Sparse Matrices in package Matrix and applications

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Outline

1. Introduction to Matrix and Sparse Matrices
   - Sparse Matrices in package `Matrix`
   - Matrix: Goals
   - 3D space of Matrix classes
2. Applications in Spatial Statistics
   - Regression with Spatially Dependent Errors: SAR(1)
3. Application - Mixed Modelling (RE)ML in R
4. Who's the best liked prof at ETH?

Introduction

- Matrix: the movie
- Matrix: the R package :

- Package Matrix: a recommended R package since R 2.9.0
- Infrastructure for other packages for several years, notably lme4[1]
- CRAN nowadays lists direct "reverse dependencies":

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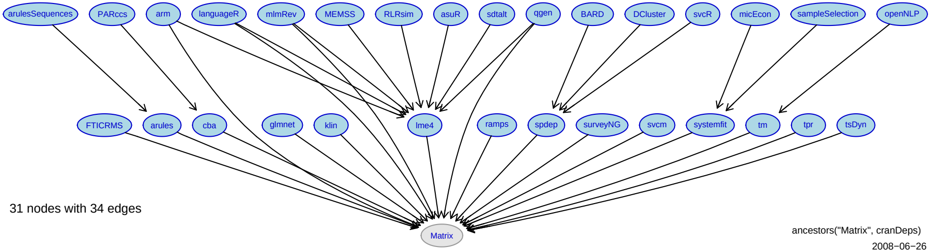
(reverse) Dependencies on Matrix

On June 26, 2008 (> one year ago), Matrix was not yet recommended, and had the following CRAN dependency graph:



i.e., 14 + 1 directly dependent packages.

Dependencies on Matrix – 2009-07

Today, quite a few more packages depend on Matrix explicitly:
CRAN → Packages → Matrix displays the following
`http://cran.r-project.org/web/packages/Matrix/`

Matrix: Sparse and Dense Matrix Classes and Methods

Classes and methods for dense and sparse matrices and operations on them using Lapack and SuiteSparse.

Version:	0.999375-29
Priority:	recommended
Depends:	R (≥ 2.9.0), stats, methods, utils, lattice
Imports:	graphics, lattice, grid, stats
Enhances:	graph, SparseM
Author:	Douglas Bates and Martin Maechler

Reverse dependencies:

Reverse depends:	FAiR, FTICRMS, GOSim, MCMCglmm, Metabonomic, arm, arules, glmnet, klin, languageR, lme4, mlmRev, pedigreemm, qgen, ramps, spdep, surveyNG, svcm, systemfit, tpr, tsDyn

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Reverse imports:	arules, cba
Reverse suggests:	R.matlab, RSiena, Rcsdp, blockmodeling, classGraph, e1071, gmodels, igraph, rattle, spam, survey
Reverse enhances:	Rcplex, Rcsdp

Dependencies on Matrix — 2009-07 — Summary

1. After one year, we have 22 (up from 15) packages depending on Matrix explicitly, plus another 12 “suggest” or “enhance” it.
2. Notably `glmnet`, Trevor Hastie’s favorite in yesterday’s keynote.
3. Most important one: lme4 and *its* dependencies

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Intro to Sparse Matrices in R package `Matrix`

- The R Package `Matrix` contains dozens of matrix classes and hundreds of method definitions.
- Has sub-hierarchies of `denseMatrix` and `sparseMatrix`.
- Very basic intro in *some* of sparse matrices:

simple example — Triplet form

The most obvious way to store a sparse matrix is the so called *"Triplet"* form; (virtual class `TsparseMatrix` in `Matrix`):

```
> A <- spMatrix(10, 20, i = c(1,3:8),
+                       j = c(2,9,6:10),
+                       x = 7 * (1:7))
> A # a  "dgTMatrix"

10 x 20 sparse Matrix of class "dgTMatrix"

 [1,] . 7 . . .  .  .  .  . . . . . . . . . . . .
 [2,] . . . . .  .  .  .  . . . . . . . . . . . .
 [3,] . . . . .  .  .  . 14 . . . . . . . . . . .
 [4,] . . . . . 21  .  .  . . . . . . . . . . . .
 [5,] . . . . .  . 28  .  . . . . . . . . . . . .
 [6,] . . . . .  .  . 35  . . . . . . . . . . . .
 [7,] . . . . .  .  .  . 42 . . . . . . . . . . .
 [8,] . . . . .  .  .  .  . 49 . . . . . . . . . .
 [9,] . . . . .  .  .  .  . . . . . . . . . . . .
[10,] . . . . .  .  .  .  . . . . . . . . . . . .
```

