Spectral simulation of a spatio-temporal random field on the three-dimensional sphere

X. Freulon, Ch. Lantuéjoul

Geosciences and Geoengineering Department
Mines Paris – PSL University
xavier.freulon@minesparis.psl.eu

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OUTLINE

SPACE-TIME MODEL ON THE SPHERE

- **Context:** Data located on earth can/should be modeled using random fields indexed on the sphere. If time is involved, the model should be indexed on the cartesian product of the sphere and the real line.
- **Aim:** to implement **kriging** and **geostatistical simulations** for prediction and uncertainty quantification
- The spectral approach
- Isotropic models on the sphere
- The Gamma mixture trick

Let Z be a **Gaussian** stationary random field in $\mathbb{R}^d$. It is defined by
- its constant mean, $\mathbb{E}\{Z(s)\} = m\ (= 0)$, and
- its covariance function, $\mathbb{C}\mathrm{ov}\{Z(s), Z(s+\mathbf{h})\} = C(\mathbf{h})$

Bochner's theorem

$$C(\mathbf{h}) = \int_{\mathbb{R}^d} e^{i<\mathbf{h},\omega>} d\chi(\omega)$$

where χ is a positive measure (**spectral measure**). If $C(\mathbf{0}) = 1$, χ is a probability distribution on $\mathbb{R}^d$

Spectral simulation

If $\Omega \sim \chi$ and $\Phi \sim \mathcal{U}_{[0,2\pi[}$,

$$Z(s) = \sqrt{2}\cos(<\Omega, s> + \Phi)$$

is a centered stationary random field with covariance function C.

But, it is a mono-chromatic wave, not Gaussian nor ergodic.

THE SPECTRAL APPROACH (2/2)

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Thanks to the **central limit theorem**, an approximate Gaussian random field can be generated as a linear combination of i.i.d. mono-chromatic waves:

$$Z(s) \approx \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \sqrt{2} \cos(< \Omega_i, s > + \Phi_i)$$

where Ω_i i.i.d. $(\sim \chi)$, and Φ_i i.i.d. $(\sim \mathcal{U}_{[0,2\pi[})$.

A continuous simulation algorithm

i) Simulation of the spectrum $(\Omega_i, \Phi_i)_{i \in 1:n}$
ii) Computation of the simulated values at target points

Note: if $d\chi(\omega) = f\, d\omega$, an auxiliary density function g ($supp(g) \supset supp(f)$) can be used to simulate the frequencies: $\Omega_i \sim g$ and $\Phi_i \sim \mathcal{U}_{[0,2\pi[)}$,

$$Z(s) \approx \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \sqrt{\frac{2f(\Omega_i)}{g(\Omega_i)}} \cos(< \Omega_i, s > + \Phi_i)$$

OUTLINE

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GEOSTATISTICS ON THE SPHERE (1/3)

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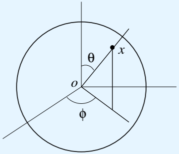
Spherical coordinates

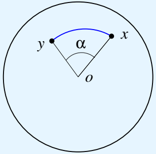
Unit sphere $\mathbb{S}_2 = \{x \in \mathbb{R}^3 : |x| = 1\}$ with center o.
Each point $x \in \mathbb{S}_2$ can be parametrized as $x = (\theta, \varphi)$ with

- $0 \leq \theta \leq \pi$ (colatitude) and
- $0 \leq \varphi < 2\pi$ (longitude).



Geodesic distance

If $x, y \in \mathbb{S}_2$, then $\alpha(x, y) = \arccos x \cdot y$.
($x \cdot y$ is the inner product of x and y in $\mathbb{R}^3$).



GEOSTATISTICS ON THE SPHERE (2/3)

- **Rotations** are used to defined *stationarity*/**isotropy** on $\mathbb{S}_2$:
  - The mean is constant
  - The covariance only depends on the geodesic distance
- Covariance functions of **isotropic** (Gaussian) random fields on the sphere are characterized by

Schoenberg theorem

$$\mathbb{C}\mathrm{ov}\{Z(s), Z(s')\} = \sum_{n=0}^{+\infty} a_n P_n(\alpha(s, s'))$$

where a_n are summable non-negative coefficients and P_n are the Legendre polynomials

The angular spectrum $\sum_{n=0}^{+\infty} a_n \delta_n$ completely characterizes the covariance function of Z

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Definitions

- The Legendre polynomials of degree $n \geq 0$ is defined by the Rodrigues'formula

$$P_n(t) = \frac{(-1)^n}{2^n n!} \frac{\partial^n}{\partial x^n}(1-t^2)^n \quad \text{for} \quad -1 \leq t \leq 1$$

