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Tools for Applied Statistics – the doBy Package

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Abstract

Keywords: .

1. Introduction

2. Introduction

The **doBy** package, (Højsgaard and Halekoh 2012) for R, (R Development Core Team 2012) contains a variety of utility functions. The package grew out of many years of work in biostatistics; in particular in agricultural sciences. This paper describes some of the functions in **doBy**. **FiXme Note: May want to mention a few other utility packages on CRAN.**

3. Data used for illustration

The description of the `doBy` package is based on the following datasets.

CO2 data The `CO2` data frame comes from an experiment on the cold tolerance of the grass species *Echinochloa crus-galli*. To limit the amount of output we modify names and levels of variables as follows

```
R> data(CO2)
R> CO2 <- transform(CO2, Treat=Treatment, Treatment=NULL)
R> levels(CO2$Treat) <- c("nchil","chil")
R> levels(CO2$Type)  <- c("Que","Mis")
```

```
R> CO2 <- subset(CO2, Plant %in% c("Qn1", "Qc1", "Mn1", "Mc1"))
R> head(CO2)
```

```
  Plant Type conc uptake Treat
1   Qn1  Que   95   16.0 nchil
2   Qn1  Que  175   30.4 nchil
3   Qn1  Que  250   34.8 nchil
4   Qn1  Que  350   37.2 nchil
5   Qn1  Que  500   35.3 nchil
6   Qn1  Que  675   39.2 nchil
```

Airquality data The `airquality` dataset contains air quality measurements in New York, May to September 1973. The months are coded as $5, \ldots, 9$. To limit the output we only consider data for two months:

```
R> airquality <- subset(airquality, Month %in% c(5,6))
R> head(airquality)
```

```
  Ozone Solar.R Wind Temp Month Day
1    41     190  7.4   67     5   1
2    36     118  8.0   72     5   2
3    12     149 12.6   74     5   3
4    18     313 11.5   62     5   4
5    NA      NA 14.3   56     5   5
6    28      NA 14.9   66     5   6
```

4. Working with groupwise data

4.1. Univariate summary statistics – The `summaryBy()` function

The `summaryBy()` function is used for calculating quantities like "the mean and variance of x and y for each combination of two factors A and B". Examples are based on the `CO2` data.

Basic usage

For example, the mean and variance of `uptake` and `conc` for each value of `Plant` is obtained by:

```
R> myfun1 <- function(x){c(m=mean(x), s=sd(x), sem=sd(x)/length(x))}
R> summaryBy(conc + uptake ~ Plant, data=CO2, FUN=myfun1)
```

```
  Plant conc.m conc.s conc.sem uptake.m uptake.s uptake.sem
1   Qn1    435  317.7    45.39    33.23    8.215     1.1735
2   Qc1    435  317.7    45.39    29.97    8.335     1.1907
3   Mn1    435  317.7    45.39    26.40    8.694     1.2420
4   Mc1    435  317.7    45.39    18.00    4.119     0.5884
```

Defining the function to return named values as above is the recommended use of `summaryBy()`. Note that the values returned by the function has been named as `m` and `s`.

If the result of the function(s) are not named, then the names in the output data in general become less intuitive:

```
R> myfun2 <- function(x){c(mean(x), var(x), sd(x)/length(x))}
R> summaryBy(conc + uptake ~ Plant, data=CO2, FUN=myfun2)

  Plant conc.FUN1 conc.FUN2 conc.FUN3 uptake.FUN1 uptake.FUN2
1   Qn1       435    100950     45.39       33.23       67.48
2   Qc1       435    100950     45.39       29.97       69.47
3   Mn1       435    100950     45.39       26.40       75.59
4   Mc1       435    100950     45.39       18.00       16.96
  uptake.FUN3
1      1.1735
2      1.1907
3      1.2420
4      0.5884
```

Using predefined functions

It is possible use a vector of predefined functions. For example

```
R> sem <- function(x){sd(x)/length(x)}
R> summaryBy(uptake~Plant, data=CO2, FUN=list(mean,sd,sem,N=length))

  Plant uptake.mean uptake.sd uptake.sem uptake.length
1   Qn1       33.23     8.215     1.1735             7
2   Qc1       29.97     8.335     1.1907             7
3   Mn1       26.40     8.694     1.2420             7
4   Mc1       18.00     4.119     0.5884             7
```

The naming of the output variables determined from what the functions returns. The names of the last two columns above are imposed by `summaryBy()` because `myfun2` does not return named values.

Copying variables out with the `id` *argument*

To get the value of the `Type` and `Treat` in the first row of the groups (defined by the values of `Plant`) copied to the output dataframe we use the `id` argument: as:

```
R> summaryBy(conc+uptake~Plant, data=CO2, FUN=myfun1, id=~Type+Treat)

  Plant conc.m conc.s conc.sem uptake.m uptake.s uptake.sem Type
1   Qn1    435  317.7    45.39    33.23    8.215     1.1735  Que
2   Qc1    435  317.7    45.39    29.97    8.335     1.1907  Que
3   Mn1    435  317.7    45.39    26.40    8.694     1.2420  Mis
```

```
4   Mc1    435  317.7    45.39    18.00    4.119     0.5884  Mis
  Treat
1 nchil
2  chil
3 nchil
4  chil
```

