Covariance functions, Bochner's theorem, and more

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PASI 2014

First part based on the book "Interpolation of Spatial Data: Some Theory for Kriging" by M. L. Stein (1999)

Outline

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Mean square properties

- Relate covariance structure of a random field and the smoothness of its realization
- Z, a random field on $\mathbb{R}^d$, is mean square continuous at $\mathbf{x}$ if

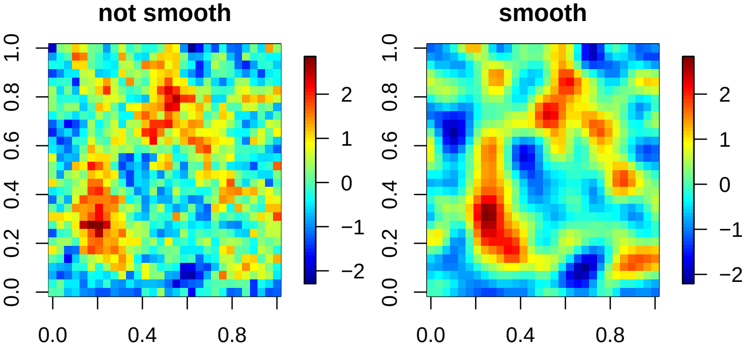
$$E\{Z(\mathbf{y}) - Z(\mathbf{x})\}^2 \to 0$$

  as $\mathbf{y} \to \mathbf{x}$
- For weakly stationary random field, mean square continuity iff its autocovariance function is continuous at the origin
- Mean square continuity does NOT imply continuity of its realizations

Mean square properties

- Z on $\mathbb{R}$ is mean square differentiable at t if there exist $Z^{'}(t) = \lim_{n\to\infty}\{Z(t+h_n) - Z(t)\}/h_n$ (in L^2) for $h_n \to 0$
- Extension to higher dimension and higher order is straightforward
- There can be analytic realizations of random field, not mean square differentiable:
  - $Z(t) = cos(Xt + Y)$, X and Y independent, X following standard Cauchy, Y following uniform on $[0, 2\pi]$
  - All realizations are obviously analytic
  - $\text{Cov}\{Z(s), Z(t)\} = exp(-|s-t|/2)$

Mean square smoothness



Spectral methods

- Define complex random fields: $Z(\mathbf{x}) = U(\mathbf{x}) + iV(\mathbf{x})$
- $Z(\mathbf{x}) = \sum_{k=1}^{n} Z_k exp(i\mathbf{w}_k^T\mathbf{x})$, $\mathbf{w}_k \in \mathbb{R}^d$,
  $Z_1, \ldots, Z_n$ are mean 0 complex random variables with
  $E(Z_i\overline{Z_j}) = 0 \ (i \neq j)$, $E|Z_i|^2 < \infty$
- Its covariance function $K(\mathbf{x}) = \sum_{k=1}^{n} f_k exp(i\mathbf{w}_k^T\mathbf{x})$
- Consider L_2 limit of the above representation

Bochner's Theorem

A complex-valued function K on $\mathbb{R}^d$ is the autocovariance function for a weakly stationary mean square continuous complex-valued random field on $\mathbb{R}^d$ iff it can be represented as

$$K(\mathbf{x}) = \int_{\mathbb{R}^d} exp(i\mathbf{w}^T\mathbf{x})F(\mathbf{dw})$$

with F a positive finite measure.
Wen F has a density wrt Lebesque measure, we have the spectral density f and

$$f(\mathbf{w}) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} exp(-i\mathbf{w}^T\mathbf{x})K(\mathbf{x})\mathbf{dx}$$

For isotropic random fields

- By Bochner's Theorem, for a weakly isotropic complex-valued random field Z on $\mathbb{R}^d$, there exists a positive finite measure F such that

$$K(|\mathbf{x}|) = \int_{\mathbb{R}^d} exp(i\mathbf{w}^T\mathbf{x})F(\mathbf{dw})$$

- Note $K(r) = \int_{\partial b_d} K(r|\mathbf{x}|)U(\mathbf{dx})$ for U uniform measure on ∂b_d

$\Rightarrow$

$$K(r) = \int_{\partial b_d}\{\int_{\mathbb{R}^d} exp(ir\mathbf{w}^T\mathbf{x})F(\mathbf{dw})\}U(\mathbf{dx})$$
$$= \int_{\mathbb{R}^d}\{\int_{\partial b_d} cos(r\mathbf{w}^T\mathbf{x})U(\mathbf{dx})\}F(\mathbf{dw})$$

