Lagrangian Spatio-Temporal Covariance Functions for Multivariate Nonstationary Random Fields

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I. Motivation

Modern-Era Retrospective Analysis for Research and Applications, version 2 (MERRA-2) reanalysis

log particulate matter (PM) data on January 1, 2018

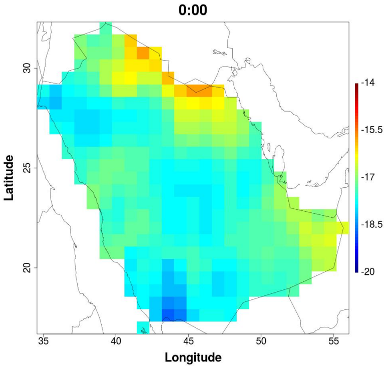

Fig. 1: log Dust Mass Concentration

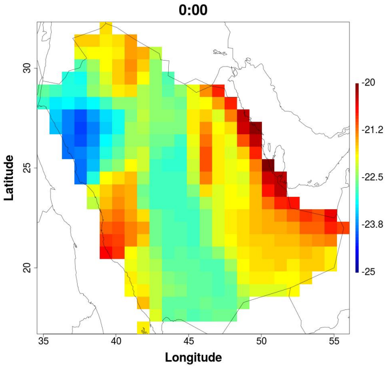

Fig. 2: log Black Carbon Concentration

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Overview

II. Review of Spatio-Temporal Geostatistics

II. Review of Spatio-Temporal Geostatistics: Univariate Spatio-Temporal Random Fields

Consider a real-valued spatio-temporal random field

$$Y(\mathbf{s}, t), \quad (\mathbf{s}, t) \in \mathbb{R}^d \times \mathbb{R},$$

where $(\mathbf{s}, t)$ is the spatio-temporal location.

Suppose that $Y(\mathbf{s}, t)$ is comprised of a deterministic and a random component, i.e.,

$$Y(\mathbf{s}, t) = \mu(\mathbf{s}, t) + Z(\mathbf{s}, t),$$

where $\mu(\cdot)$ is a trend function, and $Z(\cdot)$ a zero mean spatio-temporal random field.

II. Review of Spatio-Temporal Geostatistics: Spatio-Temporal Covariance Functions

Assuming $Z(\cdot)$ is a zero-mean Gaussian spatio-temporal random field, then $Z(\cdot)$ is completely characterized by its spatio-temporal covariance function

$$C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = \mathrm{cov}\left\{Z(\mathbf{s}_1, t_1), Z(\mathbf{s}_2, t_2)\right\}.$$

A valid spatio-temporal covariance function ensures that the resulting spatio-temporal covariance matrix of the n-dimensional vector $\mathbf{Z} = \{Z(\mathbf{s}_1, t_1), \ldots, Z(\mathbf{s}_n, t_n)\}^\top$ is positive definite, i.e., for any $n \in \mathbb{Z}^+$, for any finite set of points $(\mathbf{s}_1, t_1), \ldots, (\mathbf{s}_n, t_n)$, and for any vector $\boldsymbol{\lambda} \in \mathbb{R}^n$, we have $\boldsymbol{\lambda}^\top \boldsymbol{\Sigma} \boldsymbol{\lambda} > 0$, where $\boldsymbol{\Sigma}$ is an $n \times n$ matrix, and n is the number of spatio-temporal locations.

II. Review of Spatio-Temporal Geostatistics: Properties of Spatio-Temporal Covariance Functions

- (weakly) stationary: $C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2)$ simplifies to $C(\mathbf{h}, u)$, where $\mathbf{h} = \mathbf{s}_1 - \mathbf{s}_2$ and $u = t_1 - t_2$
- isotropy: $C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2)$ further simplifies to $C(\|\mathbf{h}\|, |u|)$, where $\|\mathbf{h}\| = \|\mathbf{s}_1 - \mathbf{s}_2\|$ and $|u| = |t_1 - t_2|$
- space-time separability: $C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = C^S(\mathbf{s}_1, \mathbf{s}_2) C^T(t_1, t_2)$, where $C^S(\mathbf{s}_1, \mathbf{s}_2)$ is a purely spatial covariance function and $C^T(t_1, t_2)$ is a purely temporal covariance function
- full symmetry: $C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = C(\mathbf{s}_1, \mathbf{s}_2; t_2, t_1)$

II. Review of Spatio-Temporal Geostatistics: Kriging

Let $Z(\mathbf{s}_0, t_0)$ be the unknown value at an unobserved spatio-temporal location $\mathbf{s}_0 \in \mathbb{R}^d$ and $t_0 \in \mathbb{R}$.

