.11
> ranges[['trt1']]
[1] 3.59 6.03

To convert values like this to data frames, the dimnames of the returned object can be combined with the values. When each element of the vector is of the same length, this operation is fairly straightforward, but the problem becomes difficult when the return values are of different lengths. In the current example, we can convert the values to a numeric matrix, and then form a data frame by combining the matrix with the dimnames:

```
> data.frame(group=dimnames(ranges)[[1]],
+ matrix(unlist(ranges),ncol=2,byrow=TRUE))
group X1 X2
1 ctrl 4.17 6.11
2 trt1 3.59 6.03
3 trt2 4.92 6.31
```

data.frame was used here instead of cbind to prevent the numeric values from being coerced to character values when they were combined with the levels of the grouping variable.

When more than one grouping variable is used with tapply, and the return value from the function used is not a scalar, the returned object is somewhat more difficult to interpret. For example, the CO2 dataset contains information about the uptake of carbon dioxide by different types of plants exposed to different treatments. Suppose we were interested in the range of CO_2 uptake for plants of each type and treatment. We can call tapply as follows:

The returned value is a matrix of lists, which explains the unusual form of the output when we display the object. Individual elements can still be accessed as expected:

```
> ranges[['Quebec','chilled']]
[1] 9.3 42.4
```

Such objects can be converted to data frames by applying expand.grid (see Section 2.8.1) to the dimnames before combining them with the values:

```
> data.frame(expand.grid(dimnames(ranges1)),
+ matrix(unlist(ranges1),byrow=TRUE,ncol=2))
        Type Treatment X1 X2
1 Quebec nonchilled 13.6 45.5
2 Mississippi nonchilled 10.6 35.5
3 Quebec chilled 9.3 42.4
4 Mississippi chilled 7.7 22.2
```

The function argument to tapply is not required; calling tapply without a function will return a vector of indices which can be used as a subscript to the array of values that tapply produces when a function is provided. For example, suppose we wish to subtract the median value of the uptake variable in the CO2 data frame, where the median is calculated separately for each Type/Treatment combination. The first step is calculating the medians for each group using tapply:

```
> meds = tapply(CO2$uptake,CO2[c('Type','Treatment')],median)
```

Next, the indices are calculated using an identical call to tapply without a function, and they are used as a subscript to the median vector:

The ave function combines these two operations in a single function call:

```
> adj.uptake = CO2$uptake -
+ ave(CO2$uptake,CO2[c('Type','Treatment')],FUN=median)
```

Since ave can accept multiple grouping variables, the function to be used for summarization must be identified using FUN=. Thus, the previous example could have been carried out with the following statement:

```
> adj.uptake = CO2$uptake -
+ ave(CO2$uptake,CO2$Type,CO2$Treatment,FUN=median)
```

When more than a single vector needs to be processed, a variety of options is available. To put the problem into context, consider the task of finding the maximum eigenvalue of the correlation matrices of the four variables from the iris dataset, broken down by the species of the plant. One solution is to use the split function, which takes a data frame and a list of grouping variables and returns a list containing data frames representing the observations for each level of the grouping variables. Such a list can then be processed using sapply or lapply to provide the final result. When working with problems like this, the first step is usually defining a function to provide the required result for a single data frame. In this case, an appropriate function could be written as follows:

```
> maxeig = function(df)eigen(cor(df))$val[1]
```

Next, the numeric values in the data frame can be passed to **split** to provide a list of data frames for further processing:

> frames = split(iris[-5],iris[5])

Finally, this result can be passed to **sapply** along with the function to do the work:

```
> sapply(frames,maxeig)
    setosa versicolor virginica
    2.058540    2.926341    2.454737
```

As always, these operations can be condensed to a single expression, although there is no great advantage in doing so. 118 8 Data Aggregation

```
> sapply(split(iris[-5],iris[5]),
+ function(df)eigen(cor(df))$val[1])
setosa versicolor virginica
2.058540 2.926341 2.454737
```

A less direct, but sometimes useful solution involves passing a vector of row indices to tapply and modifying the function used to calculate the maximum eigenvalue to operate on selected rows of the data:

Finally, the by function can be used. This generalizes the idea of tapply to operate on entire data frames broken down by a list of grouping variables. Thus, the first argument to by is a data frame, and the remaining arguments are similar to those of tapply. For the eigenvalue problem, a solution using by is as follows:

In this case, by returned a scalar, so the result can be converted to a data frame by using a combination of as.table and as.data.frame:

```
> as.data.frame(as.table(max.e))
iris.Species Freq
1 setosa 2.058540
2 versicolor 2.926341
3 virginica 2.454737
```

When there are multiple variables describing the groups to be processed, the result from by needs additional processing to get it in the form of a data frame. Consider again the CO2 dataset. Suppose we wish to find the number of observations, mean, and standard deviation of the variable uptake, broken down by Type and Treatment combinations. First, a simple function to return the required values is written. By putting together the values with data.frame instead of c, we insure that the mode of the numeric results will be preserved after we combine them with the level information for the grouping variables:

```
> sumfun = function(x)data.frame(n=length(x$uptake),
                mean=mean(x$uptake),sd=sd(x$uptake))
+
> bb = by(CO2,CO2[c('Type', 'Treatment')],sumfun)
> bb
Type: Quebec
Treatment: nonchilled
  n
      mean
              sd
1 21 35.33333 9.59637
_____
Type: Mississippi
Treatment: nonchilled
  n
      mean
               sd
1 21 25.95238 7.402136
_____
Type: Quebec
Treatment: chilled
  n
      mean
               sd
1 21 31.75238 9.644823
_____
Type: Mississippi
Treatment: chilled
  n
      mean
               sd
1 21 15.81429 4.058976
```

Each of the rows returned by the by function is in the form that we would like for a data frame containing these results, so it would be natural to use rbind to convert this result to a data frame; however, it is tedious to pass each row to the rbind function individually. In cases like this, the do.call function, first introduced in Section 6.5, can usually generalize the operation so that it will be carried out properly regardless of how many elements need to be processed. Recall that do.call takes a list of arguments and passes them to a function as if they were the argument list for the function call. In this example, the call to do.call is as follows:

With two grouping variables, the names and levels of the grouping factors are not present in the result. This can be remedied by combining a call to expand.grid with the previous result. Since all the parts being combined are data frames, they can be safely combined using cbind:

```
> cbind(expand.grid(dimnames(bb)),do.call(rbind,bb))
        Type Treatment n mean sd
1 Quebec nonchilled 21 35.33333 9.596371
2 Mississippi nonchilled 21 25.95238 7.402136
3 Quebec chilled 21 31.75238 9.644823
4 Mississippi chilled 21 15.81429 4.058976
```

8.6 The reshape Package

An alternative approach to aggregation is provided by the reshape package, available from CRAN. The functions in this package provide a unified approach to aggregation, based on an extended formula notation. The core idea behind the reshape package is to create a "melted" version of a dataset (through the melt function), which can then be "cast" (with the cast function) into an object with the desired orientation. To melt a data frame, list, or array into the appropriate melted form, it is first necessary to divide the variables into id variables and measure or analysis variables; this should generally be obvious from the nature of the data. By default, melt treats factor and integer variables as id variables, and the remaining variables as analysis variables; if your data is structured according to this convention, no additional information needs to be provided to melt. Otherwise, the id.var= or measure.var= arguments can be used; if you specify one, it will assume all the other variables are of the other type. Once a dataset is melted, it can be cast into a variety of forms.

As a simple example, consider a dataset formed from the **state.x77** data frame, combined with the **state.region** variable:

```
> states = data.frame(state.x77,state=row.names(state.x77),
+ region=state.region,row.names=1:50)
```

The state and region variables are stored as factors, so they will be automatically recognized as id variables when we melt the data:

```
> library(reshape)
> mstates = melt(states)
Using state, region as id variables
```

Notice that melt displays the names of variables that have been automatically assigned as id variables. The basic melting operation preserves the id variables, and converts the measured variables into two columns named variable (which identifies which variable is being measured) and value (which contains the actual values). You can use a name other than variable by specifying a variable_name= argument to melt.

The left-hand side of the formula passed to **cast** represents the variable(s) which will appear in the columns of the result, and the right-hand side describes the variables which will appear in the rows. Formulas used by **cast** can include a single dot (.) to represent an overall summary, or three dots ... to represent all variables not otherwise included in the formula. In the simplest case, we can reproduce the original dataset with a formula like "... ~ variable".

