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Multiple-Table Data in R with the multitable Package

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Abstract

Data frames are integral to R. They provide a standard format for passing data to model-fitting and plotting functions, and this standard makes it easier for experienced users to learn new functions that accept data as a single data frame. Still, many data sets do not easily fit into a single data frame; data sets in ecology with a so-called fourthcorner problem provide important examples. Manipulating such inherently multiple-table data using several data frames can result in long and difficult-to-read workflows. We introduce the R multitable package to provide new data storage objects called data.list objects, which extend the data.frame concept to explicitly multiple-table settings. Like data frames, data lists are lists of variables stored as vectors; what is new is that these vectors have dimension attributes that make accessing and manipulating them easier. As data.list objects can be coerced to data.frame objects, they can be used with all R functions that accept an object that is coercible to a data.frame.

Keywords: data organization, ecology, fourth-corner problem, R.

1. Introduction

The standard data management paradigm in R is based on data.frame objects, which are two-dimensional data tables with rows and columns representing replicates (sometimes also called objects) and variables (R Development Core Team 2012). Standard R workflows require that the data to be analyzed are organized into a data frame (Chambers and Hastie 1992). Hypotheses about the relationships between variables in the data frame are expressed using formula objects. Data frames and formulas are combined by passing them to functions that



Figure 1: Schematic diagram of a data structure with a fourth-corner problem.

produce analyzes (e.g., plots; fitted models; summary statistics). This framework allows scientists to concentrate on their primary interests – the relationships between variables – without explicit reference to mathematical and algorithmic details. It also provides access to those details, which are required for effective analyzes and to develop new methods of analysis within the framework. As new methods are developed, researchers simply pass their data frames to new functions in much the same way they would pass them to older functions.

Research in community ecology – the study of the distribution and abundance of multiple interacting species – sometimes involves data sets that do not easily fit within a single data frame. A common example is the fourth-corner problem (Legendre, Galzin, and Harmelin-Vivien 1997), in which three data tables are to be analyzed: a sites-by-species table of abundances or occurrences; a table of environmental variables at each site; and a table of traits for each species (Figure 1). Such data are characterized by a conspicuous (lower-right) 'fourth-corner', where there are no data. The missing data in the fourth corner are not caused by the usual problems (e.g., broken field equipment; budget restrictions; bad weather; dead subjects), but are part of the study design itself. The fourth-corner problem is a special case of a general 'multiple-table problem', which can be much more complex (e.g., could involve three-dimensional 'cubes' of data, Figure 2). The challenge of analysing such multiple-table data sets in R is that it is not obvious how to organize them into a single data.frame, which is required in standard R workflows. Our goal with the R multitable package – available from the Comprehensive R Archive Network at http://CRAN.R-project.org/package=multitable – is to provide tools that make analysing multiple-table data sets easier.

One possible solution is to develop new R analysis functions – or new software packages altogether – that are specifically designed to accept several tables as input. There have been



Figure 2: The structure of the Lac Croche zooplankton community data. The abundances of zooplankton species and several environmental variables were measured every two weeks in the summer at various basins (i.e., sites) in the lake over two years – yielding two temporal scales at which sampling took place: week within year and year. In addition, the species were characterized by a suite of traits.

several such methods developed in ecology, focusing on data with a fourth-corner problem (Dolédec, Chessel, ter Braak, and Champely 1996; Legendre *et al.* 1997; Dray and Legendre 2008; Pillar and Duarte 2010; Leibold, Economo, and Peres-Neto 2010; Ives and Helmus 2011). However, these methods do not apply to data sets that have other more complex multiple-table data structures (e.g., the zooplankton communities in Lac Croche, which are described in Figure 2; Cantin, Beisner, Gunn, Prairie, and Winter 2011). One approach to such issues would be to develop suites of data analysis functions for each new data structure. But such an approach is less than ideal as it would require that new methods be developed for each new structure, which does not take advantage of the large number of tools developed for standard R workflows (Chambers and Hastie 1992). The multitable package provides an alternative approach, by introducing a multiple-table generalization of data frames – called data lists – which can be analyzed with virtually any function that can be used to analyze a data frame. Thus, instead of providing new methods of analysis, multitable provides new methods of data management and organization.

How can data lists make data organization easier? Although practically any data set can be forced into a single data.frame by either repeating some of the data or adding missing values,



Figure 3: The **multitable** framework for using multiple-table data (in red) in R workflows (in blue). Hyper-linked section numbers indicate portions of the workflow covered by sections in this article. Data lists are used to organize and manipulate multiple-table data as a single R object, even though such data will typically be originally stored in several other sources (e.g., R objects; spreadsheets; text-based data files; database queries). When such data are ready for analysis, they can be coerced into a data frame. With the data in data frame form, they can be analyzed and visualized by combining them with any R function that accepts data.frame objects.

other structures exist that would make a particular data set easier to understand, manipulate, and analyze. Accordingly, we have designed data.list objects to provide a richer structure than data.frame objects for representing our data 'as we understand them'. This structure furnishes intuitive tools for operating on several data tables simultaneously, thereby saving time and effort that could be better spent thinking about relationships between variables. As we have discussed, there are important advantages to organizing data in data.frame objects – perhaps the most important advantage being the powerful catalogue of R functions that accept data in such a form. The multitable package provides methods for coercing data.list objects into data.frame objects, thus making standard R tools available to multiple-table data organized as a data.list object. In summary, the multitable model of data organization is to manipulate, transform, and extract subsets of our data in data.list-form, and then to coerce them into data.frame-form when we are ready to pass them to analysis functions (Figure 3).

There are several existing R packages that are designed to make data organization easier (e.g., reshape2; Wickham, 2007). The mefa and mefa4 packages have been developed to organize data with a slight generalization of the fourth-corner problem (Sólymos 2009); this generalization permits several community matrices – called segments – with identical dimensions. The multitable package has much in common with mefa, but there are noticeable differences. For example, multitable is designed to handle more general data structures than mefa or mefa4; in particular, mefa is not able to represent the relational structure of the Lac Croche data depicted in Figure 2. On the other hand, mefa provides more extensive tools for data summarization than multitable and mefa4 integrates tools for sparse-matrix computations. We therefore expect mefa and multitable to often be complementary in practice.

Our purpose is to introduce the **multitable** package, and demonstrate its utility. There are three main organizational sections, each corresponding to a part of Figure 3. Section 2 describes the structure of a simple data.list object (2.1); how to create other data lists (2.2); a simple theoretical framework for understanding data lists (2.3); and techniques for manipulating them (2.4, 2.5, 2.6, 2.7, 2.8). Section 3 illustrates the coercion of data lists to data frames. Section 4 illustrates how to use **multitable** in R workflows by summarizing (4.2); visualizing (4.3); and modeling (4.4, 4.5, 4.6) a real stream fish data set (4.1).

2. Understanding, creating, and manipulating data lists

data sources \longrightarrow data list

2.1. The structure of data lists

The **multitable** package comes with a fictitious data.list, to illustrate how these objects work.

R> library("multitable") R> data("fake.community") R> fake.community abundance: _____ , , capybara 2009 2008 1537 midlatitude 4 0 0 subtropical 0 10 0 tropical 8 0 0 7 equatorial 0 0 0 0 arctic 0 0 0 subarctic 0 , , moss 2009 2008 1537 6 midlatitude 0 0 subtropical 0 0 0 tropical 9 0 0 equatorial 0 3 0 arctic 5 0 0 subarctic 0 0 0 , , vampire 2009 2008 1537 midlatitude 0 0 0 subtropical 0 0 1 tropical 0 0 0 equatorial 0 0 0 arctic 0 0 0 0 0 subarctic 0 Replicated along: || sites || years || species ||

temperature: ____ 2009 2008 1537 midlatitude NA 10 NA 20 subtropical 25 NA tropical 48 50 NA 30 equatorial 50 NA arctic -37 -30 NA subarctic 3 0 NA Replicated along: || sites || years || precipitation: _____ 2009 2008 1537 midlatitude NA 20 NA subtropical 99 100 NA tropical 149 150 NA equatorial 199 200 NA arctic 21 20 ΝA subarctic 41 40 NA Replicated along: || sites || years || body.size: _____ capybara moss vampire 140 NA 190 Replicated along: || species || metabolic.rate: _____ capybara vampire moss 5 20 0 Replicated along: || species || homeotherm: _____ capybara vampire moss Ν Y Ν Levels: N Y Replicated along: || species || REPLICATION DIMENSIONS: sites years species 6 3 3

At first sight, this data.list object looks very different from standard data.frame objects, but on second look we can see that they are really quite similar. Just like data frames, data

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lists are composed of a number of variables – in this case, we have six variables (abundance; temperature; precipitation; body.size; metabolic.rate; and homeotherm) each identified in the printed object above by underlined names. The variables in data lists must be printed in this sequential manner, rather than as columns neatly lined up in a data frame, precisely because the variables in multiple-table data sets do not line up neatly; this is the problem multitable seeks to address.

