Sparse Matrix Techniques for Interpolation of Large Environmental and Biological Datasets

February 8, UCDHCS

Tapering and Kriging

Introduce a sparseness structure in the covariance via tapering to gain computational advantages in large interpolation problems constraint to maintaining asymptotic optimality.

In collaboration with
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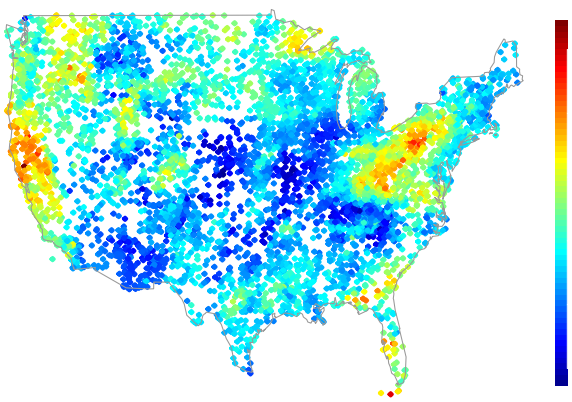
and Steve Sain (CUD)

Motivation

Precipitation anomaly in April 1948



Best Linear Unbiased Predictor

Suppose a spatial process of the form

$$Z(\mathbf{x}) = \mathbf{m}(\mathbf{x})^{\mathsf{T}}\beta + \varepsilon(\mathbf{x}), \quad \mathrm{E}(\varepsilon) = \mathbf{0}, \quad \mathrm{Cov}(\varepsilon) = \mathbf{C}$$

with observations $\mathbf{Z} = \big(Z(\mathbf{x}_1), \ldots, Z(\mathbf{x}_n)\big)^{\mathsf{T}}$, $\mathbf{x}_i \in \mathcal{D} \subset \mathbb{R}^d$.

The kriging estimator (BLUP) is

$$\hat{Z}(\mathbf{x}_0) = \lambda^{\mathsf{T}}\mathbf{Z} = \mathbf{c}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{Z}$$

where

$$\lambda = \mathbf{C}^{-1}\Big(\mathbf{I} - \mathbf{M}(\mathbf{M}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{M})^{-1}\big(\mathbf{M}^{\mathsf{T}}\mathbf{C}^{-1}\mathbf{c} - \mathbf{m}(\mathbf{x}_0)\big)\Big) = \mathbf{C}^{-1}\mathbf{c}$$

with $\mathbf{c}_i = \mathrm{Cov}\big(Z(\mathbf{x}_0), Z(\mathbf{x}_i)\big)$, and $\mathbf{M} = (\mathbf{m}(\mathbf{x}_1), \ldots, \mathbf{m}(\mathbf{x}_n)^{\mathsf{T}}$.

Motivation

Prediction at a large number of points involves either

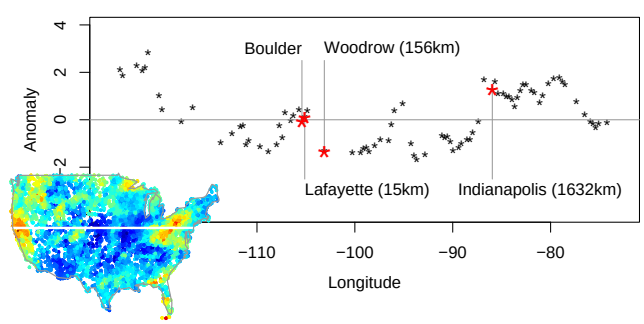
- solving one large linear system,
- solving many tiny linear systems

or, being smarter and

- "approximating" the covariance and solving "efficiently" one large linear system.

Motivation

Easy to think in one dimension: precipitation anomaly along 40° lat.



