Design Issues in Matrix package Development

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Abstract

This is a (**currently very incomplete**) write-up of the many smaller and larger design decisions we have made in organizing functionalities in the Matrix package.

Classes: There's a rich hierarchy of matrix classes, which you can visualize as a set of trees whose inner (and "upper") nodes are *virtual* classes and only the leaves are non-virtual "actual" classes.

Functions and Methods:

- setAs()
- others

1 The Matrix class structures

Take Martin's DSC 2007 talk to depict the Matrix class hierarchy; available from https://stat.ethz.ch/~maechler/R/DSC-2007_MatrixClassHierarchies.pdf

From far, there are **three** separate class hierarchies, and every **Matrix** package matrix has an actual (or "factual") class inside these three hierarchies: More formally, we have three (3) main "class classifications" for our Matrices, i.e., three "orthogonal" partitions of "Matrix space", and every Matrix object's class corresponds to an *intersection* of these three partitions; i.e., in R's S4 class system: We have three independent inheritance schemes for every Matrix, and each such Matrix class is simply defined to **contain** three *virtual* classes (one from each partitioning scheme), e.g,

The three partioning schemes are

 Content type: Classes dMatrix, lMatrix, nMatrix, (iMatrix, zMatrix) for entries of type double, logical, pattern (and not yet integer and complex) Matrices.

nMatrix only stores the *location* of non-zero matrix entries (where as logical Matrices can also have NA entries!)

- 2. structure: general, triangular, symmetric, diagonal Matrices
- 3. sparsity: denseMatrix, sparseMatrix

For example in the most used sparseMatrix class, "dgCMatrix", the three initial letters dgC each codes for one of the three hierarchies:

- d: double
- g: **g**eneral
- C: CsparseMatrix, where C is for Column-compressed.

Part of this is visible from printing getClass("<classname>"):

```
> getClass("dgCMatrix")
```

Class "dgCMatrix" [package "Matrix"]

Slots:

Name: i p Dim Dimnames x factors Class: integer integer integer list numeric list

Extends:

Class "CsparseMatrix", directly

Class "dsparseMatrix", directly

Class "generalMatrix", directly

Class "dMatrix", by class "dsparseMatrix", distance 2

Class "sparseMatrix", by class "dsparseMatrix", distance 2

Class "Matrix", by class "generalMatrix", distance 2

Another example is the "nsTMatrix" class, where nsT stands for

- n: **n** is for "pattern", boolean content where only the *locations* of the non-zeros need to be stored.
- t: triangular matrix; either Upper, or Lower.
- T: TsparseMatrix, where T is for Triplet, the simplest but least efficient way to store a sparse matrix.

From R itself, via getClass(.):

```
> getClass("ntTMatrix")
```

Class "ntTMatrix" [package "Matrix"]

Slots:

Name: i j Dim Dimnames uplo diag

```
Class: integer integer integer list character character

Extends:
Class "TsparseMatrix", directly
Class "nsparseMatrix", directly
Class "triangularMatrix", directly
Class "nMatrix", by class "nsparseMatrix", distance 2
Class "sparseMatrix", by class "nsparseMatrix", distance 2
Class "Matrix", by class "triangularMatrix", distance 2
```

1.1 Diagonal Matrices

The class of diagonal matrices is worth mentioning for several reasons. First, we have wanted such a class, because *multiplication* methods are particularly simple with diagonal matrices. The typical constructor is <code>Diagonal()</code> whereas the accessor (as for traditional matrices), <code>diag()</code> simply returns the *vector* of diagonal entries:

```
> (D4 <- Diagonal(4, 10*(1:4)))</pre>
4 x 4 diagonal matrix of class "ddiMatrix"
     [,1] [,2] [,3] [,4]
[1,]
       10
[2,]
            20
[3,]
                  30
[4,]
                        40
> str(D4)
Formal class 'ddiMatrix' [package "Matrix"] with 4 slots
  ..@ diag
              : chr "N"
  ..@ Dim
               : int [1:2] 4 4
  ..@ Dimnames:List of 2
  ....$ : NULL
  .. ..$ : NULL
  ..@ x
               : num [1:4] 10 20 30 40
> diag(D4)
[1] 10 20 30 40
We can modify the diagonal in the traditional way (via method definition for
diag<-()):
> diag(D4) <- diag(D4) + 1:4</pre>
> D4
```