- The associated Legendre function of degree $n \geq 0$ and order k, $-n \leq k \leq n$, is defined by

$$P_n^k(t) = \frac{(-1)^{n+k}}{2^n n!}(1-t^2)^{k/2} \frac{\partial^n}{\partial x^n}(1-t^2)^n \quad \text{for} \quad -1 \leq t \leq 1$$

- The spherical harmonic of degree $n \geq 0$ and order k is defined as

$$Y_{n,k}(\theta,\varphi) = \sqrt{\frac{2n+1}{4\pi}\frac{(n-k)!}{(n+k)!}}\, P_n^k(\cos\theta) e^{ik\varphi} \text{ and } Y_{n,k} = (-1)^k\, \bar{Y}_{n,k}$$

THE SPECTRAL APPROACH ON $\mathbb{S}_2$

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Let Z be a **Gaussian isotropic** random field on $\mathbb{S}^2$. It is defined by
- its constant mean, $\mathbb{E}\{Z(s)\} = m$, and
- its covariance function, $\mathbb{C}\text{ov}\{Z(s), Z(s')\} = C(\alpha(s, s'))$

Schoenberg's theorem

$$C(t) = \sum_{n=0}^{+\infty} a_n P_n(t)$$

$\mu = \sum_{n=0}^{+\infty} a_n \delta_n$ is the **spectral** measure. If $C(\mathbf{0}) = 1$, μ is a probability distribution on $\mathbb{N}_+$

Spectral simulation

If $N \sim \mu$, $K|N \sim \mathcal{U}_{\{-N,\dots,+N\}}$, and $\Phi \sim \mathcal{U}_{[0,2\pi[}$

$$Z(s) = Z(\theta, \varphi) = 2\sqrt{2\pi}\, \Re(Y_{N,K}(\theta, \varphi) e^{i\Phi}) = \frac{1}{\sqrt{2}} \tilde{P}_N^K(\cos\theta) \cos(K\varphi + \Phi)$$

is a centered isotropic random field with covariance function C

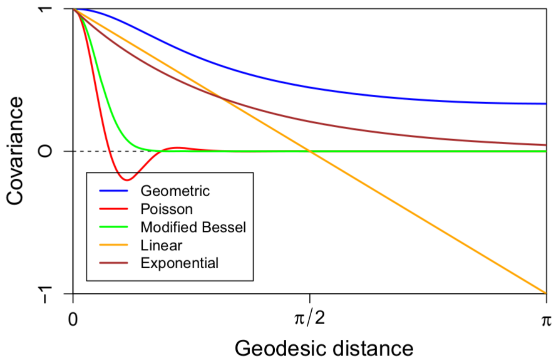
COVARIANCE FUNCTIONS ON $\mathbb{S}_2$

- **Geometric distribution:** $a_n = (1 - rho)\rho^n$
  with $0 < \rho < 1$
  $C(\alpha) = \frac{1-\rho}{\sqrt{1-2\rho\cos\alpha+\rho^2}}$

- **Poisson distribution:** $a_n = \exp(-\lambda)\lambda^n/n!$
  with $0 < \lambda$
  $C(\alpha) = \exp(\lambda(\cos\alpha - 1))J_0(\lambda\sin\alpha)$

- **Modified Bessel distribution:**
  $a_n = \sqrt{\frac{\pi}{2\lambda}}\exp(-\lambda)I_{n+1/2}(\lambda)$ with $0 < \lambda$
  $C(\alpha) = \exp(\lambda(\cos\alpha - 1)) = \exp(-\lambda 2\sin^2\frac{\alpha}{2})$
  Von Mieses covariance function

- ...



■ COMPUTING THE SPHERICAL HARMONICS

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- Normalized associated Legendre functions

$$\tilde{P}_l^m(x) = P_l^m(x) \times \sqrt{(2l+1)\frac{(l-m)!}{(l+m)!}},$$

- Two useful recursion formulae
  1. $(l, m) \longrightarrow (l+1, m+1)$

$$\tilde{P}_{l+1}^{l+1}(x) = -\sqrt{\frac{2l+3}{2l+2}}\,(1-x^2)^{1/2}\,\tilde{P}_l^l(x)$$

  2. $(l, m) \longrightarrow (l+1, m)$

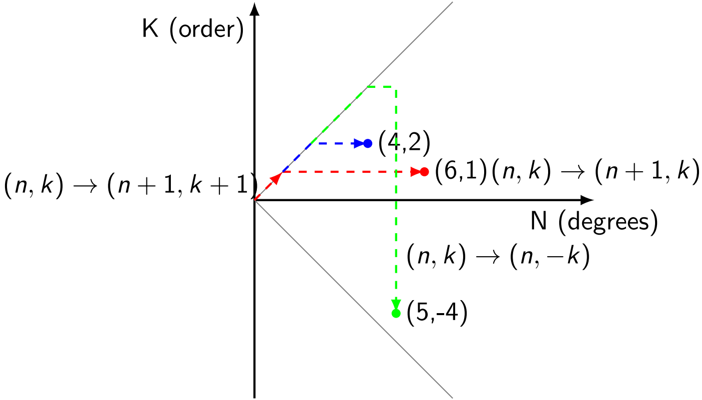
$$\tilde{P}_{l+1}^m(x) = \sqrt{\frac{(2l+3)(2l+1)}{(l+m+1)(l-m+1)}}\,x\,\tilde{P}_l^m(x) - \sqrt{\frac{(l+m)(l-m)(2l+3)}{(l+m+1)(l-m+1)(2l-1)}}\,\tilde{P}_{l-1}^m(x)$$