Under the squared-error loss criterion, the best linear unbiased predictor of $Z(\mathbf{s}_0, t_0)$ given $\mathbf{Z} = \{Z(\mathbf{s}_1, t_1), \ldots, Z(\mathbf{s}_n, t_n)\}^\top$ is the simple kriging predictor

$$\widehat{Z}(\mathbf{s}_0, t_0) = \mathrm{E}\left\{Z(\mathbf{s}_0, t_0) | Z(\mathbf{s}_1, t_1), \ldots, Z(\mathbf{s}_n, t_n)\right\}$$

with the closed form

$$\widehat{Z}(\mathbf{s}_0, t_0) = \mathbf{\Delta}_0^\top \mathbf{\Sigma}^{-1} \mathbf{Z},$$

where $\mathbf{\Delta}_0 = \{C(\mathbf{s}_0, \mathbf{s}_1; t_0, t_1), C(\mathbf{s}_0, \mathbf{s}_2; t_0, t_2), \ldots, C(\mathbf{s}_0, \mathbf{s}_n; t_0, t_n)\}^\top$.

II. Review of Spatio-Temporal Geostatistics: Multivariate Spatio-Temporal Random Fields

Consider a spatio-temporal random field

$$\mathbf{Y}(\mathbf{s},t) = \left\{Y_1(\mathbf{s},t),\dots,Y_p(\mathbf{s},t)\right\}^\top,$$

such that at each spatial location $\mathbf{s} \in \mathbb{R}^d, d \geq 1$, and at each time $t \in \mathbb{R}$, there are p variables.

Assume that $\mathbf{Y}(\mathbf{s},t)$ can be decomposed into a sum of a deterministic and a random component, i.e.,

$$\mathbf{Y}(\mathbf{s},t) = \boldsymbol{\mu}(\mathbf{s},t) + \mathbf{Z}(\mathbf{s},t),$$

where $\boldsymbol{\mu}(\cdot)$ is a trend function, and $\mathbf{Z}(\cdot)$ a zero mean multivariate spatio-temporal Gaussian random field with stationary cross-covariance function

$$C_{ij}(\mathbf{h},u) = \text{cov}\left\{Z_i(\mathbf{s},t), Z_j(\mathbf{s}+\mathbf{h},t+u)\right\}.$$

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II. Review of Spatio-Temporal Geostatistics: Properties of Spatio-Temporal Cross-Covariance Functions

- (weakly) stationary: $C_{ij}(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2)$ simplifies to $C_{ij}(\mathbf{h}, u)$, where $\mathbf{h} = \mathbf{s}_1 - \mathbf{s}_2$ and $u = t_1 - t_2$
- isotropy: $C_{ij}(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2)$ further simplifies to $C_{ij}(\|\mathbf{h}\|, |u|)$, where $\|\mathbf{h}\| = \|\mathbf{s}_1 - \mathbf{s}_2\|$ and $|u| = |t_1 - t_2|$
- space-time separability: $C_{ij}(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = C^S_{ij}(\mathbf{s}_1, \mathbf{s}_2) C^T_{ij}(t_1, t_2)$, where $C^S(\mathbf{s}_1, \mathbf{s}_2)$ is a purely spatial covariance function and $C^T(t_1, t_2)$ is a purely temporal covariance function
- full symmetry: $C_{ij}(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = C_{ij}(\mathbf{s}_1, \mathbf{s}_2; t_2, t_1)$

II. Review of Spatio-Temporal Geostatistics: Cokriging

Let $\mathbf{Z}(\mathbf{s}_0, t_0)$ be the vector of unknown values at an unobserved spatio-temporal location $\mathbf{s}_0 \in \mathbb{R}^d$ and $t_0 \in \mathbb{R}$.

