Sparse Model Matrices

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Introduction

Model matrices in the very widely used (generalized) linear models of statistics, (typically fit via lm() or glm() in R) are often practically sparse — whenever categorical predictors, factors in R, are used.

We show for a few classes of such linear models how to construct sparse model matrices using sparse matrix (S4) objects from the **Matrix** package, and typically *without* using dense matrices in intermediate steps.

1 One factor: $y \sim f1$

Let's start with an artifical small example:

```
> (ff <- factor(strsplit("statistics_is_a_task", "")[[1]], levels=c("_",letters)))
[1] s t a t i s t i c s _ i s _ a _ t a s k
Levels: _ a b c d e f g h i j k l m n o p q r s t u v w x y z
> factor(ff)  # drops the levels that do not occur
[1] s t a t i s t i c s _ i s _ a _ t a s k
Levels: _ a c i k s t
> f1 <- ff[, drop=TRUE] # the same, more transparently</pre>
```

and now assume a model

$$y_i = \mu + \alpha_{j(i)} + E_i,$$

for $i=1,\ldots,n=$ length(f1)= 20, and $\alpha_{j(i)}$ with a constraint such as $\sum_j \alpha_j=0$ ("sum") or $\alpha_1=0$ ("treatment") and j(i)=as.numeric(f1[i]) being the level number of the i-th observation. For such a "design", the model is only estimable if the levels c and k are merged, and

```
> levels(f1)[match(c("c","k"), levels(f1))] <- "ck"
> library(Matrix)
> Matrix(contrasts(f1)) # "treatment" contrasts by default -- level "_" = baseline
6 x 5 sparse Matrix of class "dgCMatrix"
    a ck i s t
    . . . . .
a 1 . . . .
ck . 1 . . .
```

```
i . . 1 . .
s . . 1 .
t . . . . 1
> Matrix(contrasts(C(f1, sum)))
6 x 5 sparse Matrix of class "dgCMatrix"
    1
    . 1 . . .
      . 1 .
ck
 -1 -1 -1 -1 -1
> Matrix(contrasts(C(f1, helmert)), sparse=TRUE) # S-plus default; much less sparse
6 x 5 sparse Matrix of class "dgCMatrix"
  -1 -1 -1 -1 -1
   1 -1 -1 -1 -1
      2 -1 -1 -1
  . . 3 -1 -1
    . . . 4 -1
where contrasts() is (conceptually) just one major ingredient in the well-known model.matrix() function
```

to build the linear model matrix X of so-called "dummy variables". Since 2007, the Matrix package has been providing coercion from a factor object to a sparseMatrix one to produce the transpose of the model matrix corresponding to a model with that factor as predictor (and no intercept):

```
> as(f1, "sparseMatrix")
6 x 20 sparse Matrix of class "dgCMatrix"
_ . . . . . . . . . . 1 . . 1 . 1 . . . .
a . . 1 . . . . . . . . . . . 1 . . 1 . .
s 1 . . . . 1 . . . 1 . . . . . . 1 .
 . 1 . 1 . . 1 . . . . . . . . . . 1 . . .
```

which is really almost the transpose of using the above sparsification of contrasts() (and arranging for nice printing),

```
> printSpMatrix( t( Matrix(contrasts(f1))[as.character(f1) ,] ),
          col.names=TRUE)
  statisticks_is_a_tasck
a . . 1 . . . . . . . . . . . 1 . . 1 .
ck . . . . . . . . 1 . . . . . . . . .
s 1 . . . . 1 . . . 1 . . . . .
```

and that is the same as the "sparsification" of model.matrix(), apart from the column names (here transposed),

```
> t( Matrix(model.matrix(~ O+ f1))) # model with*OUT* intercept
6 x 20 sparse Matrix of class "dgCMatrix"
. . 1 . . . . . . . . . . 1 . . 1 . .
f1s 1 . . . . 1 . . . 1 . . 1 . . . . . 1 .
f1t . 1 . 1 . . 1 . . . . . . . . . 1 . . .
A more realistic small example is the chickwts data set,
> str(chickwts)# a standard R data set, 71 x 2
'data.frame':
              71 obs. of 2 variables:
$ weight: num 179 160 136 227 217 168 108 124 143 140 ...
$ feed : Factor w/ 6 levels "casein", "horsebean", ...: 2 2 2 2 2 2 2 2 2 2 ...
> x.feed <- as(chickwts$feed, "sparseMatrix")</pre>
> x.feed[ , (1:72)[c(TRUE,FALSE,FALSE)]] ## every 3rd column:
6 x 24 sparse Matrix of class "dgCMatrix"
casein
      meatmeal . . . . . . . . . . . . . . . . . . 1 1 1 1 . . . .
      sovbean
```

2 One factor, one continuous: $y \sim f1 + x$

To create the model matrix for the case of one factor and one continuous predictor—called "analysis of covariance" in the historical literature— we can adopt the following simple scheme.

