

Multiple-table data in R

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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 and variables respectively. Standard R workflows require that all of the data to be analyzed is organized into a single data frame, and 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 produce analyses (e.g. plots; fitted models; summary statistics). This framework allows ecologists to concentrate on their primary interests—the relationships between ecological variables—without explicit reference to complex mathematical and algorithmic details. It also provides access to those details, which are required (1) for more effective analyses and (2) 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. Thus, by separating low-level methods development from high-level data analysis, R fosters the formation of a community of researchers where both methodologists and analysts can have mutually beneficial interactions.

However, research in my field of community ecology has led me to data sets that do not easily fit within a single data frame. A common example is the fourth-corner problem (Legendre et al. 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 (Fig. 1). Such data are characterized by a conspicuous (lower-right) ‘fourth-corner’, where there are no data. These fourth-corners of missing data 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, Fig. 2). The challenge of analyzing 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 `multitable` package is to provide tools for analyzing multiple-table data sets within this standard R framework.

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 has been a fair amount of work in this direction, focusing on

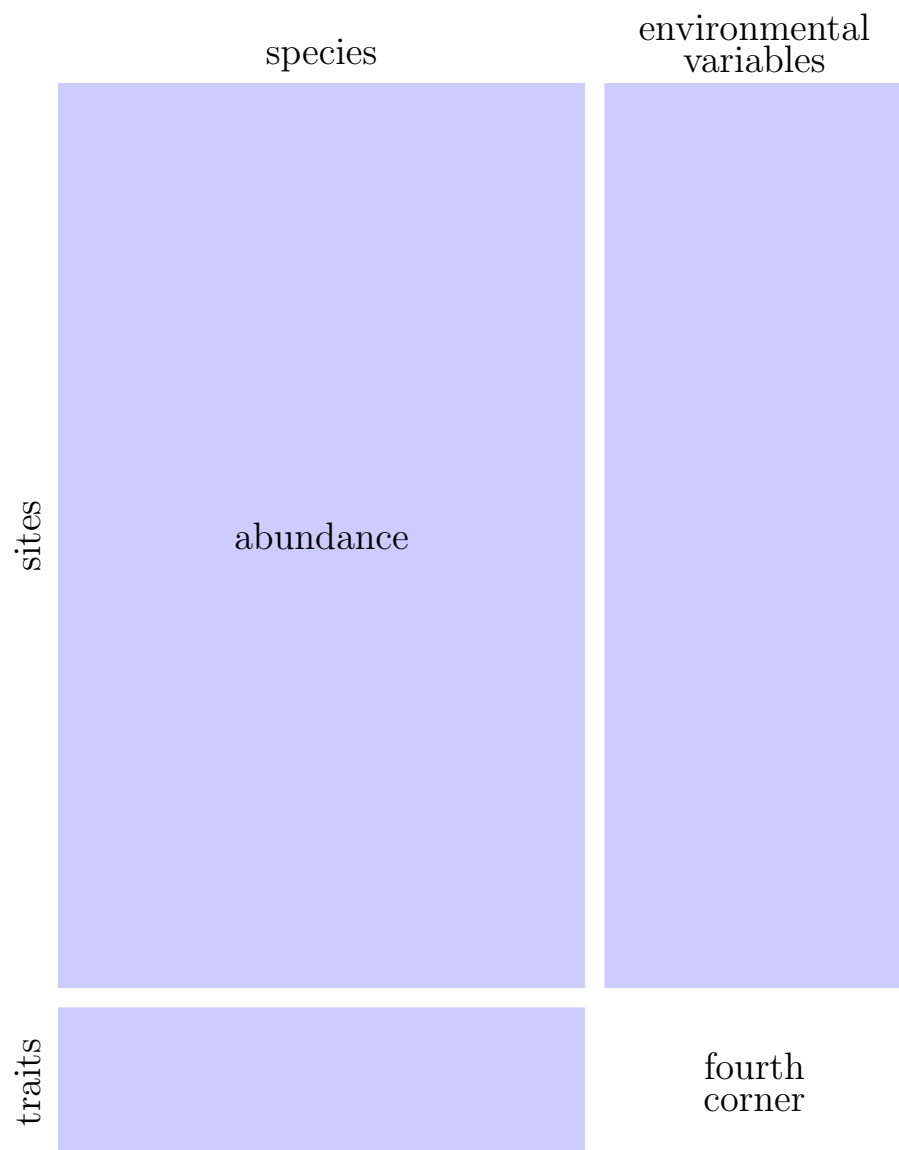


Figure 1: Fourth corner problem.