Note that **unit-diagonal** matrices (the identity matrices of linear algebra) with slot $\mathtt{diag} = "U"$ can have an empty x slot, very analogously to the unit-diagonal triangular matrices:

```
> str(I3 <- Diagonal(3)) ## empty 'x' slot
Formal class 'ddiMatrix' [package "Matrix"] with 4 slots
  ..@ diag
             : chr "U"
  ..@ Dim
             : int [1:2] 3 3
  ..@ Dimnames:List of 2
  .. ..$ : NULL
  .. ..$ : NULL
  ..@ x
              : num(0)
> getClass("diagonalMatrix") ## extending "sparseMatrix"
Virtual Class "diagonalMatrix" [package "Matrix"]
Slots:
Name:
            diag
                       Dim Dimnames
Class: character
                   integer
                                list
Extends:
Class "sparseMatrix", directly
Class "Matrix", by class "sparseMatrix", distance 2
```

Known Subclasses: "ndiMatrix", "ldiMatrix", "ddiMatrix"

Originally, we had implemented diagonal matrices as dense rather than sparse matrices. After several years it became clear that this had not been helpful really both from a user and programmer point of view. So now, indeed the "diagonalMatrix" class does also extend "sparseMatrix", i.e., is a subclass of it. However, we do not store explicitly where the non-zero entries are, and the class does not extend any of the typical sparse matrix classes, "CsparseMatrix", "TsparseMatrix", or "RsparseMatrix". Rather, the diag() onal (vector) is the basic part of such a matrix, and this is simply the x slot unless the diag slot is "U", the unit-diagonal case, which is the identity matrix.

Further note, e.g., from the ?Diagonal help page, that we provide (low level) utility function .sparseDiagonal() with wrappers .symDiagonal() and

.trDiagonal() which will provide diagonal matrices inheriting from "CsparseMatrix" which may be advantageous in *some cases*, but less efficient in others, see the help page.

2 Matrix Transformations

2.1 Coercions between Matrix classes

You may need to transform Matrix objects into specific shape (triangular, symmetric), content type (double, logical, ...) or storage structure (dense or sparse). Every useR should use as(x, <superclass>) to this end, where <superclass> is a *virtual* Matrix super class, such as "triangularMatrix" "dMatrix", or "sparseMatrix".

In other words, the user should *not* coerce directly to a specific desired class such as "dtCMatrix", even though that may occasionally work as well.

Here is a set of rules to which the Matrix developers and the users should typically adhere:

Rule 1 : as(M, "matrix") should work for all Matrix objects M.

Rule 2: Matrix(x) should also work for matrix like objects x and always return a "classed" Matrix.

Applied to a "matrix" object m, M. <- Matrix(m) can be considered a kind of inverse of m <- as(M, "matrix"). For sparse matrices however, M. well be a CsparseMatrix, and it is often "more structured" than M, e.g.,

```
> (M \leftarrow spMatrix(4,4, i=1:4, j=c(3:1,4), x=c(4,1,4,8))) \# dgTMatrix
```

4 x 4 sparse Matrix of class "dgTMatrix"

[4,] . . . 8

```
[1,] . . 4 .
[2,] . 1 . .
[3,] 4 . . .
[4,] . . . 8

> m <- as(M, "matrix")
> (M. <- Matrix(m)) # dsCMatrix (i.e. *symmetric*)
4 x 4 sparse Matrix of class "dsCMatrix"
[1,] . . 4 .
[2,] . 1 . .
[3,] 4 . . .</pre>
```

Rule 3: All the following coercions to virtual matrix classes should work:

- 1. as(m, "dMatrix")
- 2. as(m, "lMatrix")
- 3. as(m, "nMatrix")
- 4. as(m, "denseMatrix")
- 5. as(m, "sparseMatrix")
- 6. as(m, "generalMatrix")

whereas the next ones should work under some assumptions:

- as(m1, "triangularMatrix") should work when m1 is a triangular matrix, i.e. the upper or lower triangle of m1 contains only zeros.
- 2. as(m2, "symmetricMatrix") should work when m2 is a symmetric matrix in the sense of isSymmetric(m2) returning TRUE. Note that this is typically equivalent to something like isTRUE(all.equal(m2, t(m2))), i.e., the lower and upper triangle of the matrix have to be equal up to small numeric fuzz.

3 Session Info

- > toLatex(sessionInfo())
 - R Under development (unstable) (2025-03-05 r87881), x86_64-pc-linux-gnu
 - Locale: LC_CTYPE=de_CH.UTF-8, LC_NUMERIC=C, LC_TIME=en_GB.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
 - Time zone: Europe/Zurich
 - TZcode source: system (glibc)
 - Running under: Fedora Linux 40 (Forty)
 - Matrix products: default
 - BLAS: /sfs/u/maechler/R/D/r-devel/F40-64-inst/lib/libRblas.so
 - LAPACK: /usr/lib64/liblapack.so.3.12.0
 - Base packages: base, datasets, grDevices, graphics, methods, stats, utils
 - Other packages: Matrix 1.7-3
 - Loaded via a namespace (and not attached): compiler 4.5.0, grid 4.5.0, lattice 0.22-6, tools 4.5.0