Motivation

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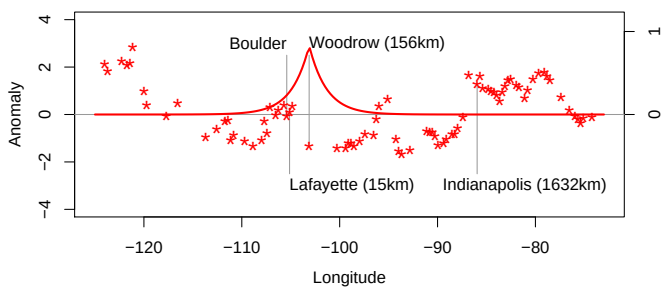
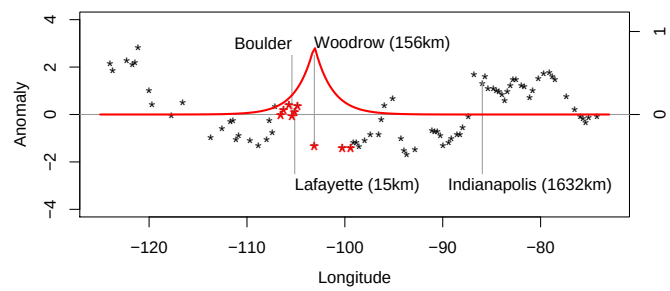
Ordinary kriging



Motivation

Easy to think in one dimension: precipitation anomaly along 40° lat.

Nearest neighbor kriging with 8 observations



Motivation

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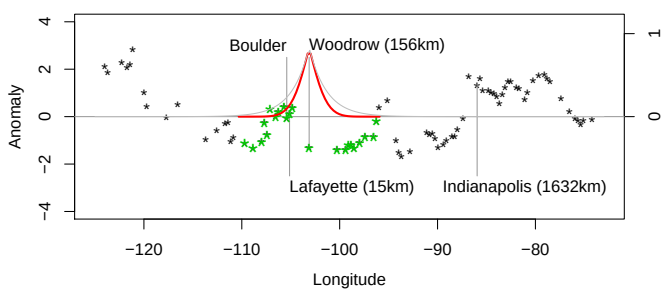
Tapering



Objective

For an isotropic and stationary process
with 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.

$$\frac{\mathrm{MSE}(\mathbf{x}^*, C_0C_\theta)}{\mathrm{MSE}(\mathbf{x}^*, C_0)} \to 1 \qquad \frac{\varrho(\mathbf{x}^*, C_0C_\theta)}{\mathrm{MSE}(\mathbf{x}^*, C_0)} \to \gamma$$

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

Matérn Covariance

We need a broad, flexible class of covariances to describe spatial processes.

Matérn class covariance

$$C_{\alpha,\nu}(h) \propto \left(\alpha h\right)^{\nu}\mathcal{K}_{\nu}\left(\alpha h\right) \qquad h = \|\mathbf{h}\|$$

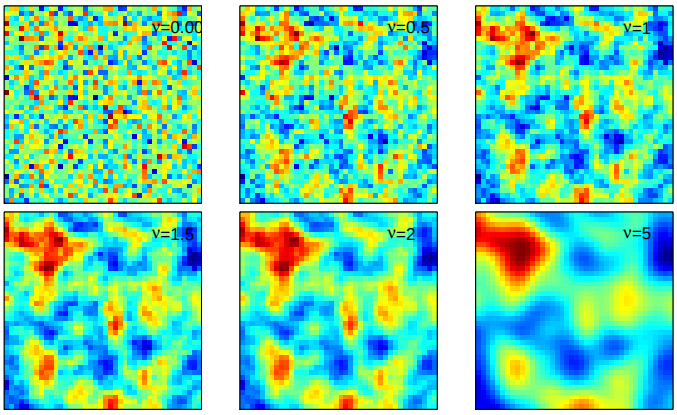
and spectral density

$$f_{\alpha,\nu}(\rho) \propto \frac{1}{\left(\alpha^2+\rho^2\right)^{\nu+d/2}} \qquad \rho = \|\boldsymbol{\omega}\|$$

Differentiability at the origin of the covariance is related to the tail behavior of the spectrum, i.e. the smoothness of the process.

The process is m times mean squared differentiable iff $m < \nu$.

Matérn Covariance



Taper Functions

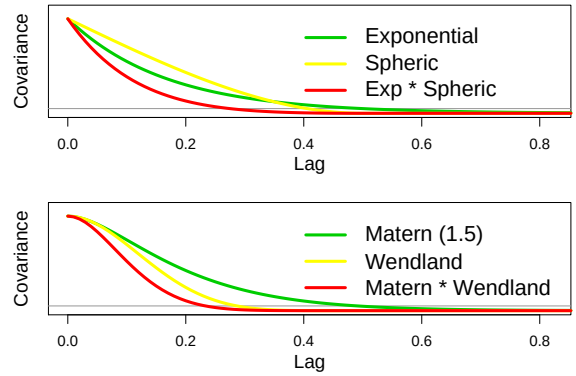
We impose on the taper C_θ the conditions