Statistics on functions of data

We may want to calculate the mean and variance for the logarithm of `uptake`, for `uptake/conc` and for `uptake` and `conc`. This can be achieved as:

```
R> summaryBy(log(uptake)+I(conc/uptake)+ conc+uptake~Plant, data=CO2,
+  FUN=myfun1)

  Plant log(uptake).m log(uptake).s log(uptake).sem conc/uptake.m
1   Qn1         3.467        0.3189         0.04555         12.12
2   Qc1         3.356        0.3446         0.04922         13.23
3   Mn1         3.209        0.4234         0.06049         14.92
4   Mc1         2.864        0.2622         0.03746         22.12
  conc/uptake.s conc/uptake.sem conc.m conc.s conc.sem uptake.m
1         7.204           1.029    435  317.7    45.39    33.23
2         7.195           1.028    435  317.7    45.39    29.97
3         7.312           1.045    435  317.7    45.39    26.40
4        12.883           1.840    435  317.7    45.39    18.00
  uptake.s uptake.sem
1    8.215     1.1735
2    8.335     1.1907
3    8.694     1.2420
4    4.119     0.5884
```

If one does not want output variables to contain parentheses then setting `p2d=TRUE` causes the parentheses to be replaced by dots (“.”).

Using '.' ans '1' in the specifications

It is possible to use the dot (”.”) on the left hand side of the formula. The dot means ”all numerical variables which do not appear elsewhere” (i.e. on the right hand side of the formula and in the `id` statement):

```
R> summaryBy(log(uptake) + I(conc/uptake) + . ~Plant, data=CO2, FUN=myfun1)

  Plant log(uptake).m log(uptake).s log(uptake).sem conc/uptake.m
1   Qn1         3.467        0.3189         0.04555         12.12
2   Qc1         3.356        0.3446         0.04922         13.23
3   Mn1         3.209        0.4234         0.06049         14.92
4   Mc1         2.864        0.2622         0.03746         22.12
```

```
  conc/uptake.s conc/uptake.sem conc.m conc.s conc.sem uptake.m
1         7.204           1.029    435  317.7    45.39    33.23
2         7.195           1.028    435  317.7    45.39    29.97
3         7.312           1.045    435  317.7    45.39    26.40
4        12.883           1.840    435  317.7    45.39    18.00
  uptake.s uptake.sem
1    8.215     1.1735
2    8.335     1.1907
3    8.694     1.2420
4    4.119     0.5884
```

The dot (".") can also be used on the right hand side of the formula where it refers to "all non–numerical variables which are not specified elsewhere":

```
R> summaryBy(log(uptake) ~ Plant + ., data=CO2, FUN=myfun1)
```

```
  Plant Type Treat log(uptake).m log(uptake).s log(uptake).sem
1   Qn1  Que nchil         3.467        0.3189         0.04555
2   Qc1  Que  chil         3.356        0.3446         0.04922
3   Mn1  Mis nchil         3.209        0.4234         0.06049
4   Mc1  Mis  chil         2.864        0.2622         0.03746
```

Using 1 on the right hand side means no grouping:

```
R> summaryBy(log(uptake) ~ 1, data=CO2, FUN=myfun1)
```

```
  log(uptake).m log(uptake).s log(uptake).sem
1         3.224        0.3971         0.01418
```

FiXme Note: Should be possible to supply first argument as a list

Preserving names of variables using `keep.names`

If the function applied to data only returns one value, it is possible to force that the summary variables retain the original names by setting `keep.names=TRUE`. A typical use of this could be

```
R> summaryBy(conc+uptake+log(uptake)~Plant,
+  data=CO2, FUN=mean, id=~Type+Treat, keep.names=TRUE)
```

```
  Plant conc uptake log(uptake) Type Treat
1   Qn1  435  33.23       3.467  Que nchil
2   Qc1  435  29.97       3.356  Que  chil
3   Mn1  435  26.40       3.209  Mis nchil
4   Mc1  435  18.00       2.864  Mis  chil
```

4.2. The `orderBy()` function

Ordering (or sorting) a data frame is possible with the `orderBy()` function. Suppose we want to order the rows of the the `airquality` data by `Temp` (in decreasing order) and by `Month` (within `Temp`). This can be achieved by:

```
R> x <- orderBy(~ -Temp + Month, data=airquality)
R> head(x)
```

```
   Ozone Solar.R Wind Temp Month Day
42    NA     259 10.9   93     6  11
43    NA     250  9.2   92     6  12
40    71     291 13.8   90     6   9
39    NA     273  6.9   87     6   8
41    39     323 11.5   87     6  10
36    NA     220  8.6   85     6   5
```

4.3. The `splitBy()` function

Suppose we want to split the `airquality` data into a list of dataframes with one dataframe for every half month. This can be achieved by:

```
R> airquality <- transform(airquality, wim=Day>15)
R> ss<-splitBy(~Month + wim, data=airquality)
R> ss
```

```
  listentry Month   wim
1   5|FALSE     5 FALSE
2    5|TRUE     5  TRUE
3   6|FALSE     6 FALSE
4    6|TRUE     6  TRUE
```

Hence for month 5, the relevant entry-name in the list is '5' and this part of data can be extracted as

```
R> ss[['5|FALSE']]
```

Information about the grouping is stored as a dataframe in an attribute called `groupid` and can be retrieved with:

```
R> attr(ss,"groupid")
```

```
  Month   wim
1     5 FALSE
2     5  TRUE
3     6 FALSE
4     6  TRUE
```

FiXme Note: listentry er dumt navn. forklar også at resultatet er en liste...