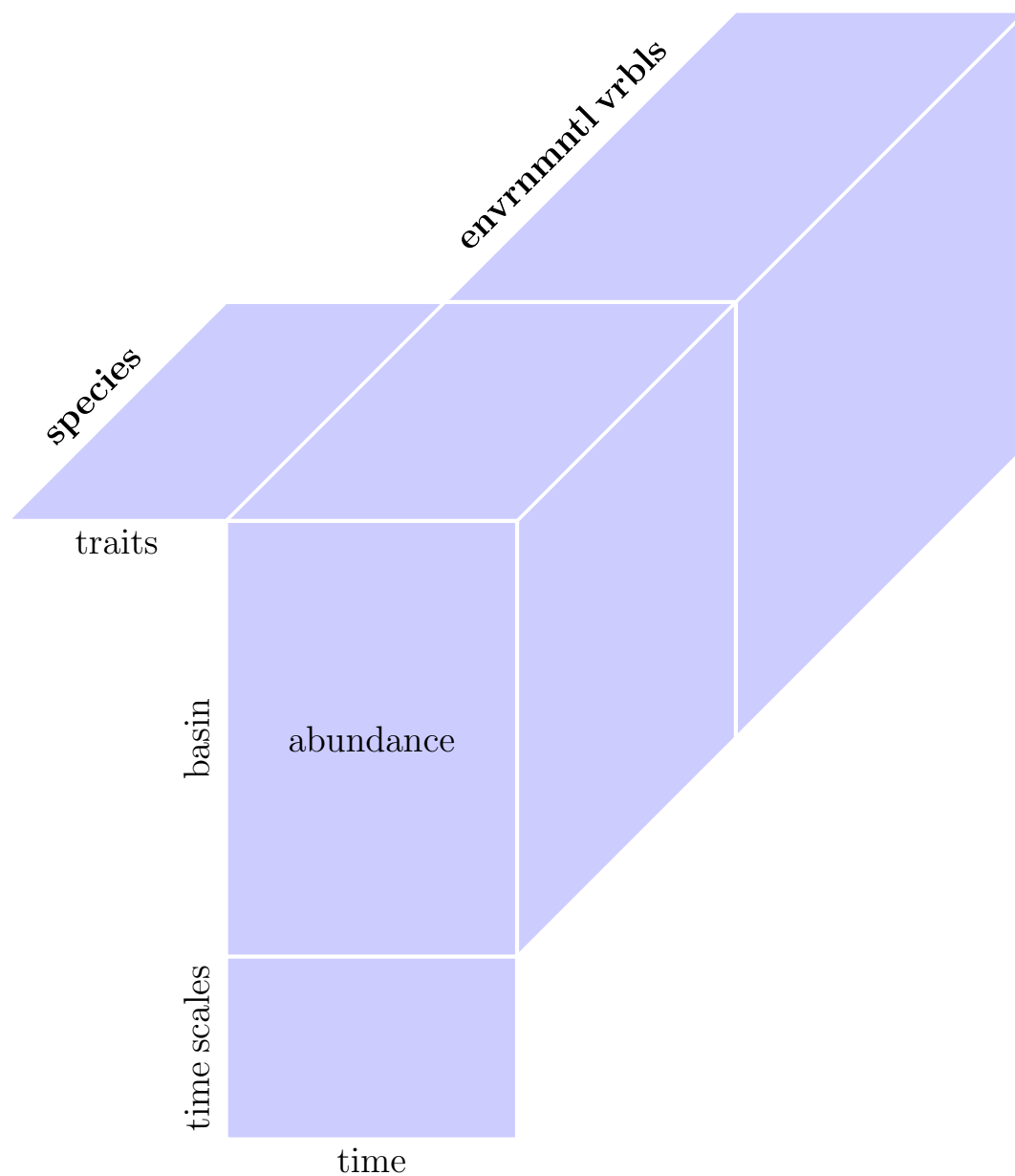


Figure 2: The structure of the Lac Croche zooplankton community data.

data with a fourth-corner problem (e.g. Chessel et al. 1996; Legendre et al. 1997; Ives and Godfray 2006; Dray and Legendre 2008; Pillar and Duarte 2010; Leibold et al. 2010; Ives and Helmus 2011). However, this work does not apply to data sets that have other more complex multiple-table data structures (e.g. zooplankton communities in Lac Croche, Fig. 2). One approach to such issues would be to build new data analysis functions for each new data structure. But such an approach is less than ideal, as it would require that new methods be learned for each new structure—it does not take advantage of the large number of tools developed within the standard R framework of data frames and formulas. 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.