When used for aggregation, an aggregation function should be supplied; if not it defers to using length. Suppose we wish to find the mean for each variable, broken down by region, with the regions appearing as a column in the output data frame:

```
> cast(mstates,region~variable,mean)
         region Population
                             Income Illiteracy Life.Exp
1
      Northeast
                  5495.111 4570.222
                                       1.000000 71.26444
2
                  4208.125 4011.938
                                       1.737500 69.70625
          South
3 North Central
                  4803.000 4611.083
                                       0.700000 71.76667
                  2915.308 4702.615
                                       1.023077 71.23462
4
           West
     Murder HS.Grad
                        Frost
                                   Area
   4.722222 53.96667 132.7778
                               18141.00
1
2 10.581250 44.34375
                     64.6250 54605.12
3
  5.275000 54.51667 138.8333 62652.00
  7.215385 62.00000 102.1538 134463.00
```

If we wanted a separate row for each variable instead of each region, we can reverse the role of those variables in the formula:

>	<pre>cast(mstates,variable~region,mean)</pre>				
	variable	Northeast	South	North Central	
1	Population	5495.111111	4208.12500	4803.00000	
2	Income	4570.222222	4011.93750	4611.08333	
3	Illiteracy	1.000000	1.73750	0.70000	
4	Life.Exp	71.264444	69.70625	71.76667	
5	Murder	4.722222	10.58125	5.27500	
6	HS.Grad	53.966667	44.34375	54.51667	
7	Frost	132.777778	64.62500	138.83333	
8	Area	18141.000000	54605.12500	62652.00000	
	Wes	st			
1	2.915308e+0)3			
2	4.702615e+0)3			
3	1.023077e+0	00			
4	7.123462e+0)1			
5	7.215385e+00				
6	6.200000e+01				
7	1.021538e+02				
8	1.344630e+0)5			

To limit the variables that are used, we can use the **subset** = argument of **cast**. Since this argument uses the melted data, we need to refer to the variable named **variable**:

```
> cast(mstates,region~variable,mean,
+ subset=variable %in% c('Population','Life.Exp'))
    region Population Life.Exp
1 Northeast 5495.111 71.26444
2 South 4208.125 69.70625
3 North Central 4803.000 71.76667
4 West 2915.308 71.23462
```

Unlike the aggregate function which does not accept functions which return vectors of values, cast allows such functions, and uses the names of the returned vector to form new variable names in its output. Alternatively, a list of functions can be provided. Suppose we wish to calculate the mean, median, and standard deviations for Population and Lif.Exp in the states data frame. Since built-in functions exist for each statistic, they can be passed to cast as a list: First, we can calculate these quantities for the entire dataset:

```
> cast(mstates,.~variable,c(mean,median,sd),
+ subset=variable %in% c('Population','Life.Exp'))
value Population_mean Population_median Population_sd
1 (all) 4246.42 2838.5 4464.491
Life.Exp_mean Life.Exp_median Life.Exp_sd
1 70.8786 70.675 1.342394
```

Since variable was specified on the right-hand side of the tilde, all of the statistics for all of the variables are listed in a single row. A more familiar form would have the variables listed in a column, once again achieved by reversing the roles of the variables in the formula:

>	cast(mstate	es,variable	e~.,c(mear	n,median,sd),	
+	subset	z=variable	%in% c('H	Population','	Life.Exp'))
	variable	mean	median	sd	
1	Population	4246.4200	2838.500	4464.491433	
2	Life.Exp	70.8786	70.675	1.342394	

To aggregate using a grouping variable, the period in the formula can be replaced by the grouping variable, in this case **region**:

> cast(mstates,region~variable,c(mean,median,sd), subset=variable %in% c('Population','Life.Exp')) + region Population_mean Population_median Population_sd Northeast 1 5495.111 3100.0 6079.565 2 South 4208.125 3710.5 2779.508 3 North Central 4803.000 4255.0 3702.828 4 2915.308 1144.0 5578.607 West Life.Exp_mean Life.Exp_median Life.Exp_sd

1	71.26444	71.23	0.7438769
2	69.70625	70.07	1.0221994
3	71.76667	72.28	1.0367285
4	71.23462	71.71	1.3519715