4.4. The `subsetBy()` function

Suppose we want to select those rows within each month for which the the wind speed is larger than the mean wind speed (within the month). This is achieved by:

```
R> subsetBy(~Month, subset=Wind > mean(Wind), data=airquality)
```

Note that the statement `Wind > mean(Wind)` is evaluated within each month.

4.5. The `transformBy` function

The `transformBy` function is analogous to the `transform` function except that it works within groups. For example:

```
R> zz<- transformBy(~Month, data=airquality, minW=min(Wind), maxW=max(Wind),
+       chg=sum(range(Wind)*c(-1,1)))
R> head(zz)
```

```
    Ozone Solar.R Wind Temp Month Day   wim minW maxW  chg
5.1    41     190  7.4   67     5   1 FALSE  5.7 20.1 14.4
5.2    36     118  8.0   72     5   2 FALSE  5.7 20.1 14.4
5.3    12     149 12.6   74     5   3 FALSE  5.7 20.1 14.4
5.4    18     313 11.5   62     5   4 FALSE  5.7 20.1 14.4
5.5    NA      NA 14.3   56     5   5 FALSE  5.7 20.1 14.4
5.6    28      NA 14.9   66     5   6 FALSE  5.7 20.1 14.4
```

4.6. The `lapplyBy()` function

The `lapplyBy()` function is a wrapper for first splitting data into a list according to the formula (using `splitBy()`) and then applying a function to each element of the list (using `apply()`). Consider the `CO2` data. Suppose that for each plant we want to find the change in `uptake` per change in `conc`:

```
R> CO2 <- orderBy(~Plant + conc, data=CO2)
R> vv <- lapplyBy(~ Plant, data=CO2,
+                 FUN = function(x){c(NA, diff(x$uptake) / diff(x$conc))})
R> str(vv)
```

```
List of 4
 $ Qn1: num [1:7] NA 0.18 0.0587 0.024 -0.0127 ...
 $ Qc1: num [1:7] NA 0.1238 0.0827 0.043 -0.014 ...
 $ Mn1: num [1:7] NA 0.1075 0.0933 0.038 0.006 ...
 $ Mc1: num [1:7] NA 0.055 0.0427 0.008 0.004 ...
```

4.7. The `sampleBy()` function

Suppose we want a random sample of 50 % of the observations from a dataframe. This can be achieved with:

```
R> sampleBy(~1, frac=0.5, data=airquality)
```

Suppose instead that we want a systematic sample of every fifth observation within each month. This is achieved with:

```
R> sampleBy(~Month, frac=0.2, data=airquality,systematic=T)
```

5. Miscellaneous

5.1. The `firstobs()` / `lastobs()` function

To obtain the indices of the first/last occurences of an item in a vector do:

```
R> x <- c(1,1,1,2,2,2,1,1,1,3)
R> firstobs(x)

[1]  1  4 10

R> lastobs(x)

[1]  6  9 10
```

The same can be done on a data frame, e.g.

```
R> firstobs(~Plant, data=CO2)

[1]  1  8 15 22

R> lastobs(~Plant, data=CO2)

[1]  7 14 21 28
```

5.2. The `which.maxn()` and `which.minn()` functions

The location of the n largest / smallest entries in a numeric vector can be obtained with

```
R> x <- c(1:4,0:5,11,NA,NA)
R> which.maxn(x,3)

[1] 11 10  4
```

```
R> which.minn(x,5)

[1] 5 1 6 2 7
```

5.3. Subsequences - subSeq()

Find (sub) sequences in a vector:

```
R> x <- c(1,1,2,2,2,1,1,3,3,3,3,1,1,1)
R> subSeq(x)

  first last slength midpoint value
1     1    2       2        2     1
2     3    5       3        4     2
3     6    7       2        7     1
4     8   11       4       10     3
5    12   14       3       13     1

R> subSeq(x, item=1)

  first last slength midpoint value
1     1    2       2        2     1
2     6    7       2        7     1
3    12   14       3       13     1

R> subSeq(letters[x])

  first last slength midpoint value
1     1    2       2        2     a
2     3    5       3        4     b
3     6    7       2        7     a
4     8   11       4       10     c
5    12   14       3       13     a

R> subSeq(letters[x],item="a")

  first last slength midpoint value
1     1    2       2        2     a
2     6    7       2        7     a
3    12   14       3       13     a
```

5.4. Recoding values of a vector - recodeVar()

```
R> x <- c("dec","jan","feb","mar","apr","may")
R> src1 <- list(c("dec","jan","feb"), c("mar","apr","may"))
R> tgt1 <- list("winter","spring")
R> recodeVar(x,src=src1,tgt=tgt1)

[1] "winter" "winter" "winter" "spring" "spring" "spring"
```

5.5. Renaming columns of a dataframe or matrix – `renameCol()`

```
R> head(renameCol(CO2, 1:2, c("kk","ll")))

   kk  ll conc uptake Treat
1 Qn1 Que   95   16.0 nchil
2 Qn1 Que  175   30.4 nchil
3 Qn1 Que  250   34.8 nchil
4 Qn1 Que  350   37.2 nchil
5 Qn1 Que  500   35.3 nchil
6 Qn1 Que  675   39.2 nchil

R> head(renameCol(CO2, c("Plant","Type"), c("kk","ll")))

   kk  ll conc uptake Treat
1 Qn1 Que   95   16.0 nchil
2 Qn1 Que  175   30.4 nchil
3 Qn1 Que  250   34.8 nchil
4 Qn1 Que  350   37.2 nchil
5 Qn1 Que  500   35.3 nchil
6 Qn1 Que  675   39.2 nchil
```