Under the squared-error loss criterion, the best linear unbiased predictor of $\mathbf{Z}(\mathbf{s}_0, t_0)$ given $\mathbf{Z} = \{\mathbf{Z}(\mathbf{s}_1, t_1)^\top, \ldots, \mathbf{Z}(\mathbf{s}_n, t_n)^\top\}^\top$ is the simple cokriging predictor

$$\widehat{\mathbf{Z}}(\mathbf{s}_0, t_0) = \mathrm{E}\left\{\mathbf{Z}(\mathbf{s}_0, t_0) | \mathbf{Z}(\mathbf{s}_1, t_1), \ldots, \mathbf{Z}(\mathbf{s}_n, t_n)\right\}$$

with the closed form

$$\widehat{\mathbf{Z}}(\mathbf{s}_0, t_0) = \mathbf{\Delta}_0^\top \mathbf{\Sigma}^{-1} \mathbf{Z},$$

where $\mathbf{\Delta}_0 = \{\mathbf{C}(\mathbf{s}_0, \mathbf{s}_1; t_0, t_1), \mathbf{C}(\mathbf{s}_0, \mathbf{s}_2; t_0, t_2), \ldots, \mathbf{C}(\mathbf{s}_0, \mathbf{s}_n; t_0, t_n)\}^\top$.

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III. The Lagrangian Framework

III. The Lagrangian Framework: Review

Waymire et al. (1987) defined a process

$$Z(\mathbf{s}, t) = \tilde{Z}(\mathbf{s} - \mathbf{v}t)$$

with spatio-temporal stationary covariance function

$$C(\mathbf{h}, u) = C^S(\mathbf{h} - \mathbf{v}u)$$

and called it the frozen field. Here $\mathbf{v}$ is called the advection velocity vector.

Cox and Isham (1988) replaced the constant velocity with a random velocity, $\mathbf{V} \in \mathbb{R}^d$, resulting in a spatio-temporal covariance function model of the form

$$C(\mathbf{h}, u) = \mathrm{E}_{\mathbf{V}}\left\{C^S(\mathbf{h} - \mathbf{V}u)\right\}.$$

We call this the non-frozen field model.

III. The Lagrangian Framework: Review

Covariance functions modeling

$$Z(\mathbf{s}, t) = \tilde{Z}(\mathbf{s} - \mathbf{v}t)$$

are termed "spatio-temporal covariance functions under the Lagrangian framework".

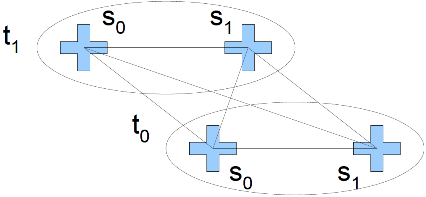

Fig. 3: Lagrangian Reference Frame (Gräler et al., 2012).

Fig. 4: Wide-angle photographs of the sky taken at 10 min intervals in Kungsbacka, Sweden on 2018-05-25. Read left to right and top to bottom. The clouds move from the lower right to the upper left (Gingsjoö, 2018).

III. The Lagrangian Framework: Contribution

The frozen field model was used to model waves, solar irradiance, cloud cover data, spread of diseases, and wind.

A survey of existing literature suggests that there is no detailed Lagrangian formulation in the nonstationary and multivariate arena.

Hence, we took significant strides towards developing and unifying the modeling of transport datasets using specialized covariance functions under the Lagrangian framework.

IV. The Univariate Nonstationary Extension

IV. Univariate Nonstationary Extension: Main Theorem

Theorem 1

Let $\mathbf{V}$ *be a random vector on* $\mathbb{R}^d$*. If* $C^S(\mathbf{s}_1, \mathbf{s}_2)$ *is a valid purely spatial nonstationary covariance function on* $\mathbb{R}^d$*, then,*

$$C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = \mathrm{E}_{\mathbf{V}}\left\{C^S(\mathbf{s}_1 - \mathbf{V}t_1, \mathbf{s}_2 - \mathbf{V}t_2)\right\}$$

for $\mathbf{s}_1, \mathbf{s}_2 \in \mathbb{R}^d$ *and* $t_1, t_2 \in \mathbb{R}$*, is a valid spatio-temporal nonstationary covariance function on* $\mathbb{R}^d \times \mathbb{R}$ *provided that the expectation exists.*

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IV. Univariate Nonstationary Extension: Example 1

