Modeling and simulating spatio-temporal multivariate and non-stationary Gaussian Random Fields: a Gaussian mixtures perspective

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Outline

Motivation

- Building covariance functions in complex settings: spatio-temporal, multivariate, nonstationary; **sometimes all at once**
- Need for algorithms for simulating GRFs (GPs) characterized by those
- Simulation algorithms are constructive arguments for defining new classes of covariance functions in these settings
- Particular focus on Gaussian mixtures

Outline

1. **Introduction:** reminders on the spectral method
2. **Building bricks:** Gaussian mixtures, geometric anisotropy, popular covariance functions; recent extensions
3. **Nonstationarity:** a general result relating to the Paciorek-Shervish construction
4. **The full combo:** new nonstationary, multivariate, spatio-temporal class

The classic "classic spectral method"

Shinozuka (1971), Matheron (1973)

Use Bochner Theorem,

$$C(\mathbf{h}) = \int_{\mathbb{R}^d} \exp(i\mathbf{h}^t\boldsymbol{\omega})d\mu(\boldsymbol{\omega}), \quad \forall \mathbf{h} \in \mathbb{R}^d.$$

Then,

$$\tilde{Z}_L(\mathbf{s}) = \sqrt{\frac{2}{L}}\sum_{l=1}^{L}\cos\left(\boldsymbol{\Omega}_l^t\mathbf{s} + \Phi_l\right), \quad \boldsymbol{\Omega}_l \sim \mu, \quad \Phi_l \sim \mathcal{U}(0, 2\pi), \quad \text{all i.i.d}$$

is approximately a GRF with expectation 0 and covariance function C

The classic ”classic spectral method”

Proof

- $E\left[\cos\left(\mathbf{\Omega}_l^t\mathbf{s}+\Phi_l\right)\right]=0$
-
$$\begin{aligned} E\left[2\cos\left(\mathbf{\Omega}_l^t\mathbf{s}+\Phi_l\right)\cos\left(\mathbf{\Omega}_l^t(\mathbf{s}+\mathbf{h})+\Phi_l\right)\right] &= E\left[\cos\left(\mathbf{\Omega}_l^t(2\mathbf{s}+\mathbf{h})+2\Phi_l\right)\right]+E\left[\cos\left(\mathbf{\Omega}_l^t\mathbf{h}\right)\right] \\ &= 0+\int_{\mathbb{R}^d}\cos(\boldsymbol{\omega}^t\mathbf{h})d\mu(\boldsymbol{\omega}) \end{aligned}$$
- Then use CLT

- Similar to the ”Random Fourier Features” (Rahimi and Recht, 2007), based on $\left(\cos(\mathbf{\Omega}_l^t\mathbf{s}),\ \sin(\mathbf{\Omega}_l^t\mathbf{s})\right)$

Extensions of the spectral method

- Multivariate (MV) (Emery et al., 2016) and non-stationary (NS) (Emery and Arroyo, 2018). Includes also NS – MV
- Saptio-temporal (ST) Allard et al. (2020)
- Spatio-temporal multivariate (ST – MV), Allard et al. (2022)

$\hookrightarrow$ Propose an algorithm and models for ”the full combo” NS – ST –MV

Extensions of the spectral method

S only –
Shinozuka,
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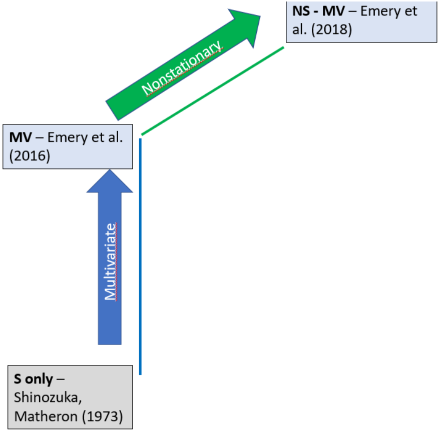
Extensions of the spectral method

