Covariance Tapering for Interpolation of Large Spatial Datasets

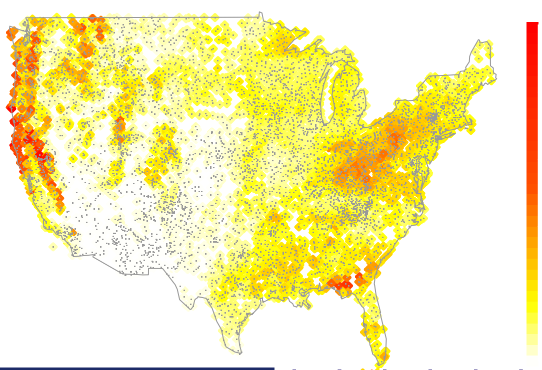
Tapering and Kriging

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

In collaboration with Marc Genton and Doug Nychka.

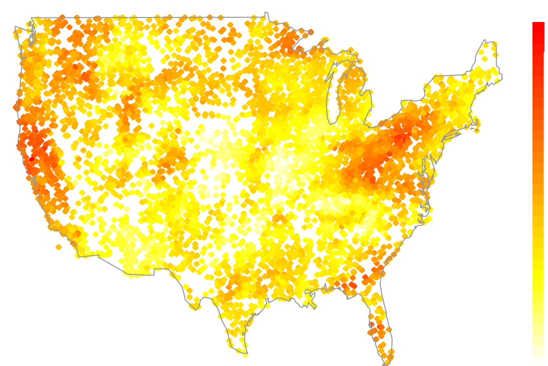
Motivation

Monthly aggregated precipitation in April 1948



Motivation

Precipitation anomaly in April 1948



Best Linear Unbiased Predictor

Suppose a spatial process of the form

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

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

The kriging estimator (BLUP) is

$$\widehat{Z}(\mathbf{x}_0) = \lambda^{\mathsf{T}}\mathbf{Z}$$

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

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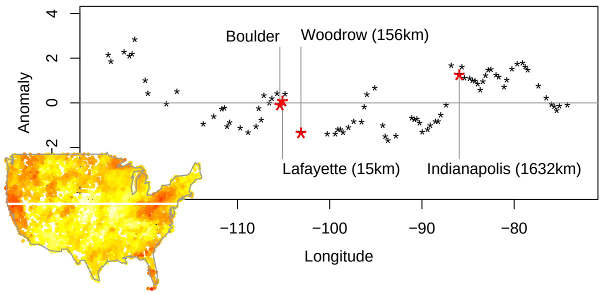
Motivation

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



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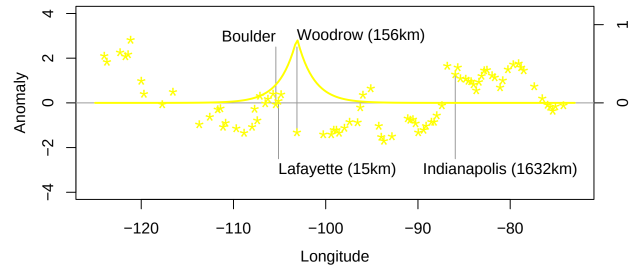
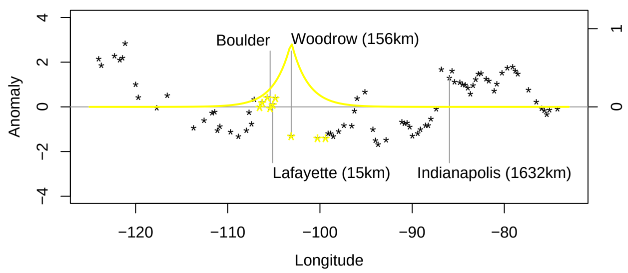
Ordinary kriging



Motivation

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

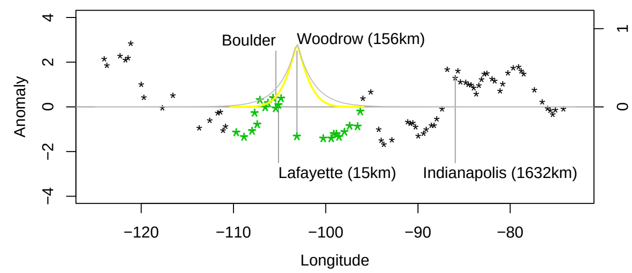
Nearest neighbor kriging with 8 observations