For isotropic random fields cont'd

- On the other hand,

$$\int_{\partial b_d} cos(r\mathbf{w}^T\mathbf{x})U(\mathbf{dx}) = \Gamma(d/2)(\frac{2}{r|\mathbf{w}|})^{(d-2)/2}J_{(d-2)/2}(r|\mathbf{w}|)$$

(J_ν: the ordinary Bessel function)

$\Rightarrow$

$$K(r) = 2^{(d-2)/2}\Gamma(d/2)\int_0^\infty (ru)^{-(d-2)/2}J_{(d-2)/2}(ru)dG(u)$$

for G nondecreasing, bounded on $[0,\infty)$, $G(0) = 0$
: Hankel transform of order $(d-1)/2$ of G

- In fact, this is if and only if

For isotropic random fields

- It is difficult to verify if any given function can be written in the Hankel transform of a function G satisfying the above condition

- A continuous isotropic covariance function
  - in $\mathbb{R}^3$: $K(r) = \int_0^\infty (ru)^{-1} sin(ru) dG(u)$
  - in "every" dimension: $K(r) = \int_0^\infty exp(-r^2u^2) dG(u)$

- **Inversion formula**: if $\int_0^\infty r^{d-1}|K(r)|dr < \infty$, there exists a nonnegative function f with $\int_0^\infty u^{d-1} f(u) du < \infty$:

$$f(u) = (2\pi)^{-d/2} \int_0^\infty (ur)^{-(d-2)/2} J_{(d-2)/2}(ur) r^{d-1} K(r) dr$$

Some examples of continuous isotropic autocovariance function

- Matérn class: $f(u) = \dfrac{2^{\nu-1}\ \phi\ \Gamma(\nu + \frac{d}{2})\ \alpha^{2\nu}}{\pi^{d/2}\ (\alpha^2 + u^2)^{\nu+d/2}}$ in the Inversion formula
- $$K(d) = \frac{\alpha}{2^{\nu-1}\Gamma(\nu)}\left(\frac{d}{\beta}\right)^{\nu}\mathcal{K}_{\nu}\left(\frac{d}{\beta}\right), \quad d = |\mathbf{s}_1 - \mathbf{s}_2|$$
- $\mathcal{K}_\nu$ is the modified Bessel function of the second kind of order ν
- Matérn class is **valid** in $\mathbb{R}^p$ for all $p \in \mathbb{N}$

Some examples of continuous isotropic autocovariance function

- Spherical model: $K(r) = c(1 - \frac{3}{2\rho}r + \frac{1}{2\rho^3}r^3)$ for $r \leq \rho$ and zero everywhere else
  - Valid up to 3 dimension
  - Spectral density has oscillation at high frequencies
  - Spectral density of $K(r) = \sigma(\alpha - |r|)_+$: $f(w) = \sigma \dfrac{1 - cos(\alpha w)}{\pi w^2}$

Smoothness of Matérn process

- The larger ν is, the smoother the resulting Matérn field is
- The Matérn field is at least m times mean square differentiable at the origin iff $\nu > m$:

$$K(d) = \begin{cases} \sum_{j=0}^{m} a_j d^{2j} - \frac{\pi\alpha}{\Gamma(2\nu+1)\sin(\nu\pi)} d^{2\nu} + O(d^{2m+2}), & \text{if } m < \nu < m+1 \\ \sum_{j=0}^{m} b_j d^{2j} + \frac{2(-1)^m\alpha}{(2m+2)!} d^{2m+2}\log(d) + O(d^{2m+2}), & \text{if } \nu = m+1, \end{cases}$$

as $d \downarrow 0$, for appropriate constants a_j and b_j, $j = 1, \ldots, m$, depending on α, ν, and β

