

Sparse Matrices and Large Data Issues

Workshop ENAR

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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.

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Sparse Matrices

What is “sparse” or a sparse matrix?

According to Wiktionary/Wikipedia:

Sparse: (Adjective)

1. *Having widely spaced intervals*
2. *Not dense; meager*

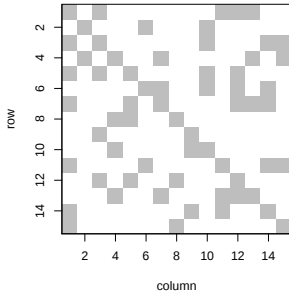
Sparse matrix:

a matrix populated primarily with zeros.

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Sparse Matrices

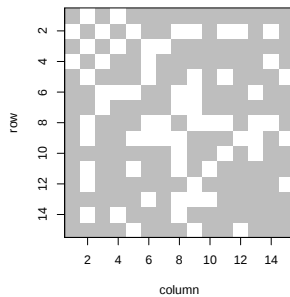
```
R> n <- 15
R> A <- array( runif(n^2), c(n,n)) + diag(n)
R> A[A < 0.75] <- 0
```



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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
```



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Sparse Matrices

Why should we use sparse matrices?

1. Savings in storage
nonzeros vs total elements
2. Savings in computing time
0.066s vs 0.003 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.

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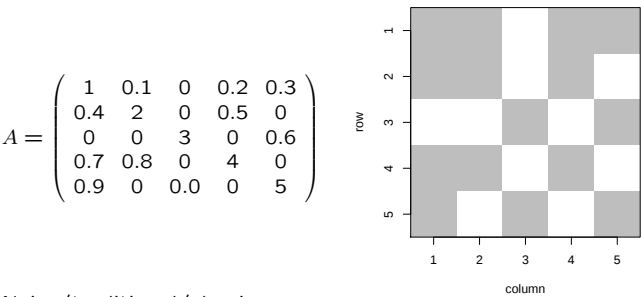
Storage Formats

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

- 1. Naive/ "traditional" /classic format:
one vector of length $n \times m$ and a dimension attribute.
- 2. Triplet format:
three vectors of length z , (i, j, a_{ij}) and a dimension attribute.
- 3. Compressed sparse row (CSR) format:
eliminate redundant row indices.
- 4. and about 10 more ...

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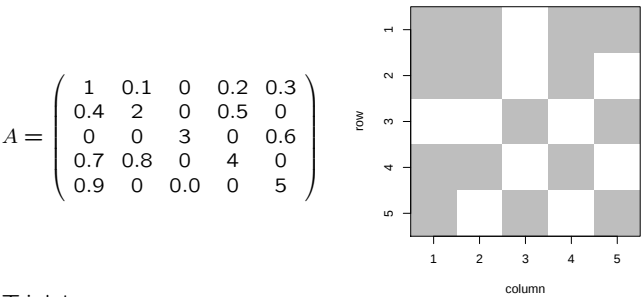
Storage Formats, Example



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

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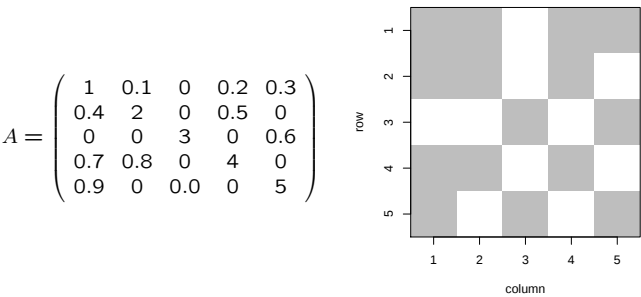
Storage Formats, Example



Triplet:
 $i :$ 1 1 1 1 2 2 2 3 3 4 4 4 5 5 5
 $j :$ 1 2 4 5 1 2 4 2 3 1 2 4 1 3 5
 $a_{ij} :$ 1 .1 .2 .3 .4 2 .5 3 .6 .7 .8 4 .9 .0 5

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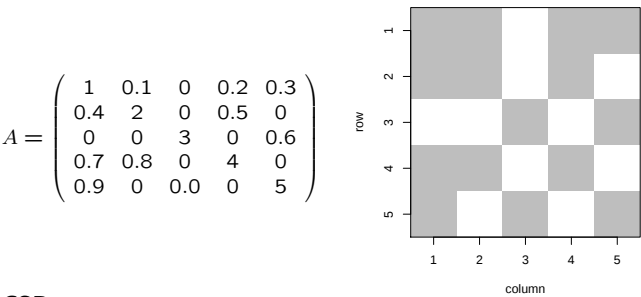
Storage Formats, Example



$i :$	1	2	3	4	5
$j :$	1 2 4 5	1 2 4	2 3	1 2 4	1 3 5
$a_{ij} :$	1 .1 .2 .3 .4	2 .5	3 .6	.7 .8 4	.9 .0 5

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Storage Formats, Example



CSR:														
$ptr :$	1	5	8	10	13	16								
$j :$	1 2 4 5	1 2 4	2 3	1 2 4	1 3 5									
$a_{ij} :$	1 .1 .2 .3 .4	2 .5	3 .6	.7 .8 4	.9 .0 5									

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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:														
$ptr :$	1	5	8	10	13	16								
$j :$	1 2 4 5	1 2 4	2 3	1 2 4	1 3 5									
$a_{ij} :$	1 .1 .2 .3 .4	2 .5	3 .6	.7 .8 4	.9 .0 5									

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(Dis)Advantages

1. Naive format:
 - No savings in storage and computation (for sparse matrices)
 - Status quo
2. Triplet format:
 - Savings in storage and computation for sparse matrices
 - Loss in storage and computation for full matrices
 - 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)

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Implications

With a new storage format new "algorithms" are required ...

Is it worthwhile???

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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 <- somecalltomagicfunctiontogetsparseformat( A)
```