The final model matrix is the concatenation of:

- 1) create the sparse 0-1 matrix m1 from the f1 main-effect
- 2) the single row/column 'x' == 'x' main-effect
- 3) replacing the values 1 in $\mathtt{m10x}$ (the x-slot of the factor model matrix), by the values of x (our continuous predictor).

3 Two (or more) factors, main effects only: y \sim f1 + f2

Let us consider the warpbreaks data set of 54 observations,

```
> data(warpbreaks)# a standard R data set
> str(warpbreaks) # 2 x 3 (x 9) balanced two-way with 9 replicates:
```

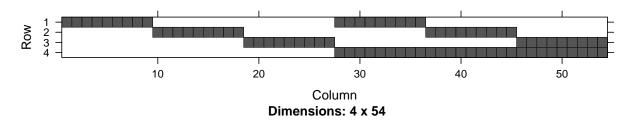
```
'data.frame': 54 obs. of 3 variables:
$ breaks : num 26 30 54 25 70 52 51 26 67 18 ...
$ wool : Factor w/ 2 levels "A", "B": 1 1 1 1 1 1 1 1 1 1 1 1 ...
$ tension: Factor w/ 3 levels "L", "M", "H": 1 1 1 1 1 1 1 1 1 1 2 ...
> xtabs(~ wool + tension, data = warpbreaks)

    tension
wool L M H
    A 9 9 9
    B 9 9 9
```

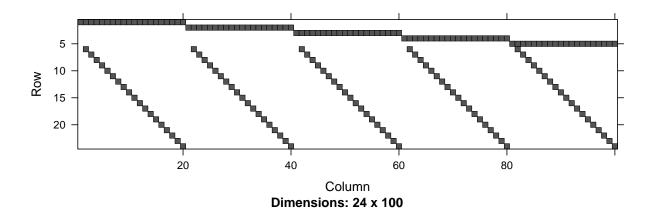
This example depicts how a model matrix would be built for the model breaks wool + tension. Since this is a main effects model (no interactions), the desired model matrix is simply the concatenation of the model matrices of the main effects. There are two here, but the principle applies to general main effects of factors.

The most sparse matrix is reached by *not* using an intercept, (which would give an all-1-column) but rather have one factor fully coded (aka "swallow" the intercept), and all others being at "treatment" contrast, i.e., here, the *transposed* model matrix, tmm, is

```
> tmm <- with(warpbreaks,
+ rBind(as(tension, "sparseMatrix"),
+ as(wool, "sparseMatrix")[-1,,drop=FALSE]))
> print( image(tmm) ) # print(.) the lattice object
```



The matrices are even sparser when the factors have more than just two or three levels, e.g., for the morley data set,



4 Interactions of two (or more) factors,.....

In situations with more than one factor, particularly with interactions, the model matrix is currently not directly available via **Matrix** functions — but we still show to build them carefully. The easiest—but not at memory resources efficient—way is to go via the dense model.matrix() result:

```
> data(npk, package="MASS")
> npk.mf <- model.frame(yield ~ block + N*P*K, data = npk)
> ## str(npk.mf) # the data frame + "terms" attribute
>
> m.npk <- model.matrix(attr(npk.mf, "terms"), data = npk)
> class(M.npk <- Matrix(m.npk))

[1] "dgCMatrix"
attr(,"package")
[1] "Matrix"
> dim(M.npk)# 24 x 13 sparse Matrix

[1] 24 13
> t(M.npk) # easier to display, column names readably displayed as row.names(t(.))
13 x 24 sparse Matrix of class "dgCMatrix"
```

```
block2
block3
     block4
block5
     block6
     N1
P1
     11...1.11...1.11...1.1.
K1
     1 . . 1 . 1 1 . . 1 . 1 . 1 1 . . . . 1 1 1 . 1 .
     . 1 . . . 1 . . . 1 . . . 1 . . . . . 1 . .
N1:P1
N1:K1
     . . . 1 . 1 . . . 1 . . . 1 . . . . 1 . 1 . . .
     1 . . . . 1 . . . 1 . . . 1 . . . . . 1 . . 1 .
P1:K1
N1:P1:K1
```

Another example was reported by a user on R-help (July 15, 2008, https://stat.ethz.ch/pipermail/r-help/2008-July/167772.html) about an "aov error with large data set".