There are several existing R packages that are designed to make data management easier (e.g. **reshape2**; etc.??). In particular, the **mefa** and **mefa4** packages have been developed to organize data with a slight generalization¹ of the fourth-corner problem. The **multitable** package has much in common with **mefa**, but there are noticeable differences. For example, **mefa** provides more extensive tools for data summarization than **multitable** and **mefa4** integrates tools for sparse-matrix computations. On the other hand, **multitable** is designed to handle more general data structures than **mefa** or **mefa4** (e.g. **mefa** cannot organize the Lac Croche data structure, Fig. 2). However, we hope that **mefa** and **multitable** will be complementary, not competitive.

The **multitable** model of data organization is illustrated in Figure 3 (**mefa** uses a similar model). In blue are the elements of the standard R workflow: data frames; formulas; functions; and analyses. The **multitable** package seeks to facilitate the use of such workflows with multiple-table data by creating tools (arrows and red boxes) for organizing and manipulating such data. These tools are based on a new kind of object, called a data list, which is used to organize multiple-table data. Data lists can be manipulated much like data frames (e.g. variables can be transformed; groups of observations extracted or removed). Our design principle was to keep the manipulation of data lists as similar as possible to the manipulation of data frames. Once data lists are ready for analysis **multitable** provides tools for coercing them into data frames, thereby entering the standard R workflow. Importantly, data, formulas, and functions are kept separate, thus preserving the benefits of using R in a standard way.

1 The structure of data lists

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

¹Several community matrices—called segments—with identical dimensions are allowed in **mefa**.

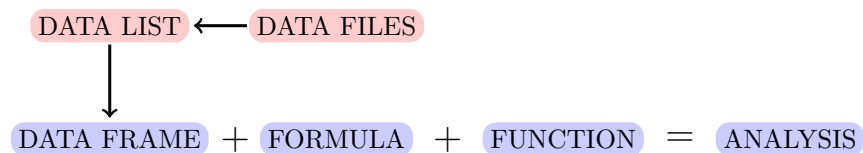


Figure 3: The `multitable` paradigm for including multiple-table data (in red) into the standard R workflow (in blue). Data lists are used to organize and manipulate multiple-table data as a single R object, even though it must be stored in multiple text-based data files. When such data are required for analysis, they are coerced into a data frame. Once in data frame form, they can be used in analyses by combining them with formulas (to specify hypothetical relationships between variables) and functions (to call computational methods).

```

> library(multitable)
> data(fake.community)
> fake.community

abundance:
-----
, , capybara

      2009 2008 1537
midlatitude    4    0    0
subtropical    0   10    0
tropical       8    0    0
equatorial     0    7    0
arctic         0    0    0
subarctic      0    0    0

, , moss

      2009 2008 1537
midlatitude    0    6    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
subarctic	0	0	0

Replicated along: || sites || years || species ||

temperature:

	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 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	NA
subarctic	41	40	NA

Replicated along: || sites || years ||

body.size:

capybara	moss	vampire
140	NA	190

Replicated along: || species ||

metabolic.rate:

capybara	moss	vampire
20	5	0

Replicated along: || species ||

homeotherm:

```

-----
copybara      moss  vampire
      Y          N      N
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 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 in 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 a `dim` (i.e. dimension) attribute, which gives it 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 indicated above after the variable itself is printed. Some variables are only replicated along two dimensions (e.g. temperature and precipitation) and others only a single 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.

```
> summary(fake.community)
```

	abundance	temperature	precipitation	body.size	metabolic.rate	homeotherm
sites	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE
years	TRUE	TRUE	TRUE	FALSE	FALSE	FALSE
species	TRUE	FALSE	FALSE	TRUE	TRUE	TRUE

This method returns a logical table 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 relates

abundance, temperature, and precipitation; whereas, the **species** dimension relates abundance, body size, metabolic rate, and homeotherm.

Note that some **FALSE** entries are bio-physical necessities, whereas some 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 physically and logically impossible to measure the precipitation of a species, and so this **FALSE** is necessarily **FALSE**.