Compare timing for different operations on A and S.

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Timing

```
R> timing( A + sqrt(A) )
[1] 0.058
R> timing( S + sqrt(S) )
[1] 0.061

R> timing( AtA <- t(A) %*% A )
[1] 0.467
R> timing( StS <- t(S) %*% S )
[1] 4.222
```

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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
```

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Timing

```
R> timing( xA <- solve(AtA, rep(1,n)) )
[1] 1.116
R> timing( xS <- solve(StS, rep(1,n)) )
[1] 1.51

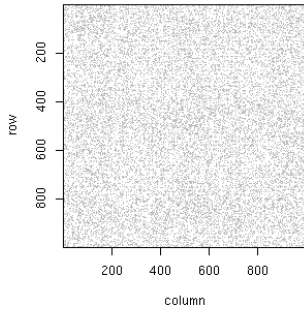
R> timing( RA <- chol(AtA) )
[1] 0.488
R> timing( RS <- chol(StS) )
[1] 1.504
```

Is it really worthwhile? What is going on?

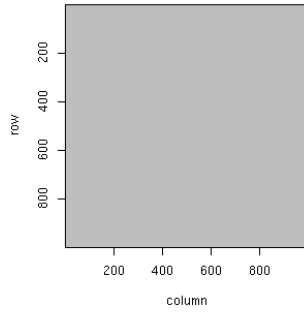
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Timing

Matrix S



Matrix StS



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Timing

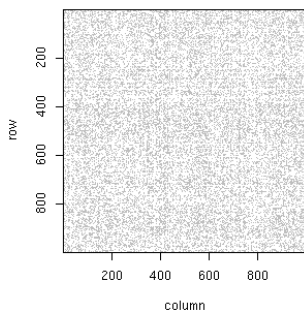
With cutoff 0.99:

```
R> timing( AtA <- t(A) %*% A )  
[1] 0.106  
R> timing( StS <- t(S) %*% S )  
[1] 0.089  
  
R> timing( RA <- chol(AtA) )  
[1] 0.494  
R> timing( RS <- chol(StS) )  
[1] 0.451
```

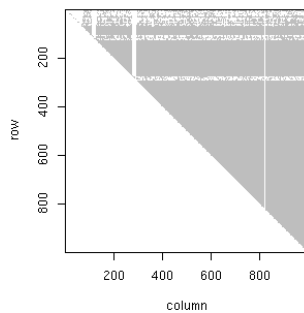
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Timing

Matrix StS



Matrix chol(StS)



Density of the factor is 41% with fill-in ratio 7.2.

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Timing

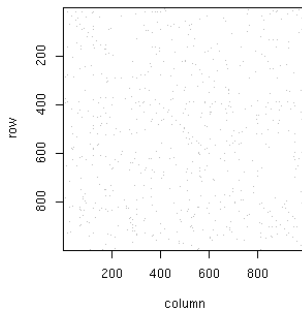
With cutoff 0.999:

```
R> timing( AtA <- t(A) %*% A )  
[1] 0.059  
R> timing( StS <- t(S) %*% S )  
[1] 0.002  
  
R> timing( RA <- chol(AtA) )  
[1] 0.466  
R> timing( RS <- chol(StS) )  
[1] 0.007
```

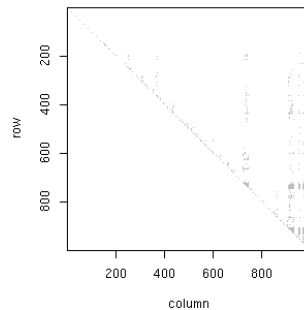
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Timing

Matrix StS



Matrix chol(StS)



Density of the factor is .6% with fill-in ratio 2.3.

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Implications

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

Is it worthwhile??? [Yes!](#)

Especially since

[spam](#): R package for sparse matrix algebra.

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What is spam?

- an R package for [sparse matrix algebra](#)
 - publicly available from CRAN, 0.15-3
 - platform independent and documented
- 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
- versatile, intuitive and simple
 - wrap an `as.spam( )` and go
 - S4 and S3 syntax
- situated between `SparseM` and `Matrix`

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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"
```

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Representation of Sparse Matrices

```
R> A
      [,1] [,2] [,3] [,4] [,5]
[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
```

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Creating Sparse Matrices

Similar coercion techniques as with `matrix`:

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

Special functions:

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

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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`;

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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)
```

Precision matrix (GMRF):

- regular grids: `nearest.dist` with different cutoffs

```
R> diag.spam(n) +  
+   (b1-b2) * nearest.dist(x, delta=1, upper=NULL) +  
+   b2 * nearest.dist(x, delta=sqrt(2), upper=NULL)
```
- irregular grids: using incidence list and `spam`

```
R> incidence <- list( i=..., j=..., values)  
R> C <- spam( incidence, n, n)
```

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Solving Linear Systems

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

To solve the system $\mathbf{Ax} = \mathbf{b}$, we

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

But we need to “ensure” that $\mathbf{U}$ is as sparse as possible!

Permute the rows and columns of $\mathbf{A}$: $\mathbf{P}^T \mathbf{A} \mathbf{P} = \mathbf{U}^T \mathbf{U}$.

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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
-

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Cholesky

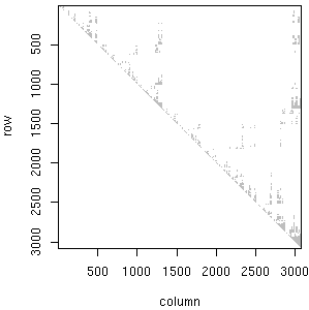
`spam` knows Cholesky!

- Several methods to construct permutation matrices $\mathbf{P}$
- `update` to perform only ‘partial’ Cholesky factors
- Flags for avoiding sanity checks

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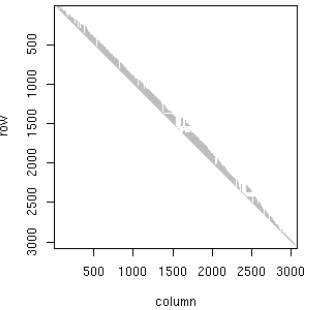
Cholesky

Cholesky factor with MMD



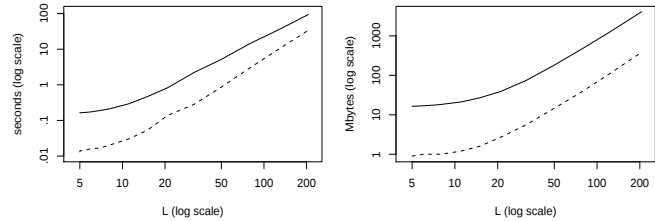
Density: 1.5%, fill-in: 4.7

RCM ordering



Density: 2.7%, fill-in: 8.1

Cholesky



Time and memory usage for 101 Cholesky factorizations (solid) and one factorization and 100 updates (dashed) of a precision matrix from different sizes L of regular $L \times L$ grids with a second order neighbor structure. (The precision matrix from $L = 200$ has $L^4 = 1.6 \cdot 10^9$ elements). See also `demo( "article-jss"`).

Cholesky

Gain of time and memory usage with different options and arguments in the case of a second order neighbor structure of a regular 50×50 grid and of the US counties. The time and memory usage for the generic call `chol` are 6.2 seconds, 174.5 Mbytes and 15.1 seconds, 416.6 Mbytes, respectively.

Options or arguments	Regular grid		US counties	
	time	memory	time	memory
Using the specific call <code>chol.spam</code>	1.001	0.992	0.954	1.004
Option <code>safemode=c(FALSE,FALSE,FALSE)</code>	0.961	1.002	0.988	0.997
Option <code>cholsymmetrycheck=FALSE</code>	0.568	0.524	0.646	0.493
Passing <code>memory=list(nnzR=..., nnzcolindices=...)</code>	0.969	0.979	0.928	0.972
All of the above	0.561	0.508	0.618	0.490
All of the above and passing <code>pivot=...</code> to <code>chol.spam</code>	0.542	0.528	0.572	0.496
All of the above and option <code>cholpivotcheck=FALSE</code>	0.510	0.511	0.557	0.489
Numeric update only using <code>update</code>	0.132	0.070	0.170	0.063

Cholesky

BTW:

efficient Cholesky factorization $\iff$ efficient determinant calculation:

$$\det(\mathbf{C}) = \det(\mathbf{U}^T) \det(\mathbf{U}) = \prod_{i=1}^n \mathbf{u}_{ii}^2$$

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Options in spam

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