'm looking to analyze a large data set: a within-Ss 2*2*1500 design with 20 Ss. However, aov() gives me an error.

And gave the following code example (slightly edited):

allocMatrix: too many elements specified

to which he got the explanation by Peter Dalgaard that the formal model matrix involved was much too large in this case, and that PD assumed, **lme4** would be able to solve the problem. However, currently there would still be a big problem with using **lme4**, because of the many levels of *fixed* effects:

Specifically¹,

```
dim(model.matrix( ~ a*b*d, data = aDat)) # 120'000 x 6000
```

where we note that $120'000 \times 6000 = 720$ mio, which is $720'000'000 * 8/2^{20} \approx 5500$ Megabytes.

Unfortunately **lme4** does not use a sparse X-matrix for the fixed effects (yet), it just uses sparse matrices for the Z-matrix of random effects and sparse matrix operations for computations related to Z.

Let us use a smaller factor d in order to investigate how sparse the X matrix would be:

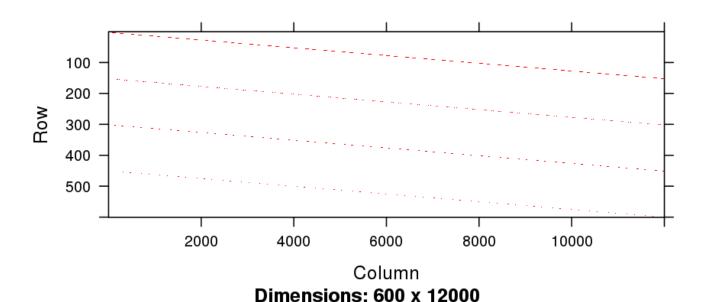
```
> d2 <- factor(1:150) # 10 times smaller
> tmp2 <- expand.grid(id=id, a=a, b=b, d=d2)
> dim(tmp2)
```

¹the following is not run in R on purpose, rather just displayed here

```
[1] 12000
> dim(mm <- model.matrix( ~ a*b*d, data=tmp2))</pre>
[1] 12000
            600
> ## is 100 times smaller than original example
> class(smm <- Matrix(mm)) # automatically coerced to sparse
[1] "dgCMatrix"
attr(,"package")
[1] "Matrix"
> round(object.size(mm) / object.size(smm), 1)
43 bytes
```

shows that even for the small d here, the memory reduction would be more than an order of magnitude.

> image(t(smm), aspect = 1/3, lwd=0, col.regions = "red")



and working with the sparse instead of the dense model matrix is considerably faster as well,

```
> x <- 1:600
> system.time(y <- smm %*% x) ## sparse is much faster
        system elapsed
  user
  0.001
          0.000
                  0.001
> system.time(y. <- mm %*\% x) ## than dense
```

```
user system elapsed 0.024 0.000 0.025
```

> identical(as.matrix(y), y.) ## TRUE

[1] TRUE

- > toLatex(sessionInfo())
 - R version 3.2.0 Patched (2015-05-29 r68442), x86_64-unknown-linux-gnu
 - Locale: LC_CTYPE=de_CH.UTF-8, LC_NUMERIC=C, LC_TIME=en_US.UTF-8, LC_COLLATE=C, LC_MONETARY=en_US.UTF-8, LC_MESSAGES=de_CH.UTF-8, LC_PAPER=de_CH.UTF-8, LC_NAME=C, LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=de_CH.UTF-8, LC_IDENTIFICATION=C
 - Base packages: base, datasets, grDevices, graphics, methods, stats, utils
 - Other packages: Matrix 1.2-1
 - Loaded via a namespace (and not attached): grid 3.2.0, lattice 0.20-31, tools 3.2.0