Outline

Non-Bayesian estimation of covariance

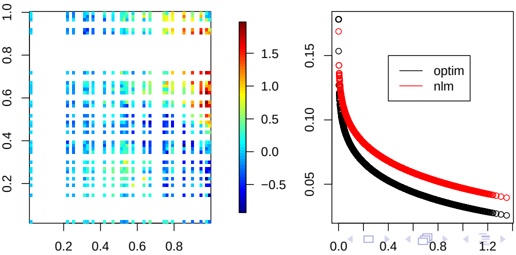
- I will only discuss likelihood methods
- Consider $Z(\mathbf{x}) = \mathbf{m}(\mathbf{x})^T\beta + \epsilon(\mathbf{x})$ with $\text{Cov}\{\epsilon(\mathbf{x}), \epsilon(\mathbf{y})\} = K_\theta(\mathbf{x}, \mathbf{y})$
- We maximize the loglikelihood of $\mathbf{Z} = (Z(\mathbf{x}_1), \ldots, Z(\mathbf{x}_n)) \sim N(M\beta, K(\theta))$
- We may use REML (Restricted maximum likelihood estimation): maximize the loglikelihood of $\mathbf{Y} = \{I - M(M^TM)^{-1}M^T\}\mathbf{Z}$ instead of $\mathbf{Z}$

Some remarks on numerical optimization

- There are R packages that provide functions for maximum likelihood estimation of covariance models (but you have to be careful using them!)
- For general covariance models, I suggest to write your own likelihood function and maximize using functions such as *optim* or *nlm*
- What you get from the functions (especially *optim*) may not be "what you want"!
- Use the two functions interchangeably, try various starting points, and check Hessians!

A simple example

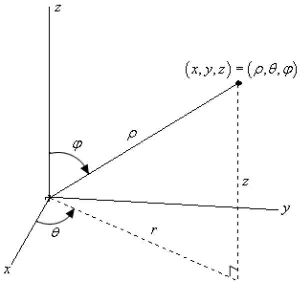
- I created a mean zero Gaussian random field on $[0,1] \times [0,1]$ with Matérn covariance structure and some nonstationarity to it
- I fitted mean zero Gaussian model with Matérn covariance structure
- Both optim and nlm claimed proper convergence and the loglikelihood values are given 660.2102 and 660.2566, respectively



Outline

On the surface of a sphere...

- Suppose $Z(\varphi,\theta)$ is a stochastic process on $\mathcal{S}^2$ ($\rho = 1$)



with mean zero and homogeneous covariance structure

- If we use a Matérn class with ϕ **distance** between $\mathbf{s}_1$ and $\mathbf{s}_2$:

$$K(\phi) = \frac{\alpha}{2^{\nu-1}\Gamma(\nu)}\left(\frac{\phi}{\beta}\right)^{\nu}\mathcal{K}_{\nu}\left(\frac{\phi}{\beta}\right)$$

On the surface of a sphere...

- Two distances on the surface of a sphere:

chordal vs **great circle** distance

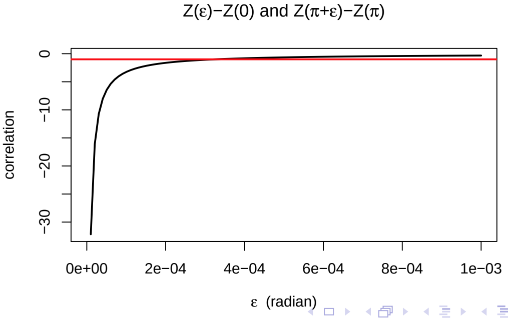
$$d = 2R \sin(\phi/2)$$

- With chordal distance, there is no difference between covariance model on the surface of a sphere and covariance model in Euclidean distance

On the surface of a sphere...

- Matérn class is positive definite if and only if $\nu \leq 0.5$ with great circle distance on 1,2,3 dimensional spheres (Gneiting 2013)

- Interesting counter example:
  - $Z(s)$, $s \in \mathcal{S}^1$
  - Z is mean zero and its covariance function is a Gaussian covariance function ($\text{Cov}\{Z(s), Z(t)\} = K(|s-t|) = e^{-|s-t|^2}$)



What has been done so far?

This is by no means a complete list!

1. "Smooth" parametric covariance models on a sphere
   - Du, Ma and Li (2013, *Mathematical Geoscience*)
   - Guinness and Fuentes (2013, *preprint*)
   - Heaton, Katzfuss, Berrett, Nychka (2014, *Environmetrics*)
   - Jeong and Jun (2013, *preprint*)
2. Nonstationary covariance models on a sphere (univariate and multivariate)
   - Jun and Stein (2007, 2008), Jun (2011, 2014)
   - ...
3. Gaussian Markov Random Field models
4. ...

Thank you!

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