Also as with data frames, the replication of variables in data lists are represented as vectors of values. The main difference between the two objects in this regard is that the vectors that represent variables in data lists have dim (i.e., dimension) attributes. These dim attributes give data.list objects further structure. In R, vectors with dim attributes are best thought of as matrices and arrays of numbers. For example, the abundance variable is replicated along three dimensions (sites; years; and species), and therefore is a three dimensional array of data. This information is displayed after the data whenever a data.list object is printed. Some variables are only replicated along two dimensions (e.g., temperature and precipitation) and others only have one dimension (e.g., body.size; metabolic.rate; and homeotherm).

Importantly however, although the variables are not replicated along all of the same dimensions, they do share dimensions; and it is this dimension sharing that allows us to relate variables to each other. To appreciate the dimension sharing of this example, we can use the summary method for data.list objects:

R> summary(fake.community)

	abundance t	emperature	precipitation	body.size
sites	TRUE	TRUE	TRUE	FALSE
years	TRUE	TRUE	TRUE	FALSE
species	TRUE	FALSE	FALSE	TRUE
	metabolic.r	ate homeotl	nerm	
sites	FA	LSE FA	ALSE	
years	FA	LSE FA	ALSE	
species	Т	RUE	TRUE	

This method returns a logical matrix with dimensions of replication as rows and variables as columns. A value of TRUE appears in cells corresponding to variables that are replicated along a particular dimension, and a value of FALSE appears otherwise. We can see that the sites and years dimensions relate abundance, temperature, and precipitation; whereas, the species dimension relates abundance, body.size, metabolic.rate, and homeotherm.

Note that some FALSE entries are biophysical necessities, whereas others are properties of the study design. For example, suppose that later in the study, the researchers decided that it was necessary to get some idea of the spatial variation in metabolic rates. It would then be possible to measure metabolic rates of the species at different sites, thereby changing the FALSE associated with the metabolic rate-sites cell to a TRUE. To the contrary, it is both physically and logically impossible to measure the precipitation of a species, so this FALSE is mandatory.

2.2. How data lists are made

Although there are several ways to create data lists, one way in particular provides a simple

framework for understanding the difference between variables and dimensions of replication – an important distinction to understand in order to use **multitable** effectively.

Consider the following data frame of species abundances counted at various sites.

R> abundance

	sites	species	abundance
1	midlatitude	capybara	4
2	subtropical	capybara	10
3	tropical	capybara	8
4	equatorial	capybara	7
5	arctic	moss	5
6	midlatitude	moss	6
7	tropical	moss	9
8	equatorial	moss	3
9	subtropical	vampire	1

We have six sites and three species, but each species is not present at each site and so there are missing site-species combinations.

Related to this **abundance** data frame we have a data frame of environmental variables at each site and a data frame of traits for each species.

R> environment

	sites	temperature	precipitation
1	subarctic	0	40
2	midlatitude	10	20
3	subtropical	20	100
4	tropical	50	150
5	equatorial	30	200

R> trait

	species	body.size	metabolic.rate
1	capybara	140	20
2	moss	5	5
3	vampire	190	0

To make things interesting to scientists with real data, we assume that our environmental data are missing from the arctic site (perhaps because data loggers did not endure harsh conditions).

The three data frames are related because they share two columns: sites and species. The specific pattern of sharing for these data can be illustrated with a bipartite graph (i.e., matching diagram; Figure 4). Columns that are shared between data frames are called *dimensions of replication* and those that are not are called *variables*. The reason for this terminology is that in standard single-table statistical settings, we are able to relate variables because they are



Figure 4: Bipartite graph of the multiple-table structure of data with a standard fourth-corner structure (Figure 1). Dimensions of replication are in blue (on the left) and tables are in red (on the right).

replicated along some common dimension. For example, one can relate pH and temperature if they are both replicated along the same set of lakes. Similarly, we can relate the variables in several tables together if they share columns (i.e., dimensions of replication).

To create a data list out of these data frames we use the data list cast, dlcast, function from **multitable**, inspired by the acast function in the **reshape2** package (Wickham 2007).

```
R> 1 <- list(abundance, environment, trait)
R > dl <- dlcast(l, fill = c(0, NA, NA))
R> summary(dl)
        abundance temperature precipitation body.size metabolic.rate
sites
             TRUE
                          TRUE
                                         TRUE
                                                   FALSE
                                                                  FALSE
             TRUE
                         FALSE
                                        FALSE
                                                    TRUE
                                                                    TRUE
species
R> dl
abundance:
 _____
            capybara moss vampire
                    0
                         5
                                  0
arctic
                    7
                         3
                                  0
equatorial
midlatitude
                    4
                         6
                                  0
subtropical
                   10
                         0
                                  1
                         9
                                  0
tropical
                    8
subarctic
                    0
                         0
                                  0
Replicated along:
                   || sites || species ||
temperature:
     arctic
             equatorial midlatitude subtropical
                                                      tropical
                                                                  subarctic
                      30
                                   10
                                                            50
         NA
                                               20
                                                                          0
Replicated along: || sites ||
```

```
precipitation:
             equatorial midlatitude subtropical
                                                      tropical
     arctic
                                                                  subarctic
         NΑ
                     200
                                   20
                                               100
                                                            150
                                                                         40
Replicated along:
                    || sites ||
body.size:
_____
capybara
              moss
                    vampire
     140
                 5
                        190
Replicated along:
                    || species ||
metabolic.rate:
capybara
             moss
                    vampire
      20
                 5
                          0
Replicated along:
                    || species ||
REPLICATION DIMENSIONS:
  sites species
      6
               З
```

This dlcast function takes one mandatory argument: a list of data frames to be combined into a data list. The optional fill argument accepts a vector with one element for each data frame, giving the value with which to fill in any structural missing values. This argument is useful because we can both (1) fill missing abundances with zeros because those site-species combinations were not observed and (2) fill missing traits and environmental variables with NA values.

Making data lists out of 'wide format' data

Researchers will often have text files or spreadsheets of data that are not stored in the same format as the three data frames in the previous example. These three data frames have two types of columns – some columns represent dimensions of replication and others represent variables. This data storage format is sometimes called 'long format' (see **?reshape**), because more sampling results in a lengthening of the data (i.e., the addition of rows) without any widening (i.e., the addition of columns). In contrast, it is common in community ecology for example to store abundance data as spreadsheets with sites as rows and species as columns (e.g., as in Figure 1). Such a data storage format is often called 'wide format', because more sampling may result in a widening of the data (e.g., more columns are required as further sampling reveals a greater diversity of species). Fortunately, the **multitable** package provides tools for reading data stored in a variety of different formats into a data list. The as.data.list, data.list, variable, variableGroup, read.multitable, and read.fourthcorner functions are all alternatives to dlcast for creating data lists.