2 Subscripting data lists

This structure relating variables and dimensions of replication, allows us to manipulate multiple variables simultaneously. In particular, **multitable** makes it possible to extract pieces of a data list while maintaining its structure. 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.

```
> 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
```


	2008	2009
midlatitude	0	0
subtropical	0	0
tropical	0	0
equatorial	0	0
arctic	0	0
subarctic	0	0

Replicated along: || sites || years || species ||

temperature:

	2008	2009
midlatitude	10	NA
subtropical	20	25
tropical	50	48
equatorial	30	50
arctic	-30	-37
subarctic	0	3

Replicated along: || sites || years ||

precipitation:

	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	moss	vampire
140	NA	190

Replicated along: || species ||

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:
```

```
  sites  years species
    6      2      3
```

This command returns the same data list of variables but without the data from 1537. In particular, for every variable replicated along the **years** dimension is subscripted appropriately. As another example, perhaps we want all of the data on the first species (i.e. capybara) in 1537 for the first three sites.

```
> fake.community[1:3, "1537", 1]
```

```
abundance:
```

```
-----
```

```
, , capybara
```

```

              1537
midlatitude    0
subtropical    0
tropical       0
```

```
Replicated along:  || sites || years || species ||
```

```
temperature:
```

```
-----
```

```

              1537
midlatitude    NA
subtropical    NA
tropical       NA
```

```
Replicated along:  || sites || years ||
```

```
precipitation:
```

```
-----
```

```

              1537
midlatitude    NA
```

```
subtropical    NA
tropical       NA
Replicated along:  || sites || years ||
```

```
body.size:
-----
capybara
      140
Replicated along:  || species ||
```

```
metabolic.rate:
-----
capybara
      20
Replicated along:  || species ||
```

```
homeotherm:
-----
capybara
      Y
Levels: N Y
Replicated along:  || species ||
```

```
REPLICATION DIMENSIONS:
  sites  years species
    3      1      1
```

Notice also that for each different subset of the data, the new replication dimensions are printed after the data.

3 Simple analysis functions

Data lists can be passed ‘as is’ to many standard functions in R that normally take data frames. In the next section I will define this class of functions in more detail, but for now consider this simple example. Perhaps we want to explore whether the interaction between body size and temperature has an influence on abundance. As a first attempt at model building, we fit a linear model using `lm`.

```
> lm(abundance ~ (body.size * temperature), data = fake.community)
```

Call:

```
lm(formula = abundance ~ (body.size * temperature), data = fake.community)
```

```

Coefficients:
      (Intercept)          body.size      temperature  body.size:temperature
      5.9804492        -0.0314760         0.1728702        -0.0009098

```

And this works just as well with mixtures of categorical and numerical data.

```
> lm(abundance ~ -1 + (homeotherm * temperature), data = fake.community)
```

Call:

```
lm(formula = abundance ~ -1 + (homeotherm * temperature), data = fake.community)
```

```

Coefficients:
      homeothermN      homeothermY      temperature
      1.008253        1.573802         0.002421
homeothermY:temperature
      0.043071

```

It also works with other ‘simple’ functions, such as `rlm` (robust linear model) in the `MASS` package.

```

> library(MASS)
> rlm(abundance ~ (body.size * temperature), data = fake.community)

```

Call:

```

rlm(formula = abundance ~ (body.size * temperature), data = fake.community)
Converged in 17 iterations

```

```

Coefficients:
      (Intercept)          body.size      temperature  body.size:temperature
      8.327288e-04        -4.382783e-06         2.775763e-05        -1.460928e-07

```

