Identication of Scale Parameter of the Matérn Model

N. Miklós Arató

Eötvös Loránd University (Budapest)

Dept. Prob. Theory & Statistics

Outline

- Matérn (Whittle) family
  - Covariance
  - Semivariogram
  - Spectral density
  - Stochastic partial differential equation
- Generalized Gaussian random fields
  - Dobrushin, Surgailis
  - Rozanov

Outline 2.

- Orthogonality and equivalence of Gaussian measures
- Levy-Baxter type theorems for stochastic elliptic differential equations
- Orthogonality and equivalence of the Matérn fields
  - Zhang
  - Anderes
  - $d=4$?
- Maximum likelihood estimation of the scale parameter for nonstationary case ($d \leq 3$)
- Orthogonality of Gaussian measures ($d=4$)

Bertil Matérn

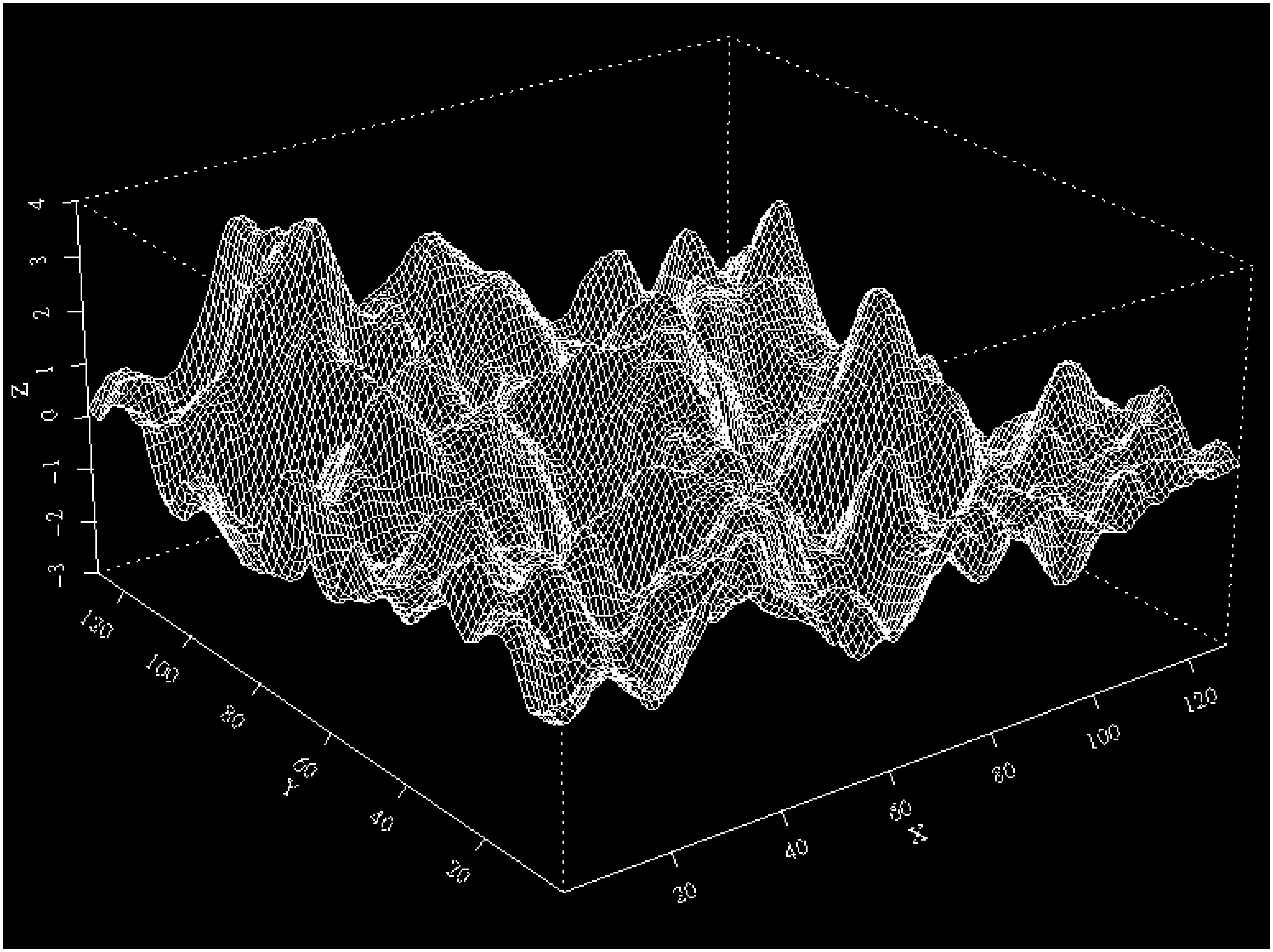
Matérn covariance model

- Matérn (1947, 1960) covariance function between locations $\mathbf{x}, \mathbf{y} \in \mathbf{R}^d$:

$$B(\mathbf{x},\mathbf{y}) = \rho_\nu(\|\mathbf{x}-\mathbf{y}\|) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}\left(\kappa\|\mathbf{x}-\mathbf{y}\|\right)^\nu K_\nu\left(\kappa\|\mathbf{x}-\mathbf{y}\|\right),$$

where

- K_ν is the modified Bessel function of the second kind and order $\nu > 0$,
- ν: smoothness parameter,
- κ: scale parameter,
- σ^2: marginal variance.



http://www2.math.umd.edu/~bnk//CLIP/clip.gauss.htm

Special cases of the Matérn model

$(\kappa=1)$

ν	$\rho_\nu(s)$	*name*
$\frac{1}{3}$	$\frac{2^{2/3}}{\Gamma(1/3)} s^{1/3} K_{1/3}(s)$	***Kármán (von Kármán)***
1	$sK_1(s)$	***Whittle***
$\frac{1}{2}$	$\exp(-s)$	***Exponential***
$\frac{3}{2}$	$(1+s)\exp(-s)$	***Second - order autoregressive***
$\frac{5}{2}$	$\left(1+s+\frac{1}{3}s^2\right)\exp(-s)$	***Third - order autoregressive***