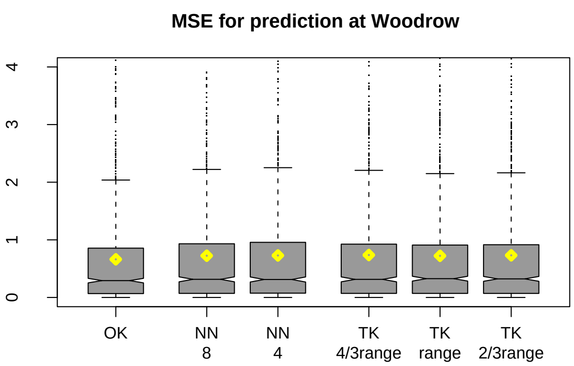
Motivation

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

Tapering with 4/3 range



Numerical Study



We Aim for . . .

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.

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

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

Matérn Covariance

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

Matérn class covariance

$$C_{\alpha,\nu}(h) \propto \big(\alpha h\big)^{\nu} \mathcal{K}_{\nu}\big(\alpha h\big), \quad h = \|\mathbf{h}\|$$

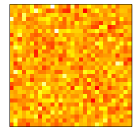
and spectral density

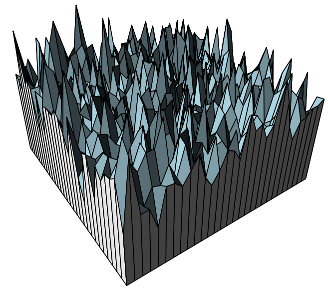
$$f_{\alpha,\nu}(\rho) \propto \frac{1}{\big(\alpha^2 + \rho^2\big)^{\nu + d/2}} \quad \rho = \|\boldsymbol{\omega}\|$$

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 $m < \nu$.

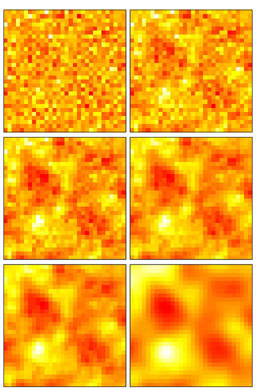
Matérn Covariance

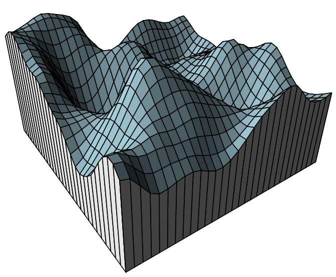




$\nu = 0.0$ (white noise)
effective range is 0.2

Matérn Covariance





$\nu = 5.0$
effective range is 0.2

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: $C_\theta(h) = \max\big(0, \frac{|h|}{\theta}\big)$
- spherical: $C_\theta(h) = \max\big(0, \frac{|h|}{\theta}\big)^2\big(1 + \frac{|h|}{\theta}\big)$
- Wu-type: $C_\theta(h) = \max\big(0, \frac{|h|}{\theta}\big)^{2k} \times$polynom in $\frac{|h|}{\theta}$ of degree $2k - 1$

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

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

we have asymptotic optimality

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

Tapered Covariances

Tapering is a form of misspecification if

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

Which taper satisfies this condition?

The taper
- has to be as differentiable at the origin as the original covariance
- has to be more differentiable throughout the domain than at the origin
- may be inflated to correct for the factor γ

Taper Theorem

Infill Condition: *Let* $\mathbf{x}^* \in \mathcal{D}$ *and* $\mathbf{x}_1, \mathbf{x}_2, \dots$ *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*

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

Conditions in Terms of Covariances

The principal irregular term (PIT) relates the tail behavior of the spectrum and the behavior at the origin of the covariance.

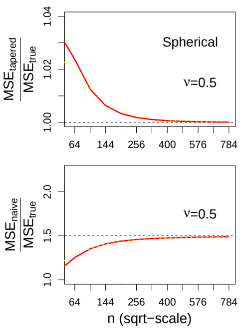
Formally, the PIT of C is the first term as a function of h in this series expansion about zero that is not raised to an even power.