The variable function provides a convenient way to add data stored in wide format to an existing data list. Consider for example, a matrix allele containing the frequencies of a particular allele (i.e., alternate form of a gene) for each species at each site,

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R> allele

	capybara	moss	vampire
arctic	NA	0.0	NA
equatorial	0.4	0.0	NA
midlatitude	0.0	0.0	NA
subtropical	0.1	NA	0
tropical	0.0	0.2	NA
subarctic	NA	NA	NA

Note that this **allele** variable is in wide format, because additional sampling could lead to a widening of the matrix. One can add such wide data to an existing data list using the **+** operator and the **variable** function,

R> dl.with.allele <- dl + variable(allele, c("sites", "species"))</pre>

The variable function creates a data list with a single variable (i.e., allele) and the + operator 'adds' it to dl. Notice that the + operator here does not have its usual arithmetic meaning, but instead means 'merge two data lists together'. The two arguments of variable give the data to be converted into a variable (the vector allele in this case) and identifies the dimensions along which the variable is replicated (which are "sites" and "species" in this case). The result of this addition of two data lists contains one more variable than dl,

```
R> summary(dl.with.allele)
```

	abundance	temperature	precipitation	body.size	<pre>metabolic.rate</pre>	allele
sites	TRUE	TRUE	TRUE	FALSE	FALSE	TRUE
species	TRUE	FALSE	FALSE	TRUE	TRUE	TRUE

2.3. Multiple-table concepts

The **multitable** package is based on a distinction between dimensions of replication and variables. One benefit of this distinction is that it provides a common framework for understanding both simple and more complex multiple-table data structures. In particular, the framework allows one to visualize the structure of complex data using bipartite graphs; for example the Lac Croche zooplankton community data (Figure 2) from Cantin *et al.* (2011) has a structure given by Figure 5. To store these data in a format amenable to **dlcast** (i.e., 'long format'), we would create one data frame for each of the groups of variables (red boxes on the right) and add a column for each dimension of replication (blue boxes on the left) associated with those variables.

Visualizing the structure of data in this way will help to clarify how it should be both organized and analyzed. One of the central themes of **multitable** is that thinking about data organization goes a long way towards clarifying how analysis should proceed. The names of what we store as variables will appear in formula objects, so that we can study the relationships between these variables. On the other hand, the information that we have for inferring these relationships will come from what we store as dimensions of replication. In single-table settings we keep



Figure 5: Bipartite graph of the Lac Croche data in Figure 2. Dimensions of replication are in blue (on the left) and tables are in red (on the right).

these two elements of data analysis separate by storing variables as columns and replicates as rows in a data.frame. The data.list concept is very similar except that replication now has a dimensionality, which allows for the storage of more complex data structures. The basic distinction between variables and replicates guides analysis in multiple-table settings just as it does in single-table settings.

To store data as a data.frame object, all variables must have the same length. This requirement ensures that the variables can be related to each other along the single dimension of replication defined by the rows of the data frame. The analogous requirement for storing data in a data.list object is that at least one variable must be replicated along all of the dimensions present in the data set. This requirement ensures two important properties: (1) every variable can be related to at least one other variable along at least one dimension of replication and (2) at least one variable will be relatable to all other variables, a property that is necessary for a response variable. For example, the Lac Croche data (Figure 5) meets this requirement because the abundance variable is replicated along all three dimensions of replication. Therefore, all other variables must at least share one dimension with the abundance variable (e.g., the traits and abundance share the species dimension).

2.4. Subscripting data lists

When analyzing data, it is often of interest to extract a part of the data. For example, examining the data suggests that 1537 might have been an outlying year relative to 2008 and 2009. We can exclude data from 1537 just as we would with a single R array:

```
R> fake.community[, c("2008", "2009"), ]
```

abundance:

, , capybara

	2008	2009						
midlatitude	0	4						
subtropical	10	0						
tropical	0	8						
equatorial	7	0						
arctic	0	0						
subarctic	0	0						
, , moss								
	2008	2009						
midlatitude	6	0						
subtropical	0	0						
tropical	0	9						
equatorial	3	0						
arctic	0	5						
subarctic	0	0						
, , vampire								
	0000	0000						
midlotitudo	2008	2009						
aubtropical	0	0						
tropical	0	0						
equatorial	0	0						
arctic	0	0						
subarctic	0	0						
Suburovio	Ũ	Ŭ						
Replicated a	along:	:	sites		years		species	
temperature	:							
	2008	2000						
midlatitudo	10	2009 NA						
subtropical	20	25						
tropical	50	20 48						
equatorial	30	50						
arctic	-30	-37						
subarctic	0	3						
Replicated a	along:	: 11	sites	11	vears	11		
	0		2000	• •	J 0 0 2 2	• •		
precipitatio	on: 							
	2008	2009						
midlatitude	20	NA						
subtropical	100	99						

```
tropical
             150 149
equatorial
             200
                 199
arctic
              20
                  21
subarctic
              40
                  41
Replicated along: || sites || years ||
body.size:
_____
capybara
                  vampire
            moss
     140
              NA
                      190
                   || species ||
Replicated along:
metabolic.rate:
_____
capybara
           moss
                  vampire
      20
               5
                         0
Replicated along: || species ||
homeotherm:
_____
capybara
            moss
                  vampire
      Y
               Ν
                        Ν
Levels: N Y
Replicated along:
                  || species ||
REPLICATION DIMENSIONS:
  sites
         years species
     6
              2
                     3
```

This command returns the same data list of variables but without the data from 1537. Note that every variable replicated along the **years** dimension is subscripted appropriately, while variables that are not replicated along this dimension are unchanged. As another example, perhaps we want all of the data from the first three sites, in 1537, for the first species (i.e., capybara). The following line would produce such a data list:

```
R> fake.community[1:3, "1537", c(TRUE, FALSE, FALSE)]
```

This example illustrates that data list subscripting can be done with integers (e.g., 1:3), character strings (e.g., "1537"), and logical vectors (e.g., c(TRUE, FALSE, FALSE)).

The previous subscripting examples operated on all variables in the data list simultaneously. However, it is often useful to be able to extract subsets of the variables themselves. Such variable extraction can be done by passing a single subscripting vector that refers to variables instead of dimensions of replication,

```
R> fake.community[c("temperature", "precipitation")]
```

temperature:

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	2009	2008	1537		
midlatitude	NA	10	NA		
subtropical	25	20	NA		
tropical	48	50	NA		
equatorial	50	30	NA		
arctic	-37	-30	NA		
subarctic	3	0	NA		
Replicated a	along	:	sites	years	
precipitatio	on: 				
	2009	2008	1537		
midlatitude	NA	20	NA		
subtropical	99	100	NA		
tropical	149	150	NA		
equatorial	199	200	NA		
arctic	21	20	NA		
subarctic	41	40	NA		
Replicated a	along	:	sites	years	
REPLICATION sites years	DIMEN	ISIONS	5:		
6 3					

If subscripting results in a data list with only a single dimension of replication, then the default behaviour is to coerce to a data frame; for example,

R> fake.community[5:6]

	metabolic.rate	homeotherm
capybara	20	Y
moss	5	Ν
vampire	0	Ν

To suppress this behaviour, use,

R> fake.community[5:6, drop = FALSE]

metabolic.rate:

----capybara moss vampire 20 5 0 Replicated along: || species ||

homeotherm:

```
capybara moss vampire
Y N N
Levels: N Y
Replicated along: || species ||
REPLICATION DIMENSIONS:
species
3
```

The drop argument refers to whether or not the the dimensional structure of the data list should be dropped, because a data frame is sufficient to organize the results of a data list with only a single dimension of replication.

It is important to distinguish between the two ways in which data lists can be subscripted: extraction of subsets of (1) dimensions of replication and (2) variables. We refer to these two subscripting techniques as array-like and list-like – array-like because when R arrays are subscripted, subsets of dimensions are extracted; and list-like because when R lists are subscripted, subsets of variables are extracted. Both the array-like and list-like subscripting functions are designed to behave as similarly as possible to standard **base** R array and list subscripting. See the Extract.data.list help file for more details.