If the roles of **region** and **variable** were reversed, there would be one variable for each combination of **region** and **mean**, **median**, and **sd**, which might not be convenient for display or further manipulation. To provide added flexibility, the vertical bar (1) can be used to cause **cast** to produce a list instead of a data frame. To create a list with a separate data summary for each region, we can specify **region** after the vertical bar, and replace it with a period in the formula:

```
> cast(mstates,variable~.|region,
+
               c(mean,median,sd),
               subset=variable%in%c('Population','Life.Exp'))
+
$Northeast
    variable
                         median
                                           sd
                   mean
1 Population 5495.11111 3100.00 6079.5651457
2
    Life.Exp
               71.26444
                          71.23
                                    0.7438769
$South
    variable
                   mean median
                                          sd
1 Population 4208.12500 3710.50 2779.508251
2
    Life.Exp
               69.70625
                          70.07
                                    1.022199
$'North Central'
    variable
                         median
                                          sd
                   mean
1 Population 4803.00000 4255.00 3702.827593
2
    Life.Exp
               71.76667
                          72.28
                                    1.036729
$West
    variable
                   mean
                         median
                                          sd
1 Population 2915.30769 1144.00 5578.607015
2
    Life.Exp
               71.23462
                          71.71
                                    1.351971
```

Note that this creates a separate list element for each region, and that the contents of these elements are similar to those created with the formula "variable ~ ." in a previous example.

The principles in the previous example extend readily to the case with more than one id variable. Consider once again the ChickWeight data frame. The variables in this dataset are weight, Time, Chick, and Diet. The last three variables represent id variables, with weight being the only measure variable. Since Time is stored as a numeric variable, it is necessary to explicitly provide either the id or measure variables to the melt function:

> mChick = melt(ChickWeight,measure.var='weight')

To create a data frame with the median value of weight for each level of Diet and Time, the following call to cast can be used:

>	head(cast(mChick,Diet				Time	~	<pre>variable,median))</pre>
	Diet	Time	weight				
1	1	0	41				
2	1	2	49				
3	1	4	56				
4	1	6	67				
5	1	8	79				
6	1	10	93				

Notice that the variable specified last on the left-hand side (Time) is the one that varies the fastest.

To create a separate column for the median at each time, Time can be moved to the right-hand side of the formula:

>	cast(mChio	ck,Diet ~	Time +	variable	,mean)	
	Diet 0_we	eight 2_w	reight	4_weight	6_weight	8_weight
1	1	41.4	47.25	56.47368	66.78947	79.68421
2	2	40.7	49.40	59.80000	75.40000	91.70000
3	3	40.8	50.40	62.20000	77.90000	98.40000
4	4	41.0	51.80	64.50000	83.90000	105.60000
	10_weight	12_weight	14_wei	ight 16_w	eight 18_we	eight 20_weight
1	93.05263	108.5263	123.3	3889 144	.6471 158	9412 170.4118
2	108.50000	131.3000	141.9	9000 164	.7000 187	7000 205.6000
3	117.10000	144.4000	164.5	5000 197	.4000 233	1000 258.9000
4	126.00000	151.4000	161.8	3000 182	.0000 202	9000 233.8889
	21_weight					
1	177.7500					
2	214.7000					
3	270.3000					
4	238.5556					

To create a list, with one element for each Diet, and the median of weight for each Time, use the vertical bar as follows:

> cast(mChick,Time ~ variable|Diet,mean) \$'1' Time weight 1 0 41.40000 2 2 47.25000 3 56.47368 4 4 6 66.78947 5 8 79.68421 6 10 93.05263 . . .

\$ʻ	4'	
	Time	weight
1	0	41.0000
2	2	51.8000
3	4	64.5000
4	6	83.9000
5	8	105.6000
6	10	126.0000

.

•

In the previous example there were valid values for each combination of the id variables. If this is not the case, the default behavior of cast is to only include combinations actually encountered in the data. To include all possible combinations, use the add.missing=TRUE argument. For example, suppose we remove one combination of Diet and Time from ChickWeight:

```
> xChickWeight = subset(ChickWeight,
+
                  !(Diet == 1 & Time == 4))
> mxChick = melt(xChickWeight,measure.var='weight')
> head(cast(mxChick,Diet + Time ~ variable,median))
  Diet Time weight
          0
     1
                 41
1
2
     1
          2
                 49
3
     1
          6
                 67
4
     1
          8
                 79
5
     1
         10
                 93
6
         12
     1
                106
```

