Sparse Matrices Methods and Kriging

Applications to Large Spatial Data Sets

SAMSI

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Outline

What are sparse matrices?

How to work with sparse matrices?

Sparse positive definite matrices in statistics.

Sparse matrices and fields.

Thanks NSF!
DMS-0621118
Outline

What are sparse matrices?

How to work with sparse matrices?

Sparse positive definite matrices in statistics.

Sparse matrices and fields.
Sparse Matrices

What is “sparse” or a sparse matrix?

According to Wiktionary/Wikipedia:

Sparse: (Adjective)
1. Having widely spaced intervals
2. Not dense; meager

Sparse matrix:
a matrix populated primarily with zeros.
Sparse Matrices

R> n <- 15
R> A <- array( runif(n^2), c(n,n)) + diag(n)
R> A[A < 0.75] <- 0
Sparse Matrices

R> n <- 15
R> A <- array( runif(n^2), c(n,n)) + diag(n)
R> A[A < 0.75] <- 0
R> AtA <- t(A) %*% A
Sparse Matrices

Why should we use sparse matrices?
Sparse Matrices

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1. Savings in storage

2. Savings in computing time
Sparse Matrices

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1. Savings in storage
   nonzeros vs total elements

2. Savings in computing time
   0.066sec vs 0.003sec for $1,000 \times 1,000$ matrix multiplication
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To exploit the savings need to exploit the sparsity.
Sparse Matrices

Why should we use sparse matrices?

1. Savings in storage
   nonzeros vs total elements

2. Savings in computing time
   0.066sec vs 0.003sec for $1,000 \times 1,000$ matrix multiplication

To exploit the savings need to exploit the sparsity.

We need a clever storage format and fast algorithms.
Storage Formats

Let $A = (a_{ij}) \in \mathbb{R}^{n \times m}$ and $z$ the number of its nonzero elements.

1. Naive/"traditional”/classic format:
   one vector of length $n \times m$ and a dimension attribute.
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3. Compressed sparse row (CSR) format:
   eliminate redundant row indices.
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3. Compressed sparse row (CSR) format:
   eliminate redundant row indices.

4. and about 10 more . . .
Storage Formats, Example

\[ A = \begin{pmatrix}
1 & 0.1 & 0 & 0.2 & 0.3 \\
0.4 & 2 & 0 & 0.5 & 0 \\
0 & 0 & 3 & 0 & 0.6 \\
0.7 & 0.8 & 0 & 4 & 0 \\
0.9 & 0 & 0.0 & 0 & 5
\end{pmatrix} \]
Storage Formats, Example

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0.7 & 0.8 & 0 & 4 & 0 \\
0.9 & 0 & 0.0 & 0 & 5
\end{pmatrix}
\]

Naive/traditional/classic:
1, .4, 0, .7, .9, .1, 2, 0, .8, 0, 0, 0, 3, 0, .0, .2, .5, 0, 4, 0, .3, 0, .6, 0, 5
Storage Formats, Example

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0 & 0 & 3 & 0 & 0.6 \\
0.7 & 0.8 & 0 & 4 & 0 \\
0.9 & 0 & 0.0 & 0 & 5 
\end{pmatrix} \]

Triplet:

\[ i : \quad 1 \quad 1 \quad 1 \quad 1 \quad 2 \quad 2 \quad 2 \quad 3 \quad 3 \quad 4 \quad 4 \quad 4 \quad 5 \quad 5 \quad 5 \]

\[ j : \quad 1 \quad 2 \quad 4 \quad 5 \quad 1 \quad 2 \quad 4 \quad 2 \quad 3 \quad 1 \quad 2 \quad 4 \quad 1 \quad 3 \quad 5 \]

\[ a_{ij} : \quad 1 \quad .1 \quad .2 \quad .3 \quad .4 \quad 2 \quad .5 \quad 3 \quad .6 \quad .7 \quad .8 \quad 4 \quad .9 \quad 0 \quad 5 \]
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0.9 & 0 & 0.0 & 0 & 0.5
\end{pmatrix} \]

\[ i : \quad 1 \quad 2 \quad 4 \quad 5 \quad 1 \quad 2 \quad 4 \quad 2 \quad 3 \quad 1 \quad 2 \quad 4 \quad 1 \quad 3 \quad 5 \]

\[ j : \quad 1 \quad 2 \quad 4 \quad 5 \]