2.5. Assigning new values to variables in data lists

Often we need to alter the values of variables before passing data frames to functions. This is easily done with variables in data lists as well. For example, we note that fake.community has a lot of missing values. Suppose that these missing measurements were observed in a subsequent sampling campaign. We can replace these missing values with the new observations using the standard logic of R replacement.

```
R> fake.community$precipitation[is.na(fake.community$precipitation)] <-
+ c(30, 5, 50, 75, 50, 2, 7)</pre>
```

2.6. Creating transformed variables in data lists

Another common task in data analysis is to create new variables that are transformed versions of older variables in the data set. For example, suppose we want to make a log transformation of the abundance data. If fake.community was a data frame, one could create a new logged version of abundance with the following command,

```
R> fake.community$log.precipitation <- log(fake.community$precipitation)
```

However, because fake.community is a data list rather than a data frame, this command results in the following error: can't add variables this way...try using [[instead of \$...and don't forget to specify match.dimids or shape. The reason why this command works for data frames but not data lists, is that the dimensional structure of data lists must also be specified for this new variable. A simple approach to such a specification is to use the shape argument, which identifies an existing variable with the same shape (i.e., dimensions of replication) as the new variable,

```
R> fake.community[["log.precipitation", shape = "precipitation"]] <-
     log(fake.community$precipitation)
+
R> fake.community["log.precipitation"]
log.precipitation:
_____
                2009
                         2008
                                   1537
midlatitude 3.401197 2.995732 1.6094379
subtropical 4.595120 4.605170 3.9120230
tropical
            5.003946 5.010635 4.3174881
equatorial 5.293305 5.298317 3.9120230
arctic
            3.044522 2.995732 0.6931472
            3.713572 3.688879 1.9459101
subarctic
Replicated along: || sites || years ||
REPLICATION DIMENSIONS:
sites years
    6
          3
```

2.7. Creating variables to identify replicates

It is often useful to construct variables that identify replicates. For example, if one of the dimensions of replication of a data list varies across spatial locations (e.g., sites), it is often of interest to examine potential site effects. A site ID variable will be required to construct models with such a site effect. Therefore, **site** must be considered both a dimension of replication and a variable. The **dims_to_vars** function in the **multitable** package is a convenience function for creating variables out of dimensions of replication,

```
R> fake.community <- dims_to_vars(fake.community)
R> summary(fake.community)
```

	abundance	temperature	precip	itatior	ı body	.size	metabolic.rate
sites	TRUE	TRUE		TRUE	2 1	FALSE	FALSE
years	TRUE	TRUE		TRUE	2 1	FALSE	FALSE
species	TRUE	FALSE		FALSE	2	TRUE	TRUE
	homeotherm	log.precipi	itation	sites	years	speci	es
sites	FALSE		TRUE	TRUE	FALSE	FAL	.SE
years	FALSE		TRUE	FALSE	TRUE	FAL	SE
species	TRUE		FALSE	FALSE	FALSE	TF	UE

Note that this manipulated data list now contains variables associated with the three dimensions of replication (i.e., sites; years; and species). For example, here is the variable associated with the species dimension,

R> fake.community["species", drop = FALSE]

```
species:
------
capybara moss vampire
capybara moss vampire
Levels: capybara moss vampire
Replicated along: || species ||
REPLICATION DIMENSIONS:
species
3
```

2.8. Melting and recasting data lists

We now describe a fairly advanced technique. Occasionally it is difficult to manipulate a data list into the desired form. For example, note that an identical set of variables are replicated along both sites and years in the following subset of the fake.community data,

```
R> data("fake.community")
R> fake.community <- fake.community[1:3, 1:2, 1:2][1:4]
R> summary(fake.community)
```

	abundance	temperature	precipitation	body.size
sites	TRUE	TRUE	TRUE	FALSE
years	TRUE	TRUE	TRUE	FALSE
species	TRUE	FALSE	FALSE	TRUE

When two dimensions share the same variables it is always possible to collapse them into a single dimension, without loss of information. In other words, instead of three dimensions (e.g., sites; years; and species) one could have two dimensions (e.g., sites.years and species). Below in Section 4.6 we will give an example of where it would be useful to collapse dimensions in this way. Here we show how to actually do the collapsing.

In future versions of **multitable** there may be a **collapse** function. In the meantime, we can use a **multitable** implementation of the melt-cast approach to complex data manipulations that has become popular via the **reshape2** package (Wickham 2007). The basic principle of **reshape2** is that it is often difficult to go from one type of structure to another – rather it can be easier to 'melt' away the structure and then 'cast' the molten data into a new form.

The dlmelt function in multitable allows one to remove structure from data lists. This function is similar to the melt function in the reshape2 package, which converts many different kinds of data into 'long' (i.e., database-like) format (see Section 2.2). However, it is not possible to melt a data list into a single long-format data frame without repeating many of its entries – a result of the multiple-table structure of data lists. Therefore, dlmelt first separates variables into groups such that all variables in a group can be stored together in a single data frame. The common feature that variables in such a group share is that they are all replicated along the same dimensions. For example,

R> dlm <- dlmelt(fake.community)</pre>

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This dlm object is a list of three data frames,

R> summary(dlm)

	Length	Class	Mode
<pre>sites.years.species</pre>	4	data.frame	list
sites.years	4	data.frame	list
species	2	data.frame	list

each containing the variables replicated along the dimensions indicated by the names of the data frames. The first two lines of the three data frames are,

R > lapply(dlm, head, n = 2)

\$sites.years.species

asites.years.species				
	abundance	sites	years	species
midlatitude.2009.capybara	4	midlatitude	2009	capybara
subtropical.2009.capybara	0	subtropical	2009	capybara
\$sites.years			• .	

	temperature	precipitation	sites	years
midlatitude.2009	NA	NA	midlatitude	2009
subtropical.2009	25	99	subtropical	2009

\$species

	body.size	species
capybara	140	capybara
moss	NA	moss

The columns of each of these data frames give both variables and dimensions of replication. We could recast this melted multiple-table data set and get the original data list back, with the following command,

R> dlcast(dlm)

But what we want is to collapse the **sites** and **years** dimensions together before recasting. To do this, we need to make new columns representing the collapsed dimension of replication, and delete the columns associated with original un-collapsed dimensions. These new columns can be created with the **interaction** and **within** functions in **base** R,

```
R> dlm$sites.years.species <- within(dlm$sites.years.species, {
    sites.years <- interaction(sites, years, drop = TRUE)
    sites <- years <- NULL
    })
R> dlm$sites.years <- within(dlm$sites.years, {
        sites.years <- interaction(sites, years, drop = TRUE)
        sites <- years <- NULL
        sites <- years <- NULL
    })</pre>
```

Recasting can then be applied to produce the reshaped data list,

```
R> dl <- dlcast(dlm)
R> summary(dl)
```

	abundance	temperature	precipitation	body.size
species	TRUE	FALSE	FALSE	TRUE
sites.years	TRUE	TRUE	TRUE	FALSE

3. Coercing data lists to data frames

 $\frac{\text{data list}}{\text{data frame}} \longrightarrow \frac{\text{data frame}}{\text{data frame}}$

A pivotal point in any workflow using **multitable** is the coercion of a data list to a data frame – this is the point at which the variety of R tools for single-table data, become available to multiple-table data. Because this coercion is so pivotal, the syntax required to execute it is as simple as possible. See Table 1.

```
R> data("fake.community")
```

```
R> fake.community.df <- as.data.frame(fake.community)</pre>
```

R> fake.community.df

	abundance	temperature	precipitation	body.size	metabolic.rate	
midlatitude.2009.capybara	4	NA	NA	140	20	
<pre>subtropical.2009.capybara</pre>	0	25	99	140	20	
tropical.2009.capybara	8	48	149	140	20	
equatorial.2009.capybara	0	50	199	140	20	
arctic.2009.capybara	0	-37	21	140	20	
subarctic.2009.capybara	0	3	41	140	20	
midlatitude.2008.capybara	0	10	20	140	20	
subtropical.2008.capybara	10	20	100	140	20	
tropical.2008.capybara	0	50	150	140	20	
equatorial.2008.capybara	7	30	200	140	20	
arctic.2008.capybara	0	-30	20	140	20	
subarctic.2008.capybara	0	0	40	140	20	
midlatitude.1537.capybara	0	NA	NA	140	20	
subtropical.1537.capybara	0	NA	NA	140	20	
tropical.1537.capybara	0	NA	NA	140	20	
equatorial.1537.capybara	0	NA	NA	140	20	
arctic.1537.capybara	0	NA	NA	140	20	
subarctic.1537.capybara	0	NA	NA	140	20	
midlatitude.2009.moss	0	NA	NA	NA	5	
subtropical.2009.moss	0	25	99	NA	5	

Table 1: The fake.community data.list object that has been coerced into a data.frame. Some rows and columns are omitted for brevity. The resulting data frame contains one column for each variable and one row for each combination of replicates across the three dimensions of replication; Table 1 shows this data frame, without the last column so that it can fit on one page. This as.data.frame method for data lists is essentially a database join operation. Notice that the row names are automatically generated to be informative about the dimensions of replication that have been collapsed into a single dimension. Unlike the corresponding data list object, the data frame has redundancy. For example, because body.size is only replicated along species there are only three unique body.size values, one for each of the three species. These three values are repeated so that all of the variables can be stored side-by-side in a single data frame.