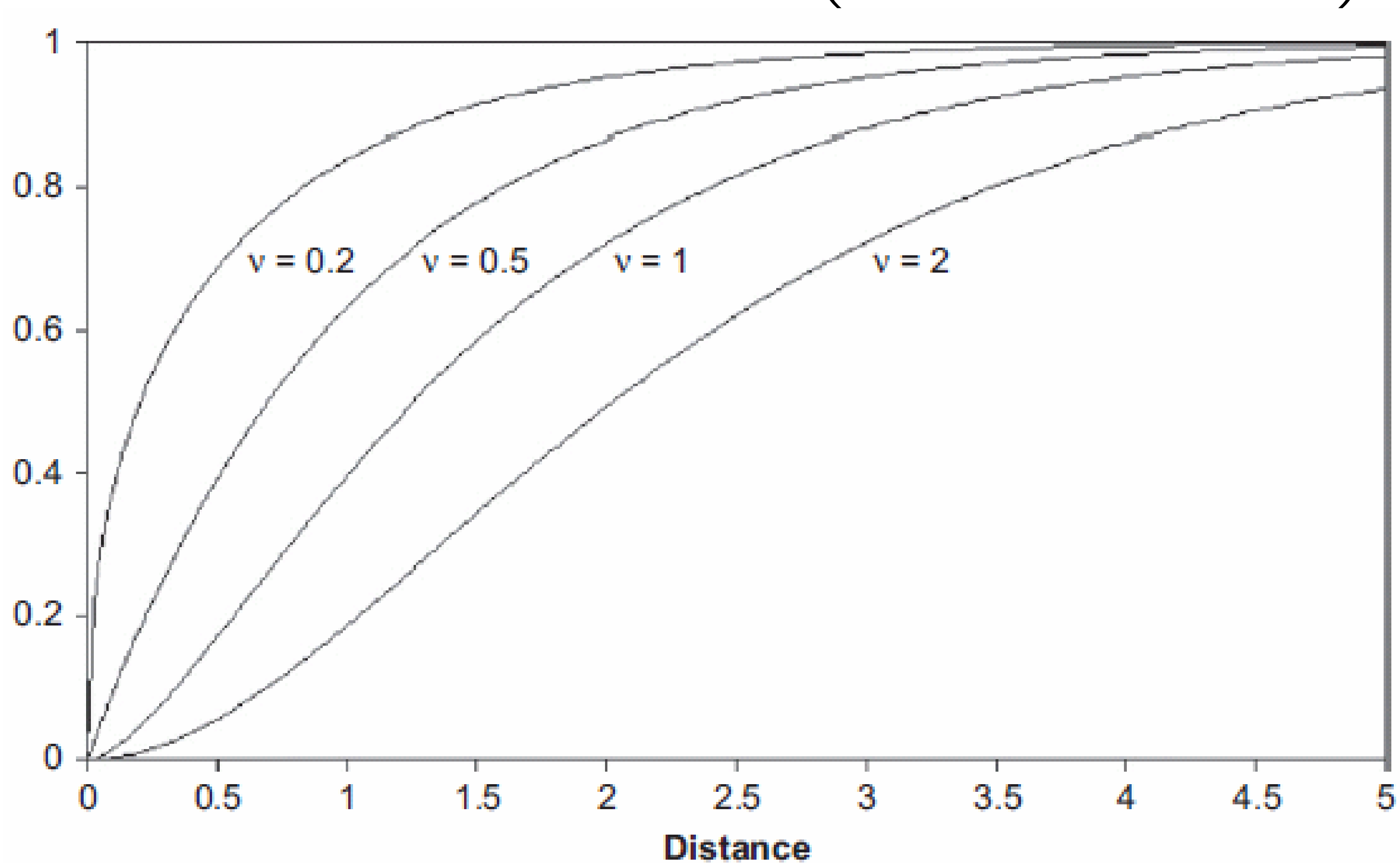
Uses of the Matérn model

- Environmental applications (temperature data)
- Hydrological spatial processes
- Geostatistics (gravitational fiels, geodetic networks, satellite sensor images, soil science, topography)
- Machine learning

Semivariogram

- In geostatistics:

$$\gamma_\nu(s) = \sigma^2 - \rho_\nu(s) = \sigma^2\left(1 - \frac{(\kappa s)^\nu K_\nu(\kappa s)}{2^{\nu-1}\Gamma(\nu)}\right),$$



Spectral density

$$f_{\nu}(\mathbf{u}) = \frac{\sigma^2 \kappa^{2\nu}}{\pi^{d/2}\left(\kappa^2 + \|\mathbf{u}\|^2\right)^{\nu+d/2}},$$

$$B(\mathbf{x},\mathbf{y}) = \int_{\mathbf{R}^d} \exp\left(i(\mathbf{x}-\mathbf{y})^T \mathbf{u}\right) f_{\nu}(\mathbf{u}) d\mathbf{u}$$

Linear fractional SPDE

- Whittle (1954, 1963):
  - ξ is a zero-mean Gaussian random field and
  - ξ is a solution of the equation:

$$(\kappa^2 - \Delta)^{(\nu + d/2)/2} \xi = \eta \text{ in } \mathbf{R}^d \quad (\eta : \text{Gaussian white noise})$$

$$\Rightarrow$$

$$\text{cov}(\xi(\mathbf{x}), \xi(\mathbf{y})) = \rho_\nu\left(\left\|\mathbf{x} - \mathbf{y}\right\|\right)$$

Dobrushin, Surgailis (1979)

$T \subseteq \mathbf{R}^d$ open domain, X is a Gaussian generalized random field on T if

$\{X(\varphi), \varphi \in C_0^\infty(T)\}$ is a system of Gaussian random variables,

X is linear and $X(\varphi)$ in probability as $\varphi \to 0$.

$$A\varphi = \sum_{|\alpha|,|\beta| \le p} (-1)^\alpha D^\alpha (a_{\alpha,\beta}(\mathbf{t}) D^\beta \varphi), \varphi \in C_0^\infty(T),$$

is a symmetric, uniformly strongly elliptic operator $\Rightarrow$

$\exists X$ Gaussian g.r.f. with mean zero

and $R(\varphi,\psi) = E(X(\varphi)X(\psi)) = \int_T \varphi(\mathbf{u})\left(\left(\overline{A}\right)^{-1}\psi\right)(\mathbf{u})d\mathbf{u}$, where

$\overline{A}$ is the Friedrichs' extension of A.