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0.9 & 0 & 0.0 & 0 & 5
\end{pmatrix} \]

CSR:

\[
\begin{array}{l}
\text{ptr :} \\
1 & 5 & 8 & 10 & 13 & 16 \\
\text{j :} \\
1 & 2 & 4 & 5 & 1 & 2 & 4 & 2 & 3 & 1 & 2 & 4 & 1 & 3 & 5 \\
\text{a}_{ij} : \\
1 & .1 & .2 & .3 & .4 & 2 & .5 & 3 & .6 & .7 & .8 & 4 & .9 & .0 & 5
\end{array}
\]
Compressed Sparse Row Format

1. the nonzero values row by row

2. the (ordered) column indices of nonzero values

3. the position in the previous two vectors corresponding to new rows, given as pointers

4. the column dimension of the matrix.

CSR:

<table>
<thead>
<tr>
<th>ptr</th>
<th>1</th>
<th>5</th>
<th>8</th>
<th>10</th>
<th>13</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>j</td>
<td>1</td>
<td>2</td>
<td>4</td>
<td>5</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>a_{ij}</td>
<td>1</td>
<td>.1</td>
<td>.2</td>
<td>.3</td>
<td>.4</td>
<td>2</td>
</tr>
</tbody>
</table>

...
(Dis)Advantages

1. Naive format:
   No savings in storage and computation (for sparse matrices)
   Status quo
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   Savings in storage and computation for sparse matrices
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(Dis)Advantages

1. Naive format:
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   Intuitive

3. Compressed sparse row (CSR) format:
   Apart from intuitive, same as triplet
   Faster element access
   Many available algorithms
   Arbitrary choice for “row” vs “column” format (CSC)
Implications

With a new storage format new “algorithms” are required . . .

Is it worthwhile???
Timing

Setup:

R> timing <- function(expr)
+ as.vector( system.time( for (i in 1:N) expr)[1])

R> N <- 1000         # how many operations
R> n <- 999          # matrix dimension
R> cutoff <- 0.9     # what will be set to 0

R> A <- array( runif(n^2), c(n,n))
R> A[A < cutoff] <- 0

R> S <- somecalltomagicfunctiontogetsparsesformat( A)

Compare timing for different operations on A and S.
Timing

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R> cutoff <- 0.9    # what will be set to 0

R> A <- array( runif(n^2), c(n,n))
R> A[A < cutoff] <- 0

R> S <- as.spam(A)

Compare timing for different operations on A and S.
Timing

R> timing( A + sqrt(A) )
[1] 0.058
R> timing( S + sqrt(S) )
[1] 0.065

R> timing( AtA <- t(A) %*% A )
[1] 1.567
R> timing( StS <- t(S) %*% S )
[1] 3.422
Timing

R> timing( A[1,2] <- .5 )
[1] 0.007
R> timing( S[1,2] <- .5 )
[1] 0.018

R> timing( A[n,n-1] <- .5 )
[1] 0.001
R> timing( S[n,n-1] <- .5 )
[1] 0.012
Timing

R> timing( xA <- solve(AtA, rep(1,n)) )
[1] 0.626
R> timing( xS <- solve(StS, rep(1,n)) )
[1] 0.831
R> timing( RA <- chol(AtA) )
[1] 0.301
R> timing( RS <- chol(StS) )
[1] 0.824
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Is it really worthwhile? What is going on?
Timing

Matrix S

[Image of a matrix with rows and columns labeled]
Timing

Matrix $S$

Matrix $StS$
Timing

With cutoff 0.99:

R> timing(AtA <- t(A) %*% A )
[1] 1.536
R> timing( StS <- t(S) %*% S )
[1] 0.076

R> timing( RA <- chol(AtA) )
[1] 0.304
R> timing( RS <- chol(StS) )
[1] 0.451
Density of the factor is 41% with fill-in ratio 7.2.
Timing

With cutoff 0.999:

R> timing( AtA <- t(A) %*% A )
[1] 1.549
R> timing( StS <- t(S) %*% S )
[1] 0.004

R> timing( RA <- chol(AtA) )
[1] 0.304
R> timing( RS <- chol(StS) )
[1] 0.004
Density of the factor is .6% with fill-in ratio 2.3.
Implications

With a new storage format new “algorithms” are required . . .

Is it worthwhile??? Yes!
Implications

With a new storage format new “algorithms” are required . . .

Is it worthwhile? Yes!

Especially since

spam: R package for sparse matrix algebra.
Outline

What are sparse matrices?

How to work with sparse matrices?

Sparse positive definite matrices in statistics.

Sparse matrices and fields.
What is spam?

- an R package for **sparse** matrix algebra
  - publicly available from CRAN, 0.15-4
  - platform independent and documented
What is spam?

- an R package for sparse matrix algebra
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- storage economical and fast
  - uses “old Yale sparse format”
  - most routines are in Fortran, adapted for spam
  - balance between readability and overhead
  - flags for “expert” users
What is **spam**?

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- versatile, intuitive and simple
  - wrap an **as.spam()** and go
  - **?xyz.spam** for help
  - **S4** and **S3** syntax
What is `spam`?

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- versatile, intuitive and simple
  - wrap an `as.spam()` and go
  - `?xyz.spam` for help
  - S4 and S3 syntax

- situated between SparseM and Matrix
Representation of Sparse Matrices

spam defines a S4 class spam containing the vectors: “entries”, “colindices”, “rowpointers” and ”dimension”.

R> slotNames( "spam")
[1] "entries" "colindices" "rowpointers" "dimension"

R> getSlots( "spam")
  entries  colindices  rowpointers  dimension
 "numeric" "integer"  "integer"  "integer"
### Representation of Sparse Matrices

```r
R> A

[1,] 1.0 0.1 0 0.2 0.3
[2,] 0.6 2.0 0 0.5 0.0
[3,] 0.0 0.0 3 0.0 0.6
[4,] 0.7 0.8 0 4.0 0.0
[5,] 0.9 0.0 1 0.0 5.0

Class 'spam'
R> slotNames(A)

[1] "entries"  "colindices"  "rowpointers"  "dimension"

R> A@entries

[1] 1.0 0.1 0.2 0.3 0.6 2.0 0.5 3.0 0.6 0.7 0.8 4.0 0.9 1.0 5.0

R> A@colindices

[1] 1 2 4 5 1 2 4 3 5 1 2 4 1 3 5

R> A@rowpointers

[1] 1 5 8 10 13 16

R> A@dimension

[1] 5 5
```
Creating Sparse Matrices

Similar coercion techniques as with `matrix`:

- `spam(...)`
- `as.spam(...)`

Special functions:

- `diag.spam(...)`
- `nearest.dist(...)`
Methods for spam

- Similar behavior as with matrices
  plot; dim; determinant; %*%; +; ...

- Slightly enhanced behavior
  print; dim<-; chol;

- Specific behavior
  Math; Math2; Summary; ...