Spatially Varying Parameters Model (Paciorek & Schervish, 2006)

$$C^S(\mathbf{s}_1,\mathbf{s}_2) = \sigma(\mathbf{s}_1,\mathbf{s}_2)\mathscr{M}_\nu\left[\left\{(\mathbf{s}_1-\mathbf{s}_2)^\top \mathbf{D}(\mathbf{s}_1,\mathbf{s}_2)^{-1}(\mathbf{s}_1-\mathbf{s}_2)\right\}^{1/2}\right],$$

Here $\mathscr{M}_\nu$ is the univariate Matérn stationary correlation with smoothness parameter $\nu > 0$, i.e., $\mathscr{M}_\nu(\mathbf{h}) = \frac{2^{1-\nu}}{\Gamma(\nu)}(\|\mathbf{h}\|)^\nu \mathscr{K}_\nu(\|\mathbf{h}\|)$, $\sigma(\mathbf{s}_1,\mathbf{s}_2)$ is the spatially varying variance parameter, and $\mathbf{D}(\mathbf{s}_1,\mathbf{s}_2)$ is a positive definite matrix which serves as the spatially varying scale parameter.

Lagrangian Spatio-Temporal Spatially Varying Parameters Model

$$C(\mathbf{s}_1,\mathbf{s}_2;t_1,t_2) = \mathrm{E}_{\mathbf{V}}\Big\{\sigma(\mathbf{s}_1-\mathbf{V}t_1,\mathbf{s}_2-\mathbf{V}t_2)\mathscr{M}_\nu\Big(\big[\{\mathbf{s}_1-\mathbf{s}_2-\mathbf{V}(t_1-t_2)\}^\top \times\mathbf{D}(\mathbf{s}_1-\mathbf{V}t_1,\mathbf{s}_2-\mathbf{V}t_2)^{-1}\{\mathbf{s}_1-\mathbf{s}_2-\mathbf{V}(t_1-t_2)\}\big]^{1/2}\Big)\Big\}$$

IV. Univariate Nonstationary Extension: Example 1

Lagrangian Spatio-Temporal Spatially Varying Parameters Model

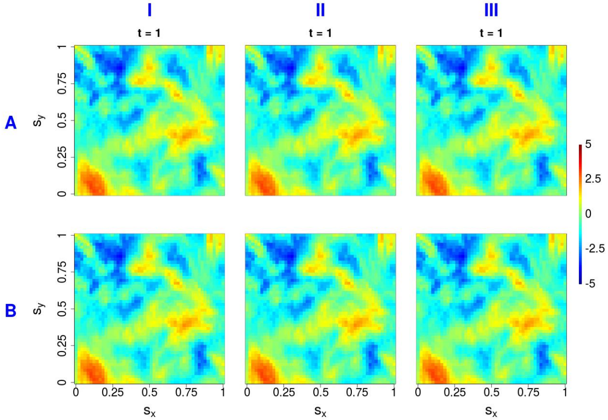

Fig. 5: Simulations on the unit square with $\mathbf{V} \sim \mathcal{N}_d(\boldsymbol{\mu}_{\mathbf{V}}, \boldsymbol{\Sigma}_{\mathbf{V}})$.
A: $\boldsymbol{\mu}_{\mathbf{V}} = (0,0)^\top$, B: $\boldsymbol{\mu}_{\mathbf{V}} = (0.1,0.1)^\top$
I: $\boldsymbol{\Sigma}_{\mathbf{V}} = 0.001 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, II: $\boldsymbol{\Sigma}_{\mathbf{V}} = 0.1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, III: $\boldsymbol{\Sigma}_{\mathbf{V}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