5.6. Time since an event - `timeSinceEvent()`

Consider the vectors

```
R> yvar <- c(0,0,1,0,0,0,0,0,1,0,0,0,1,1,0,0,0)
R> (tvar <- seq_along(yvar) + c(0.1,0.2))

 [1]  1.1  2.2  3.1  4.2  5.1  6.2  7.1  8.2  9.1 10.2 11.1 12.2 13.1
[14] 14.2 15.1 16.2 17.1
```

Imagine that a non–zero element in `yvar` indicates an event which takes place at the corresponding time point in `tvar` (which by default is assumed to contain equidistant values)

Now we find time since event as

```
R> tse<- timeSinceEvent(yvar,tvar)
```

```
   yvar tvar abs.tse sign.tse ewin run tae  tbe
1     0  1.1     2.0     -2.0    1  NA  NA -2.0
2     0  2.2     0.9     -0.9    1  NA  NA -0.9
3     1  3.1     0.0      0.0    1   1 0.0  0.0
4     0  4.2     1.1      1.1    1   1 1.1 -4.9
5     0  5.1     2.0      2.0    1   1 2.0 -4.0
6     0  6.2     2.9     -2.9    2   1 3.1 -2.9
7     0  7.1     2.0     -2.0    2   1 4.0 -2.0
8     0  8.2     0.9     -0.9    2   1 5.1 -0.9
9     1  9.1     0.0      0.0    2   2 0.0  0.0
10    0 10.2     1.1      1.1    2   2 1.1 -2.9
11    0 11.1     2.0      2.0    2   2 2.0 -2.0
12    0 12.2     0.9     -0.9    3   2 3.1 -0.9
13    1 13.1     0.0      0.0    3   3 0.0  0.0
14    1 14.2     0.0      0.0    4   4 0.0  0.0
15    0 15.1     0.9      0.9    4   4 0.9   NA
16    0 16.2     2.0      2.0    4   4 2.0   NA
17    0 17.1     2.9      2.9    4   4 2.9   NA
```

The output reads as follows:

- `abs.tse` and `sign.tse`: Absolute and signed time since (nearest) event.
- `ewin`: Event window: Gives a symmetric window around each event. **FiXme Note: ewin beregnes forkert**
- `run`: The value of `run` is set to 1 when the first event occurs and is increased by 1 at each subsequent event.
- `tae` and `tbe`: Time after and before event.

We may now find times for which time since an event is at most 1 as

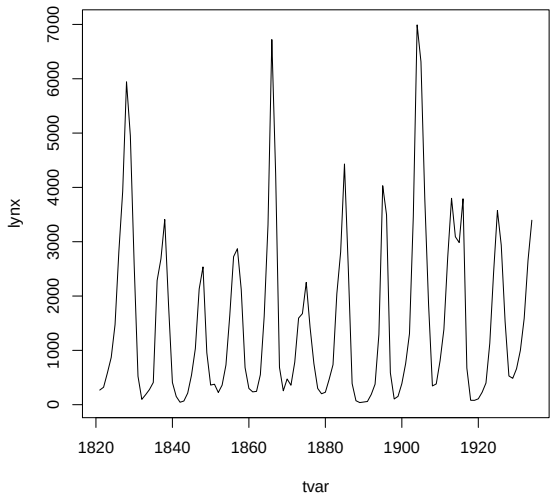
```
R> tse$tvar[tse$abs.tse<=1]
```

```
[1]  2.2  3.1  8.2  9.1 12.2 13.1 14.2 15.1
```

5.7. Example: Using `subSeq()` and `timeSinceEvent()`

Consider the `lynx` data:

```
R> lynx <- as.numeric(lynx)
R> tvar <- 1821:1934
R> plot(tvar,lynx,type='l')
```



Suppose we want to estimate the cycle lengths. One way of doing this is as follows:

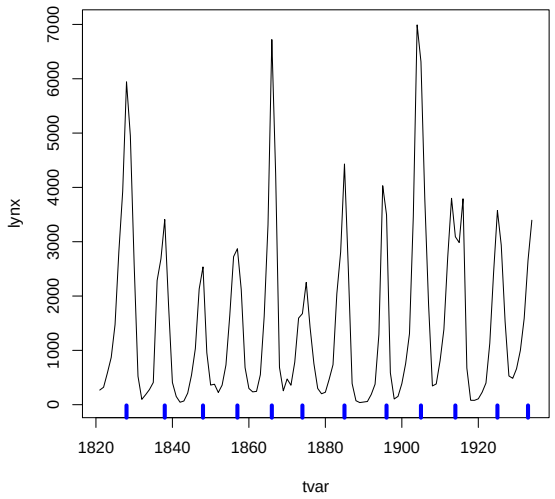
```
R> yyy <- lynx>mean(lynx)
R> head(yyy)
```

```
[1] FALSE FALSE FALSE FALSE FALSE  TRUE
```

```
R> (sss <- subSeq(yyy,item=TRUE))
```

```
   first last slength midpoint value
1      6   10       5        8  TRUE
2     16   19       4       18  TRUE
3     27   28       2       28  TRUE
4     35   38       4       37  TRUE
5     44   47       4       46  TRUE
6     53   55       3       54  TRUE
7     63   66       4       65  TRUE
8     75   76       2       76  TRUE
9     83   87       5       85  TRUE
10    92   96       5       94  TRUE
11   104  106       3      105  TRUE
12   112  114       3      113  TRUE
```

```
R> plot(tvar,lynx,type='l')
R> rug(tvar[sss$midpoint],col='blue',lwd=4)
```



