

# 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 2.10
- A prerequisite for other packages for several years, notably **lavaan**
- C++ provides fast direct / sparse dependencies

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- Infrastructure for other packages for several years, notably `lme4`<sup>1</sup>
- CRAN nowadays lists direct “reverse dependencies”:

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(using `S4` | re-implemented from scratch the 4<sup>th</sup> time)

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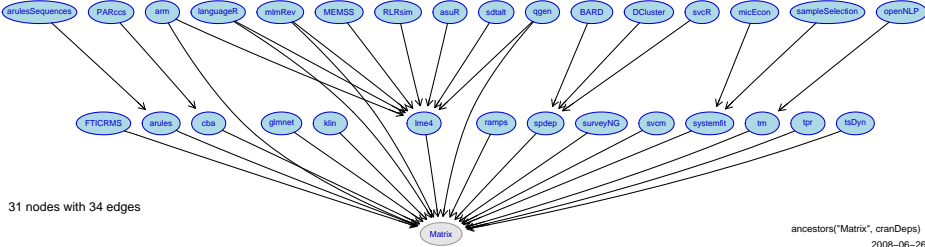
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# (reverse) Dependencies on Matrix

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



31 nodes with 34 edges

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 ( $\geq 2.9.0$ ), 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](#), [MCMCglimm](#), [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, slightly 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 **double**, **logical**, **pattern** (and not yet **integer** 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  $\text{crossprod}(x,y) \text{ — } x^T y$
- 3  $\text{tcrossprod}(x,y) \text{ — } x y^T$
- 4  $x + y \text{ — "Arith" group methods}$
- 5  $x <= y \text{ — "Compare" group methods}$

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 allows 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 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,

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

## 3-way Partitioning of Matrix space — 2

The three partitioning schemes are

- 1 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`

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")
```

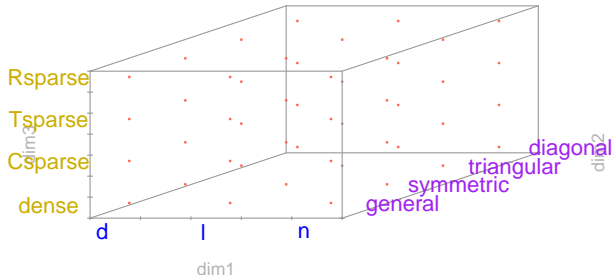
```
> d3 <- c("dense", c("Csparse", "Tsparse", "Rsparse"))
```

```
> clGrid <- expand.grid(dim1 = d1, dim2 = d2, dim3 = d3, KEEP.OUT.A...
```

```
> 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" ...
```

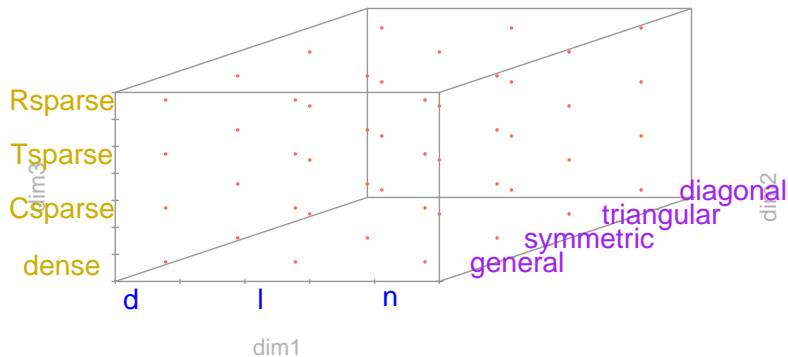
```
> substring(M3cl,1,3)
```