- The spherical harmonics

$$Y_{n,k}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}\tilde{P}_n^k(\cos\theta)e^{ik\varphi} \text{ and } Y_{n,-k}(\theta,\varphi) = \frac{(-1)^k}{\sqrt{4\pi}}\tilde{P}_n^k(\cos\theta)e^{-ik\varphi}$$

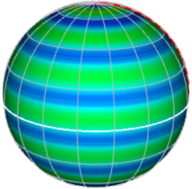
■ COMPUTING THE SIMULATION VALUES

i) Simulation of the spectrum $(N_i, K_i, \Phi_i)_{i \in 1:p}$ (e.g. $\{(5,-4),(4,2)),(6,1)\}$)
ii) Computing the spherical harmonics for the leaves of the tree

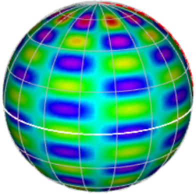


■ EXAMPLE OF SPHERICAL HARMONICS

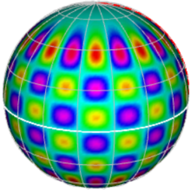
$N = 15, K = 0$



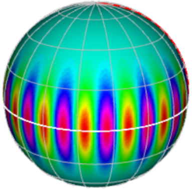
$N = 15, K = 0$



$N = 15, K = 10$



$N = 15, K = 15$



THE GAMMA MIXTURE TRICK

Aim: to define a "*pseudo Matern's*" family on the sphere (i.e. to be able to control the regularity and the scale of the random field)

- On $\mathbb{R}^d$, a **Matern's** covariance is a Gamma mixture of Gaussian covariances

$$\mathcal{M}(\mathbf{h};\nu,Q) = \int_{\mathbb{R}_+} g_\nu(r)dr\,\exp(-\frac{\nu}{2r}\|\mathbf{h}\|_Q^2) = \frac{2^{1-\nu}}{\Gamma(\nu)}(\sqrt{2\nu}\|h\|_Q)^\nu K_\nu(\sqrt{2\nu}\|h\|_Q)$$

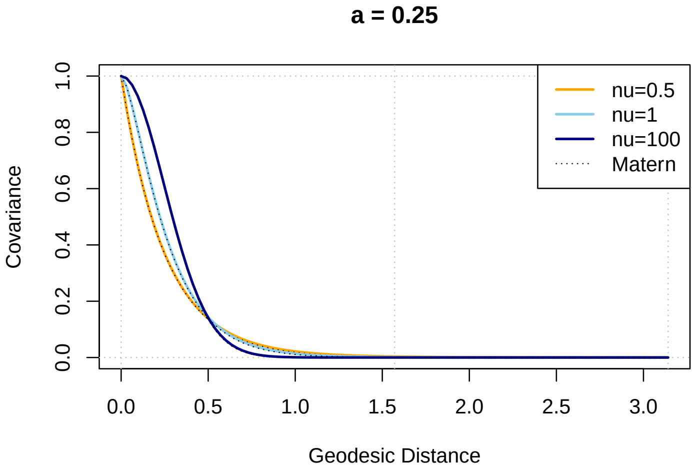
  where g_ν is the gamma pdf and Q is the geometrical anisotropy paramaters on $\mathbb{R}^d$

- As the **Von Mieses** covariance *looks like* a **Gaussian** covariance, the mixture trick defines a covariance function on $\mathbb{S}_2$

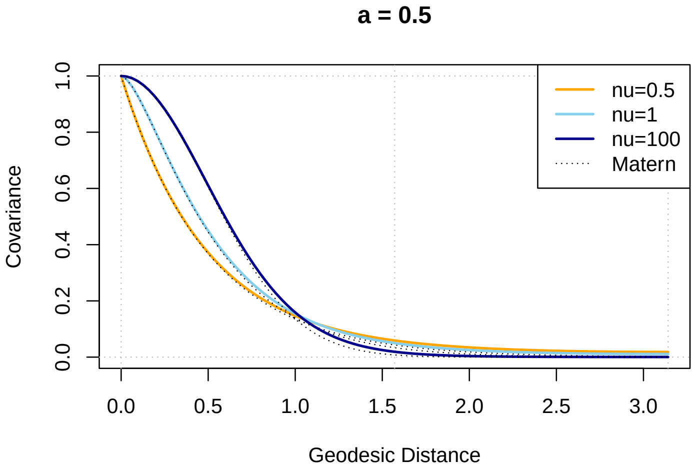
$$\tilde{\mathcal{M}}(\mathbf{h};\nu,a) = \int_{\mathbb{R}_+} g_\nu(r)dr\,\exp\{-\frac{\nu}{2r}\frac{4}{a^2}\sin^2\frac{\alpha}{2}\} = \frac{2^{1-\nu}}{\Gamma(\nu)}(\sqrt{2\nu}d_\alpha)^\nu K_\nu(\sqrt{2\nu}d_\alpha)$$