Extensions of the spectral method



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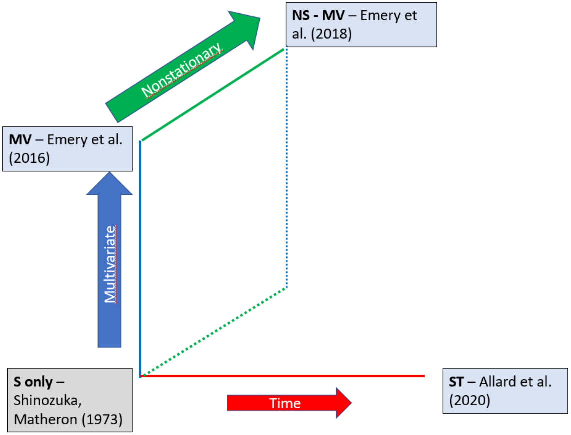

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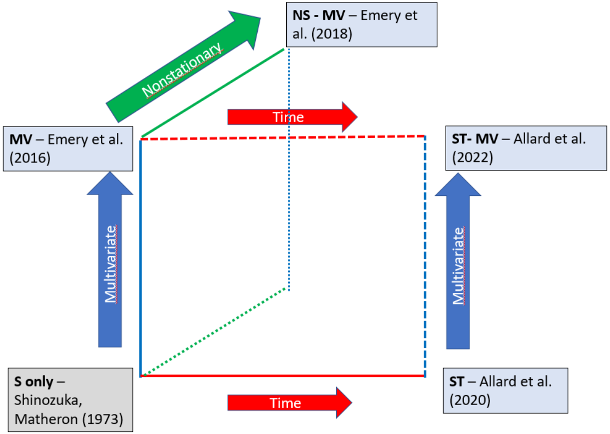

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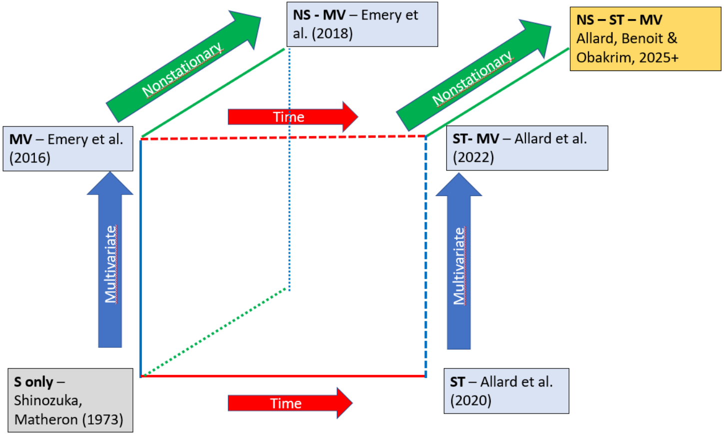

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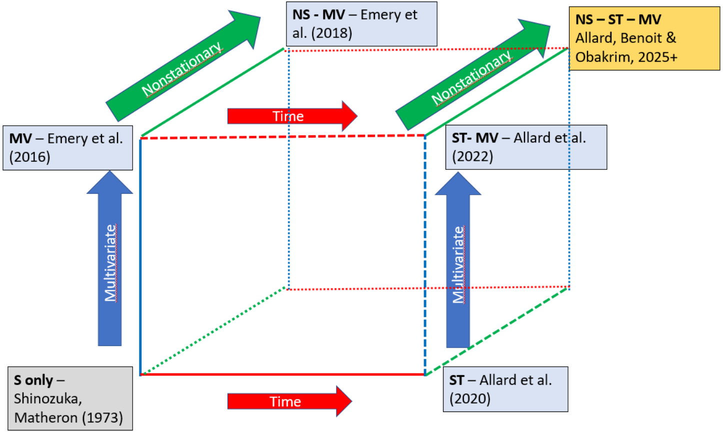

Outline

Gaussian mixtures

Schoenberg (1938)