3.1. Faster iterative coercion of data lists to data frames

On occasion, one may wish to iteratively coerce a sequence of data lists to data frames. For example, in a randomization test one might loop over a number of random subscripts of a data list (Section 4.5). One may find that such an iterative procedure takes too long to run. Fortunately, we can exploit the fact that each replicated data list has the same relational structure (i.e., the same replication dimensions and variables) to reduce computation times. In particular, much of the computational effort involved in coercing data lists to data frames can be done once for all data lists with the same structure; we refer to this initial computation as 'molding'.

Molding begins by taking a 'mold' of the original data list,

```
R> data("fake.community")
R> fc.mold <- data.list.mold(fake.community)</pre>
```

With such a mold, the as.data.frame operation can be computed much faster than without one. In particular, this command,

```
R> as.data.frame(fake.community, mold = fc.mold)
```

is faster than this one,

```
R> as.data.frame(fake.community)
```

To demonstrate the computational savings of molding, consider the following two simple functions that each coerce the **fake.community** data list to a data frame one hundred times.

```
R> with_molding <- function(){
    fake.community.mold <- data.list.mold(fake.community)
    for(i in 1:100) as.data.frame(fake.community,
        mold = fake.community.mold)
    + }
R> without_molding <- function(){
    for(i in 1:100) as.data.frame(fake.community)
    + }
</pre>
```

The only difference between these functions is that a mold is created outside of the loop, and therefore should be faster. This first function is indeed faster as the following timing shows,

This output indicates that the function without molding took ≈ 1.5 times as long. For more on this technique see the help file for data.list.mold in the multitable package, and the randomization test in Section 4.5.





4.1. Stream fish data

Now that we have described how data lists are created and manipulated using a simple example, we move on to analyzing a small yet real data set on stream fish communities in Texas (Higgins 2009) that comes pre-loaded with **multitable**.

R> data("higgins")

The relational structure of this data set is given in Figure 6, and can be accessed in more detail using the summary and dim functions,

```
R> summary(higgins)
```

	abundance	width	temp	${\tt depth}$	velocity	${\tt substrate}$	habitat
species	TRUE	FALSE	FALSE	FALSE	FALSE	FALSE	FALSE
seasons	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE
rivers	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE	TRUE
	trophic 1	ife.his	story				
species	TRUE		TRUE				
seasons	FALSE	I	FALSE				
rivers	FALSE	Η	FALSE				
R> dim(h	niggins)						
species	seasons	rivers					
24	4	3					

22



Figure 6: Bipartite graph of the **higgins** stream fish data. Dimensions of replication are in blue (on the left) and tables are in red (on the right). Sample sizes along each dimension of replication are given as n; and numbers of variables in each variable group are given as m.

One 100-m stretch of each of three rivers (tributaries of the Colorado River) were sampled once in each of the four seasons. Abundances of 24 fish species were measured as numbers of individuals captured by electro-fishing; we abbreviate species names following Higgins (2009). Two categorical traits (trophic status and life history) were obtained from the stream fish literature to characterize each of the 24 species. Trophic status characterizes species' diet and is described by four levels in this data set (herbivore; omnivore; insectivore; and piscivore). Life history describes the strategy by which a species' individuals allocate limited resources amongst themselves, and is based on a three-way classification of strategies (equilibrium, or large investment in relatively few individual offspring; opportunistic, or small size and rapid maturation; and periodic, or pulsed production of large numbers of small offspring); some species are also described as intermediate between two categories. Six environmental variables (stream width (m), temperature (°C), depth (cm), and velocity (m s⁻¹), and two dimensionless measures of river bed substrate and fish habitat) were measured at each river in each season.

4.2. Marginal summaries

A common task in data exploration is to compute marginal summaries (e.g., means and quantiles). In R this is commonly done using the apply family of functions or more recently with packages such as **plyr** (Wickham 2011). In general these functions 'apply' another function to various parts of an R object. Here we demonstrate how to use existing apply functions to summarize data lists and introduce a new function: data list apply, dlapply. The dlapply function is designed to be intuitive for anyone familiar with the standard apply function in base R – the arguments for the two functions are identical,

- apply(X, MARGIN, FUN, ...)
- dlapply(X, MARGIN, FUN, ...)

The dlapply function attempts to use apply on each variable in a data list, in order to return another data list replicated along the marginal dimensions of replication (i.e., the dimensions specified in MARGIN). However, the rich structure of data lists often makes it impossible to completely marginalize in this way. Still, dlapply is extremely useful because it not only marginalizes as many of the variables in a data list as possible, but also provides informative messages about why some variables are unable to be marginalized, allowing our thoughts to be centred on data analysis rather than the details of marginalization. For example, to obtain the median values of the variables in higgins for each species, we set MARGIN = 1 because species is the first dimension and set FUN = median,

```
R> dlapply(higgins, 1, median)
```

omitting width because it is not replicated along MARGIN omitting temp because it is not replicated along MARGIN omitting depth because it is not replicated along MARGIN omitting velocity because it is not replicated along MARGIN omitting substrate because it is not replicated along MARGIN omitting habitat because it is not replicated along MARGIN omitting trophic because of the following error: Error in median.default(newX[, i], ...) : need numeric data omitting life.history because of the following error: Error in median.default(newX[, i], ...) : need numeric data

abundance:

amna caan caca cicy cyve dini etle etsp gaaf icpu leau lecy legu lema 0.0 3.5 0.0 0.0 34.5 10.0 11.5 6.0 41.0 1.5 12.5 9.5 0.0 10.5 leme mido mipu misa moco noam nost peca pivi pyol 14.0 0.0 1.0 0.0 0.5 1.0 7.0 6.0 0.0 0.0 Replicated along: || species ||

REPLICATION DIMENSIONS: species 24

The species median abundances are given as a single-variable data list and the messages explain why the other variables did not marginalize. All of the environmental variables are not replicated along species and so it is impossible to find species medians for them. While the trophic and life.history traits are replicated along species, their medians cannot be computed because they are factors. Note that these messages are *not* errors, even though the word 'error' frequently appears in them; reporting on which variables were unable to be marginalized because of an error in the function, FUN, being applied is part of the normal behaviour of dlapply.

Sometimes results are more visually pleasing when dlapply is wrapped in a call to as.data.frame, particularly when the resulting data list is large,

```
R> as.data.frame(dlapply(higgins, c(2, 3), median))
```

```
omitting trophic because it is not replicated along MARGIN omitting life.history because it is not replicated along MARGIN
```

	abundance	width	temp	depth	velocity	${\tt substrate}$	habitat
<pre>spring.pedernales</pre>	1.0	20.43	23.32	47.62	3.00	3.68	2.70
<pre>summer.pedernales</pre>	0.0	19.19	28.42	34.28	2.88	3.72	2.49
fall.pedernales	8.0	21.88	15.00	36.68	4.14	3.83	2.57
winter.pedernales	0.5	22.37	15.28	35.32	3.13	3.68	2.49
spring.san.saba	0.5	30.56	20.32	32.38	1.20	4.78	2.71
summer.san.saba	1.0	23.04	26.25	20.86	0.00	4.63	2.64
fall.san.saba	4.0	35.12	11.73	29.43	0.00	4.63	2.49
winter.san.saba	5.5	37.66	11.44	34.21	1.37	4.64	2.37
<pre>spring.south.llano</pre>	2.5	14.45	21.54	46.64	0.25	3.34	2.72
<pre>summer.south.llano</pre>	1.0	11.91	25.49	34.42	0.00	2.93	2.83
fall.south.llano	10.0	13.05	11.42	37.90	0.00	3.31	2.58
winter.south.llano	6.0	14.28	12.18	45.90	0.05	2.94	2.58

The result here gives the median values of several variables for each season-river combination. One clear pattern in the median **abundances** is that the three rivers have more fish in fall and winter than in spring and summer.