IV. Univariate Nonstationary Extension: Example 1

Lagrangian Spatio-Temporal Spatially Varying Parameters Model

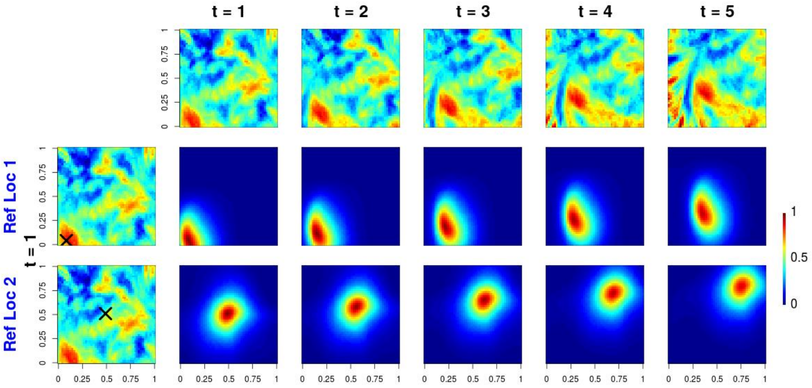

Fig. 6: Heatmaps of $C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2)$ observed at two reference locations marked with "×" when $\mathbf{V} \sim \mathcal{N}_d(\boldsymbol{\mu}_\mathbf{V}, \boldsymbol{\Sigma}_\mathbf{V})$ with $\boldsymbol{\mu}_\mathbf{V} = (0.1, 0.1)^\top$ and $\boldsymbol{\Sigma}_\mathbf{V} = 0.001 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

IV. Univariate Nonstationary Extension: Example 2

Deformation Model

$$C^S(\mathbf{s}_1, \mathbf{s}_2) = \tilde{C}^S\left\{\|\mathbf{f}(\mathbf{s}_1) - \mathbf{f}(\mathbf{s}_2)\|\right\},$$

where $\tilde{C}^S(\cdot)$ is a valid purely spatial stationary covariance function on $\mathbb{R}^d$ and $\mathbf{f}: \mathbb{R}^d \rightarrow \mathbb{R}^d$ represents deterministic non-linear smooth bijective function of the original space onto the deformed space.

Lagrangian Spatio-Temporal Deformation Model

$$C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = \mathrm{E}_{\mathbf{V}}\left[\tilde{C}^S\left\{\|\mathbf{f}(\mathbf{s}_1 - \mathbf{V}t_1) - \mathbf{f}(\mathbf{s}_2 - \mathbf{V}t_2)\|\right\}\right]$$

IV. Univariate Nonstationary Extension: Example 2

Lagrangian Spatio-Temporal Deformation Model

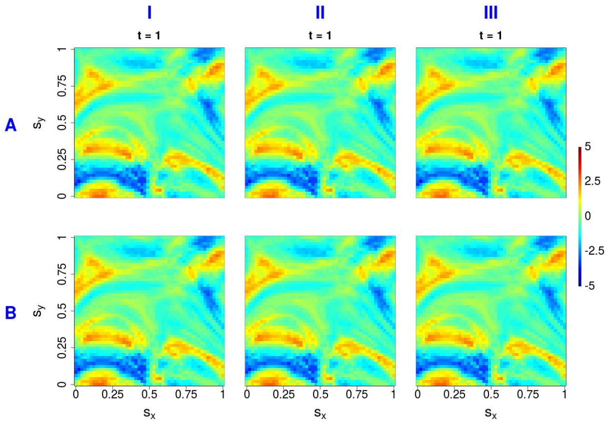

Fig. 7: Simulations on the unit square with $\mathbf{V} \sim \mathcal{N}_d(\boldsymbol{\mu}_\mathbf{V}, \boldsymbol{\Sigma}_\mathbf{V})$.
A: $\boldsymbol{\mu}_\mathbf{V} = (0,0)^\top$, B: $\boldsymbol{\mu}_\mathbf{V} = (0.1,0.1)^\top$
I: $\boldsymbol{\Sigma}_\mathbf{V} = 0.001\begin{pmatrix}1&0\\0&1\end{pmatrix}$, II: $\boldsymbol{\Sigma}_\mathbf{V} = 0.1\begin{pmatrix}1&0\\0&1\end{pmatrix}$, III: $\boldsymbol{\Sigma}_\mathbf{V} = \begin{pmatrix}1&0\\0&1\end{pmatrix}$.