```
[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"
```

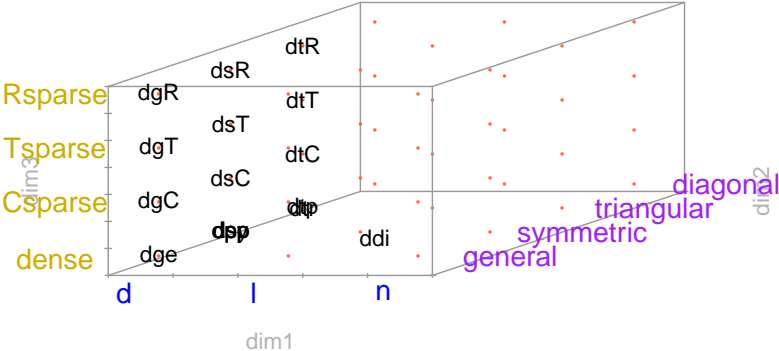
```
> M3cl <- M3cl[M3cl != "corMatrix"] # corMatrix not desired in follow
```



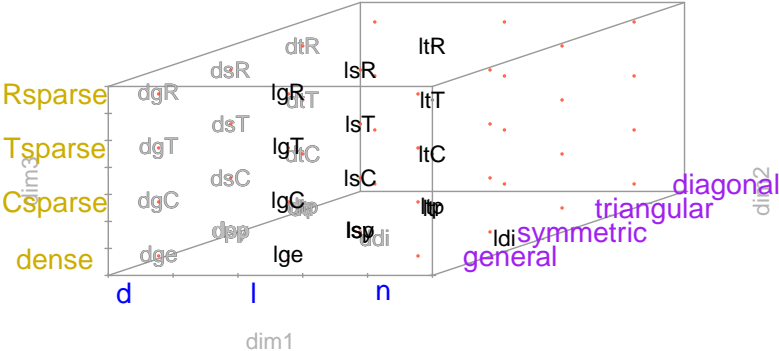
# 3D space of Matrix classes



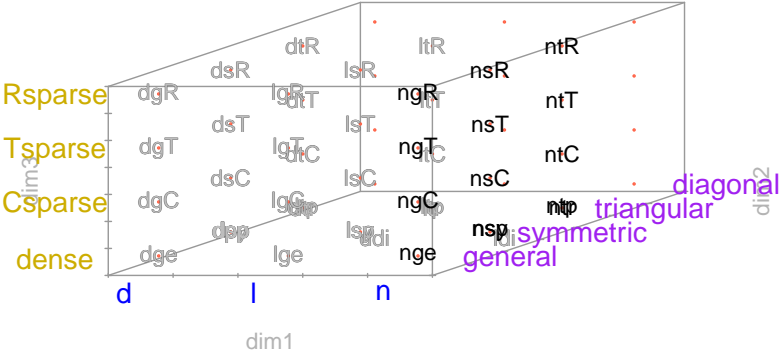
# Matrix 3d space: filled (2)



# Matrix 3d space: filled (3)



# Matrix 3d space: filled (4)



# Spatially Dependent Errors — SAR(1)

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

## Simultaneous Autoregression

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

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

Compute Cholesky / Determinant of  $\mathbf{A} + \rho \mathbf{I}$  for large sparse symmetric  $\mathbf{A}$ :  
 $\implies$  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  $determinant(\mathbf{A}) =: |\mathbf{A}|$

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

## 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
4.180   0.064   4.608

> ## 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))$mo

  user  system elapsed
0.656   0.000   0.715

> 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))$mo

  user  system elapsed
0.772   0.036   0.867
```

## 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
0.400   0.000   0.415

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

  user  system elapsed
0.384   0.000   0.406

> 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

$$\mathbf{U}_\theta \mathbf{U}_\theta^\top + \mathbf{I}, \quad (3)$$

for many  $\theta$  values (= the relative variance components) and (often very large), very sparse matrix  $\mathbf{U}_\theta$  where only the *non-zeros* of  $\mathbf{U}$  depend on  $\theta$ , 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  $\mathbf{L}$  ( $\mathbf{L}\mathbf{L}^\top = \mathbf{U}\mathbf{U}^\top + \mathbf{I}$ ),
- 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: Who's the best prof?

Hence, for “political” reasons, want  $d$  as a **fixed** effect.

## Model for ETH teacher ratings

Want  $d$  (“teacher\_ID”,  $\approx 1000$  levels) as **fixed** effect. Consequently, in

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

have  $\mathbf{X}$  as  $n \times 1000$  (roughly),  $\mathbf{Z}$  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*  $\mathbf{X}$  (fixed effects) in addition to the indispensably sparse  $\mathbf{Z}$  (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

– Sparse Matrices

– `Matrix` will contain `sparseModel.matrix()`

– `Matrix` will contain `trajSparse` (`traj`, `sparsesolve`)

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

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Matrix will contain sparse model matrices  
nlminb will contain only sparse matrix operations

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- 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.

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