Define $\mathcal{C}_\infty$ the class of continuous isotropic covariance functions valid on $\mathbb{R}^d$, $\forall d \geq 1$. Then, $\phi \in \mathcal{C}_\infty$ if and only if

$$\phi(\mathbf{h}) = \int_{\mathbb{R}^+} \exp(-||\mathbf{h}||^2 \xi) f(\xi) d\xi$$

$f(\xi)$ is the **Gaussian scale mixture**

Proposition

$$\mu(\omega) = (2\sqrt{\pi})^{-d} \int_0^{+\infty} \exp(-||\omega||^2/4\xi)\xi^{-d/2} f(\xi)\, d\xi$$

In **purple**, spectral density of a Gaussian covariance with scale parameter $\xi^{-1/2}$.

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Geometric anisotropy

Geometric anisotropy in $\mathbb{R}^2$ (Chilès and Delfiner, 2012)

$$\boldsymbol{\Sigma}^{-1/2} = \begin{pmatrix} r_1 & 0 \\ 0 & r_2 \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}, \tag{1}$$

For the Gaussian covariance, one gets:

$$C_G(\mathbf{h}) = \exp\left(-\mathbf{h}^t \boldsymbol{\Sigma}^{-1} \mathbf{h}\right); \qquad \mu_G(\boldsymbol{\omega}) = (2\sqrt{\pi})^{-d} |\boldsymbol{\Sigma}|^{1/2} \exp\left(-\boldsymbol{\omega}^t \boldsymbol{\Sigma} \boldsymbol{\omega}/4\right)$$

Simulation algorithms for stationary univariate spatial GRFs

`Spectral simulation`

Require: $C \in \mathcal{C}_\infty$ and μ
Require: A set of points, $\mathcal{S} \in \mathbb{R}^d$
Require: A large number L

1: **for** $l = 1$ to L **do**
2: **Simulate $\Omega_l \sim \mu$**
3: Simulate $\Phi_l \sim \mathcal{U}(0, 2\pi)$
4: **end for**
5: For each $\mathbf{s} \in \mathcal{S}$ return

$$\tilde{Z}(\mathbf{s}) = \sqrt{\frac{2}{L}} \sum_{l=1}^{L} \cos\left(\boldsymbol{\Sigma}^{-1/2} \boldsymbol{\Omega}_l^t \mathbf{s} + \Phi_l\right)$$

`Gaussian mixture simulation`

Require: $C \in \mathcal{C}_\infty$ and f
Require: A set of points, $\mathcal{S} \in \mathbb{R}^d$
Require: A large number L

1: **for** $l = 1$ to L **do**
2: **Simulate $\xi_l \sim f$**
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Some covariance functions

Matérn covariance

$$C_{\mathcal{M}}(\mathbf{h}) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}(\kappa||\mathbf{h}||)^{\nu} K_{\nu}(\kappa||\mathbf{h}||)$$

$$\mu_{\mathcal{M}}(\boldsymbol{\omega}) \propto \frac{1}{(1+||\boldsymbol{\omega}||^2/\kappa^2)^{\nu+d/2}}$$

$$f_{\mathcal{M}}(\xi) = \left(\frac{\kappa^2}{4}\right)^{\nu} \frac{\xi^{-1-\nu}}{\Gamma(\nu)} e^{-\kappa^2/4\xi}.$$