- C_θ is a positive definite function in $\mathbb{R}^d$
- $C_\theta(h) = 0$ for $h > \theta$

For example:

- triangular: $C_\theta(h) = \left(1 - \frac{|h|}{\theta}\right)_+$ $\qquad (x)_+ = \max(0, x)$
- spherical: $C_\theta(h) = \left(1 - \frac{|h|}{\theta}\right)_+^2 \left(1 + \frac{|h|}{\theta}\right)$
- Wendland-type: $C_\theta(h) = \left(1 - \frac{|h|}{\theta}\right)_+^{\ell+k} \cdot$polynom in $\frac{|h|}{\theta}$ of deg k

Examples



Misspecified Covariances

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

Suppose the true covariance C_0 and spectrum f_0. If we krig with the misspecified covariance C_1 characterized by f_1 then under the **Tail Condition**

$$\frac{f_1(\omega)}{f_0(\omega)} = \gamma \quad 0 < \gamma < \infty \quad \text{as } \|\omega\| \to \infty \qquad \text{and } \ldots$$

we have asymptotic optimality

$$\frac{\mathrm{MSE}(\mathbf{x}^*, C_1)}{\mathrm{MSE}(\mathbf{x}^*, C_0)} \to 1 \qquad \frac{\varrho(\mathbf{x}^*, C_1)}{\mathrm{MSE}(\mathbf{x}^*, C_0)} \to \gamma$$

Tapered Covariances

Tapering is a form of misspecification if

$$\frac{\mathcal{F}\big(C_{\alpha,\nu}(h) C_\theta(h)\big)}{\mathcal{F}\big(C_{\alpha,\nu}(h)\big)} \to \gamma \text{ as } \|\omega\| \to \infty$$

Which taper satisfies this condition?

The taper has to be

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

Taper Theorem

Infill Condition: *Let* $\mathbf{x}^* \in \mathcal{D}$ *and* $\mathbf{x}_1, \mathbf{x}_2, \ldots$ *be a dense sequence in* $\mathcal{D}$.

Taper Condition: *Let* f_θ *be the spectral density of the taper covariance,* C_θ*, and for some* $\epsilon > 0$ *and* $M < \infty$

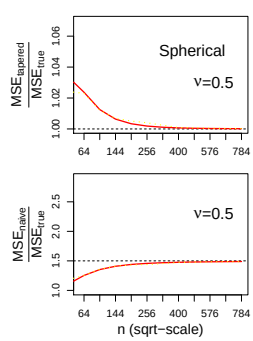
$$f_\theta(\rho) < \frac{M}{(1 + \rho^2)^{\nu + d/2 + \epsilon}}$$

Taper Theorem: *Assume that* $C_{\alpha,\nu}$ *is a Matérn covariance with smoothness parameter* ν *and the Infill and Taper Conditions hold. Then*

$$\lim_{n\to\infty} \frac{\mathrm{MSE}(\mathbf{x}^*, C_{\alpha,\nu} C_\theta)}{\mathrm{MSE}(\mathbf{x}^*, C_{\alpha,\nu})} = 1 \qquad \lim_{n\to\infty} \frac{\varrho(\mathbf{x}^*, C_{\alpha,\nu} C_\theta)}{\mathrm{MSE}(\mathbf{x}^*, C_{\alpha,\nu})} = 1 (= \gamma)$$

Simulation Study

When does infill asymptotics kick in?

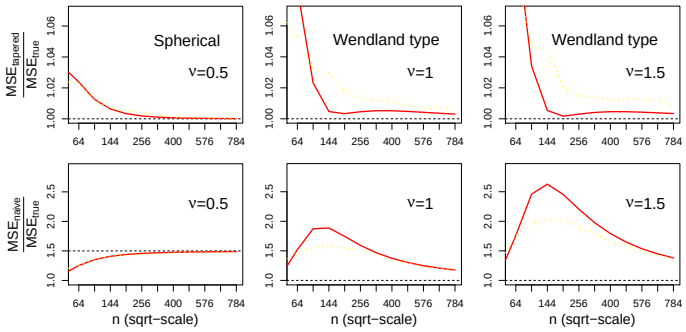


Simulation setup:

- n equispaced or random (100 samples) observations in $[0, 1]^2$
- $C_{\alpha,\nu}$: Matérn covariance, eff. range 0.4
- C_θ: spherical and Wendland-type, range $\theta = 0.4$
- prediction on $(0.5, 0.5)$.