Less didactical, slighly more recommended: `A1 <- sparseMatrix(.....)`

simple example – 2 –

```
> str(A) # note that *internally* 0-based indices (i,j) are used
Formal class 'dgTMatrix' [package "Matrix"] with 6 slots
  ..@ i       : int [1:7] 0 2 3 4 5 6 7
  ..@ j       : int [1:7] 1 8 5 6 7 8 9
  ..@ Dim     : int [1:2] 10 20
  ..@ Dimnames:List of 2
  .. ..$ : NULL
  .. ..$ : NULL
  ..@ x       : num [1:7] 7 14 21 28 35 42 49
  ..@ factors : list()
> A[2:7, 12:20] <- rep(c(0,0,0,(3:1)*30,0), length = 6*9)
> A >= 20  ##  <--- what result do you expect ?
```

simple example – 3 –

```
> A >= 20 # -> logical sparse; nice show() method

10 x 20 sparse Matrix of class "lgTMatrix"

 [1,] . . . . . . . . . . . . . . . . . . . .
 [2,] . . . . . . . . . . . . . | | | . . . .
 [3,] . . . . . . . . . . . . . . | | | . . .
 [4,] . . . . . | . . . . . . . . . | | | . .
 [5,] . . . . . . | . . . . | . . . . | | | .
 [6,] . . . . . . . | . . . | | . . . . | | |
 [7,] . . . . . . . . | . . | | | . . . . | |
 [8,] . . . . . . . . . | . . . . . . . . . .
 [9,] . . . . . . . . . . . . . . . . . . . .
[10,] . . . . . . . . . . . . . . . . . . . .
```

sparse *compressed* form

Triplet representation: easy for us humans, but can be both made smaller *and* more efficient for (column-access heavy) operations:
The "column compressed" sparse representation:

```
> Ac <- as(t(A), "CsparseMatrix")
> str(Ac)
```

```
Formal class 'dgCMatrix' [package "Matrix"] with 6 slots
  ..@ i       : int [1:30] 1 13 14 15 8 14 15 16 5 15 ...
  ..@ p       : int [1:11] 0 1 4 8 12 17 23 29 30 30 ...
  ..@ Dim     : int [1:2] 20 10
  ..@ Dimnames:List of 2
  .. ..$ : NULL
  .. ..$ : NULL
  ..@ x       : num [1:30] 7 30 60 90 14 30 60 90 21 30 ...
  ..@ factors : list()
```

Column *index* slot `j`
replaced by a column *pointer* slot `p`.

R Package Matrix: Compelling reasons for S4

1. Classes for Matrices: well-defined inheritance hierarchies:
   1. Content kind: Classes `dMatrix`, `lMatrix`, `nMatrix`, (`iMatrix`, `zMatrix`) for contents of **d**ouble, **l**ogical, patter**n** (and not yet **i**nteger and complex) Matrices, where `nMatrix` only stores the *location* of non-zero matrix entries (where as logical Matrices can also have `NA` entries)
   2. sparsity: `denseMatrix`, `sparseMatrix`
   3. structure: general, triangular, symmetric, diagonal Matrices
2. Inheritance: Visualisation via graphs
3. **Multiple** Inheritance (of classes)
4. **Multiple** Dispatch (of methods)

Multiple Dispatch in S4 .... for Matrix operations

Methods for "Matrix"-matrices: Often 2 matrices involved..

1. `x %*% y`
2. `crossprod(x,y)` — $\mathbf{x}^\mathsf{T}\mathbf{y}$
3. `tcrossprod(x,y)` — $\mathbf{x}\mathbf{y}^\mathsf{T}$
4. `x + y` — `"Arith"` *group methods*
5. `x <= y` — `"Compare"` *group methods*

and many many more.

S4 >> S3

- S4 - multiple dispatch: Find method according to classes of *both* (or more) arguments.
- S3 - single dispatch: e.g., "ops.Matrix": only first argument counts.