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IV. Univariate Nonstationary Extension: Example 2

Lagrangian Spatio-Temporal Deformation Model

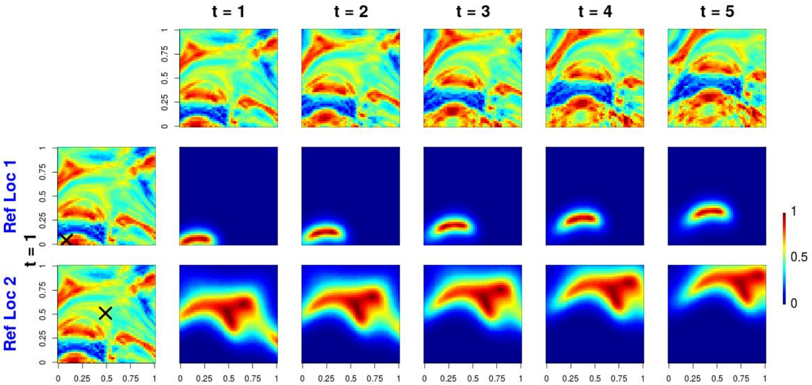

Fig. 8: Heatmaps of $C(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2)$ observed at two reference locations marked with "×" when $\mathbf{V} \sim \mathcal{N}_d(\boldsymbol{\mu}_\mathbf{V}, \boldsymbol{\Sigma}_\mathbf{V})$ with $\boldsymbol{\mu}_\mathbf{V} = (0.1, 0.1)^\top$ and $\boldsymbol{\Sigma}_\mathbf{V} = 0.001 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

IV. Univariate Nonstationary Extension: Two-Step Maximum Likelihood Estimation

Deformation Models

To estimate: $\mathbf{f}(\cdot)$, purely spatial parameters of $\tilde{C}^S(\cdot)$, advection velocity parameters

Spatially Varying Parameters Models

To estimate: spatially varying parameters and advection velocity parameters

Approach: Two-step maximum likelihood estimation with partial warps parameterization of the thin-plate splines to model the nonstationary parameters

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IV. Univariate Nonstationary Extension: Maximum Likelihood Estimation

Suppose $\mathbf{Z} = \left\{Z(\mathbf{s}_1, t_1), Z(\mathbf{s}_2, t_2), \ldots, Z(\mathbf{s}_n, t_n)\right\}^\top$ is a zero mean observation vector where $n \in \mathbb{Z}^+$ is the total number of space-time locations. Inference is performed through maximizing the log-likelihood

$$l(\boldsymbol{\Theta}; \mathbf{Z}) = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log|\boldsymbol{\Sigma}(\boldsymbol{\Theta})| - \frac{1}{2}\mathbf{Z}^\top \boldsymbol{\Sigma}(\boldsymbol{\Theta})^{-1}\mathbf{Z}$$

with respect to all the parameters collected in $\boldsymbol{\Theta} \in \mathbb{R}^q$.

Here $\boldsymbol{\Sigma}(\boldsymbol{\Theta})$ is the $n \times n$ covariance matrix formed by a parametric spatio-temporal nonstationary covariance function.

IV. Univariate Nonstationary Extension: Likelihood Approximations in the Temporal Domain

The log-likelihood function can be approximated as follows:

$$l(\boldsymbol{\Theta}; \mathbf{Z}_1, \ldots, \mathbf{Z}_T) \approx l(\boldsymbol{\Theta}; \mathbf{Z}_{1,t^*}) + \sum_{j=t^*+1}^{T} l(\boldsymbol{\Theta}; \mathbf{Z}_j | \mathbf{Z}_{j-t^*,j-1}),$$

where $\mathbf{Z}_{a,b} = \left(\mathbf{Z}_a^\top, \ldots, \mathbf{Z}_b^\top\right)^\top \in \mathbb{R}^{Nt^*}$, for $a < b$, and t^* specifies the number of consecutive temporal locations included in the conditional distribution and $l(\boldsymbol{\Theta}; \mathbf{Z}_j | \mathbf{Z}_{j-t^*,j-1})$ is the log-likelihood function based only on the vector of space-time observations $\mathbf{Z}_{j-t^*,j-1} = \left(\mathbf{Z}_{j-t^*}^\top, \ldots, \mathbf{Z}_{j-1}^\top\right)^\top$. Here $\mathbf{Z}_t = \{Z(\mathbf{s}_1, t), \ldots, Z(\mathbf{s}_N, t)\}^\top \in \mathbb{R}^N$, for $t = 0, \ldots, T-1$, N and T are the number of spatial and temporal locations, respectively, and $n = N \times T$.

