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, `factor`s 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
```

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  .  .  .  .
a   .  1  .  .  .
ck  .  .  1  .  .
i   .  .  .  1  .
s   .  .  .  .  1
t  -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
a   1 -1 -1 -1 -1
ck  .  2 -1 -1 -1
i   .  .  3 -1 -1
s   .  .  .  4 -1
t   .  .  .  .  5
```

where `contrasts()` is (conceptually) just one major ingredient in the well-known `model.matrix()` function to build the linear model matrix $\mathbf{X}$ 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 . .
ck . . . . . . . . 1 . . . . . . . . . . 1
i  . . . . 1 . . 1 . . . 1 . . . . . . . .
s  1 . . . . 1 . . . 1 . . 1 . . . . . 1 .
t  . 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)
```

```
   s t a t i s t i ck s _ i s _ a _ t a s ck
a  . . 1 . . . . .  . . . . . . 1 . . 1 .  .
ck . . . . . . . .  1 . . . . . . . . . .  1
i  . . . . 1 . . 1  . . . 1 . . . . . . .  .
s  1 . . . . 1 . .  . 1 . . 1 . . . . . 1  .
t  . 1 . 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(~ 0+ f1))) # model with*OUT* intercept

6 x 20 sparse Matrix of class "dgCMatrix"

f1_  . . . . . . . . . . 1 . . 1 . 1 . . . .
f1a  . . 1 . . . . . . . . . . . 1 . . 1 . .
f1ck . . . . . . . . 1 . . . . . . . . . . 1
f1i  . . . . 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")
> x.feed[ , (1:72)[c(TRUE,FALSE,FALSE)]] ## every  3rd  column:

6 x 24 sparse Matrix of class "dgCMatrix"

casein    . . . . . . . . . . . . . . . . . . . . . . . . 1 1 1 1
horsebean 1 1 1 1 . . . . . . . . . . . . . . . . . . . . . . . .
linseed   . . . . 1 1 1 1 . . . . . . . . . . . . . . . . . . . .
meatmeal  . . . . . . . . . . . . . . . . . . . . 1 1 1 1 . . . .
soybean   . . . . . . . . . 1 1 1 1 . . . . . . . . . . . . . . .
sunflower . . . . . . . . . . . . . 1 1 1 1 . . . . . . . . . . .

>
```

2 One factor, one continuous: `y ~ 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 `m1@x` (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 ~ 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:
```

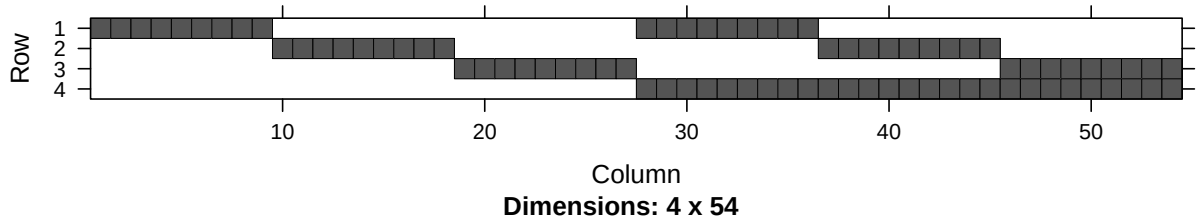
```
'data.frame':        54 obs. of  3 variables:
 $ breaks : num  26 30 54 25 70 52 51 26 67 18 ...
 $ wool   : Factor w/ 2 levels "A","B": 1 1 1 1 1 1 1 1 1 1 ...
 $ tension: Factor w/ 3 levels "L","M","H": 1 1 1 1 1 1 1 1 1 2 ...
```

```
> 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.

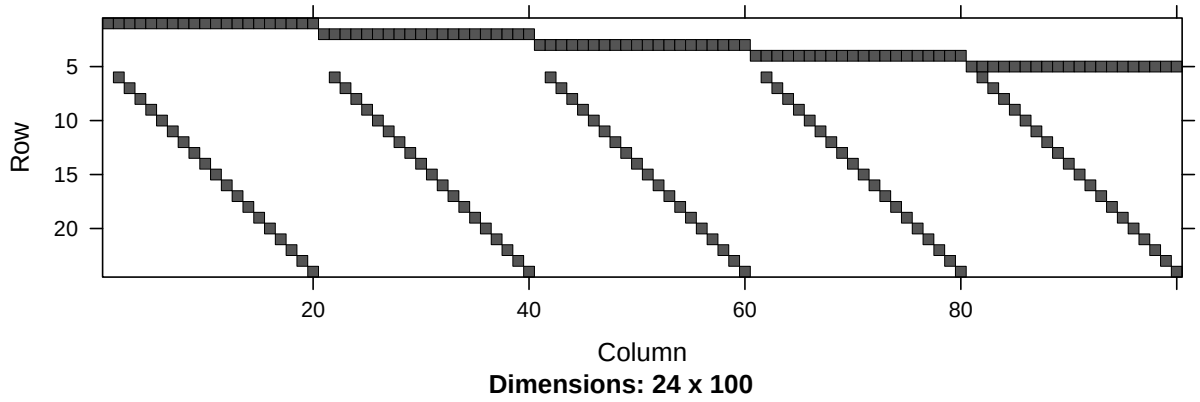
The most sparse matrix is reached by *not* using an intercept, (which would give an all-1-column) but rather have one factor fully coded (aka "swallow" the intercept), and all others being at `"treatment"` contrast, i.e., here, the *transposed* model matrix, `tmm`, is