While median returns a single value, we often want to apply a function that returns several values in a vector (e.g., the quantile function). This is easily done with dlapply (omitting several variables to save space),

```
R> dlapply(higgins[1:2], 3, quantile)
```

abundance:

	pedern	ales	san.saba	a south	.llano	
0%	-	0	()	0.0	
25%		0	()	0.0	
50%		1	4	2	2.5	
75%		9	13	3	13.5	
100%		187	529)	212.0	
Repli	cated	along	յ։ գւ	lantile	rivers	3
width	1 :					
	-					
	pedern	ales	san.saba	a south	.llano	
0%	19.	1900	23.040) 1:	1.9100	
25%	20.	1200	28.680) 11	2.7650	
50%	21.	1550	32.840) 13	3.6650	
75%	22.	0025	35.755	5 14	4.3225	
100%	22.	3700	37.660) 14	4.4500	
Repli	cated	along	յ։ գւ	antile	rivers	3
REPL1	CATION	I DIME	INSIONS:			
quant	cile	river	s			
	5		3			

We see that when the length of the return value of FUN is greater than one, a new dimension of replication is created with the name of FUN to store this additional information. However, if this new dimension of replication is not the same length for each variable, then a data list cannot be created that contains all of the results. For example, the following command results in an error,

R> dlapply(higgins[1:2], 3, summary)

Error in dlapply(higgins[c(1, 2, 8)], 3, summary) : results could not be combined into a data list

The reason for this error is that the summary function does not summarize each type of object in the same way. In this example, summary is applied along a margin of a numerical array, a numerical matrix, and a factor; the output in each of these cases is too different to be combined back into a single data list. However, data lists are also standard R lists,

R> is.list(higgins) && is.data.list(higgins)

[1] TRUE

Therefore, functions such as summary can be applied to complex data lists using the standard list apply function, lapply, in base R,

R> lapply(higgins[c("abundance", "width", "trophic")], summary)

\$abundance

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
0.00	0.00	1.00	17.18	12.25	529.00
\$width					
peder	nales	san.	saba	south.	llano
Min.	:19.19	Min.	:23.04	Min.	:11.91
1st Qu.	:20.12	1st Qu.	:28.68	1st Qu.	:12.77
Median	:21.16	Median	:32.84	Median	:13.66
Mean	:20.97	Mean	:31.59	Mean	:13.42
3rd Qu.	:22.00	3rd Qu.	:35.76	3rd Qu.	:14.32
Max.	:22.37	Max.	:37.66	Max.	:14.45
\$trophic	:				
hrbvr om	nvr insct	t pscvr			
1	4 13	3 6			

The summary function gives different types of results depending on the class of the object being summarized. For matrices such as higgins\$width, summary returns various quantiles and means of the matrix columns, representing the three tributaries in this case. For other arrays such as higgins\$abundance, summary gives these statistics over the entire array. For factors such as higgins\$trophic, summary counts the number of observations in each category.

In short, dlapply attempts to repeatedly summarize data list margins by passing each variable to the standard apply function and then combining the successfully marginalized variables back into a data list. If this combination fails, dlapply will throw an error; in such a case, consider using the **base** R apply functions for lists (i.e., lapply; sapply; rapply) or the **plyr** package (i.e., laply; ldply; llply; l_ply).

4.3. Data list visualization

Many standard plotting functions in the base R graphics package combine formula and data.frame objects to produce plots. Because data.list objects are readily coerced into data frames, these functions can also be used to visualize data lists. For example, the boxplot command can be used to visualize the variation in the abundances of each of the species across seasons and rivers (Figure 7),

```
R> data("higgins")
R> boxplot(sqrt(abundance) ~ species,
+     data = as.data.frame(dims_to_vars(higgins)), horizontal = TRUE, las = 1,
+     xaxt = "n", xlab = "abundance (square-root scale)", ylab = "species")
R> tickmarks <- with(higgins, pretty(sqrt(abundance)))
R> axis(1, at = tickmarks, labels = tickmarks<sup>2</sup>)
```

Note the use of the dims_to_vars function, which is required because a dimension of replication (i.e., species) is referred to in the formula (see Section 2.7). Figure 7 shows that while many species are rare across all rivers and seasons (e.g., pyol; amna), some vary widely in abundance (e.g., dini; cyve).

One of the most challenging aspects of data with more than one dimension of replication is visualizing this higher dimensional structure. For example, a single dimension of replication is naturally represented on a scatterplot as variation in the x-y position of the points. But other aesthetics beyond x-y position – such as color or shape – are required to visualize multidimensional replication on a single scatterplot. We have found that the faceting (i.e., trellising) technique is an effective tool for visualizing multiple dimensions of replication, when at least one of the dimensions is short (i.e., less than 30 replicates). Faceting is used to display subsets of the data in different panels, so that differences between the subsets can be more easily perceived (Wickham 2009). In the multiple-table context, dimensions of replication may be used to define these subsets.

To illustrate faceting in a multiple-table context, we ask whether environmental variables interact with species traits to affect abundance in the higgins data set. Visualizing all of the possible trait-by-environment interactions is virtually impossible, and so we begin by considering a trait and environmental variable that have been hypothesized to interact in many stream fish communities: stream width and fish species life history (Goldstein and Meador 2004). Figure 8 provides a visualization of the dependence of abundance (y-position) on both width (x-position) and life.history (point shape). Each panel is associated with a particular species – therefore, faceting represents the species dimension of replication. Within panels, each point represents a particular river in a particular season – therefore, the position of the points within each scatterplot represents both the seasons and rivers dimensions of replication. Fitted model curves are also plotted for each species to help visualize any systematic trends in the scatterplots.



Figure 7: Boxplots showing spatio-temporal variation of the abundances of species in the higgins data.

Figure 8 illustrates that the width-abundance relationship is variable along the species dimension of replication. However, this variation is not clearly related to the life.history trait that characterizes species, although perhaps equilibrium-periodic species appear more likely than other species to have a flat width-abundance relationship. This possibility is investigated further in Sections 4.4-4.5 on statistical analysis.

The code for producing Figure 8 follows the same pattern as most applications of **multitable**: a data list is manipulated, it is converted to a data frame, and another R function is used to operate on the resulting data frame. Figure 8 requires two manipulations. Because we intend to use dimensions of replication to define the pattern of faceting, the dimnames of the data list must be accessible as variables; therefore, the higgins data must first be passed through the dims_to_vars function (Section 2.7),

```
R> data("higgins")
R> higgins <- dims_to_vars(higgins)</pre>
```

The order of the panels in Figure 8 is not arbitrary; the **species** dimension is ordered by **life.history**. This ordering helps to clarify whether certain types of species have similar



Figure 8: Visual exploration of the interaction between width and life.history on abundance in the higgins data. Faceting is used to represent the species dimension of replication.

width-abundance relationships, because the panels for similar species are adjacent in the faceted plot. To do this, the species variable must be converted into an ordered factor, with ordering determined by life.history; the with and reorder functions are useful for this purpose,

R> higgins\$species <- with(higgins, reorder(species, life.history))</pre>

The higgins data are now ready to be coerced into a data frame. Before doing so, we load the ggplot2 package,

R> library("ggplot2")

which we used to produce Figure 8. Because our focus is on describing **multitable**, we will not explain each **ggplot2** command in detail. However, the syntax of **ggplot2** functions should be readable to anyone familiar with R in general. One of the benefits of **ggplot2** is that the code for producing a plot can be broken into manageable pieces, which are added together to create the full plot (Wickham 2009). We begin by producing a **ggplot** object, **p**, for the higgins data,

R> p <- ggplot(as.data.frame(higgins))</pre>

In the next step we specify the pattern of faceting, which will represent replication along the **species** dimension,

```
R> p <- p + facet_wrap(~ species, ncol = 4)</pre>
```

Here the + operator does not have its usual arithmetic meaning, but rather indicates that the property of faceting by species should be added to the plot object, p. Setting ncol = 4 reflects a purely aesthetic choice to organize the plots into 4 columns of 6 species each. Having specified that replication along the **species** dimension will be represented by faceting, we now specify that the remaining dimensions (**seasons** and **rivers**) will be represented by points,

R> p <- p + geom_point(aes(x = width, y = abundance, shape = life.history))

This command also indicates that the x-y position of the points will describe the width and abundance variables, whereas the shape of the points will describe life.history. To help guide the eye we plot a fitted quadratic predictive model of the width-abundance relationship in each panel using the bayesglm function from the arm package (Gelman *et al.* 2012); the standard glm function in the stats package yielded unrealistically large coefficients, whereas bayesglm automatically shrinks coefficients towards zero resulting in a much better smoothing of the data.

```
R> library("arm")
R> p <- p + stat_smooth(aes(x = width, y = abundance), se = FALSE,
+ method = "bayesglm", family = poisson, form = y ~ x + I(x^2),
+ colour = "black", alpha = 0.4, geom = "line")</pre>
```

Finally, the **abundance** data are put on a square-root scale, to help visually homogenize residual variance.

```
R> p <- p + scale_y_continuous(trans = "sqrt",
+ breaks = trans_breaks("sqrt", function(x) x<sup>2</sup>))
```

And then the plot is produced (Figure 8),

R> print(p)

4.4. Generalized linear model example

Figure 8 suggested that abundance might have been affected by an interaction between width

and life.history, because the abundances of species with an equilibrium-periodic life history had weaker relationships with width than other species. To explore this possibility we conducted a variety of formal statistical analyzes, which also help to demonstrate how models can be fitted to data lists in much the same way that they are fitted to data frames.