IV. Univariate Nonstationary Extension: Application

Modern-Era Retrospective Analysis for Research and Applications, version 2 (MERRA-2) reanalysis hourly log PM2.5 data on January 2017

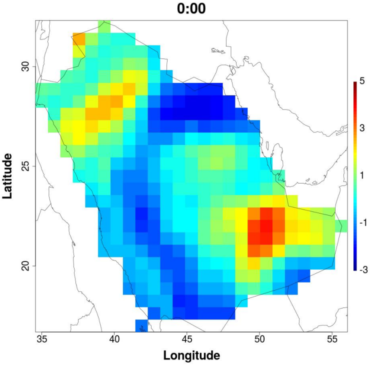

Fig. 9: log Dust Mass Concentration Residuals

IV. Univariate Nonstationary Extension: Application

We fit six different spatio-temporal covariance functions with Matérn spatial margins.

- M1: Non-frozen Lagrangian spatio-temporal stationary covariance
- M2: Non-frozen Lagrangian spatio-temporal spatially varying parameters model
- M3: Non-frozen Lagrangian spatio-temporal deformation model
- M4: Non-Lagrangian spatio-temporal stationary covariance
- M5: Non-Lagrangian spatio-temporal nonstationary model I
- M6: Non-Lagrangian spatio-temporal nonstationary model II

IV. Univariate Nonstationary Extension: Application

Table 1: A summary of the models fitted to the log PM2.5 residuals and their corresponding AIC, BIC, and MSE. The lower the values, the better. The best scores are in bold. The number of parameters (NumParams) are also reported.

Model	NumParams	AIC	BIC	MSE
M1 (S)	8	−597,266	−597,179	0.209
M2 (NS)	38	−602,736	−602,430	0.208
M3 (NS)	28	**−607,148**	**−606,733**	**0.207**
M4 (S)	4	−591,474	−591,430	0.213
M5 (NS)	34	−595,644	−595,272	0.211
M6 (NS)	44	−596,082	−595,601	0.211

M3: Non-frozen Lagrangian spatio-temporal deformation model

IV. Univariate Nonstationary Extension: Simulation Study

Lagrangian vs. Non-Lagrangian Stationary Models

When $\mathbf{V} \sim \mathcal{N}_d(\boldsymbol{\mu}_\mathbf{V}, \boldsymbol{\Sigma}_\mathbf{V})$ and C^S is the stationary squared exponential covariance function,

$$C(\mathbf{h}, u) = \frac{1}{\sqrt{|\mathbf{I}_d + \boldsymbol{\Sigma}_\mathbf{V} u^2|}} \exp\left\{-a\left(\mathbf{h} - \boldsymbol{\mu}_\mathbf{V} u\right)^\top \left(\mathbf{I}_d + \boldsymbol{\Sigma}_\mathbf{V} u^2\right)^{-1} \left(\mathbf{h} - \boldsymbol{\mu}_\mathbf{V} u\right)\right\},$$

where $a > 0$ is a scale parameter in space and $\boldsymbol{\mu}_\mathbf{V}$ and $\boldsymbol{\Sigma}_\mathbf{V}$ are the Lagrangian parameters (Schlather, 2010).

When $\boldsymbol{\mu}_\mathbf{V} = \mathbf{0}$ and $\boldsymbol{\Sigma}_\mathbf{V} = \sigma^2_\mathbf{V} \mathbf{I}_d$, $\sigma^2_\mathbf{V} > 0$, the Lagrangian model above reduces to

$$C(\mathbf{h}, u) = \frac{1}{(1 + \sigma^2_\mathbf{V} u^2)^{d/2}} \exp\left\{-\frac{a\|\mathbf{h}\|^2}{1 + \sigma^2_\mathbf{V} u^2}\right\},$$

which is a spatio-temporal isotropic covariance function under the Gneiting class (Gneiting, 2002).