Create the 'event vector'

```
R> yvar <- rep(0,length(lynx))
R> yvar[sss$midpoint] <- 1
R> tse <- timeSinceEvent(yvar,tvar)
R> head(tse,20)
```

```
   yvar tvar abs.tse sign.tse ewin run tae tbe
1     0 1821       7       -7    1  NA  NA  -7
2     0 1822       6       -6    1  NA  NA  -6
3     0 1823       5       -5    1  NA  NA  -5
4     0 1824       4       -4    1  NA  NA  -4
5     0 1825       3       -3    1  NA  NA  -3
6     0 1826       2       -2    1  NA  NA  -2
7     0 1827       1       -1    1  NA  NA  -1
8     1 1828       0        0    1   1   0   0
9     0 1829       1        1    1   1   1  -9
10    0 1830       2        2    1   1   2  -8
11    0 1831       3        3    1   1   3  -7
12    0 1832       4        4    1   1   4  -6
13    0 1833       5        5    1   1   5  -5
14    0 1834       4       -4    2   1   6  -4
15    0 1835       3       -3    2   1   7  -3
16    0 1836       2       -2    2   1   8  -2
17    0 1837       1       -1    2   1   9  -1
18    1 1838       0        0    2   2   0   0
19    0 1839       1        1    2   2   1  -9
20    0 1840       2        2    2   2   2  -8
```

We get two different (not that different) estimates of period lengths:

```
R> len1 <- tapply(tse$ewin, tse$ewin, length)
```

```
 1  2  3  4  5  6  7  8  9 10 11 12
13 10  9  9  9  9 11 10  9 10 10  5
```

```
R> len2 <- tapply(tse$run,  tse$run, length)
```

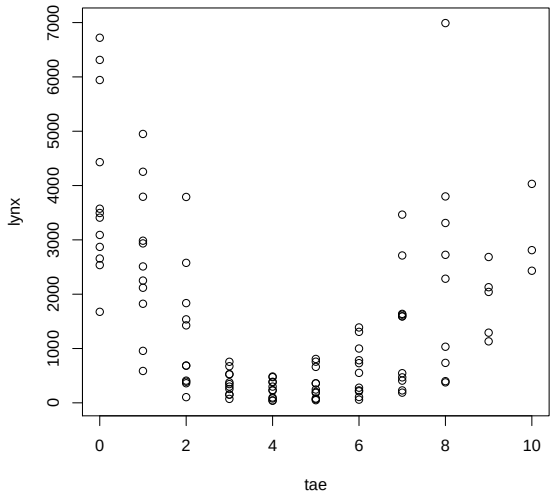
```
 1  2  3  4  5  6  7  8  9 10 11 12
10 10  9  9  8 11 11  9  9 11  8  2
```

```
R> c(median(len1),median(len2),mean(len1),mean(len2))
```

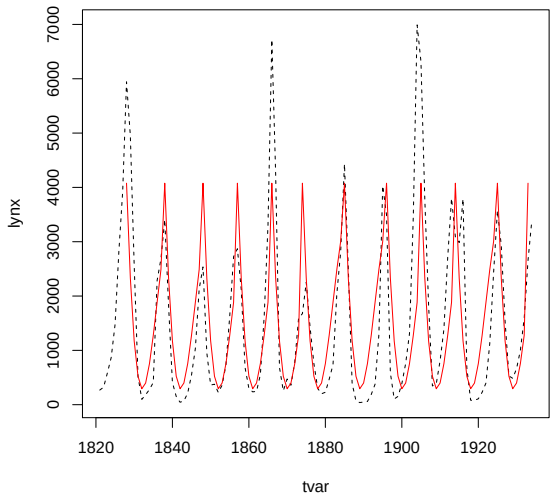
```
[1] 9.500 9.000 9.500 8.917
```

We can overlay the cycles as:

```
R> tse$lynx <- lynx
R> tse2 <- na.omit(tse)
R> plot(lynx~tae, data=tse2)
```




```
R> plot(tvar,lynx,type='l',lty=2)
R> mm <- lm(lynx~tae+I(tae^2)+I(tae^3), data=tse2)
R> lines(fitted(mm)~tvar, data=tse2, col='red')
```



5.8. The `esticon()` function

Consider a linear model which explains `Ozone` as a linear function of `Month` and `Wind`:

```
R> data(airquality)
R> airquality <- subset(airquality, Month %in% c(5,6,7))
R> airquality <- transform(airquality, Month=factor(Month))
R> m<-lm(Ozone ~ Month * Wind, data=airquality)
R> coefficients(m)
```

```
(Intercept)      Month6      Month7        Wind Month6:Wind
     50.748     -41.793      68.296      -2.368       4.051
Month7:Wind
     -4.663
```

When a parameter vector β of (systematic) effects have been estimated, interest is often in a particular estimable function, i.e. linear combination $\lambda^\top \beta$ and/or testing the hypothesis $H_0 : \lambda^\top \beta = \beta_0$ where λ is a specific vector defined by the user.

Suppose for example we want to calculate the expected difference in ozone between consequtive months at wind speed 10 mph (which is about the average wind speed over the whole period).

The `esticon` function provides a way of doing so. We can specify several λ vectors at the same time. For example

For a linear normal model, one would typically prefer to do a likelihood ratio test instead. However, for generalized estimating equations of glm–type (as dealt with in the packages **geepack** and **gee**) there is no likelihood. In this case `esticon` function provides an operational alternative.