For most model fitting functions in R, the hypothesized relationships between variables is specified via a formula object. For example, a simple formula including the effect of the interaction between width and life.history on abundance is given by,

R> form <- abundance ~ -1 + life.history + (scale(width):life.history)

The overall intercept has been removed (with -1) so that each life.history class has its own intercept. The scale command was used to standardize width to have mean zero and standard deviation one, which simplifies the interpretation of the estimated coefficients. We fitted this formula to the higgins data using the glm function with a poisson error distribution, which is a good first choice for count data. Because glm takes data in the form of a data frame, data lists can also be fitted by first passing them through as.data.frame,

```
R> higgins.glm <- glm(form, family = poisson, data = as.data.frame(higgins))
R> printCoefmat(summary(higgins.glm)$coefficients, signif.stars = FALSE)
```

	Estimate	Std. Error	z value	Pr(> z)
life.historyeqlbr	2.564697	0.033109	77.4613	< 2.2e-16
life.historyeqlbr.perdc	1.111861	0.067897	16.3756	< 2.2e-16
life.historyopprt.eqlbr	3.510256	0.029166	120.3560	< 2.2e-16
life.historyopprt.perdc	3.311290	0.030468	108.6820	< 2.2e-16
life.historyperdc	2.125420	0.052921	40.1625	< 2.2e-16
life.historyeqlbr:scale(width)	0.234802	0.030539	7.6886	1.488e-14
<pre>life.historyeqlbr.perdc:scale(width)</pre>	0.137218	0.064942	2.1129	0.03461
<pre>life.historyopprt.eqlbr:scale(width)</pre>	-0.218340	0.030926	-7.0600	1.665e-12
<pre>life.historyopprt.perdc:scale(width)</pre>	0.771661	0.022881	33.7250	< 2.2e-16
life.historyperdc:scale(width)	-0.935271	0.057963	-16.1357	< 2.2e-16

A striking aspect of this fitted model is that all of the coefficients are significant, and most are highly significant. However, these strong results are caused by inflated type I error rates related to the fact that repeated measurements have been taken on each species. Repeated measurements are *always* an important consideration when analyzing data with multiple dimensions of replication; in a three-dimensional data list, such as ours for example, replication along two of the dimensions (e.g., **seasons** and **rivers**) induces repeated measurements of the replicates along the other (i.e., **species**). However, these inevitable repeated measurements will only inflate type I error if the deviations from model expectations tend to be more similar for observations associated with the same replicate along a particular dimension of replication – a form of autocorrelation. To visually explore this possibility, a good option is to plot the expected versus observed values of the response variable, faceted by a dimension of replication. For example, we plot **abundance** against its fitted values and facet by **species** (with 1:1 lines to guide the eye) (Figure 9),

```
R> higgins[["fitted", shape = "abundance"]] <-
+ array(fitted.values(higgins.glm), dim(higgins))</pre>
```



Figure 9: Observed abundances in the higgins data versus the abundances expected from a fitted generalized linear model with Poisson error structure and formula, abundance ~ -1 + life.history + (scale(width):life.history). Each panel is for a single species, with 1:1 lines to aide visual interpretation.

```
R> ggplot(as.data.frame(higgins)) +
+ facet_wrap(~ species, ncol = 4) +
+ geom_point(aes(x = fitted, y = abundance)) +
+ geom_abline(intercept = 0, slope = 1) +
+ scale_y_continuous(trans = "sqrt",
+ breaks = trans_breaks("sqrt", function(x) x^2)) +
+ scale_x_continuous(trans = "sqrt",
+ breaks = trans_breaks("sqrt", function(x) x^2))
```

Autocorrelation is clearly visible in the panels for species within which all observed abundances lie below the 1:1 line (i.e., amna; legu; mido; misa; pyol; caca). The biological interpretation of this autocorrelation is that life.history does not completely determine each species' relationship with width, and therefore that width must interact with other traits to affect abundance.

Despite this autocorrelation issue, the parameter estimates themselves suggest that there may in fact be an interaction between life.history and width. In particular, the width coefficient for equilibrium-periodic species is smaller in magnitude than for the others. Furthermore, some life.history strategies were associated with positive width coefficients (i.e., equilibrium; equilibrium-periodic; and opportunistic-periodic) whereas the other two were associated with negative width coefficients (i.e., opportunistic-equilibrium and periodic). But, will this interaction be significant after properly accounting for autocorrelation? There are two general approaches to addressing this question: mixed modeling and randomization testing, which is considered next.

4.5. Randomization tests

As in all randomization tests, the first step is to compute the statistics of the observed data, which in this case are the five coefficients defining the interaction between life.history and width.

R> coef.obs <- coefficients(higgins.glm)[6:10]

These observed coefficients will be compared with a distribution of coefficients for randomized data. Next we decide on the number of randomizations,

R> B <- 500

and allocate an array to store the randomized coefficients,

```
R> coef.B <- array(0, c(B, length(coef.obs), 2))
R> dimnames(coef.B) <- list(1:B, names(coef.obs),
+ c("species", "seasons.rivers"))</pre>
```

This array, coef.B, has one dimension for the B randomizations of the data, one for the number of coefficients in the model, and a third dimension for the number of null models to be considered; with more than a single dimension of replication, several null models are often required (e.g., Dray and Legendre 2008; Cormont, Vos, van Turnhout, Foppen, and ter Braak 2011). When sample sizes are sufficiently large, it is ideal to compute one null model for each dimension of replication. The null model for each dimension permutes the indices of the response variable (i.e., abundance in this case) for that dimension. This is the approach suggested by Dray and Legendre (2008). However, the seasons and rivers dimensions are very short (i.e., 4 and 3), which translates into only 24 and 6 possible permutations for these dimensions. Therefore, we consider only two null models: permute the (1) species dimension and (2) seasons and rivers dimensions.

Because randomization tests involving data lists require the repeated coercion of data lists to data frames, we use the molding technique to speed up computation (Section 3.1). In this example, the savings in speed are modest, but they can be much greater in larger problems. Molding begins by taking a mold of the initial data list,

R> mold.higgins <- data.list.mold(higgins)</pre>

Both null models require a three-line loop over the B permutations,

```
R> higgins.tmp <- higgins
R> for(i in 1:B) {
    higgins.tmp$abundance <- higgins$abundance[sample(24), , ]
    df.tmp <- as.data.frame(higgins.tmp, mold = mold.higgins)
    coef.B[i, , 1] <- glm(form, family = poisson, df.tmp)$coefficients[6:10]
    + }</pre>
```

The first line permutes the **species** dimension of the response variable; the second coerces the permuted data list to a data frame; and the third computes and stores the coefficients estimated from the permuted data. The second null model is computed similarly,

```
R> higgins.tmp <- higgins
R> for(i in 1:B) {
    higgins.tmp$abundance <- higgins$abundance[, sample(4), sample(3)]
    df.tmp <- as.data.frame(higgins.tmp, mold = mold.higgins)
    coef.B[i, , 2] <- glm(form, family = poisson, df.tmp)$coefficients[6:10]
    + }</pre>
```

To avoid issues with two-sided tests, we assess the magnitudes of the coefficients irrespective of their signs,

```
R> coef.B.abs <- abs(coef.B)
R> coef.obs.abs <- abs(coef.obs)</pre>
```

Simple estimates of p values can now be computed by processing coef.B.abs using standard R commands,

```
R> pvalues <- apply(sweep(coef.B.abs, 2, coef.obs.abs, ">="), c(2,3), mean)
R> round(cbind(coef.obs, pvalues), 3)
```

	<pre>coef.obs</pre>	species	<pre>seasons.rivers</pre>
life.historyeqlbr:scale(width)	0.235	0.626	0.336
<pre>life.historyeqlbr.perdc:scale(width)</pre>	0.137	0.780	0.532
<pre>life.historyopprt.eqlbr:scale(width)</pre>	-0.218	0.708	0.274
<pre>life.historyopprt.perdc:scale(width)</pre>	0.772	0.122	0.474
life.historyperdc:scale(width)	-0.935	0.072	0.192

With these more accurate p values, we can see that there is very little evidence for an interaction between width and life.history. A mixed-model approach that more directly accounts for repeated measurements on species might be beneficial here. Although such an approach is beyond our scope here, the consistent logic of **multitable** applies: manipulate the data list, coerce it to a data frame, and pass the data frame to a mixed-model fitting function.