Hence

$$2: \text{ Simulate } \quad \xi_l \sim IG(\nu, \kappa^2/4)$$

Cauchy covariance

$$C_{\mathcal{C}}(\mathbf{h}) = \left(1 + a||\mathbf{h}||^2\right)^{-\nu}$$

$$\mu_{\mathcal{C}} = \text{Unknown}$$

$$f_{\mathcal{C}}(\xi) = a^{-\nu}\Gamma(\nu)^{-1}\xi^{\nu-1}e^{-\xi/a}$$

Hence

$$2: \text{ Simulate } \quad \xi_l \sim G(\nu, a).$$

Some covariance functions

Matérn covariance

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C_{\mathcal{M}}(\mathbf{h}) &= \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}(\kappa||\mathbf{h}||)^{\nu} K_{\nu}(\kappa||\mathbf{h}||) \\
\mu_{\mathcal{M}}(\boldsymbol{\omega}) &\propto \frac{1}{(1+||\boldsymbol{\omega}||^2/\kappa^2)^{\nu+d/2}} \\
f_{\mathcal{M}}(\xi) &= \left(\frac{\kappa^2}{4}\right)^{\nu} \frac{\xi^{-1-\nu}}{\Gamma(\nu)} e^{-\kappa^2/4\xi}.
\end{aligned}
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Hence

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Cauchy covariance

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C_{\mathcal{C}}(\mathbf{h}) &= \left(1 + a||\mathbf{h}||^2\right)^{-\nu} \\
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\end{aligned}
$$

Hence

$$2: \text{ Simulate } \quad \xi_l \sim G(\nu, a).$$

ST extension

Allard et al. (2020)

Gneiting covariance

$$C(\mathbf{h}, u) = \frac{1}{(\gamma(u) + 1)^{\delta + bd/2}} \phi \left(\frac{||\mathbf{h}||}{(\gamma(u) + 1)^{b/2}} \right)$$

with $b \in [0, 1]$ and $\delta > 0$.

- Define $W(t) \sim \mathrm{GP}(0, \gamma)$ with $W(0) = 0$
- Define $Z_T(t) \sim \mathrm{GP}(0, C_T)$ with

$$C_T(u) = \frac{1}{(\gamma(u) + 1)^{\delta}}$$

Simulation for univariate stationary Gneiting ST GRFs

Require: $C \in \mathcal{C}_\infty$ and associated f ; spatial anisotropy $\boldsymbol{\Sigma}^{-1/2}$
Require: Variogram γ
Require: Parameters $b \in [0,1]$ and $\delta > 0$
Require: A set of points, $\mathcal{S} \in \mathbb{R}^d \times \mathbb{R}$; a large number L

for $l = 1$ to L **do**
  Simulate a RF $Z_{T,l}$ with covariance function $C_T(u) = (1+\gamma(u))^{-\delta}$
  Simulate a RF W_l with Gaussian increments and variogram $\gamma_b = (1+\gamma)^b - 1$
  Simulate $\xi_l \sim f$
  Simulate $\mathbf{V}_l \sim \mathcal{N}_d(0, \mathbf{I}_d)$
  set $\boldsymbol{\Omega}_l = \sqrt{2\xi_l}\boldsymbol{\Sigma}^{-1/2}\mathbf{V}_l$
  Simulate $\Phi_l \sim \mathcal{U}(0, 2\pi)$
end for
For each $(\mathbf{s}, t) \in \mathcal{S}$ return

$$\tilde{Z}_L(\mathbf{s}, t) = \sqrt{\frac{2}{L}} \sum_{l=1}^{L} Z_{T,l}(t) \cos\left(\boldsymbol{\Omega}_l^t \mathbf{s} + \frac{\|\mathbf{V}_l\|}{\sqrt{2}} W_l(t) + \Phi_l\right)$$

ST – MV extension

Allard et al. (2022)

Multivariate Gneiting

$$C_{ij}(\mathbf{h},u) = \frac{\sigma_{ij}}{(\gamma_{ij}(u)+1)^{\delta+bd/2}}\phi_{ij}\left(\frac{\mathbf{\Sigma}^{-1/2}\mathbf{h}}{(\gamma_{ij}(u)+1)^{b/2}}\right)$$

with $\phi_{ij}(\mathbf{h}) = \int_0^\infty e^{-\xi||\mathbf{h}||^2}(f_{ij}(\xi)d\xi$ and $f_{ij} = \sqrt{f_{ii}f_{jj}}$.
For example, for a Matérn covariance: $2\nu_{ij} = \nu_{ii} + \nu_{ii}$ and $2\kappa_{ij}^2 = \kappa_{ii}^2 + \kappa_{ii}^2$