```

Degrees of freedom: 22 total; 18 residual
(32 observations deleted due to missingness)
Scale estimate: 5.92e-15

```

Therefore, in many cases, data lists enter the standard R workflow in exactly the same manner as data frames.

4 Coercing data lists to data frames

The reason that unmodified data lists can be passed to some functions that are expecting data frames, is that these functions try to coerce whatever data object they receive into a data frame. When the `multitable` package is loaded, these functions can find a method for making such a conversion. This method can be accessed by users directly via the `as.data.frame` function from the R base package. For example, we can pass the `fake.community` data to `as.data.frame`.

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

	abundance	temperature	precipitation	body.size	metabolic.rate
midlatitude.2009.capybara	4	NA	NA	140	20
subtropical.2009.capybara	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
tropical.2009.moss	9	48	149	NA	5
equatorial.2009.moss	0	50	199	NA	5
arctic.2009.moss	5	-37	21	NA	5
subarctic.2009.moss	0	3	41	NA	5
midlatitude.2008.moss	6	10	20	NA	5
subtropical.2008.moss	0	20	100	NA	5
tropical.2008.moss	0	50	150	NA	5
equatorial.2008.moss	3	30	200	NA	5
arctic.2008.moss	0	-30	20	NA	5
subarctic.2008.moss	0	0	40	NA	5
midlatitude.1537.moss	0	NA	NA	NA	5
subtropical.1537.moss	0	NA	NA	NA	5
tropical.1537.moss	0	NA	NA	NA	5
equatorial.1537.moss	0	NA	NA	NA	5
arctic.1537.moss	0	NA	NA	NA	5
subarctic.1537.moss	0	NA	NA	NA	5
midlatitude.2009.vampire	0	NA	NA	190	0
subtropical.2009.vampire	0	25	99	190	0
tropical.2009.vampire	0	48	149	190	0
equatorial.2009.vampire	0	50	199	190	0
arctic.2009.vampire	0	-37	21	190	0
subarctic.2009.vampire	0	3	41	190	0
midlatitude.2008.vampire	0	10	20	190	0

subtropical.2008.vampire	0	20	100	190	0
tropical.2008.vampire	0	50	150	190	0
equatorial.2008.vampire	0	30	200	190	0
arctic.2008.vampire	0	-30	20	190	0
subarctic.2008.vampire	0	0	40	190	0
midlatitude.1537.vampire	0	NA	NA	190	0
subtropical.1537.vampire	1	NA	NA	190	0
tropical.1537.vampire	0	NA	NA	190	0
equatorial.1537.vampire	0	NA	NA	190	0
arctic.1537.vampire	0	NA	NA	190	0
subarctic.1537.vampire	0	NA	NA	190	0
homeotherm					
midlatitude.2009.capybara	Y				
subtropical.2009.capybara	Y				
tropical.2009.capybara	Y				
equatorial.2009.capybara	Y				
arctic.2009.capybara	Y				
subarctic.2009.capybara	Y				
midlatitude.2008.capybara	Y				
subtropical.2008.capybara	Y				
tropical.2008.capybara	Y				
equatorial.2008.capybara	Y				
arctic.2008.capybara	Y				
subarctic.2008.capybara	Y				
midlatitude.1537.capybara	Y				
subtropical.1537.capybara	Y				
tropical.1537.capybara	Y				
equatorial.1537.capybara	Y				
arctic.1537.capybara	Y				
subarctic.1537.capybara	Y				
midlatitude.2009.moss	N				
subtropical.2009.moss	N				
tropical.2009.moss	N				
equatorial.2009.moss	N				
arctic.2009.moss	N				
subarctic.2009.moss	N				
midlatitude.2008.moss	N				
subtropical.2008.moss	N				
tropical.2008.moss	N				
equatorial.2008.moss	N				
arctic.2008.moss	N				
subarctic.2008.moss	N				
midlatitude.1537.moss	N				
subtropical.1537.moss	N				
tropical.1537.moss	N				
equatorial.1537.moss	N				

arctic.1537.moss	N
subarctic.1537.moss	N
midlatitude.2009.vampire	N
subtropical.2009.vampire	N
tropical.2009.vampire	N
equatorial.2009.vampire	N
arctic.2009.vampire	N
subarctic.2009.vampire	N
midlatitude.2008.vampire	N
subtropical.2008.vampire	N
tropical.2008.vampire	N
equatorial.2008.vampire	N
arctic.2008.vampire	N
subarctic.2008.vampire	N
midlatitude.1537.vampire	N
subtropical.1537.vampire	N
tropical.1537.vampire	N
equatorial.1537.vampire	N
arctic.1537.vampire	N
subarctic.1537.vampire	N

5 Theory

Data lists are based on a distinction between

The `multitable` package coerce multiple-table data into a single data frame?

This model of data organization is made possible by new objects, called data lists. These data list objects organize and relate data from multiple tables, which were stored in multiple text-based data files. Once in data list form, handling multiple-table data is much like handling single-table data in data frames; in fact data lists are much like the data frames that you have come to love!

Like data lists

6 Reading multiple data files into a data list

7 Manipulating data lists

8 Simple analyses with data lists

9 Coercing data lists to data frames