4.6. Analyzing data lists with multivariate methods

So far we have used data lists by manipulating them, converting to a data frame, and passing to a function to produce an analysis or visualization. In the context of multivariate analysis, it is often useful to cut out the middle step and pass a data list directly to a function. In most univariate methods, both the response and explanatory variables are vectors; in contrast, the response variables of many multivariate methods are matrices while the explanatory variables are vectors. Because data lists are – unlike data frames – able to store both matrix- and vector-valued variables, they are well suited for use in multivariate analyzes.

As an example of using a data list in a multivariate analysis, we use the adonis (analysis of dissimilarities) function (Anderson 2001; McArdle and Anderson 2001) in the vegan package (Oksanen *et al.* 2012) to analyze the relationships between abundance and the environmental variables in the higgins data. However, abundance is a three dimensional array, and adonis – like many other multivariate methods requires a matrix-valued response variable. Therefore, higgins must be manipulated before it is ready to be analyzed. In particular, we collapse the seasons and rivers dimensions of replication into a single dimension, seasons.rivers. In Section 2.8 we described how to collapse dimensions using the melt-recast concept, and so we use this technique here,

```
R> data("higgins")
R> higgins.melt <- dlmelt(higgins)
R> higgins.melt$species.seasons.rivers <-
+
     within(higgins.melt$species.seasons.rivers, {
       seasons.rivers <- interaction(seasons, rivers, drop = TRUE)</pre>
+
       seasons <- rivers <- NULL
+
   })
+
R> higgins.melt$seasons.rivers <-
     within(higgins.melt$seasons.rivers,
+
       seasons.rivers <- interaction(seasons, rivers, drop = TRUE)</pre>
+
   )
+
R> higgins <- dlcast(higgins.melt)
```

This new version of higgins has only two dimensions of replication, with abundance as a matrix and the environmental variables as one-dimensional vectors,

R> summary(higgins)

abundance width temp depth velocity substrate habitat seasons species TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE seasons.rivers rivers trophic life.history FALSE TRUE TRUE species TRUE FALSE FALSE seasons.rivers

We can now call adonis within an environment defined by higgins,

```
R> library("vegan")
R> dl.adonis <- with(higgins, adonis(
+ t(abundance) ~ width + temp + depth + velocity + substrate + habitat,
+ strata = higgins$species
+ ))
R> print(dl.adonis$aov.tab, signif.stars = FALSE)
```

	\mathtt{Df}	SumsOfSqs	MeanSqs	F.Model	R2	Pr(>F)
width	1	0.80370	0.80370	6.3398	0.28374	0.001
temp	1	0.28776	0.28776	2.2699	0.10159	0.046
depth	1	0.19041	0.19041	1.5020	0.06722	0.193
velocity	1	0.43200	0.43200	3.4078	0.15252	0.011
substrate	1	0.23012	0.23012	1.8152	0.08124	0.104
habitat	1	0.25466	0.25466	2.0088	0.08991	0.082
Residuals	5	0.63385	0.12677		0.22378	
Total	11	2.83250			1.00000	

Terms added sequentially (first to last)

The fact that width and velocity have significant effects indicate that these factors might be important in structuring these stream fish communities. However, taken together with the previous results using Poisson generalized linear models, these results also indicate that these effects are not well understood in terms of the life.history trait.

5. Conclusion

The structure of data.list objects is sufficiently rich to give rise to a wider variety of uses than can be described in detail here. Our intention was to illustrate the basic features and concepts of the **multitable** package, and to demonstrate its utility. Our long-term goal with the **multitable** project in general is to make standard analyzes in R simpler to conduct on complex multiple-table data.

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References

- Anderson MJ (2001). "A New Method for Non-Parametric Multivariate Analysis of Variance." Austral Ecology, 26, 32–46.
- Cantin A, Beisner BE, Gunn JM, Prairie YT, Winter JG (2011). "Effects of Thermocline Deepening on Lake Plankton Communities." *Canadian Journal of Fisheries and Aquatic Science*, 68, 260–276.
- Chambers JM, Hastie TJ (1992). *Statistical Models in S*. Wadsworth and Brooks, Pacific Grove, California.

- Cormont A, Vos CC, van Turnhout CAM, Foppen RPB, ter Braak CJF (2011). "Using Life-History Traits to Explain Bird Population Responses to Changing Weather Variability." *Climate Research*, 49, 59–71.
- Dolédec S, Chessel D, ter Braak CJF, Champely S (1996). "Matching Species Traits to Environmental Variables: A New Three-Table Ordination Method." *Environmental and Ecological Statistics*, 3, 143–166.
- Dray S, Legendre P (2008). "Testing the Species Traits-Environment Relationships: The Fourth-Corner Problem Revisited." *Ecology*, **89**, 3400–3412.
- Gelman A, Su YS, Yajima M, Hill J, Pittau MG, Kerman J, Zheng T (2012). arm: Data Analysis Using Regression and Multilevel/Hierarchical Models. R package version 1.5-08, URL http://CRAN.R-project.org/package=arm.
- Goldstein RM, Meador MR (2004). "Comparisons of Fish Species Traits from Small Streams to Large Rivers." Transactions of the American Fisheries Society, 133, 971–983.
- Higgins CL (2009). "Spatiotemporal Variation in Functional and Taxonomic Organization of Stream-Fish Assemblages in Central Texas." Aquatic Ecology, 43, 1133–1141.
- Ives AR, Helmus MR (2011). "Generalized Linear Mixed Models for Phylogenetic Analyses of Community Structure." *Ecological Monographs*, 81, 511–523.
- Legendre P, Galzin R, Harmelin-Vivien ML (1997). "Relating Behavior to Habitat: Solutions to the Fourth-Corner Problem." *Ecology*, 78, 547–562.
- Leibold MA, Economo EP, Peres-Neto PR (2010). "Metacommunity Phylogenetics: Separating the Roles of Environmental Filters and Historical Biogeography." *Ecology Letters*, 13, 1290–1299.
- McArdle BH, Anderson MJ (2001). "Fitting Multivariate Models to Community Data: A Comment on Distance-Based Redundancy Analysis." *Ecology*, 82, 290–297.
- Oksanen J, Blanchet FG, Kindt R, Legendre P, Minchin PR, O'Hara RB, Simpson GL, Solymos P, Stevens MHH, Wagner H (2012). *vegan: Community Ecology Package*. R package version 2.0-5, URL http://CRAN.R-project.org/package=vegan.
- Pillar VD, Duarte LDS (2010). "A Framework for Metacommunity Analysis of Phylogenetic Structure." *Ecology Letters*, 13, 587–596.
- R Development Core Team (2012). R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0, URL http: //www.R-project.org/.
- Sólymos P (2009). "Processing Ecological Data in R with the **mefa** Package." Journal of Statistical Software, **29**(8), 1–28. URL http://www.jstatsoft.org/v29/i08/.
- Wickham H (2007). "Reshaping Data with the **reshape** Package." Journal of Statistical Software, **21**(12), 1-20. URL http://www.jstatsoft.org/v21/i12/.
- Wickham H (2009). *ggplot2:* Elegant Graphics for Data Analysis. Springer-Verlag, New York.

Wickham H (2011). "The Split-Apply-Combine Strategy for Data Analysis." Journal of Statistical Software, 40(1), 1-29. URL http://www.jstatsoft.org/v40/i01/.

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