X can be extend to the Sobolev space $H_0^{-p}(T)$

Dobrushin, Surgailis stationary case

$T = \mathbf{R}^d$ open domain, X is a stationary Gaussian g.r.f

with the spectral density $f(\mathbf{u}) = \dfrac{1}{(2\pi)^d P(i\mathbf{u})}$, where

$$P(i\mathbf{u}) = \sum_{|\alpha|,|\beta| \le p} (-1)^\alpha a_{\alpha,\beta} (i\mathbf{u})^\alpha (i\mathbf{u})^\beta, P(i\mathbf{u}) = P(-i\mathbf{u}),$$

$$P(i\mathbf{u}) \ge c\left(1 + \|\mathbf{u}\|^2\right)^p, \ \mathbf{u} \in \mathbf{R}^d.$$

Corresponding operator :

$$A\varphi = \sum_{|\alpha|,|\beta| \le p} (-1)^\alpha a_{\alpha,\beta} D^\alpha (D^\beta \varphi), \varphi \in C_0^\infty(\mathbf{R}^d).$$

SPDE (Rozanov)

I. $A\varphi = \sum_{|\alpha|,|\beta|\le p} (-1)^{\alpha} D^{\alpha}(a_{\alpha,\beta}(\mathbf{t}) D^{\beta}\varphi) = \sum_{|\alpha|\le 2p} b_{\alpha}(\mathbf{t}) D^{\alpha}\varphi, \varphi \in C_0^{\infty}(T),$

is a positive elliptic operator.

δ is a Gaussian g.r.f. with mean zero and

$\mathrm{E}\big(\delta(\varphi)\delta(\psi)\big) = \int_T \varphi(\mathbf{u})\big(A\psi\big)(\mathbf{u})\, d\mathbf{u}.$

$A\xi = \delta$ in T, if

ξ is a Gaussian g.r.f. with mean zero and $\xi\big(A\varphi\big) = \delta(\varphi), \varphi \in C_0^{\infty}(T).$

II. ξ is a Gaussian g.r.f. with mean zero and

$E\big(\xi(\varphi)\xi(\psi)\big) = \int_T \varphi(\mathbf{u})\Big(\big(\overline{A}\big)^{-1}\psi(\mathbf{u})\Big) d\mathbf{u},\ \varphi, \psi \in C_0^{\infty}(T) \Rightarrow$

$A\xi = \delta$ in T.

Orthogonality and equivalence of Gaussian measures

- General results:
  - Feldman
  - Hajek
  - Golosov, Tempelman
- Isotropic fields:
  - Yadrenko
- Etc.

Theorem (Rozanov 1968., p. 46-49.)

Let (Ω, A) be a measurable space with two probability measures Q_1 and Q_2. Let U be a Hilbert space and $\xi : U \times \Omega \to \mathbf{R}$ be a Gaussian linear cont. functional with zero mean with respect to both measures and the covariance functions fulfill $E_{Q_i}\left(\xi(u)\xi(v)\right) = \left\langle u, B_i v \right\rangle_U, \forall u, v \in U, i = 1,2,$ where B_i are linear continuous operators and there exists $\varepsilon > 0$ for which $\left\langle B_1 u, u \right\rangle_U \geq \varepsilon \|u\|_U^2 \ \forall u \in U$.

Then the measures Q_1 and Q_2 are equivalent if and only if the operator $\left(I\text{-}B_1^{-1}B_2\right)$ is a Hilbert - Schmidt operator with eigenvalues $\left(1-\sigma_k^2\right) \neq 1$. In this case the Radon - Nikodym derivative is given by

$$\frac{dQ_1}{dQ_2} = \lim_{n\to\infty} \frac{1}{\prod_{k=1}^{n} \sigma_k} \exp\left\{-\frac{1}{2}\sum_{k=1}^{n} \frac{1-\sigma_k^2}{\sigma_k^2} \xi^2(u_k)\right\}, \text{ where}$$

$\{u_k\}_{k=1}^{\infty}$ is a complete orthonormal system of eigenvectors of the operator $\left(I\text{-}B_1^{-1}B_2\right)$.