Observe that another function for calculating contrasts as above is the `contrast` function in the **Design** package but it applies to a narrower range of models than `esticon` does.

6. Acknowledgements

Credit is due to Dennis Chabot, Gabor Grothendieck, Paul Murrell, Jim Robison-Cox and Erik Jørgensen for reporting various bugs and making various suggestions to the functionality in the **doBy** package.

7. A simulated dataset

Consider these data:

```
R> library(doBy)
R> dd <- expand.grid(A=factor(1:3),B=factor(1:3),C=factor(1:2))
R> dd$y <- rnorm(nrow(dd))
R> dd$x <- rnorm(nrow(dd))^2
R> dd$z <- rnorm(nrow(dd))
R> head(dd,10)
```

```
   A B C        y        x        z
1  1 1 1 -0.61706 0.413575 -1.07969
2  2 1 1 -0.24555 0.500546 -1.16123
3  3 1 1 -1.82130 0.887302 -0.54921
4  1 2 1  0.11152 0.089367  1.08098
5  2 2 1  0.13153 0.853216 -0.03592
6  3 2 1 -1.09549 0.003458  0.86814
7  1 3 1 -0.83327 0.092064  3.49082
8  2 3 1 -0.17350 0.658494  0.24181
9  3 3 1  1.15572 1.364387 -1.33347
10 1 1 2  0.02867 1.746930 -0.05263
```

Consider the additive model

$$y_i = \beta_0 + \beta^1_{A(i)} + \beta^2_{B(i)} + \beta^3_{C(i)} + e_i \tag{1}$$

where $e_i \sim N(0, \sigma^2)$. We fit this model:

```
R> mm <- lm(y~A+B+C, data=dd)
R> coef(mm)
```

```
(Intercept)          A2          A3          B2          B3
    -1.4421      0.9119      0.7429      0.5020      1.0404
         C2
     1.1759
```

Notice that the parameters corresponding to the factor levels `A1`, `B1` and `C2` are set to zero to ensure identifiability of the remaining parameters.

8. Linear functions of parameters, contrasts

For a regression model with parameters $\beta = (\beta^1, \beta^2, \ldots, \beta^P)$ we shall refer to a weighted sum of the form

$$\sum_j w_j \beta^j$$

as a contrast. Notice that it is common in the litterature to require that $sum_j w_j = 0$ for the sum $\sum_j w_j \beta^j$ to be called a contrast but we do not follow this tradition here.

The effect of changing the factor A from `A2` to `A3` can be found as

```
R> w <- c(0,-1,1,0,0,0)
R> sum(coef(mm)*w)

[1] -0.1691
```

The `esticon()` function provides this estimate, the standard error etc. as follows:

```
R> esticon(mm, w)

  beta0 Estimate Std.Error t.value DF Pr(>|t|)  Lower  Upper
1     0  -0.1691    0.4978 -0.3396 12     0.74 -1.254 0.9155
```

9. Population means

Population means (sometimes also called marginal means) are in some sciences much used for reporting marginal effects (to be described below). Population means are known as lsmeans in SAS jargon. Population means is a special kind of contrasts as defined in Section 8.

The model (1) is a model for the conditional mean $\mathbb{E}(y|A, B, C)$. Sometimes one is interested in quantities like $\mathbb{E}(y|A)$. This quantity can not formally be found unless B and C are random variables such that we may find $\mathbb{E}(y|A)$ by integration.

However, suppose that A is a treatment of main interest, B is a blocking factor and C represents days on which the experiment was carried out. Then it is tempting to average $\mathbb{E}(y|A, B, C)$ over B and C (average over block and day) and think of this average as $\mathbb{E}(y|A)$.

9.1. A brute–force calculation

The population mean for $A = 1$ is

$$\beta^0 + \beta^1_{A1} + \frac{1}{3}(\beta^2_{B1} + \beta^2_{B2} + \beta^2_{B3}) + \frac{1}{2}(\beta^3_{C1} + \beta^3_{C2}) \tag{2}$$

Recall that the parameters corresponding to the factor levels `A1`, `B1` and `C2` are set to zero to ensure identifiability of the remaining parameters. Therefore we may also write the population mean for $A = 1$ as

$$\beta^0 + \frac{1}{3}(\beta^2_{B2} + \beta^2_{B3}) + \frac{1}{2}(\beta^3_{C2}) \tag{3}$$

This quantity can be estimated as:

```
R> w <- c(1, 0, 0, 1/3, 1/3, 1/2)
R> coef(mm)*w

(Intercept)          A2          A3          B2          B3
    -1.4421      0.0000      0.0000      0.1673      0.3468
         C2
     0.5880

R> sum(coef(mm)*w)

[1] -0.34
```

We may find the population mean for all three levels of A as

```
R> W <- matrix(c(1, 0, 0, 1/3, 1/3, 1/2,
+                1, 1, 0, 1/3, 1/3, 1/2,
+                1, 0, 1, 1/3, 1/3, 1/2),nr=3, byrow=TRUE)
R> W

     [,1] [,2] [,3]   [,4]   [,5] [,6]
[1,]    1    0    0 0.3333 0.3333  0.5
[2,]    1    1    0 0.3333 0.3333  0.5
[3,]    1    0    1 0.3333 0.3333  0.5

R> W %*% coef(mm)

        [,1]
[1,] -0.3400
[2,]  0.5719
[3,]  0.4028
```

Notice that the matrix W is based on that the first level of A is set as the reference level. If the reference level is changed then so must W be.