- γ is a pseudo-vaiogram with $\gamma_{ij}(u) = 0.5\, Var\left[W_i - W_j\right]$
- Define $(W_1,\dots,W_p)$ a p-variate GP $(0,\gamma)$ with $W_i = 0$
- Define $(Z_{T,1},\dots,Z_{T,p})$ a p-variate GP $(0,[C_{T,ij}]_{ij=1,p})$ with

$$C_{T,ij}(u) = \sigma_{ij}\left(\gamma_{ij}(u)+1\right)^{-\delta}$$

Simulation for p-variate stationary Gneiting ST GRFs

Require: C Matérn or Cauchy and associated f_{ii}; spatial anisotropy $\mathbf{\Sigma}^{-1/2}$
Require: Pseudo variogram γ; parameters $b \in [0,1]$ and $\delta > 0$
Require: A covariance matrix $\boldsymbol{\sigma} = \boldsymbol{L}\boldsymbol{L}^t$
Require: A pdf f, with support equal to $(0,\infty)$
Require: A set of points, $\mathcal{S} \in \mathbb{R}^d \times \mathbb{R}$; a large number L

1: **for** $l = 1$ to L **do**
2: Simulate a p-variate GRF $\boldsymbol{Z}_{T,l}$ with matrix-valued covariance function $\boldsymbol{C}_T(u) = (1+\gamma(u))^{-\delta}$
3: Simulate a p-variate RF $\boldsymbol{W}_l = [W_{l,i}]_{i=1}^p$ with Gaussian direct and cross-increments, with 0 mean and pseudo-variogram $\gamma_b = (1+\gamma)^b - 1$
4: Simulate $\xi_l \sim f$
5: Simulate $\boldsymbol{V}_l \sim \mathcal{N}_d(0, \mathbf{I}_d)$; set $\mathbf{\Omega}_l = \sqrt{2\xi_l}\mathbf{\Sigma}^{-1/2}\mathbf{V}_l$; simulate $\Phi_l \sim \mathcal{U}(0, 2\pi)$
6: Simulate $\mathbf{A}_l \sim \mathcal{N}_p(0, \boldsymbol{\sigma})$
7: **end for**
8: For each $(\mathbf{s}, t) \in \mathcal{S}$ return

$$\tilde{Z}_{L,i}(\mathbf{s},t) = \sqrt{\frac{2}{L}} \sum_{l=1}^{L} Z_{T,l,i}(t) \sqrt{\frac{f_{ii}(\xi_l)}{f(\xi_l)}} A_{l,i} \cos\left(\mathbf{\Omega}_l^t \mathbf{s} + \frac{\|\mathbf{V}_l\|}{\sqrt{2}} W_{l,i}(t) + \Phi_l\right), \qquad i = 1, \dots, p$$

Outline

State of the art

Non-stationary spatial models

Let $\phi \in \mathcal{C}_\infty$ and $\mathbf{\Sigma}^{-1/2}(\mathbf{s})$ ansiotropy matrices, $\mathbf{s} \in \mathbb{R}^d$. Then,

$$\phi_{NS}(\mathbf{s}, \mathbf{s}') = |\mathbf{\Sigma}_\mathbf{s}|^{1/4} |\mathbf{\Sigma}_{\mathbf{s}'}|^{1/4} |\mathbf{\Sigma}_{\mathbf{s},\mathbf{s}'}|^{-1/2} \phi\left(\sqrt{(\mathbf{s}-\mathbf{s}')^t \mathbf{\Sigma}_{\mathbf{s},\mathbf{s}'}^{-1} (\mathbf{s}-\mathbf{s}')}\right),$$

is a nonstationary covariance on $\mathbb{R}^d$, with $\mathbf{\Sigma}_{\mathbf{s},\mathbf{s}'} = \left(\mathbf{\Sigma}_\mathbf{s} + \mathbf{\Sigma}_{\mathbf{s}'}\right)/2$, (Paciorek and Schervish, 2006; Emery and Arroyo, 2018).