Levy-Baxter type theorems for stochastic elliptic differential equations

*I*n 1988 Goryainov proved that observing a stationary Gaussian g.r.f with the spectral density $f(\mathbf{u}) = \dfrac{1}{P(i\mathbf{u})}$, where P is an elliptic positive polynomial, in an arbitrary small neigborhood of a point t_0, one can estimate with probability 1 the coefficients b_α, $|\alpha| > 2p - \dfrac{d}{2}$.

Corollary: if $d > 4$ we can estimate with probability 1 the coefficients κ (scale) and σ^2(marginal variance) in the Matérn model (if the smoothing parameter is integer).

Arató N. M. (1989 - 1990) proved a similar result for the nonstationary case: if $P\xi = \delta \; in \; T \subseteq \mathbf{R}^d$ than observing ξ in an arbitrary small neigborhood of a point $t_0 \in \mathrm{T}$, one can estimate with probability 1 the coefficients

$$b_\alpha(t_0), \; |\alpha| > 2p - \frac{d}{2}.$$

We constructed explicitly test functions $\varphi_{m,n} \in C_0^\infty(S), S \subseteq T$ neigborhood of t_0 and statistics $\sum_m \left(\xi(\varphi_{m,n})\right)^2 \xrightarrow[n\to\infty]{} b_\alpha(t_0) \; a.s.$

Equivalence of the measures

- Inoue (1976) and Sokolova (1983) proved that the probability measures corresponding to different elliptic operators and Gaussian fields with covariance

$$\int_T \varphi(\mathbf{u}) \left(\left(\overline{A_i} \right)^{-1} \psi \right) (\mathbf{u}) \, d\mathbf{u}$$

are equivalent if $\deg(A_1 - A_2) < 2p - d/2$.

Estimation of the parameters of the Matérn field

- Zhang (2004) proved that observing Matérn field in a bounded set there do not exists consistent estimators of the marginal variance and scale parameter ($d \leq 3$).
- Anderes (2010) constructed consistent estimators for the marginal variance and scale parameter ($d > 4$).
- d=4 ???

d (dimension)=4, ν (smoothing parameter) is integer

Statement :

Let (Ω, A) be a measurable space with two probability measures Q_1 and Q_2. Let $T \subset \mathbf{R}^d$ be a bounded domain and $\xi : T \times \Omega \to \mathbf{R}$ be a Gaussian (Matérn) mean zero field with respect to both measures and the covariance functions fulfill

$$E_{Q_i}\left(\xi(\mathbf{x})\xi(\mathbf{y})\right) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}\left(\kappa_i \|\mathbf{x}-\mathbf{y}\|\right)^{\nu} K_{\nu}\left(\kappa_i \|\mathbf{x}-\mathbf{y}\|\right), \forall \mathbf{x},\mathbf{y} \in T, i = 1, 2,$$

Then the probability measures Q_1 and Q_2 are orthogonal if $d \geq 4$ and ν is integer.

Sketch of the proof

Dobrushin - Surgailis, Rozanov $\Rightarrow$

$\sigma_i^2 \kappa_i^{2\nu} (\kappa - \Delta)^{\nu + d/2} \xi = \delta$ in T, where

$E_{Q_i}\left(\delta_i(\varphi)\delta_i(\psi)\right) = \int \varphi(\mathbf{x}) \sigma_i^2 \kappa_i^{2\nu} (\kappa_i - \Delta)^{\nu + d/2} \psi(\mathbf{x}) d\mathbf{x},$

$\forall \varphi, \psi \in C_0^\infty(T).$

Goryanov, Arató N.M. $\Rightarrow$

we can determine $\sigma_i^2 \kappa_i^{2\nu}$ with probability 1.