  with $d_\alpha = |\frac{2}{a}\sin\frac{\alpha}{2}|$, $\nu > 0$ the regularity parameter and $a > 0$ the scale parameter.

■ EXAMPLES:

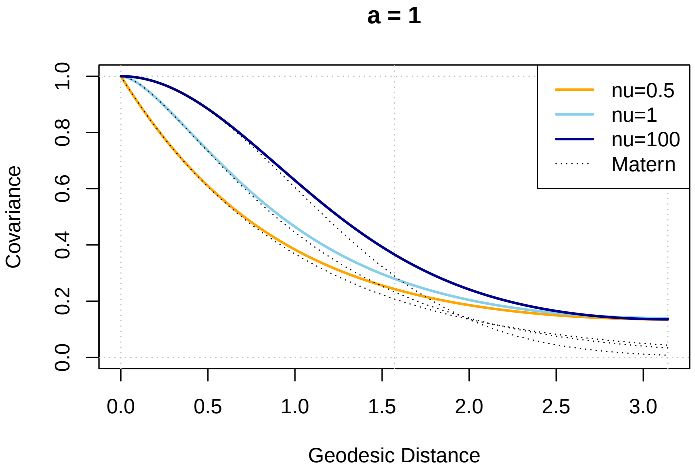

a = 0.25
nu=0.5
nu=1
nu=100
Matern
Covariance
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Geodesic Distance

■ EXAMPLES:



a = 0.5
1.0
0.8
0.6
0.4
0.2
0.0
Covariance
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Geodesic Distance
nu=0.5
nu=1
nu=100
Matern

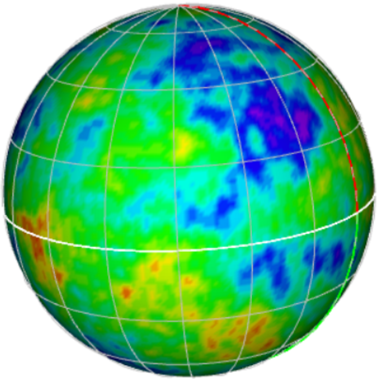
■ EXAMPLES:

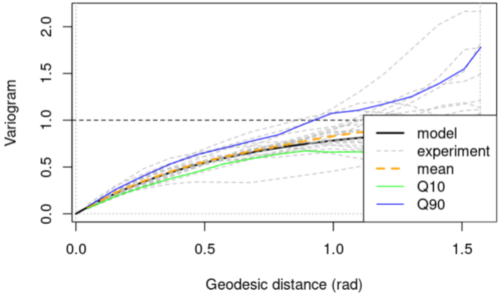


a = 1
nu=0.5
nu=1
nu=100
Matern
Covariance
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Geodesic Distance

■ SIMULATION:

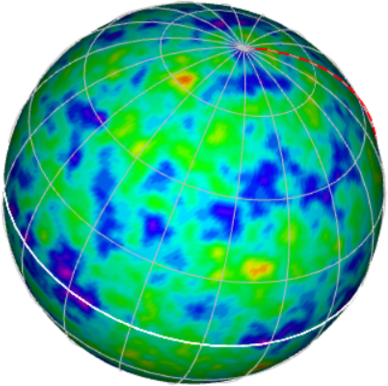
$$a = \pi/5 \text{ and } \nu = 1/2$$

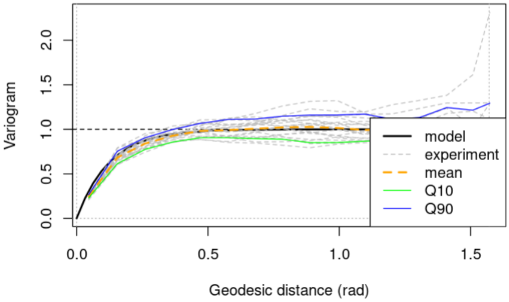




■ SIMULATION:

$$a = \pi/25 \text{ and } \nu = 1/2$$





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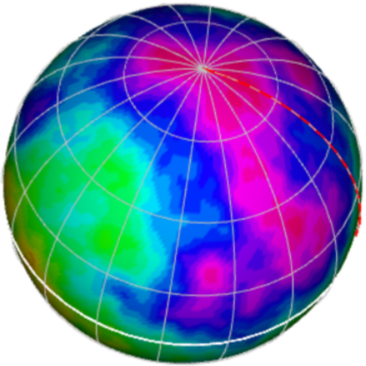
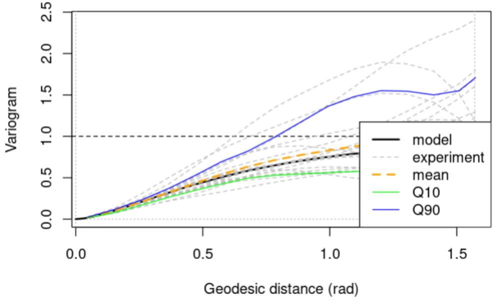
$a = \pi/5$ and $\nu = 1$

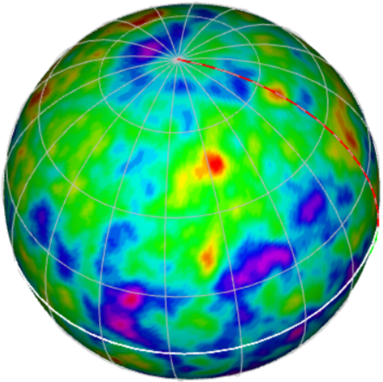


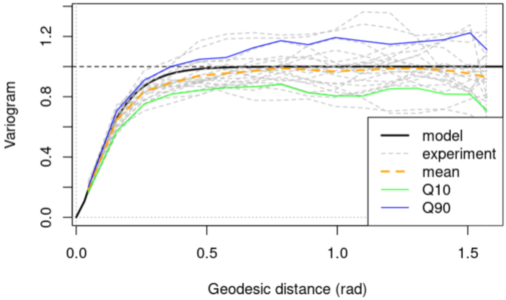


Spectral simulation of a spatio-temporal random field on the three-dimensional sphere

■ SIMULATION:

$$a = \pi/25 \text{ and } \nu = 1$$





Spectral simulation of a spatio-temporal random field on the three-dimensional sphere

OUTLINE

I. Introduction

II. Isotropic random fields on the sphere

III. Gamma mixture for space-time models
- Matern model
- Cauchy model

IV. Conclusions and perspectives

A SEPARABLE RANDOM FIELD ON $\mathbb{S}_2 \times \mathbb{R}$

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Building block: Z is a RF, isotropic on $\mathbb{S}_2$ and stationary in $\mathbb{R}$

- $\mathbb{E}\{Z(s,t)\} = m$
- $\mathbb{C}\text{ov}\{Z(s,t), Z(s',t')\} = C^S(\alpha(s,s')) \times C^T(t-t')$
- Spectral simulation using n components:

$$Z(s,t) = Z(\theta,\varphi,t) \approx \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \tilde{P}_{N_i}^{K_i}(\cos\theta) \times \cos(K_i\,\varphi + \phi_i^{(1)}) \times \cos(\Omega_i\,t + \phi_i^{(2)})$$

with n spectral components, **i.i.d.**

- $N_i \sim \chi^S$, the angular measure of C^S and $K_i|N_i \sim \mathcal{U}_{\{-N_i,\dots,N_i\}}$
- $\Omega_i \sim \chi^T$, the spectral measure of C^T
- $\Phi_i^{(1)}, \Phi_i^{(2)}$ are random phases, uniformly distributed on $[0, 2\pi[$

BEYOND THE SEPARABLE MODEL?

- **On** $\mathbb{S}_2$: a gamma mixture of Von Mieses isotropic covariance, $\tilde{\mathcal{M}}_{\nu,a}$ (as seen before)
- **On** $\mathbb{R}$: a gamma mixture of powered exponential covariance functions, gives the following models:
  - **The Matern's model** ($\nu > 0$ and $a > 0$)

$$C^T_{\nu,a}(\tau) = \int_{\mathbb{R}_+} g_{\nu,1}(r)\, e^{-\frac{\nu}{2r}|\frac{\tau}{a}|^2} dr = \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu}\,|\frac{\tau}{a}|\right)^{\nu} K_\nu\left(\sqrt{2\nu}\,|\frac{\tau}{a}|\right)$$

  - **The Cauchy model** ($\nu > 0$, $a > 0$, and $\gamma \in (0, 2]$)

$$C^T_{\nu,a,\gamma}(\tau) = \int_{\mathbb{R}_+} g_{\nu,1}(r) e^{-r|\frac{\tau}{a}|^\gamma} dr = \frac{1}{(1 + |\frac{\tau}{a}|^\gamma)^\nu}$$

- Using a **common** mixing parameter to link the space and time to generate non-separable models