Goals of Matrix package

1. interface to LAPACK= state-of-the-art numerical linear algebra for *dense* matrices
   - making use of special structure for *symmetric* or *triangular* matrices (e.g. when solving linear systems)
   - setting and keep such properties alows more optimized code in these cases.
2. Sparse matrices for large designs: regression, mixed models, etc
3. . . . . . . [omitted in this talk]

Hence, quite a few *different classes* for matrices.

many Matrix classes ...

```
> library(Matrix)
> length(allCl <- getClasses("package:Matrix"))

[1] 98

> ## Those called "...Matrix" :
> length(M.Cl <- grep("Matrix$",allCl, value = TRUE))

[1] 70
```

i.e., *many* ..., each inheriting from root class "Matrix"

```
> str(subs <- showExtends(getClassDef("Matrix")@subclasses,
+                              printTo=FALSE))

List of 2
 $ what: chr [1:76] "compMatrix" "triangularMatrix" "dMatrix" "iMatrix" ...
 $ how : chr [1:76] "directly" "directly" "directly" "directly" ...

> ## even more... :  All those above and these in addition:
> subs$what[ ! (subs$what %in% M.Cl)]

[1] "Cholesky"      "pCholesky"     "BunchKaufman"  "pBunchKaufman"
```

...... a bit messy ...

3-way Partitioning of “Matrix space”

Logical organization of our Matrices: 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 inheritence schemes for every Matrix, and each such Matrix class is simply defined to `contain` three *virtual* classes (one from each partitioning scheme), e.g,

```
setClass("dgCMatrix",
      contains= c("CsparseMatrix", "dsparseMatrix", "generalMatrix"),
      validity= function(..) .....)
```

3-way Partitioning of Matrix space — 2

The three partioning schemes are

1. Content type: Classes `dMatrix`, `lMatrix`, `nMatrix`, (`iMatrix`, `zMatrix`) for entries of type **d**ouble, **l**ogical, patter**n** (and not yet **i**nteger 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`

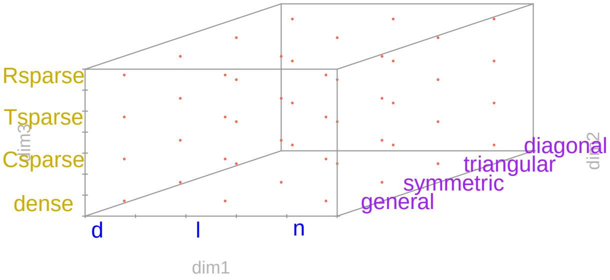
First two schemes: a slight generalization from LAPACK for dense matrices.

3D space of Matrix classes

three-way partitioning of Matrix classes visualized in 3D space, dropping the final `Matrix`, e.g., "d" instead of "dMatrix":

```
> d1 <- c("d", "l", "n")
> d2 <- c("general", "symmetric", "triangular", "diagonal")
> d3 <- c("dense", c("Csparse", "Tsparse", "Rsparse"))
> clGrid <- expand.grid(dim1 = d1, dim2 = d2, dim3 = d3, KEEP.OUT.AT
> clGr <- data.matrix(clGrid)
> library(scatterplot3d)
```

used for visualization:



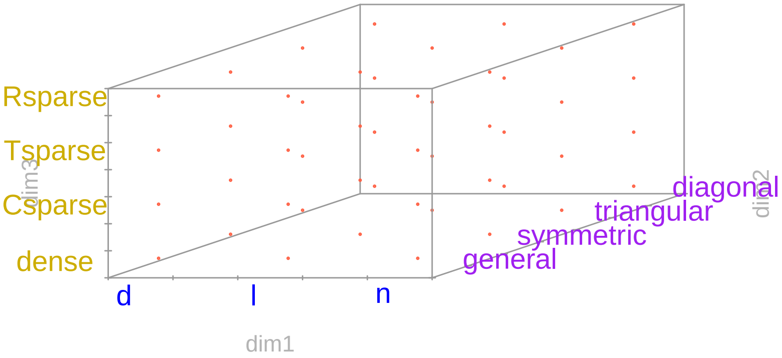
3-fold classification — Matrix naming scheme

1. *"Actual"* classes: Matrix objects are of those; the above "points in 3D space"
2. *Virtual* classes: e.g. the above coordinate axes categories.
   Superclasses of actual ones
   cannot have objects of, but —importantly— many *methods* for these virtual classes.