- It is the covariance function of

$$Z(\mathbf{s}) = \sqrt{\frac{2\mu_\mathbf{s}(\mathbf{\Omega})}{\mu_0(\mathbf{\Omega})}} \cos(\mathbf{\Omega}^t \mathbf{s} + \Phi), \quad \mathbf{\Omega} \sim \mu_0$$

- Univariate and multivariate simulation algorithms in Emery and Arroyo (2018)

A more general result

- Consider f belongs to the exponential family

$$f(\xi;\boldsymbol{\theta}) = h(\boldsymbol{\theta}) \exp\left(-\ell(\boldsymbol{\theta})^t \boldsymbol{T}(\xi)\right)$$

- Includes Gamma (Cauchy cov.), Inverse Gamma (Matérn cov.), Beta, Gaussian, Inverse Gaussian, etc.

Theorem (Allard et al., 2025+)

Let $C(\cdot,\theta)$ be an isotropic statioanry covariance function defined by $f(\cdot;\theta)$. Then,

$$C^*(\mathbf{s},\mathbf{s}') = |\boldsymbol{\Sigma}_{\mathbf{s}}|^{1/4}|\boldsymbol{\Sigma}_{\mathbf{s}'}|^{1/4}|\boldsymbol{\Sigma}_{\mathbf{s},\mathbf{s}'}|^{-1/2} C(\boldsymbol{\Sigma}_{\mathbf{s},\mathbf{s}'}{}^{-1/2}(\mathbf{s}-\mathbf{s}');\boldsymbol{\theta}_{\mathbf{s},\mathbf{s}'}),$$

is a nonstationary covariance on $\mathbb{R}^d$, where $\boldsymbol{\theta}_{\mathbf{s},\mathbf{s}'}$ is such that

$$\ell(\boldsymbol{\theta}_{\mathbf{s},\mathbf{s}'}) = \frac{\ell(\boldsymbol{\theta}_{\mathbf{s}}) + \ell(\boldsymbol{\theta}_{\mathbf{s}'})}{2}.$$

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Construction and example

- It is the covariance function of

$$Z(\mathbf{s}) = \sqrt{2f(\xi;\boldsymbol{\theta}_{\mathbf{s}})/f_1(\xi)}\sqrt{\mu^G_{\boldsymbol{\Sigma}_{\mathbf{s}}}(\boldsymbol{\Omega})/\mu^G_{\boldsymbol{I}_d}(\boldsymbol{\Omega})}\cos(\boldsymbol{\Omega}^t\mathbf{s}+\Phi),$$

- Matérn $\to$ the covariance in Emery and Arroyo (2018)
- Cauchy $\to$ since $f_C(\xi;(\nu,a)) = a^{-\nu}\Gamma(\nu)^{-1}\xi^{\nu-1}e^{-\xi/a}$, we get $\ell(\theta) = (1-\nu, 1/a)^t$, $\boldsymbol{T}(\xi) = (\ln\xi,\xi)^t$ and $h(\theta) = a^{-\nu}\Gamma(\nu)^{-1}$. Hence,

$$\ell(\theta_{\mathbf{s},\mathbf{s}'}) = \left(1-(\nu_{\mathbf{s}}+\nu'_{\mathbf{s}})/2,\ ({a_{\mathbf{s}}}^{-1}+{a'_{\mathbf{s}}}^{-1})/2\right)^t, \quad h(\theta_{\mathbf{s},\mathbf{s}'}) = \frac{1}{\Gamma\left((\nu_{\mathbf{s}}+\nu'_{\mathbf{s}})/2\right)}\left(\frac{2a_{\mathbf{s}}a'_{\mathbf{s}}}{a_{\mathbf{s}}+a'_{\mathbf{s}}}\right)^{-(\nu_{\mathbf{s}}+\nu'_{\mathbf{s}})/2}$$