9.2. Using `esticon()`

Given that one has specified W, the `esticon()` function in the `doBy` package be used for the calculations above and the function also provides standard errors, confidence limits etc:

```
R> esticon(mm, W)

  beta0 Estimate Std.Error t.value DF Pr(>|t|)  Lower  Upper
1     0  -0.3400     0.352  -0.966 12   0.3531 -1.107 0.4269
2     0   0.5719     0.352   1.625 12   0.1302 -0.195 1.3388
3     0   0.4028     0.352   1.145 12   0.2747 -0.364 1.1697
```

10. Using popMatrix() and popMeans()

Writing the matrix W is somewhat tedious and hence error prone. In addition, there is a potential risk of getting the wrong answer if the the reference level of a factor has been changed. The `popMatrix()` function provides an automated way of generating such matrices. The above `W` matrix is constructed by

```
R> pma <- popMatrix(mm,effect='A')
R> summary(pma)

     (Intercept) A2 A3     B2     B3  C2
[1,]           1  0  0 0.3333 0.3333 0.5
[2,]           1  1  0 0.3333 0.3333 0.5
[3,]           1  0  1 0.3333 0.3333 0.5
grid:
'data.frame':        3 obs. of  1 variable:
 $ A: chr  "1" "2" "3"
at:
 NULL
```

The `popMeans()` function is simply a wrapper around first a call to `popMatrix()` followed by a call to (by default) `esticon()`:

```
R> pme <- popMeans(mm, effect='A')
R> pme

  beta0 Estimate Std.Error t.value DF Pr(>|t|)  Lower  Upper A
1     0  -0.3400     0.352  -0.966 12   0.3531 -1.107 0.4269 1
2     0   0.5719     0.352   1.625 12   0.1302 -0.195 1.3388 2
3     0   0.4028     0.352   1.145 12   0.2747 -0.364 1.1697 3
```

More details about how the matrix was constructed is provided by the `summary()` function:

```
R> summary(pme)

  beta0 Estimate Std.Error t.value DF Pr(>|t|)  Lower  Upper A
1     0  -0.3400     0.352  -0.966 12   0.3531 -1.107 0.4269 1
2     0   0.5719     0.352   1.625 12   0.1302 -0.195 1.3388 2
3     0   0.4028     0.352   1.145 12   0.2747 -0.364 1.1697 3
Call:
NULL
Contrast matrix:
Length  Class   Mode
     0   NULL   NULL
```

The `effect` argument requires to calculate the population means for each level of A aggregating across the levels of the other variables in the data.

Likewise we may do:

```
R> popMatrix(mm,effect=c('A','C'))

     (Intercept) A2 A3     B2     B3 C2
[1,]           1  0  0 0.3333 0.3333  0
[2,]           1  1  0 0.3333 0.3333  0
[3,]           1  0  1 0.3333 0.3333  0
[4,]           1  0  0 0.3333 0.3333  1
[5,]           1  1  0 0.3333 0.3333  1
[6,]           1  0  1 0.3333 0.3333  1
```

This gives the matrix for calculating the estimate for each combination of `A` and `C` when averaging over `B`. Consequently

```
R> popMeans(mm)

  beta0 Estimate Std.Error t.value DF Pr(>|t|)   Lower  Upper
1     0   0.2116    0.2032   1.041 12   0.3183 -0.2312 0.6543
```

gives the "total average".

10.1. Using the `at` argument

We may be interested in finding the population means at all levels of A but only at $C = 1$. This is obtained by using the `at` argument:

```
R> popMatrix(mm,effect='A', at=list(C='1'))

     (Intercept) A2 A3     B2     B3 C2
[1,]           1  0  0 0.3333 0.3333  0
[2,]           1  1  0 0.3333 0.3333  0
[3,]           1  0  1 0.3333 0.3333  0
```

Notice here that average is only taken over B. Another way of creating the population means at all levels of (A, C) is therefore

```
R> popMatrix(mm,effect='A', at=list(C=c('1','2')))

     (Intercept) A2 A3     B2     B3 C2
[1,]           1  0  0 0.3333 0.3333  0
[2,]           1  1  0 0.3333 0.3333  0
[3,]           1  0  1 0.3333 0.3333  0
[4,]           1  0  0 0.3333 0.3333  1
[5,]           1  1  0 0.3333 0.3333  1
[6,]           1  0  1 0.3333 0.3333  1
```

We may have several variables in the `at` argument:

```
R> popMatrix(mm,effect='A', at=list(C=c('1','2'), B='1'))

     (Intercept) A2 A3 B2 B3 C2
[1,]           1  0  0  0  0  0
[2,]           1  1  0  0  0  0
[3,]           1  0  1  0  0  0
[4,]           1  0  0  0  0  1
[5,]           1  1  0  0  0  1
[6,]           1  0  1  0  0  1
```

10.2. Ambiguous specification when using the `effect` and `at` arguments

There is room for an ambiguous specification if a variable appears in both the `effect` and the `at` argument, such as

```
R> popMatrix(mm,effect=c('A','C'), at=list(C='1'))

     (Intercept) A2 A3     B2     B3 C2
[1,]           1  0  0 0.3333 0.3333  0
[2,]           1  1  0 0.3333 0.3333  0
[3,]           1  0  1 0.3333 0.3333  0
```

This ambiguity is due to the fact that the `effect` argument asks for the populations means at all levels of the variables but the `at` chooses only specific levels.