```
R> powerboost() # in spam_0.15-4
```

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

eps	drop	printsize
2.220446e-16	FALSE	100
imagesize	trivalues	cex
10000	FALSE	1200
safemode	dopivoting	cholsymmetrycheck
TRUE, TRUE, TRUE	TRUE	TRUE
cholpivotcheck	cholupdatesingular	cholincreasefactor
TRUE	warning	1.25, 1.25
nearestdistincreasefactor	nearestdistnnz	
1.25	160000, 400	

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Limits of spam

What can spam not do (yet)?

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

But, please, comments to rfurrer@mines.edu!

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Sparse Matrices in Statistics

Where do large matrices occur?

- Location matrices
- Design matrices
- Covariance matrices
- Precision matrices

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Sparse Matrices in Statistics

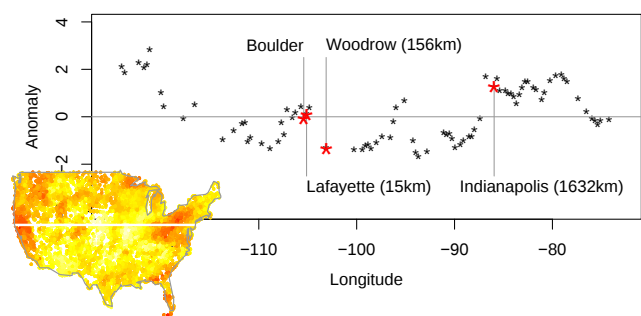
- Covariance matrices:
Compactly supported covariance functions
Tapering
- Precision matrices:
(Gaussian) Markov random fields
(Tapering???)

We have symmetric positive definite (spd) matrices.

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Motivation

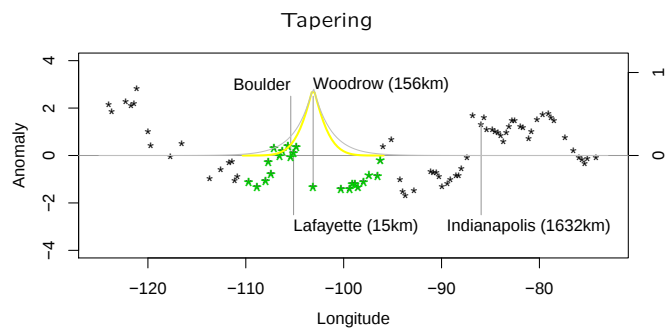
Precipitation anomaly along 40° lat.



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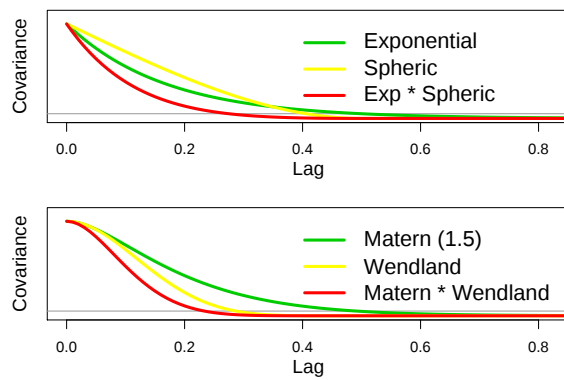
Motivation

Precipitation anomaly along 40° lat.



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Examples



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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**.

$$\frac{\text{MSE}(\mathbf{x}^*, C_0 C_\theta)}{\text{MSE}(\mathbf{x}^*, C_0)} \rightarrow 1 \quad \frac{\varrho(\mathbf{x}^*, C_0 C_\theta)}{\text{MSE}(\mathbf{x}^*, C_0)} \rightarrow \gamma$$

$$\varrho(\mathbf{x}^*, C) = C(0) - \mathbf{c}^{*T} \mathbf{C}^{-1} \mathbf{c}^*$$

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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

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

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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.

`fields` uses `spam` as default package!

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Example `mKrig`

With appropriate covariance function:

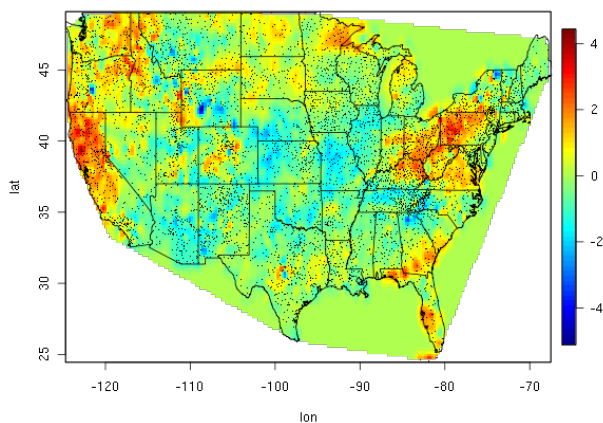
```
R> x <- USprecip[ precipsubset, 1:2] # locations
R> Y <- USprecip[ precipsubset, 4]   # anomaly