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Outline

A simulation algorithm for NS MV S-T GRFs

Require: A family of scale mixtures, $f(\cdot;\boldsymbol{\theta})$, belonging to the exponential family
Require: A set of points, $\mathcal{S} \in \mathbb{R}^d \times \mathbb{R}$
Require: Parameters $\boldsymbol{\theta}_{ii,\mathbf{x}}$ and anisotropy matrices $\boldsymbol{\Sigma}_{ii,\mathbf{x}}^{-1/2}$; covariance matrices $\boldsymbol{\sigma}_{\mathbf{x}} = \boldsymbol{L}_{\mathbf{x}}\boldsymbol{L}_{\mathbf{x}}^t$
Require: Pseudo variogram γ; $\delta > 0$

1: Set $f_1 := f(\boldsymbol{\theta})$ for $\boldsymbol{\theta} = \mathbf{1}$
2: **for** $l = 1$ to L **do**
3: Simulate a p-variate RF $\boldsymbol{Z}_{T,l}$ with matrix-valued covariance function $\boldsymbol{C}_T(t) = (1+\gamma(t))^{-\delta}$
4: Simulate a p-variate RF $\boldsymbol{W}_l = [W_{l,i}]_{i=1}^p$ with pseudo-variogram γ
5: Simulate $\xi_l \sim f_1$
6: Simulate $\boldsymbol{V}_l \sim \mathcal{N}_d(0, \mathbf{I}_d)$; set $\boldsymbol{\Omega}_l = \sqrt{2\xi_l}\mathbf{V}_l$
7: Simulate $\Phi_l \sim \mathcal{U}(0, 2\pi)$; Simulate $\boldsymbol{A}_l \sim \mathcal{N}_p(0, \boldsymbol{I}_p)$
8: **end for**
9: For each $\mathbf{x} = (\mathbf{s}, t) \in \mathcal{S}$, and for $i = 1, \dots, p$ return

$$\tilde{Z}_{L,i}(\mathbf{s}, t) = \sqrt{\frac{2}{L}} \sum_{l=1}^{L} Z_{T,l,i}(t) \sqrt{\frac{f_{ii,\mathbf{x}}(\xi_l)}{f_1(\xi_l)}} \sqrt{\frac{\mu^G_{\boldsymbol{\Sigma}_{ii,\mathbf{x}}}(\sqrt{2}\mathbf{V}_l)}{\mu^G_{\mathbf{I}_d}(\sqrt{2}\mathbf{V}_l)}} (\boldsymbol{L}_{\mathbf{x}}\boldsymbol{A}_l)_i \cos\left(\boldsymbol{\Omega}_l^t \mathbf{s} + \frac{\|\mathbf{V}_l\|}{\sqrt{2}} W_i(t) + \Phi_l\right)$$

Nonstationary multivariate space-time model

Theorem (Allard et al., 2025+)

Let us denote $\mathbf{x} = (\mathbf{s}, t)$. Then,

$$C_{ij}(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = |\boldsymbol{\Sigma}_{ii,\mathbf{x}_1}|^{1/4} |\boldsymbol{\Sigma}_{jj,\mathbf{x}_2}|^{1/4} \frac{\sigma_{ij,\mathbf{x}_1\mathbf{x}_2}}{|\boldsymbol{\Lambda}_{ij,\mathbf{x}_1,\mathbf{x}_2}|^{1/2}} \phi_{ij}\left(\boldsymbol{\Lambda}_{ij,\mathbf{x}_1,\mathbf{x}_2}^{-1/2}(\mathbf{s}_1 - \mathbf{s}_2); \boldsymbol{\theta}_{\mathbf{x}_1,\mathbf{x}_2}\right)$$

where $\boldsymbol{\Lambda}_{ij,\mathbf{x}_1,\mathbf{x}_2} = (\boldsymbol{\Sigma}_{ii,\mathbf{x}_1} + \boldsymbol{\Sigma}_{jj,\mathbf{x}_2})/2 + \gamma_{ij}(t_1 - t_2)\boldsymbol{I}_d$.