By using add.missing=TRUE, observations for the missing combinations will be created, with a missing value for the analysis variable:

```
> head(cast(mxChick,Diet + Time ~ variable,median,
             add.missing=TRUE))
+
  Diet Time weight
1
     1
           0
                  41
2
     1
           2
                  49
3
     1
           4
                  NA
4
           6
                  67
     1
5
     1
           8
                  79
6
     1
          10
                  93
```

In each of the preceding examples, the dataset was first melted, then repeated calls to cast were carried out. If only a single call to cast is needed, the recast function combines the melt and cast steps into a single call:

> head(recast(xChickWeight,measure.var='weight',

+			Diet ·	+ Time ~ variable,median,
+	add.missing=TRUE))			
	Diet	Time	weight	
1	1	0	41	
2	1	2	49	
3	1	4	NA	
4	1	6	67	
5	1	8	79	
6	1	10	93	

8.7 Loops in R

In previous sections, the apply family of functions (and associated wrappers) has been presented as the first choice for most repetitive tasks, such as operating on each element of a list, or performing a computation for nonoverlapping subgroups of the data. The major factor in this decision has to do with the simplicity of the functions, as well as their ability to properly use any names which have been assigned to their input arguments. But this way of programming may be awkward and unfamiliar, and many people would like to leverage their knowledge of other programming languages into R by using more familiar programming constructs like loops. An examination of some of the apply-style functions' source code will show that these functions internally use loops to actually get their work done, so arguments against loops based solely on efficiency do not carry much weight. The real problem with loops is that there are some very intuitive operations that may be implemented with loops that turn out to be extremely inefficient in R. In this and the following sections, we'll access the efficiency of different approaches to common problems with the use of the system.time function. This function accepts any valid R expression, and returns a vector of length five, containing the user CPU time, the system CPU time, the elapsed time, and the user and system times from any subprocesses. The first value shown, user CPU, is usually the most useful measure of efficiency, and will vary less than the other values when the same task is repeated several times. Since the argument handling in functions uses equal signs to identify keywords, the one restriction when using system.time is that assignment statements which are to be timed must use the "gets" form of the assignment operator, namely, <- instead of the equal sign.

Before looking at the cases to avoid, let's consider a simple example: finding the mean of each column of a matrix. This problem is so common that the rowMeans function is provided for an extremely efficient solution:

```
> dat = matrix(rnorm(1000000),10000,100)
> system.time(mns <- rowMeans(dat))
[1] 0.008 0.000 0.010 0.000 0.000</pre>
```

Another solution is to use apply:

```
> system.time(mns <- apply(dat,2,mean))
[1] 0.032 0.020 0.056 0.000 0.000</pre>
```

Next, we can use a loop to calculate the mean of each column separately. Notice that in this case, we need to initialize the result vector **mns** to accommodate the answer:

```
> system.time({m <- ncol(dat)
+ for(i in 1:m)mns[i] <- mean(dat[,i])})
[1] 0.032 0.004 0.036 0.000 0.000</pre>
```

There really isn't that much of a difference in execution time (the loop uses slightly less system time). The main advantage of apply in this case is that it eliminates the need to worry about the result vector, and, if the matrix were named, those names would be passed on to the result.

Keep in mind that the previous example still took advantage of vectorization: each column mean was calculated from a single call to **mean**. It is almost always a mistake to loop over each element of a matrix. Consider the following function, which calculates the mean of each column of the matrix by adding together every element and then dividing by the column length:

```
> slowmean = function(dat){
+
    n = dim(dat)[1]
+
    m = dim(dat)[2]
    mns = numeric(m)
+
+
    for(i in 1:n){
       sum = 0;
+
       for(j in 1:m)sum = sum + dat[j]
+
+
       mns[i] = sum / n
    }
+
+
    return(mns)
+}
> system.time(mns <- slowmean(dat))</pre>
[1] 2.100 0.000 2.097 0.000 0.000
```

Without any vectorization, the computation is much slower than the other solutions. This illustrates that unless some kind of vectorization is used, computations in R will be very slow.

Before leaving this problem, it should be mentioned that, for any given problem, there may be unique solutions available. For example, the mean of each column of a matrix can be calculated directly using matrix expressions as follows:

```
> system.time({m = dim(dat)[1];mns = rep(1,m) %*% dat / m})
[1] 0.020 0.000 0.021 0.000 0.000
```

This represents an improvement over the apply and loop-based solutions, but is still not as efficient as the colMeans solution.