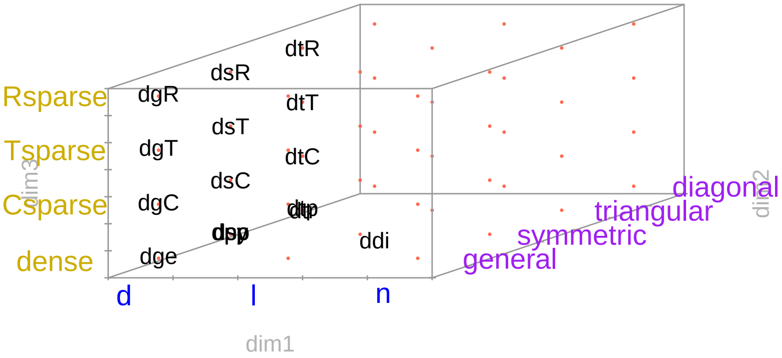
Actual classes follow a "simple" terse naming convention:

```
> str(M3cl <- grep("^...Matrix$",M.Cl, value = TRUE))

 chr [1:47] "corMatrix" "ddiMatrix" "dgCMatrix" "dgeMatrix" ...

> substring(M3cl,1,3)

 [1] "cor" "ddi" "dgC" "dge" "dgR" "dgT" "dpo" "dpp" "dsC" "dsp" "dsR" "dsT
[13] "dsy" "dtC" "dtp" "dtr" "dtR" "dtT" "ldi" "lgC" "lge" "lgR" "lgT" "lsC
[25] "lsp" "lsR" "lsT" "lsy" "ltC" "ltp" "ltr" "ltR" "ltT" "ngC" "nge" "ngR
[37] "ngT" "nsC" "nsp" "nsR" "nsT" "nsy" "ntC" "ntp" "ntr" "ntR" "ntT"

> M3cl <- M3cl[M3cl != "corMatrix"] # corMatrix not desired in foll
```

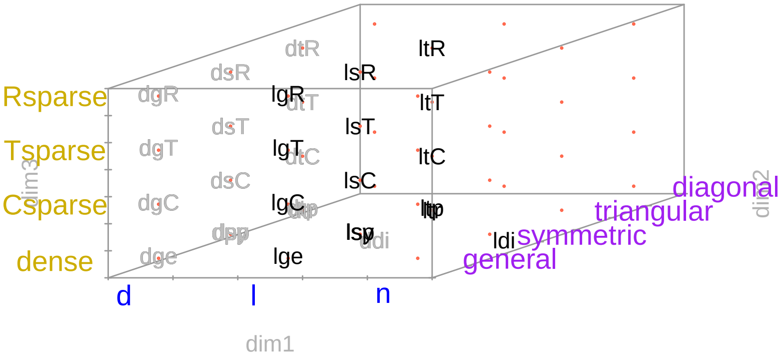
3D space of Matrix classes



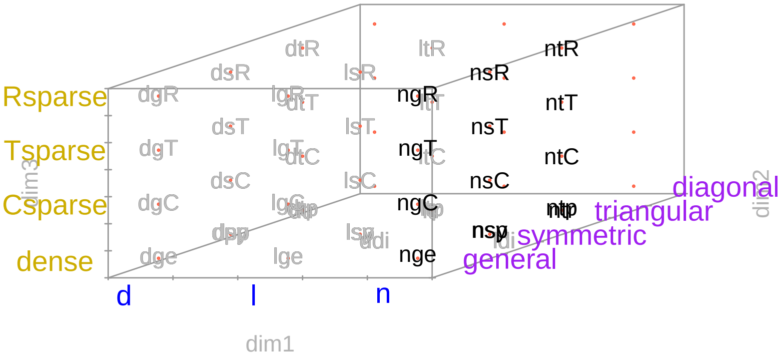
Matrix 3d space: filled (2)



Matrix 3d space: filled (3)



Matrix 3d space: filled (4)



Spatially Dependent Errors — SAR(1)

Regression with spatially dependent errors; observations at *locations* $i, \quad i = 1, \ldots, n$, n in the thousands, possibly 100'000s.