- Proof: it is the covariance resulting from the Algorithm above

Temporal trace

Theorem (Allard et al., 2025+)

$$C_{T\,ij}(\mathbf{s}_1, \mathbf{s}_1; t_1, t_2) = |\boldsymbol{\Sigma}_{ii,\mathbf{x}_1}|^{1/4} |\boldsymbol{\Sigma}_{jj,\mathbf{x}_2}|^{1/4} \frac{\sigma_{ij,\mathbf{x}_1\mathbf{x}_1}}{|\boldsymbol{\Sigma}_{ij,\mathbf{x}_1} + \gamma_{ij}(t_1 - t_2)\boldsymbol{I}_d|^{1/2}}$$

where $\boldsymbol{\Sigma}_{ij,\mathbf{x}_1} = (\boldsymbol{\Sigma}_{ii,\mathbf{x}_1} + \boldsymbol{\Sigma}_{jj,\mathbf{x}_1})/2$

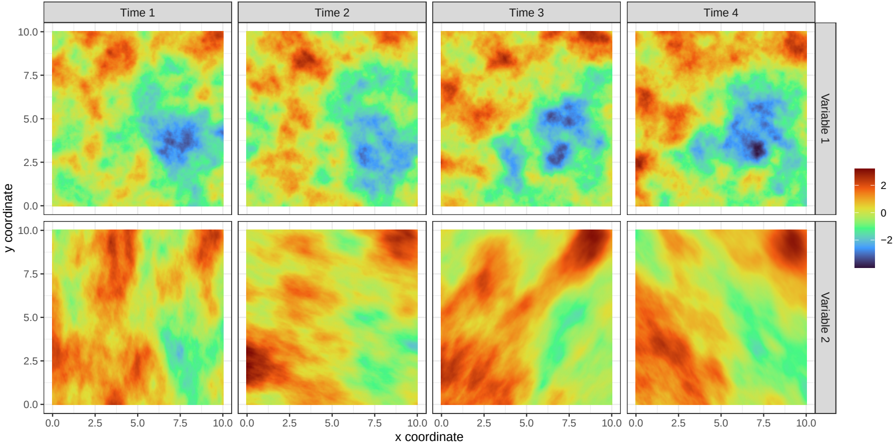
- The temporal correlation trace is thus

$$|\boldsymbol{\Sigma}_{ij,\mathbf{x}_1} + \gamma_{ij}(u)\boldsymbol{I}_d|^{-1/2}$$

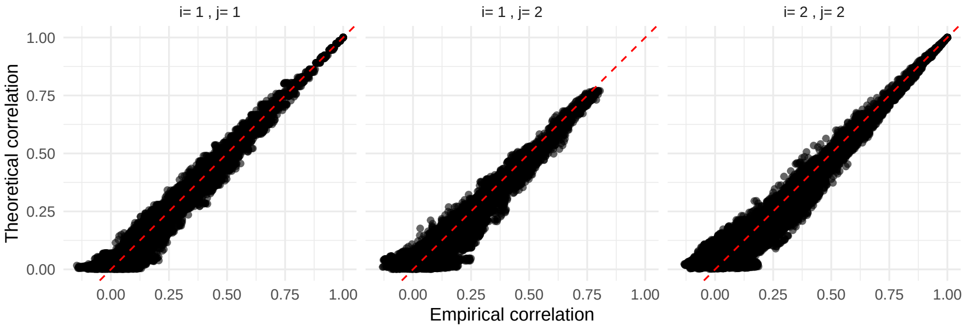
- It is non stationary in space !

The **spatial trace** is identical to the construction in Paciorek and Schervish (2006).

Illustration



Illustration



Final words

- We propose a change of perspective: from spectral representation to Gaussian mixture representation
- It paves the way to general theorem allowing for the construction of a new and wide class of nonstationary covariance functions
- Two well separated steps: i) stochastic generation; ii) projection onto $\mathcal{S}$
- The second step is massively parallelizable
- Possible extensions to non Euclidean spaces

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