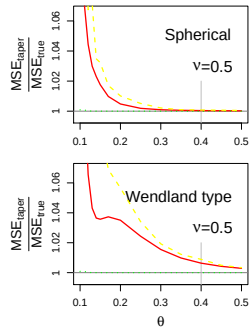
Simulation Study

When does infill asymptotics kick in?



Simulation Study

What is an efficient taper?

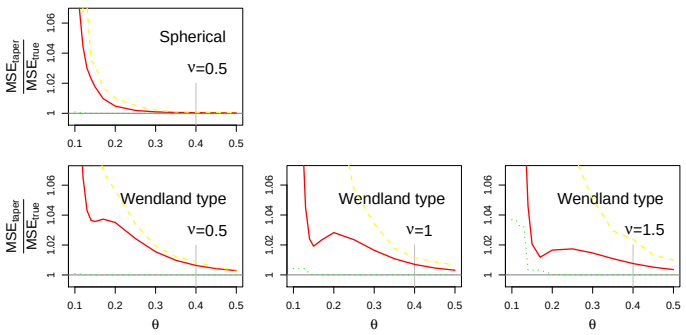


Simulation setup:

- $n = 400$ equispaced or random observations in $[0,1]^2$
- $C_{\alpha,\nu}$: Matérn covariance, eff. range 0.4
- C_θ: spherical, Wendland-type, range θ
- NN-kriging with neighborhood θ
- prediction on $(0.5, 0.5)$.

Simulation Study

What is an efficient taper?



Recap

To summarize we have discussed

- the BLUP, requiring solutions of linear systems
  $\rightsquigarrow$ one point $\mathbf{c}^\mathsf{T}\mathbf{C}^{-1}\mathbf{Z}$, field $\widetilde{\mathbf{C}}^\mathsf{T}\mathbf{C}^{-1}\mathbf{Z}$
- optimal covariances, decay exponentially
  $\rightsquigarrow$ no zeros in $\mathbf{C}$, $\mathbf{c}$ or $\widetilde{\mathbf{C}}$
- that tapering preserves optimality,
  $\rightsquigarrow$ covariance matrices are sparse

Is there a computational gain?

Computational Efficiency

To solve the system $\mathbf{Cx} = \mathbf{Z}$, we

- perform a Cholesky factorisation $\mathbf{C} = \mathbf{LL}^\mathsf{T}$
- solve two triangular systems $\mathbf{Lu} = \mathbf{Z}$ and $\mathbf{L}^\mathsf{T}\mathbf{x} = \mathbf{u}$

Use a special format to store sparse matrices:

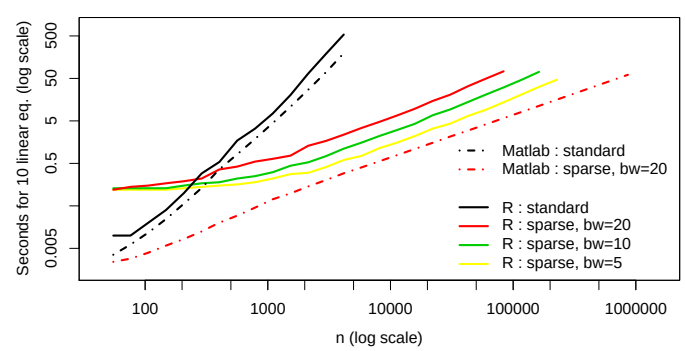
$$8z + 4z + 4n + 1 \text{ bytes} \quad \text{vs} \quad 8 \times n^2 \text{ bytes}$$

and $z \approx n \times \#$ tapered neighbors.

The Cholesky factor of a sparse matrix "is" sparse.

Matlab and R contain a toolbox and libraries (SparseM and KriSp).

Computational Efficiency

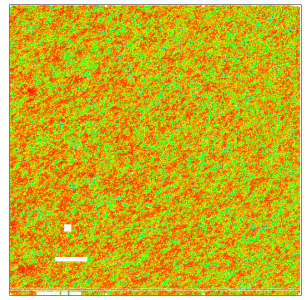


Computational Efficiency

Linux powered 2.6 GHz Xeon processor with 2 Gbytes RAM.
R with KriSp, SparseM, Fields and Base libraries.