- New methods
  display; ordering;
Create Covariance Matrices

Covariance matrix:

- nearest.dist and applying a covariance function:
  
  R> C <- nearest.dist(x, diag=TRUE, upper=NULL)
  
  R> C@entries <- Wendland(C@entries, dim=2, k=1)
Create Covariance Matrices

Covariance matrix:

nearest.dist and applying a covariance function:

\[
R> C <- \text{nearest.dist}(x, \text{diag}=\text{TRUE}, \text{upper}=\text{NULL}) \\
R> C@entries <- \text{Wendland}(C@entries, \text{dim}=2, k=1)
\]

Precision matrix (GMRF):

— regular grids: nearest.dist with different cutoffs

\[
R> \text{diag.spam}(n) + \\
+ (b_1-b_2) * \text{nearest.dist}(x, \text{delta}=1, \text{upper}=\text{NULL}) + \\
+ b_2 * \text{nearest.dist}(x, \text{delta}=\sqrt{2}, \text{upper}=\text{NULL})
\]

— irregular grids: using incidence list and spam

\[
R> \text{incidence} <- \text{list}(i=\ldots, j=\ldots, \text{values}) \\
R> C <- \text{spam}(\text{incidence}, n, n)
\]
Solving Linear Systems

A key feature of spam is to solve efficiently linear systems.

To solve the system $Ax = b$, we

- perform a Cholesky factorisation $A = U^T U$
- solve two triangular systems $U^T z = b$ and $U x = z$

But we need to “ensure” that $U$ is as sparse as possible!
Solving Linear Systems

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But we need to “ensure” that $U$ is as sparse as possible!

Permute the rows and columns of $A$: $P^T A P = U^T U$. 
Cholesky

Some technical details about a Cholesky decomposition:

[1] Determine permutation and permute the input matrix $\mathbf{A}$ to obtain $\mathbf{P}^T \mathbf{A} \mathbf{P}$

[2] Symbolic factorization:
   the sparsity structure of $\mathbf{U}$ is constructed

[3] Numeric factorization:
   the elements of $\mathbf{U}$ are computed
BTW:
efficient Cholesky factorization

$\iff$

efficient determinant calculation:

$$\det(C) = \det(U^T) \det(U) = \prod_{i=1}^{n} U_{ii}^2$$
Cholesky

spam knows Cholesky!

— Several methods to construct permutation matrices $P$

none, MMD, RCM
Cholesky

spam knows Cholesky!

— Several methods to construct permutation matrices $P$

**Cholesky factor with MMD**

Density: 1.5%, fill-in: 4.7

**RCM ordering**

Density: 2.7%, fill-in: 8.1
Cholesky

spam knows Cholesky!

— Several methods to construct permutation matrices \( \mathbf{P} \)

— update to perform only ‘partial’ Cholesky factors

\[
\text{update( choleskyobject, covariancematrix)}
\]

Performing the numerical decomposition only, [3]
Cholesky

spam knows Cholesky!

— Several methods to construct permutation matrices $P$
— update to perform only ‘partial’ Cholesky factors
— Passing arguments and flags for avoiding sanity checks

Using the specific call `chol.spam`

Passing `memory=list(nnzR=..., nnzcolindices=...), pivot=...`

Options `safemode=c(FALSE,FALSE,FALSE), cholsymmetrycheck=FALSE, cholpivotcheck=FALSE`
Options in spam

For “experts”, flags to speed up the code:

R> powerboost()

R> noquote( format( spam.options() ) )

<table>
<thead>
<tr>
<th>Option</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>eps</td>
<td>2.220446e-16</td>
</tr>
<tr>
<td>drop</td>
<td>FALSE</td>
</tr>
<tr>
<td>printsizhe</td>
<td>100</td>
</tr>
<tr>
<td>imagesize</td>
<td>10000</td>
</tr>
<tr>
<td>trivalues</td>
<td>FALSE</td>
</tr>
<tr>
<td>cex</td>
<td>1200</td>
</tr>
<tr>
<td>safemode</td>
<td>TRUE, TRUE, TRUE</td>
</tr>
<tr>
<td>dopivoting</td>
<td>TRUE</td>
</tr>
<tr>
<td>cholpivots</td>
<td>TRUE</td>
</tr>
<tr>
<td>cholupdatesingular</td>
<td>TRUE</td>
</tr>
<tr>
<td>cholincreasefactor</td>
<td>1.25, 1.25</td>
</tr>
<tr>
<td>nearestdistincreasefactor</td>
<td>1.25</td>
</tr>
<tr>
<td>nearestdistnnz</td>
<td>160000, 400</td>
</tr>
</tbody>
</table>
Limits of spam

What can spam not do (yet)?