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='.')
R>
```

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Example `mKrig`



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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)

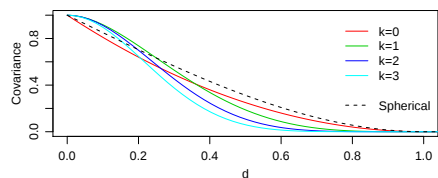
R> sum( ( out.q$z-out.p$z)^2, na.rm=T)
[1] 1.616783e-20
```

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

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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.

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Tapering

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

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Tapering

Compare the predicted surfaces without and with tapering:

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

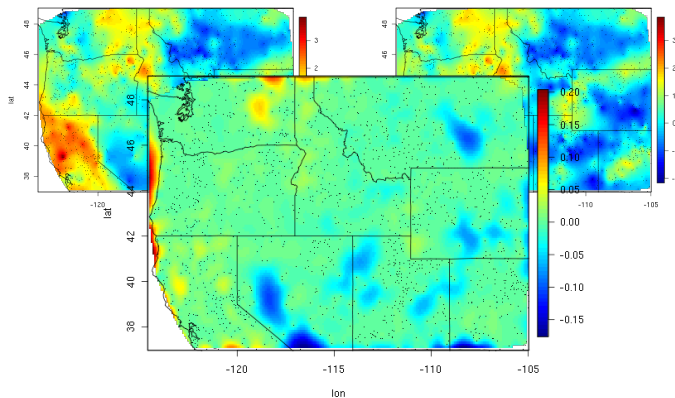
R> out2 <- mKrig( xr,Yr, m=1, theta=1.5,
+               cov.function="stationary.taper.cov",
+               Taper.args = list(k=0, theta=3))
R> out2.p <- predict.surface( out2, nx=220, ny=120 )
```

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

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Tapering

Exponential covariance and with tapering



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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.

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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")
```

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And Beyond?

Parallelization:

`nws`, `snow`, `Rmpi`, ...

Memory “Outsourcing”:

Matrices are not (entirely) kept in memory:

`ff`, `filehash`, `biglm`, ...

(S+ has the library `BufferedMatrix`)

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References

Furrer, R., Genton, M. G. and Nychka, D. (2006). Covariance Tapering for Interpolation of Large Spatial Datasets. *Journal of Computational and Graphical Statistics*, 15(3), 502–523.

Furrer, R. and Sain, S. R. (2009). Spatial Model Fitting for Large Datasets with Applications to Climate and Microarray Problems. *Statistics and Computing*, 19(2), 113–128, doi:10.1007/s11222-008-9075-x.

Furrer, R. and Sain, S. R. (2008). `spam`: A Sparse Matrix R Package with Emphasis on MCMC Methods for Gaussian Markov Random Fields. Submitted.

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