Action		Time (sec) Classic	Classic optim.	Sparse	Sparse +FFT
Reading data, variable setup		0.54	0.54	0.54	0.54
Creating the matrix $\mathbf{C}$		41.34	21.59	6.35	6.35
Solving $\mathbf{Cx} = \mathbf{Z}$	Cholesky	169.09	169.09	0.28	0.28
	Backsolve	6.13	6.13	0.03	0.03
Multiplying $\tilde{\mathbf{C}}^{\mathsf{T}}$ with $\mathbf{C}^{-1}\mathbf{Z}$		4638.01	1830.86	733.82	26.99
Creating the figure		6.19	6.19	6.19	6.19
Total		**1.4h**	**34min**	**12min**	**41sec**

Application: Microarrays



Building a profile of differentially expressed genes relating to cerebral vascular malformation
(Shenkar et al., Neurosurgery, 2003)

Application: Microarrays

Additive mixed-effects "spatial" process:

$$\mathbf{Y} = \text{fixed effects} + \text{remaining random structure}$$
$$= \mathbf{X}\beta + \mathbf{h} + \varepsilon$$

where $\mathbf{h}$ represents a random, zero-mean spatial process
ε represents a random error process orthonormal to $\mathbf{h}$
$\mathbf{X}$ includes chip specific and gene specific (across chip) terms

$$\mathbf{X} = \begin{bmatrix} \mathbf{1\,R\,C} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{G} \\ \mathbf{0} & \mathbf{1\,R\,C} & & \vdots & \vdots \\ \vdots & & \ddots & \mathbf{0} & \vdots \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{1\,R\,C} & \mathbf{G} \end{bmatrix}$$

where $\mathbf{R}$ and $\mathbf{C}$ represent row and column effects
$\mathbf{G}$ indicate gene effects

Application: Microarrays

Additive mixed-effects "spatial" process:

$$\begin{array}{ccccccccc} \mathbf{Y} & = & & & & \mathbf{X} & \beta & + & \mathbf{h} & + & \varepsilon \end{array}$$

$$\begin{bmatrix} \mathbf{Y}_1 \\ \vdots \\ \mathbf{Y}_k \end{bmatrix} = \begin{bmatrix} \mathbf{1\,R\,C} & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{G} \\ \mathbf{0} & \mathbf{1\,R\,C} & & \vdots & \vdots \\ \vdots & & \ddots & \mathbf{0} & \vdots \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{1\,R\,C} & \mathbf{G} \end{bmatrix} \begin{bmatrix} \beta_{\text{Chip }1} \\ \vdots \\ \beta_{\text{Chip }k} \\ \beta_{\text{Gene}} \end{bmatrix} + \begin{bmatrix} \mathbf{h}_{\text{Chip }1} \\ \vdots \\ \mathbf{h}_{\text{Chip }k} \end{bmatrix} + \begin{bmatrix} \epsilon_{\text{Chip }1} \\ \vdots \\ \epsilon_{\text{Chip }k} \end{bmatrix}$$

Estimation via backfitting:

estimate iteratively $\begin{cases} \text{fixed effects } \beta \text{ (regression step)} \\ \text{the spatial process } \mathbf{h} \text{ (kriging step)} \end{cases}$

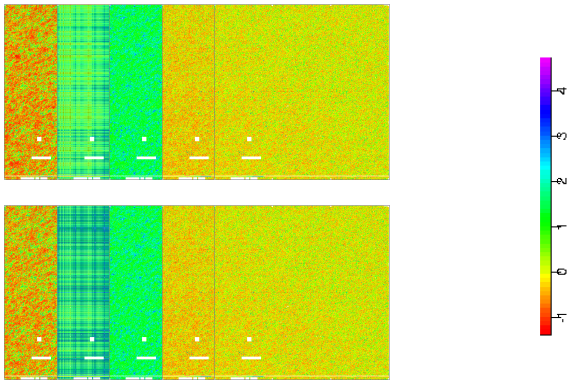
Application: Microarrays

$\mathbf{Y}$ − mean = row effects + column effects + spatial process + gene effects + error

Chip 1

Difference

Chip 2



Discussion

Completed:

- Efficient methodological approach
- Spatial models with drift and/or nugget effect
- Rule of thumb: 16–24 observation in taper range

In progress:

- Relate the tail behavior of the spectrum and the behavior at the origin of the covariance
- Apply to other statistical problems, like microarrays

In prospection:

- Nonstationarity, MLE, ...