- LU decompositions
- SVD/eigendecompositions
- Non-double elements
- ...

But, please, comments to reinhard.furrer@math.uzh.ch!
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Sparse Matrices in Statistics

Where do large matrices occur?

- Location matrices
- Design matrices
Sparse Matrices in Statistics

Where do large matrices occur?

- Location matrices
- Design matrices
- Covariance matrices
- Precision matrices
Sparse Matrices in Statistics

- Covariance matrices:
  Compactely supported covariance functions
  Tapering

- Precision matrices:
  (Gaussian) Markov random fields
  (Tapering???)

We have symmetric positive definite (spd) matrices.
Motivation

Precipitation anomaly along 40° lat.
Motivation

Precipitation anomaly along 40° lat.

Ordinary kriging
Motivation

Precipitation anomaly along 40° lat.

Nearest neighbor kriging with 8 observations
Motivation

Precipitation anomaly along 40° lat.

Tapering

Longitude

Anomaly

Boulder

Woodrow (156km)

Lafayette (15km)

Indianapolis (1632km)
Examples

![Graph showing covariance against lag for Exponential and Spheric models.](chart)

- **Covariance**
- **Lag**
- **Exponential**
- **Spheric**
Examples

Covariance vs Lag for Exponential, Spheric, and Exp * Spheric models.
Examples

Covariance vs. Lag

1. Exponential
   - 
   - 
2. Spheric
   - 
   - 
3. Exp * Spheric
   - 
   - 

Covariance vs. Lag

1. Matern (1.5)
   - 
   - 
2. Wendland
   - 
   -
Examples

Covariance vs Lag

- Exponential
- Spheric
- Exp * Spheric

Covariance vs Lag

- Matern (1.5)
- Wendland
- Matern * Wendland
Objective

For an isotropic and stationary process with Matérn covariance $C_0(h)$, find a taper $C_\theta(h)$, such that kriging with the product $C_0(h)C_\theta(h)$ is asymptotically optimal.
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For an isotropic and stationary process with Matérn covariance $C_0(h)$, find a taper $C_\theta(h)$, such that kriging with the product $C_0(h)C_\theta(h)$ is asymptotically optimal.

\[
\frac{\text{MSE}(x^*, C_0C_\theta)}{\text{MSE}(x^*, C_0)} \to 1
\]

\[
\frac{\varrho(x^*, C_0C_\theta)}{\text{MSE}(x^*, C_0)} \to \gamma
\]

\[
\varrho(x^*, C) = C(0) - c^T C^{-1} c^*
\]
Misspecified Covariances

In a series of (Annals) papers, Stein gives asymptotic results for misspecified covariances.

Under appropriate conditions, tapering is a form of misspecification.

The taper has to be

- as differentiable at the origin as the original covariance
- more differentiable throughout the domain than at the origin
Tapering

Tapering is an (asymptotically and computationally) efficient technique to create sparse covariance matrices.

Taper range can be justified by computing resources. However, 20–30 locations within the taper range is often sufficient.

“Classical” tapers are:

- spherical: $C_\theta(h) = \left(1 - \frac{|h|}{\theta}\right)^2 \left(1 + \frac{|h|}{\theta}\right)$

- Wendland-type: $C_\theta(h) = \left(1 - \frac{|h|}{\theta}\right)^{\ell+k} \cdot \text{polynomial in } \frac{|h|}{\theta} \text{ of deg } k$
Positive Definite Matrices

A (large) covariance (often) appears in:

- drawing from a multivariate normal distribution
- calculating/maximizing the (log-)likelihood
- linear/quadratic discrimination analysis
- PCA, EOF, . . .