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$$C(\alpha,\tau) = \int_{\mathbb{R}_+} g_{\nu,1}(r)\, \exp\{-\frac{\nu}{2r}(|\frac{2}{a_s}\sin\frac{\alpha}{2}|^2 + |\frac{\tau}{a_t}|^2)\}\, dr$$

with $\nu > 0$ and $(a_s, a_t) > 0$

- **Space trace** is a *pseudo* Matern's covariance on $\mathbb{S}_2$

$$C^S_{\nu,a_s}(\alpha) = \int_{\mathbb{R}_+} g_{\nu,1}(r)\exp\{-\frac{\nu}{2r}\frac{4}{a_s^2}\sin^2\frac{\alpha}{2}\}dr = \frac{2^{1-\nu}}{\Gamma(\nu)}(\sqrt{2\nu}\, d_\alpha)^\nu K_\nu(\sqrt{2\nu}\, d_\alpha)$$

  with $d_\alpha = |\frac{2}{a_s}\sin\frac{\alpha}{2}|$

- **Time trace** is a Matern's covariance on $\mathbb{R}$

$$C^T_{\nu,a_t}(\tau) = \int_{\mathbb{R}_+} g_{\nu,1}(r)\, e^{-\frac{\nu}{2r}|\frac{\tau}{a_t}|^2} dr = \frac{2^{1-\nu}}{\Gamma(\nu)}\left(\sqrt{2\nu}\,|\frac{\tau}{a_t}|\right)^\nu K_\nu\left(\sqrt{2\nu}\,|\frac{\tau}{a_t}|\right)$$

- It is a *quasi* geometrical anisotropy!

THE CAUCHY'S MODEL

$$C(\alpha,\tau) = \int_{\mathbb{R}_+} g_{\nu,1}(r)\ \exp\{-\frac{\nu}{2r}|\frac{2}{a_s}\sin\frac{\alpha}{2}|^2 - r|\frac{\tau}{a_t}|^\gamma\}\ dr$$

with $\nu > 0$, $\gamma \in (0,2]$, and $(a_s, a_t) > 0$

- **Space trace** is a *pseudo* Matern's covariance on $\mathbb{S}_2$

$$C^S_{\nu,a_s}(\alpha) = \int_{\mathbb{R}_+} g_{\nu,1}(r)\exp\{-\frac{\nu}{2r}|\frac{2}{a_s}\sin\frac{\alpha}{2}|^2\}dr = \frac{2^{1-\nu}}{\Gamma(\nu)}(\sqrt{2\nu}\,d_\alpha)^\nu K_\nu(\sqrt{2\nu}\,d_\alpha)$$

with $d_\alpha = |\frac{2}{a_s}\sin\frac{\alpha}{2}|$

- **Time trace** is a Cauchy's covariance on $\mathbb{R}$

$$C^T_{\nu,a_t,\gamma}(\tau) = \int_{\mathbb{R}_+} g_{\nu,1}(r)e^{-r|\frac{\tau}{a_t}|^\gamma}dr = \frac{1}{(1+|\frac{\tau}{a_t}|^\gamma)^\nu}$$

SPACE-TIME SIMULATION

- Simulation of n spectral components, **i.i.d.**:
  - $R_i \sim g_{\nu,1}$
  - $N_i \sim \chi^S$, the angular measure of the **Von Mieses** covariance with $\lambda = \frac{\nu}{R_i a_s^2}$
  - $K_i | N_i, R_i \sim \mathcal{U}_{\{-N_i,\ldots,N_i\}}$
  - $\Omega_i \sim \chi^T$, the spectral measure of a **Time** trace covariance
    i) Matern's case: $\Omega_i | R_i \sim \mathcal{N}(0, \sqrt{\nu / R_i})$
    ii) Cauchy's case: $\Omega_i | R_i \ldots$ using stable random variables
  - $\Phi_i^{(1)}, \Phi_i^{(2)}$ are random phases, uniformly distributed on $[0, 2\pi[$
- Computation of the simulation value at the target locations:

$$Z(s,t) = Z(\theta, \varphi, t) \approx \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \tilde{P}_{N_i}^{K_i}(\cos\theta) \times \cos(K_i\,\varphi + \phi_i^{(1)}) \times \cos(\Omega_i\, t + \phi_i^{(2)})$$