Simultaneous Autoregression

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{u} \quad \text{where} \quad \boldsymbol{u} = \lambda \mathbf{W}\boldsymbol{u} + \boldsymbol{\epsilon}. \tag{1}$$

- $\mathbf{W}$: matrix (W_{ij}) of "distance-based contiguities" of locations i and j $(W_{ii} \equiv 0)$.
- λ: SAR(1) parameter; estimate via MLE, ($\boldsymbol{\beta}$ profiled out).
- $\boldsymbol{u} \sim \mathcal{N}\left(\mathbf{0}, \sigma^2 (\boldsymbol{I} - \lambda \mathbf{W})^{-1} (\boldsymbol{I} - \lambda \mathbf{W}^{\mathsf{T}})^{-1}\right)$
- For log likelihood, need to compute determinant $|\boldsymbol{I} - \lambda \mathbf{W}| = (-\lambda)^n \left| -\mathbf{W} + \frac{1}{\lambda}\boldsymbol{I} \right|$ for many λ.

Compute Cholesky / Determinant of $\boldsymbol{A} + \rho \boldsymbol{I}$ for large sparse symmetric $\boldsymbol{A}$:
$\Longrightarrow$ Fast Cholesky Update

SAR(1) – fast Likelihood from Cholesky Update

Data provided by Roger Bivand, as a relevant test case:

```
> data(USCounties, package="Matrix")
> dim(USCounties)

[1] 3111 3111

> (n <- ncol(USCounties))

[1] 3111

> IM <- .symDiagonal(n)
> nWC <- -USCounties
> set.seed(1)
> rho <- sort(runif(50,  0, 1)) ## rho = 1 / lambda
```

and now compute *determinant(A)* $=: |\boldsymbol{A}|$

$$|\boldsymbol{I} - \lambda \mathbf{W}| \propto \left| -\mathbf{W} + \frac{1}{\lambda}\boldsymbol{I} \right| \quad \text{for many} \lambda\ 's. \tag{2}$$

SAR(1) – Cholesky Update – 2 –

```
> ## Determinant : Direct Computation
> system.time(MJ <- sapply(rho, function(x)
+         determinant(IM - x * USCounties, logarithm = TRUE)$modulus
```

```
   user  system elapsed
  3.620   0.124   4.006
```

```
> ## Determinant : "high-level" Update of the Cholesky {Simplicial /
> C1 <- Cholesky(nWC, Imult = 2)
> system.time(MJ1 <- n * log(rho) +
+    sapply(rho, function(x) c(determinant(update(C1, nWC, 1/x))$mod
```

```
   user  system elapsed
  0.700   0.012   0.722
```

```
> stopifnot(all.equal(MJ, MJ1))
> C2 <- Cholesky(nWC, super = TRUE, Imult = 2) ## <<-- "Supernodal"
> system.time(MJ2 <- n * log(rho) +
+    sapply(rho, function(x) c(determinant(update(C2, nWC, 1/x))$mod
```

```
   user  system elapsed
  0.804   0.020   0.859
```

SAR(1) – Cholesky Update – 3 –

```
> stopifnot(all.equal(MJ, MJ2))
> ## Determinant : "low-level" Update of the Cholesky {Simplicial /
> system.time(MJ3 <- n*log(rho) + Matrix::ldetL2up(C1, nWC,1/rho))

   user  system elapsed
  0.404   0.012   0.454

> stopifnot(all.equal(MJ, MJ3))
> system.time(MJ4 <- n*log(rho) + Matrix::ldetL2up(C2, nWC,1/rho))

   user  system elapsed
  0.384   0.008   0.405

> stopifnot(all.equal(MJ, MJ4))
```

Findings:

1. Using Cholesky update: order of magnitude faster
2. Simplicial (`super= FALSE`) ↔ Supernodal (`super= TRUE`) : no big difference here
3. An even faster method for Det(Chol(.)) yields another 50% speed.

Mixed Modelling - (RE)ML Estimation in pure R

In (linear) mixed effects, the evaluation of the (RE) likelihood or equivalently deviance, needs repeated Cholesky decompositions of

$$\boldsymbol{U}_\theta \boldsymbol{U}_\theta^\mathsf{T} + \boldsymbol{I}, \tag{3}$$

for many θ values ($=$ the relative variance components) and (often very large), very sparse matrix $\boldsymbol{U}_\theta$ where only the *non*-zeros of $\boldsymbol{U}$ depend on θ, i.e., the sparsity pattern is given (by the observational design).
Sophisticated (fill-reducing) Cholesky done in two phases:

1. "symbolic" decomposition: Determine the non-zero entries of $\boldsymbol{L}$ ($\boldsymbol{L}\boldsymbol{L}^\mathsf{T} = \boldsymbol{U}\boldsymbol{U}^\mathsf{T} + \boldsymbol{I}$),
2. numeric phase: compute these entries.
   Phase 1: typically takes much longer; only needs to happen *once*.
   Phase 2: "update the Cholesky Factorization"

Who's the best liked prof at ETH?

