Design Issues in Matrix package Development

Martin Maechler and Douglas Bates R Core Development Team maechler@stat.math.ethz.ch, bates@r-project.org

Spring 2008 (typeset on March 17, 2011)

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 class hierarchy.

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:

```
> 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
> D4
4 x 4 diagonal matrix of class "ddiMatrix"
     [,1] [,2] [,3] [,4]
[1,]
       11
[2,]
            22
[3,]
                  33
[4,]
                       44
   Note that unit-diagonal matrices (the identity matrices of linear algebra)
with slot 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 "denseMatrix"
Virtual Class "diagonalMatrix" [package "Matrix"]
Slots:
```

Dim Dimnames

Name:

diag

Class: character integer list

Extends:

Class "sparseMatrix", directly
Class "Matrix", by class "sparseMatrix", distance 2

Known Subclasses: "ddiMatrix", "ldiMatrix"

We have implemented diagonal matrices as *dense* rather than sparse matrices, for the following reasons:

- 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.
- 2. given '1)', it does not make much sense to store *where* the matrix is non-zero. This contrasts with all sparse matrix implementations, and hence we did not want to call a diagonal matrix "sparse".

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 <- 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"

[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 . . .
[4,] . . . 8</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 version 2.12.2 (2011-02-25), 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=C, 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

- \bullet Other packages: Matrix 0.999375-48, lattice 0.19-17
- Loaded via a name space (and not attached): grid 2.12.2, tools 2.12.2