But all boils down to solving a linear system and possibly calculating the determinant . . .

‘Sparse PCA’ is sparse in a different sense . . .
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Sparse Matrices and fields

- fields is not bound to a specific sparse matrix format

- All heavy lifting is done in mKrig or Krig.engine.fixed

- For a specific sparse format, requires the methods: chol, backsolve, forwardsolve and diag as well as elementary matrix operations need to exist

- If available uses operators to handle diagonal matrices quickly

⇝ The covariance matrix has to stem from particular class.
Sparse Matrices and fields

- fields is not bound to a specific sparse matrix format
- All heavy lifting is done in mKrig or Krig.engine.fixed
- For a specific sparse format, requires the methods: chol, backsolve, forwardsolve and diag as well as elementary matrix operations need to exist
- If available uses operators to handle diagonal matrices quickly

⇝ The covariance matrix has to stem from particular class.

fields uses spam as default package!
**Example mKrig**

With appropriate covariance function:

```r
R> x <- USprecip[ precipsubset, 1:2] # locations
R> Y <- USprecip[ precipsubset, 4] # anomaly

R> out <- mKrig(x,Y, m=1, cov.function="wendland.cov",theta=1.5)

R> out.p <- predict.surface( out, nx=220, ny=120)
R> surface(out.p, type='I')
R> US(add=T)
R> points(x,pch='.')
```
Example mKrig
Example Krig

R> out <- Krig( x,Y, m=1, cov.function="wendland.cov",theta=1.5,
+ lambda=0)

R> out.q <- predict.surface( out, nx=220, ny=120)

R> sum( ( out.q$z-out.p$z)^2, na.rm=T)
[1] 1.616783e-20

Krig/predict is slower (here 2.1/3.7 vs 10.4/3.9 seconds).
Wendland family

wendland.cov (based on Wendland) produces a spam matrix. All matrix functions are appropriately overloaded . . .

To create sparse covariance matrices based on other covariance functions, use wendland.cov as skeleton.
Tapering can be performed with stationary.taper.cov.
Arguments are (selection):

Covariance = "Exponential"

Taper = "Wendland"

Taper.args = NULL: arguments for the taper function

Dist.args = NULL: arguments passed to nearest.dist

... : arguments passed to covariance function

All arguments can also be passed from mKrig/Krig
Tapering

Compare the predicted surfaces without and with tapering:

R> out1 <- mKrig( x, y, m=1, theta=1.5 )
R> out1.p <- predict.surface( out1, nx=220, ny=120 )

R> out2 <- mKrig( x, y, m=1, theta=1.5,
+ cov.function="stationary.taper.cov",
+ Taper.args = list(k=0, theta=3))
R> out2.p <- predict.surface( out2, nx=220, ny=120 )

(timing yields 4/22 and 1/9 seconds)
Tapering

Exponential covariance

and with tapering
Tapering

Exponential covariance and with tapering
Asides . . .

The following arguments of mKrig/Krig are linked to spam:

- Dist.args: arguments passed to nearest.dist
- chol.args: arguments passed to chol

Use their help for fine tuning.

predict.se.Krig, predict.surface.se.Krig are very inefficient because nrow(x) equations need to be solved.
How Big is Big?

Upper limit to create a large matrix is the minimum of:

(1) available memory (machine and OS/shell dependent)
   Error: 'cannot allocate vector of size'

(2) addressing capacity \((2^{31} - 1)\)
   Error: 'cannot allocate vector of length'

However, R is based on passing by value, calls create local copies
(often 3–4 times the space of the object is used).

R> help("Memory-limits")
And Beyond?

Parallelization:
nws, snow, Rmpi, ...

Memory “Outsourcing”:
Matrices are not (entirely) kept in memory:
ff, filehash, biglm, ...

(S+ has the library BufferedMatrix)
References