Conjecture: *Assume a polynomial isotropic covariance function* C_θ *in* $\mathbb{R}^d$ *that is integrable with PIT* Bh^μ*. Then the PIT and the tail behaviour are related by*

$$\lim_{\rho\to\infty} \rho^{\mu+d} f_\theta(\rho) = \left| B \cdot \frac{\mu!}{2}\Big(\frac{2}{\pi}\Big)^{(d+1)/2} \right|$$

Simulation Study

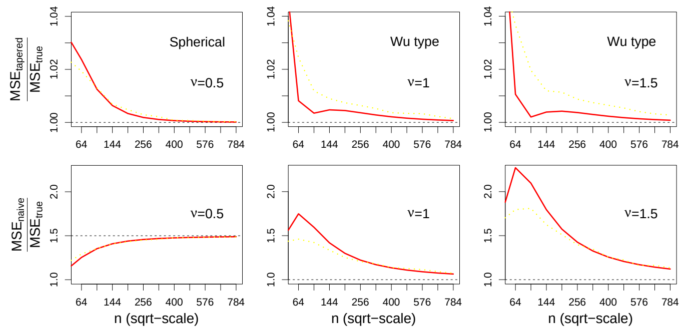
When does infill asymptotics kick in?



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

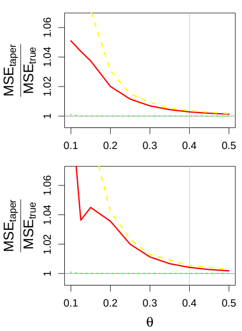
Simulation Study

When does infill asymptotics kick in?



Simulation Study

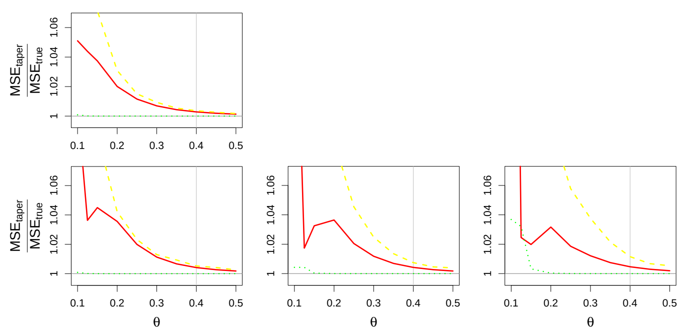
What is an efficient taper?



Simulation setup:
- n equispaced or 100 random observations in $[0,1]^2$
- $C_{\alpha,\nu}$: Matérn covariance, eff. range 0.4
- C_θ: spherical, Wu 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:

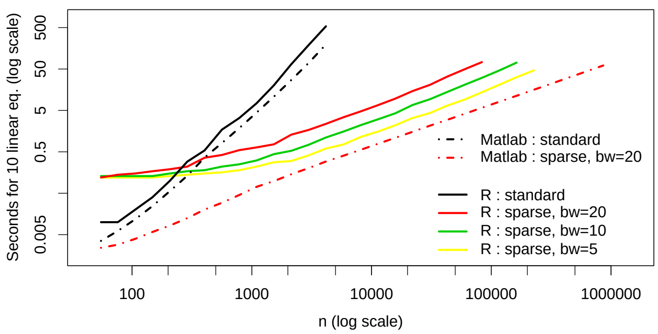
$$8z + 4z + 4n + 1 \text{ bytes} \quad \text{vs} \quad 8 \times n^2 \text{ bytes}$$

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

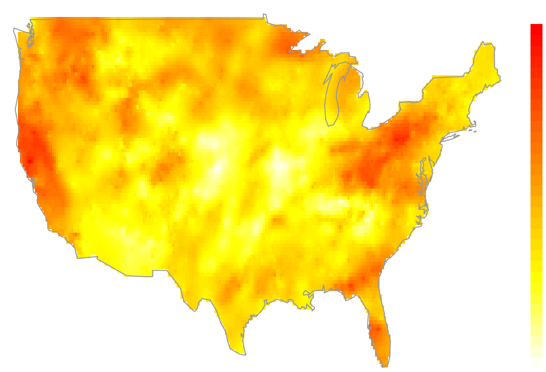
The Cholesky factor of a sparse matrix "is" sparse.

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

Computational Efficiency



Application



Computational Gain

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

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

Discussion

- Spatial models with drift and/or nugget effect
  - $\rightsquigarrow$ theoretical aspect: io.
  - $\rightsquigarrow$ practical aspect: io with backfitting
- Nonstationarity
  - $\rightsquigarrow$ future work
- Conjecture
  - $\rightsquigarrow$ should hold for many covariances
- Apply to other statistical problems
  - $\rightsquigarrow$ Microarrays, . . .