This ambiguity is resolved as follows: Any variable in the `at` argument is removed from the `effect` argument such as the statement above is equivalent to

```
R> popMatrix(mm,effect='A', at=list(C='1'))
```

10.3. Using covariates

Next consider the model where a covariate is included:

```
R> mm2 <- lm(y~A+B+C+C:x, data=dd)
R> coef(mm2)

(Intercept)          A2          A3          B2          B3
    -1.4475      0.4126      0.3106      0.6511      0.8274
         C2        C1:x        C2:x
     1.9525      0.6242     -0.5630
```

In this case we get

```
R> popMatrix(mm2,effect='A', at=list(C='1'))
```

```
     (Intercept) A2 A3     B2     B3 C2   C1:x C2:x
[1,]           1  0  0 0.3333 0.3333  0 0.6603    0
[2,]           1  1  0 0.3333 0.3333  0 0.6603    0
[3,]           1  0  1 0.3333 0.3333  0 0.6603    0
```

Above, x has been replaced by its average and that is the general rule for models including covariates. However we may use the `at` argument to ask for calculation of the population mean at some user-specified value of x, say 12:

```
R> popMatrix(mm2,effect='A', at=list(C='1',x=12))

     (Intercept) A2 A3     B2     B3 C2 C1:x C2:x
[1,]           1  0  0 0.3333 0.3333  0   12    0
[2,]           1  1  0 0.3333 0.3333  0   12    0
[3,]           1  0  1 0.3333 0.3333  0   12    0
```

10.4. Using transformed covariates

Next consider the model where a transformation of a covariate is included:

```
R> mm3 <- lm(y~A+B+C+C:log(x), data=dd)
R> coef(mm3)

(Intercept)          A2          A3          B2          B3
  -1.248531    0.792032    0.737053    0.664020    1.055321
         C2  C1:log(x)  C2:log(x)
   0.955725    0.152552   -0.008265
```

In this case we can not use `popMatrix()` (and hence `popMeans()` directly. Instead we have first to generate a new variable, say `log.x`, with `log.x`= $\log(x)$, in the data and then proceed as

```
R> dd <- transform(dd, log.x = log(x))
R> mm3 <- lm(y~A+B+C+C:log.x, data=dd)
R> popMatrix(mm3,effect='A', at=list(C='1'))

     (Intercept) A2 A3     B2     B3 C2 C1:log.x C2:log.x
[1,]           1  0  0 0.3333 0.3333  0   -1.267        0
[2,]           1  1  0 0.3333 0.3333  0   -1.267        0
[3,]           1  0  1 0.3333 0.3333  0   -1.267        0
```

11. The `engine` argument of `popMeans()`

The `popMatrix()`is a function to generate a linear tranformation matrix of the model parameters with emphasis on constructing such matrices for population means. `popMeans()` invokes

by default the `esticon()` function on this linear transformation matrix for calculating parameter estimates and confidecne intervals. A similar function to `esticon()` is the `glht` function of the `multcomp` package.

The `glht()` function can be chosen via the `engine` argument of `popMeans()`:

```
R>  library(multcomp)
R> g<-popMeans(mm,effect='A', at=list(C='1'),engine="glht")
R> g

         General Linear Hypotheses

Linear Hypotheses:
       Estimate
1 == 0  -0.9280
2 == 0  -0.0161
3 == 0  -0.1851
```

This allows to apply the methods available on the `glht` object like

```
R> summary(g,test=univariate())

         Simultaneous Tests for General Linear Hypotheses

Fit: lm(formula = y ~ A + B + C, data = dd)

Linear Hypotheses:
       Estimate Std. Error t value Pr(>|t|)
1 == 0  -0.9280     0.4064   -2.28    0.041 *
2 == 0  -0.0161     0.4064   -0.04    0.969
3 == 0  -0.1851     0.4064   -0.46    0.657
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
(Univariate p values reported)

R> confint(g,calpha=univariate_calpha())

         Simultaneous Confidence Intervals

Fit: lm(formula = y ~ A + B + C, data = dd)

Quantile = 2.179
95% confidence level


Linear Hypotheses:
       Estimate lwr     upr
```

```
1 == 0 -0.9280  -1.8135 -0.0424
2 == 0 -0.0161  -0.9016  0.8695
3 == 0 -0.1851  -1.0706  0.7004
```

which yield the same results as the `esticon()` function.
By default the functions will adjust the tests and confidence intervals for multiplicity

```
R> summary(g)

         Simultaneous Tests for General Linear Hypotheses

Fit: lm(formula = y ~ A + B + C, data = dd)

Linear Hypotheses:
       Estimate Std. Error t value Pr(>|t|)
1 == 0  -0.9280     0.4064   -2.28     0.11
2 == 0  -0.0161     0.4064   -0.04     1.00
3 == 0  -0.1851     0.4064   -0.46     0.95
(Adjusted p values reported -- single-step method)

R> confint(g)

         Simultaneous Confidence Intervals

Fit: lm(formula = y ~ A + B + C, data = dd)

Quantile = 2.732
95% family-wise confidence level


Linear Hypotheses:
       Estimate lwr     upr
1 == 0 -0.9280  -2.0383  0.1824
2 == 0 -0.0161  -1.1264  1.0943
3 == 0 -0.1851  -1.2954  0.9252
```

12. Discussion

13. Acknowledgements

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References

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