This illustrates that loops, in and of themselves, are not necessarily inefficient in R, but they should certainly take advantage of any vectorization possible to keep them competitive with other techniques.

To understand the kinds of loops which cause problems in R, it's worthwhile to recall how matrices are stored in R, namely, as a one-dimensional vector, with the columns of the matrix "stacked" on top of each other. A very common operation is to build up a matrix iteratively, by starting with an empty matrix, and using the **rbind** function to grow the matrix one row at a time. There are two problems with this approach. First, the size of the matrix changes at each iteration, requiring additional time to be spent in memory allocations. More importantly, since adding a row changes the size of each column in the matrix, all of the matrix elements need to be rearranged in memory each time a new row is added. These repeated memory allocations and rearrangements very quickly take their toll on the efficiency of a program.

Consider the trivial task of creating a matrix, each of whose rows represent the numbers from 1 to 100. Because of recycling rules, this can be achieved as follows:

```
> system.time(m <- matrix(1:100,10000,100,byrow=TRUE))
[1] 0.022 0.003 0.025 0.000 0.000</pre>
```

Performing the same operation by incrementally building the matrix is much slower:

```
> buildrow = function(){
+   res = NULL
+   for(i in 1:10000)res = rbind(res,1:100)
+   res
+ }
> system.time(buildrow())
[1] 239.236 21.446 260.707 0.000 0.000
```

Two forces are slowing the computation: first, the size of **res** is changing each time a new row is added to the matrix, causing R to reallocate memory at each iteration. In addition, since R stores its matrices internally by columns, the addition of a row to the matrix means that every column in the matrix needs to be extended, resulting in large amounts of data being moved around in memory. By this reasoning, it would be faster to build the matrix by columns of equal size, since less rearrangement of the data will be necessary:

```
> buildcol = function(){
+   res = NULL
+   for(i in 1:10000)res = cbind(res,1:100)
+   t(res)
+ }
> system.time(buildcol())
[1] 142.666 20.596 163.289 0.000 0.000
```

While this does represent a speedup, it is still far from an optimal solution. What makes the first technique so fast is that when the matrix function is used, the size of the result can be determined before the data is generated. We can provide the same advantage to a loop-based solution as follows:

```
> buildrow1 = function(){
+ res = matrix(0,10000,100)
+ for(i in 1:10000)res[i,] = 1:100
+ res
+ }
> system.time(buildrow1())
[1] 0.242 0.015 0.257 0.000 0.000
```

Even if we didn't know how many rows the matrix would contain, it would still be faster to allocate more rows than we need, and then truncate the matrix at the end. For example, let's include only 50% of the rows by checking the value of a random number before adding that row to the output matrix. First, we'll start with a NULL matrix:

```
> somerow1 = function(){
+ res = NULL
+ for(i in 1:10000)if(runif(1) < .5)res = rbind(res,1:100)
+ res
+ }
> system.time(somerow1())
[1] 51.007 6.062 57.125 0.000 0.000
```

Next, we'll allocate a matrix large enough to hold all the rows, then truncate it at the end:

```
> somerow2 = function(){
+
    res = matrix(0, 10000, 100)
+
    k = 0
+
    for(i in 1:10000)if(runif(1) < .5){</pre>
         k = k + 1
+
         res[k,] = 1:100
+
    }
+
    res[1:k,]
+
+ }
> system.time(somerow2())
[1] 0.376 0.027 0.404 0.000 0.000
```

Provided there is enough memory for the initial allocation, creating a sufficiently large matrix before beginning to build it will generally be much faster than repeatedly calling rbind.

If a situation arises where it is difficult or impossible to allocate an appropriate matrix before building the rows, we can take advantage of the fact that lists in R are stored very differently than matrices. In particular, the

memory used by list elements does not have to be contiguous, which means that adding elements to a list doesn't require as much manipulation of data within memory as the corresponding operation on a matrix. The strategy is to build a list of the rows that will eventually become the matrix, and then use do.call to pass all of the rows to rbind in a single operation:

```
> somerow3 = function(){
+   res = list()
+   for(i in 1:10000)if(runif(1) < .5)res = c(res,list(1:100))
+   do.call(rbind,res)
+ }
> system.time(somerow3())
[1] 33.308 0.247 33.575 0.000 0.000
```

While nowhere near as fast as more optimal methods, this technique may prove useful in those situations where the size of the final result may be difficult to determine.