- Private donation for encouraging excellent teaching at ETH
- Student union of ETH Zurich organizes survey to award prizes: Best lecturer — of ETH, and of each of the 14 departments.
- Smart Web-interface for survey: Each student sees the names of his/her professors from the last 4 semesters and all the lectures that applied.
- ratings in $\{1, 2, 3, 4, 5\}$.
- high response rate

Who's the best prof — data

```
> md <- within(read.csv("~/R/MM/Pkg-ex/lme4/puma-lmertest.csv"), {
+      s       <- factor(s) # Student_ID
+      d       <- factor(d) # Lecturer_ID ("d"ozentIn)
+      dept    <- factor(dept)
+      service <- factor(service)
+      studage <- ordered(studage)## *ordered* factors
+      lectage <- ordered(lectage) })
> str(md)
```

```
'data.frame': 73421 obs. of  7 variables:
 $ s      : Factor w/ 2972 levels "1","2","3","4",..: 1 1 1 1 2 2 3 3 3 3 .
 $ d      : Factor w/ 1128 levels "1","6","7","8",..: 525 560 832 1068 62 4
 $ studage: Ord.factor w/ 4 levels "2"<"4"<"6"<"8": 1 1 1 1 1 1 1 1 1 1 ...
 $ lectage: Ord.factor w/ 6 levels "1"<"2"<"3"<"4"<..: 2 1 2 2 1 1 1 1 1 1
 $ service: Factor w/ 2 levels "0","1": 1 2 1 2 1 1 2 1 1 1 ...
 $ dept   : Factor w/ 15 levels "1","2","3","4",..: 15 5 15 12 2 2 14 3 3 3
 $ y      : int  5 2 5 3 2 4 4 5 5 4 ...
```

Modelling the ETH teacher ratings

Model: The rating depends on

- students (`s`) (rating subjectively)
- teacher (`d`) – main interest
- department (`dept`)
- "service" lecture or "own department student", (`service`: 0/1).
- semester of student at time of rating (`studage`$\in \{2, 4, 6, 8\}$).
- how many semesters back was the lecture (`lectage`).

Main question: $\boxed{\text{Who's the best prof?}}$

Hence, for "political" reasons, want `d` as a **fixed** effect.

Model for ETH teacher ratings

Want `d` ("teacher_ID", ≈ 1000 levels) as **fixed** effect. Consequently, in

$$y = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{Z}\boldsymbol{b} + \boldsymbol{\epsilon}$$

have $\boldsymbol{X}$ as $n \times 1000$ (roughly), $\boldsymbol{Z}$ as $n \times 5000$, $n \approx 70'000$.

```
> fm0 <- lmer2(y ~ d + dept*service + studage + lectage + (1|s),
+                  data = md, sparseX = TRUE)
```

`sparseX = TRUE`: *sparse* $\boldsymbol{X}$ (fixed effects) in addition to the indispensably sparse $\boldsymbol{Z}$ (random effects).

Unfortunately: Here, the above "sparseX - lmer" ends in

```
Error ... Cholmod error 'not positive definite' at file:../Cholesky/......
```

Good News: Newly in `Matrix`:

`sparse.model.matrix()`

- which `lmer()` can use,
- or you can use for "truly sparse" least squares (i.e. no intermediately dense design matrix)
- something we plan to provide in Matrix 1.0-0.

Summary

- Recommended R package "Matrix"
- *Sparse* Matrices: in increasing number of applications
- S4 classes and methods are the natural implementation tools
- lme4 is going to contain an alternative "pure R" version of ML and REML, you can pass to `nlminb()` (or `optim()` if you must :-). UseRs can easily extend these R functions to more flexible models or algorithms.
- Matrix 1.0-0
  - will happen
  - will contain `sparse.model.matrix()`
  - will contain truly sparse `lm(*, sparse=TRUE)`

That's all folks — with thanks for your attention!

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