```
> 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,

```
> data(morley) # a standard R data set
> morley$Expt <- factor(morley$Expt)
> morley$Run <- factor(morley$Run)
> str(morley)

'data.frame':        100 obs. of  3 variables:
 $ Expt : Factor w/ 5 levels "1","2","3","4",..: 1 1 1 1 1 1 1 1 1 1 ...
 $ Run  : Factor w/ 20 levels "1","2","3","4",..: 1 2 3 4 5 6 7 8 9 10 ...
 $ Speed: int  850 740 900 1070 930 850 950 980 980 880 ...

> t.mm <- with(morley,
+              rBind(as(Expt, "sparseMatrix"),
+                    as(Run,  "sparseMatrix")[-1,]))
> print(  image(t.mm)  ) # print(.) the lattice object
```



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"
```

```
(Intercept) 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
block2      . . . . 1 1 1 1 . . . . . . . . . . . . . . . .
block3      . . . . . . . . 1 1 1 1 . . . . . . . . . . . .
block4      . . . . . . . . . . . . 1 1 1 1 . . . . . . . .
block5      . . . . . . . . . . . . . . . . 1 1 1 1 . . . .
block6      . . . . . . . . . . . . . . . . . . . . 1 1 1 1
N1          . 1 . 1 1 1 . . . 1 1 . 1 1 . . 1 . 1 . 1 1 . .
P1          1 1 . . . 1 . 1 1 1 . . . 1 . 1 1 . . 1 . 1 1 .
K1          1 . . 1 . 1 1 . . 1 . 1 . 1 1 . . . 1 1 1 . 1 .
N1:P1       . 1 . . . 1 . . . 1 . . . 1 . . 1 . . . . 1 . .
N1:K1       . . . 1 . 1 . . . 1 . . . 1 . . . . 1 . 1 . . .
P1:K1       1 . . . . 1 . . . 1 . . . 1 . . . . . 1 . . 1 .
N1:P1:K1    . . . . . 1 . . . 1 . . . 1 . . . . . . . . . .
```

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):

```
> id <- factor(1:20)
> a <- factor(1:2)
> b <- factor(1:2)
> d <- factor(1:1500)
> aDat <- expand.grid(id=id, a=a, b=b, d=d)
> aDat$y <- rnorm(length(aDat[, 1])) # generate some random DV data
> dim(aDat) # 120'000 x 5  (120'000 = 2*2*1500 * 20 = 6000 * 20)

[1] 120000      5
```

and then continued with

```
m.aov <- aov(y ~ a*b*d + Error(id/(a*b*d)), data=aDat)
```

which yields the following error:

```
Error in model.matrix.default(mt, mf, contrasts) :
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:

Specifically[1],

```
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:

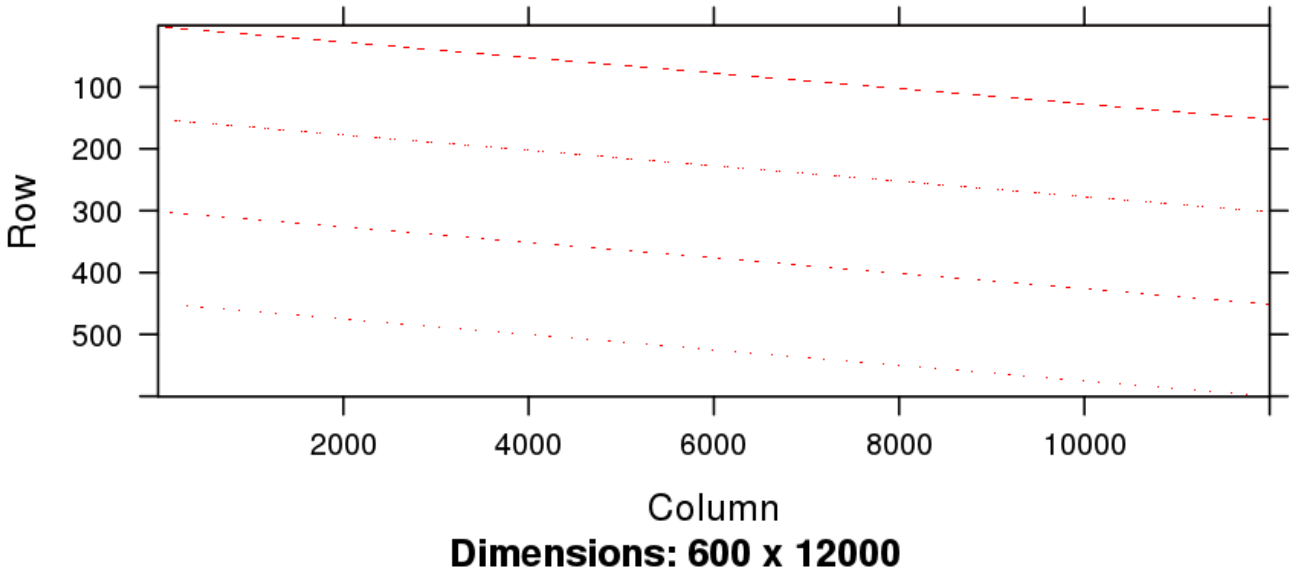
```
> d2 <- factor(1:150) # 10 times smaller
> tmp2 <- expand.grid(id=id, a=a, b=b, d=d2)
> dim(tmp2)
```

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

```
[1] 12000     4

> dim(mm <- model.matrix( ~ a*b*d, data=tmp2))

[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

   user  system elapsed
  0.001   0.001   0.003

> system.time(y. <- mm %*% x) ## than dense
```

```
   user  system elapsed
  0.055   0.015   0.069
```

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

```
[1] TRUE
```

```
> toLatex(sessionInfo())
```

- R version 3.2.0 beta (2015-04-01 r68134), `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 1.2-0
- Loaded via a namespace (and not attached): grid 3.2.0, lattice 0.20-31, tools 3.2.0