$\Rightarrow$ we can assume that $\sigma_i^2 \kappa_i^{2\nu} = 1.$

The g.r.f. δ_1 can be extend to Sobolev space $U = H_0^{\nu + d/2}$

with the equivalent norm $\|u\| = \int_T u(\mathbf{x})(\kappa_1 - \Delta)^{\nu + d/2} u(\mathbf{x}) d\mathbf{x}$

$\Rightarrow E_{Q_1}\left(\delta(u)\delta(v)\right) = \langle u, v \rangle_U$

$$E_{Q_2}\left(\delta(u)\delta(v)\right)=\left\langle u,(\kappa_2-\Delta)^{-(\nu+d/2)}(\kappa_1-\Delta)^{\nu+d/2}v\right\rangle_U \Rightarrow$$

$$B_1=I, B_2=(\kappa_2-\Delta)^{-(\nu+d/2)}(\kappa_1-\Delta)^{\nu+d/2},$$

$$I-B_1^{-1}B_2=I-(\kappa_2-\Delta)^{-(\nu+d/2)}(\kappa_1-\Delta)^{\nu+d/2}.$$

We can choose a complete orthogonal system $\{u_k\}_{k=1}^{\infty}$ in $H_0^{\nu+d/2}$:

$$-\Delta u_k=\lambda_k u_k \text{ in } T,$$

$$\alpha_0 k^{2/d}<\lambda_k<\alpha_1 k^{2/d}, \text{ for } k\geq k_0, \ (\alpha_0,\alpha_1,k_0>0).$$

$$u=\sum_k c_k u_k \in U:$$

$$\left(I-B_1^{-1}B_2\right)u=\left(I-(\kappa_2-\Delta)^{-(\nu+d/2)}(\kappa_1-\Delta)^{\nu+d/2}\right)u=$$

$$\sum_k\left(1-\left(\frac{\kappa_1+\lambda_k}{\kappa_2+\lambda_k}\right)^{\nu+d/2}\right)c_k u_k$$

eigenvalues $(1-\sigma_k^2)$ of the $I - B_1^{-1}B_2$

are $1-\left(\frac{\kappa_1+\lambda_k}{\kappa_2+\lambda_k}\right)^{\nu+d/2}$ and

$$\sum_k (1-\sigma_k^2)^2 = \sum_k \left(1-\left(\frac{\kappa_1+\lambda_k}{\kappa_2+\lambda_k}\right)^{\nu+d/2}\right)^2 = \infty \text{ if } d \geq 4.$$

Nonstationary case (and $\nu+d/2$ is integer)

Statement:

Let (Ω, A) be a measurable space with two probability measures Q_1 and Q_2. Let $T \subset \mathbf{R}^d$ be a bounded domain and $\xi : T \times \Omega \to \mathbf{R}$ be a Dobrushin - Surgailis field with respect to both measures and $(\kappa_i\text{-}\Delta)^{\nu+d/2}$ differential operators.

Then the probability measures Q_1 and Q_2 are equivalent if and only if $d < 4$.

At the case $d < 4$

the Radon - Nikodym derivative is the following

$$\frac{dQ_2}{dQ_1} =$$

$$\lim_{n\to\infty}\left\{\left(\prod_{k=1}^{n}\frac{\kappa_2+\lambda_k}{\kappa_1+\lambda_k}\right)^{(\nu+d/2)/2}\exp\left(-\frac{1}{2}\sum_{k=1}^{n}\frac{\left(\kappa_2+\lambda_k\right)^{\nu+d/2}-\left(\kappa_1+\lambda_k\right)^{\nu+d/2}}{\left(\kappa_1+\lambda_k\right)^{\nu+d/2}}\xi^2(u_k)\right)\right\},$$

where $\{u_k\}_{k=1}^{\infty}$ is a complete orthonormal system of the eigenfunctions of the operator - Δ.

Maximum likelihood estimation of the mean

If we observe in a sphere T the random field $m+\xi$ where m is an unknown constant and ξ is a Matérn field ($\alpha=(\nu+d/2)/2$ is integer) then the maximum likelihood estimator of the m has the following form.

$$\hat{m} = q\int_T \xi(\mathbf{x})d\mathbf{x} + q_0 \int_{\partial T} \xi(\mathbf{x})d\mathbf{x} + \sum_{i=1}^{\alpha-1} q_i \int_{\partial T} \left(\partial_{n,i}\xi\right)(\mathbf{x})d\mathbf{x},$$

$\partial_{n,1}\xi,\ldots,\partial_{n,\alpha-1}\xi$: generalized normal derivatives of ξ

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