■ SPACE-TIME MATERN'S MODEL ON $\mathbb{S}_2$

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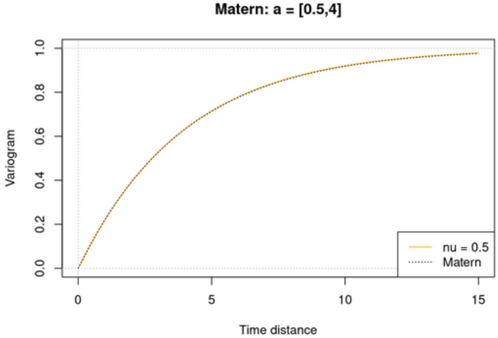
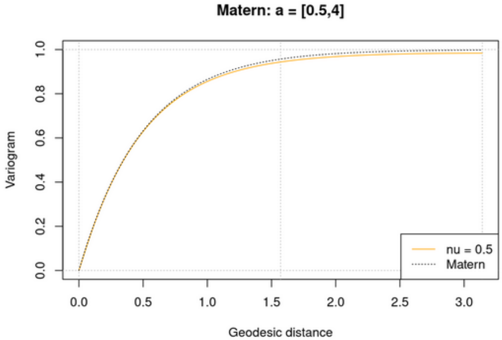
The trace covariance functions: $\nu = 1/2$ and $a = (1/2, 4)$

Covariance function on $\mathbb{R}$



Covariance function on $\mathbb{S}_2$



■ SPACE-TIME MATERN'S MODEL ON $\mathbb{S}_2$

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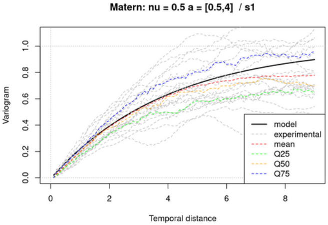
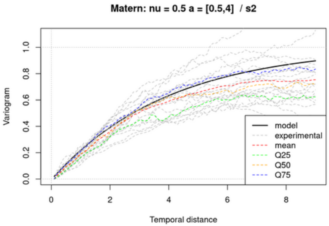
Time variogram: $\nu = 1/2$ and $a = (1/2, 4)$

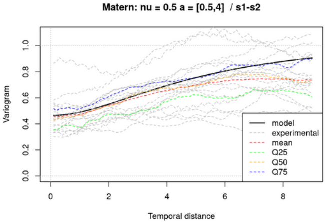
$Z(s_1, \cdot)$



$Z(s_2, \cdot)$



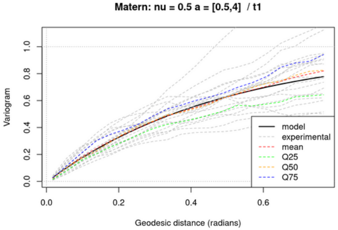
$(Z(s_1, \cdot), Z(s_2, \cdot))$



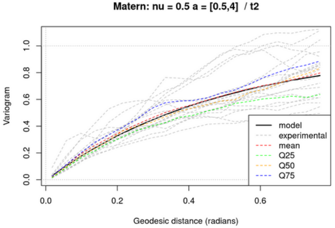
SPACE-TIME MATERN'S MODEL ON $\mathbb{S}_2$

Space variogram: $\nu = 1/2$ and $a = (1/2, 4)$

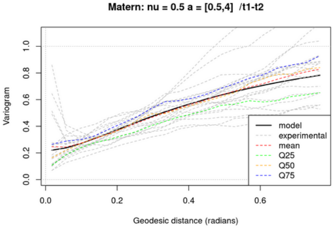
$Z(\cdot, t_1)$



$Z(\cdot, t_2)$



$(Z(\cdot, t_1), Z(\cdot, t_2))$



■ SPACE-TIME CAUCHY'S MODEL ON $\mathbb{S}_2$

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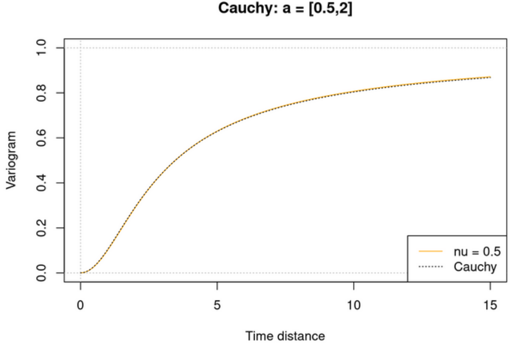
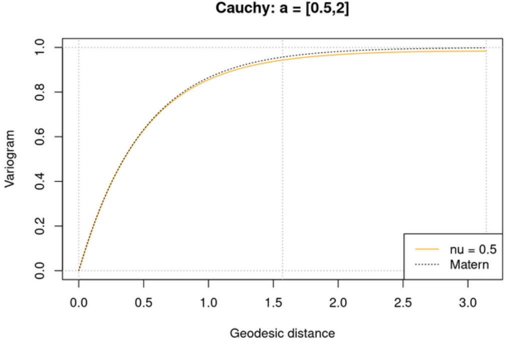
The trace variograms: $\nu = 1/2$ and $a = (1/2, 4)$

Covariance function on $\mathbb{R}$



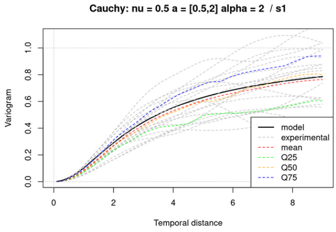
Covariance function on $\mathbb{S}_2$



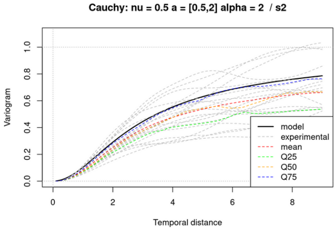
■ SPACE-TIME CAUCHY'S MODEL ON $\mathbb{S}_2$

Time variogram: $\nu = 1/2$ and $a = (1/2, 4)$

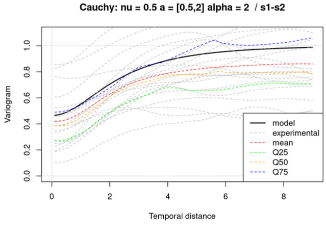
$Z(s_1, \cdot)$



$Z(s_2, \cdot)$



$(Z(s_1, \cdot), Z(s_2, \cdot))$



■ SPACE-TIME CAUCHY'S MODEL ON $\mathbb{S}_2$

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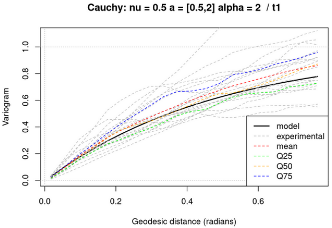
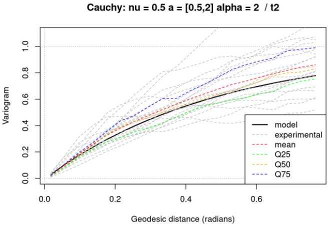
Space variogram: $\nu = 1/2$ and $a = (1/2, 4)$

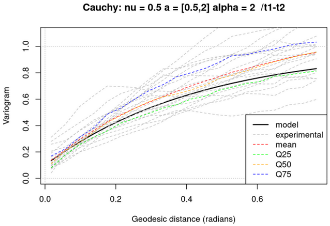
$Z(\cdot, t_1)$



$Z(\cdot, t_2)$



$(Z(\cdot, t_1), Z(\cdot, t_2))$



CONTROLING THE SEPARABILITY?

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$$C(\alpha,\tau) = \frac{1}{(1+|\frac{\tau}{a_t}|^\gamma)^{\beta-\nu}} \int_{\mathbb{R}_+} g_{\nu,1}(r)\ \exp\{-\frac{\nu}{2r}|\frac{2}{a_s}\sin\frac{\alpha}{2}|^2 - r|\frac{\tau}{a_t}|^\gamma\}\, dr$$

with $\beta > 0$, $0 \leq \nu \leq \beta$, $\gamma \in (0,2]$, and $(a_s, a_t) > 0$

- **Space trace** is a *pseudo* Matern's covariance on $\mathbb{S}_2$, $C^S_{\nu,a_s}(\alpha) = \frac{2^{1-\nu}}{\Gamma(\nu)}(\sqrt{2\nu}\, d_\alpha)^\nu K_\nu(\sqrt{2\nu}\, d_\alpha)$ with $d_\alpha = |\frac{2}{a_s}\sin\frac{\alpha}{2}|$
- **Time trace** is a Cauchy's covariance on $\mathbb{R}$, $C^T_{\nu,a_t,\gamma}(\tau) = \frac{1}{(1+|\frac{\tau}{a_t}|^\gamma)^\beta}$

The components $\tilde{\Omega}_i$ and $\Phi_i^{(3)}$ of the Cauchy covariance on the real line, $(1+|\frac{\tau}{a_t}|^\gamma)^{-(\beta-\nu)}$, are simulated independently, and then combined:

$$\frac{1}{\sqrt{n}}\sum_{i=1}^{n} \tilde{P}_{N_i}^{K_i}(\cos\theta) \times \cos(K_i\,\varphi + \phi_i^{(1)}) \times \cos(\Omega_i\, t + \phi_i^{(2)}) \times \sqrt{2}\cos(\tilde{\Omega}_i\, t + \phi_i^{(3)})$$

OUTLINE

■ CONCLUSIONS AND PERSPECTIVES

1. Covariance with parameters to control the scales and the regularity
2. Simulation using a spectral approach (see also Alegria et al. (2020))
3. Implementation in **gstlearn**?

REFERENCES

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- **Allard, D., Emery, X., Lacaux, C., & Lantuéjoul, C.** (2020). Simulating space-time random fields with nonseparable Gneiting-type covariance functions. Statistics and Computing, 30(5), 1479-1495.
- **Lantuéjoul, C., Freulon, X., & Renard, D.** (2019). Spectral simulation of isotropic Gaussian random fields on a sphere. Mathematical Geosciences, 51(8), 999-1020.