IV. Univariate Nonstationary Extension: Simulation Study

Lagrangian vs. Non-Lagrangian Stationary Models

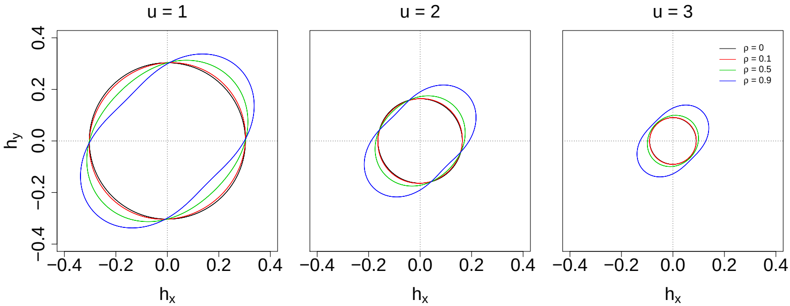

Fig. 10: Values of the non-frozen Lagrangian covariance model for $\rho_{\mathbf{V}} = 0, 0.1, 0.5$, and 0.9, at temporal lags $u = 1, 2$, and 3, at every $\mathbf{h} = (h_x, h_y)^\top$ such that $\|\mathbf{h}\|_2 = 1$. Note that $\rho_{\mathbf{V}} = 0$ (black) corresponds to the non-Lagrangian model.

IV. Univariate Nonstationary Extension: Simulation Study

Lagrangian vs. Non-Lagrangian Nonstationary Models

The Loss of Efficiency (LOE) and Misspecification of the Mean Square Error (MOM) at space-time location $(\mathbf{s}, t)$ are given by:

$$\text{LOE}(\mathbf{s}, t) = \frac{\mathrm{E}_{tr,m}(\mathbf{s}, t)}{\mathrm{E}_{tr}(\mathbf{s}, t)} - 1 \quad \text{and} \quad \text{MOM}(\mathbf{s}, t) = \frac{\mathrm{E}_{m}(\mathbf{s}, t)}{\mathrm{E}_{tr,m}(\mathbf{s}, t)} - 1,$$

where $\mathrm{E}_{tr}(\mathbf{s}, t)$ and $\mathrm{E}_{m}(\mathbf{s}, t)$ are the mean square errors of the predictors under the true, tr, and misspecified, m, models, respectively. $\mathrm{E}_{tr,m}(\mathbf{s}, t)$, on the other hand, is the mean square error, with respect to the true model, of the predictor that is derived from the misspecified model.

IV. Univariate Nonstationary Extension: Simulation Study

Lagrangian vs. Non-Lagrangian Nonstationary Models

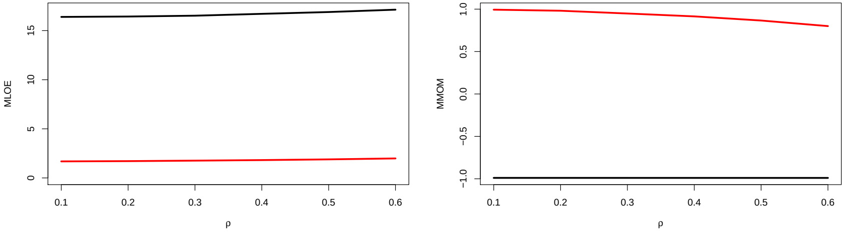

Fig. 11: Medians of the MLOE and MMOM when C_{NS}^{G} is fitted to D_{NS}^{LGR} (black) and when C_{NS}^{LGR} is fitted to D_{NS}^{G} (red) at different values of $\rho_{\mathbf{V}}$.

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V. The Multivariate Nonstationary Extension

V. Multivariate Nonstationary Extension: Main Theorem

Theorem 2

Let $\mathbf{V}$ *be a random vector on* $\mathbb{R}^d$*. If* $\mathbf{C}^S(\mathbf{s}_1, \mathbf{s}_2)$ *is a valid purely spatial matrix-valued nonstationary covariance function on* $\mathbb{R}^d$*, i.e.,* $\mathbf{C}^S(\mathbf{s}_1, \mathbf{s}_2) = \{C^S_{ij}(\mathbf{s}_1, \mathbf{s}_2)\}_{i,j=1}^{p}$*, then*

$$\mathbf{C}(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = \mathrm{E}_{\mathbf{V}}\{\mathbf{C}^S(\mathbf{s}_1 - \mathbf{V}t_1, \mathbf{s}_2 - \mathbf{V}t_2)\}$$

for $\mathbf{s}_1, \mathbf{s}_2 \in \mathbb{R}^d$ *and* $t_1, t_2 \in \mathbb{R}$*, is a valid spatio-temporal matrix-valued nonstationary covariance function on* $\mathbb{R}^d \times \mathbb{R}$ *provided that the expectation exists.*

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V. Multivariate Nonstationary Extension: Example 1

Bivariate Lagrangian Spatio-Temporal Spatially Varying Parameters Model

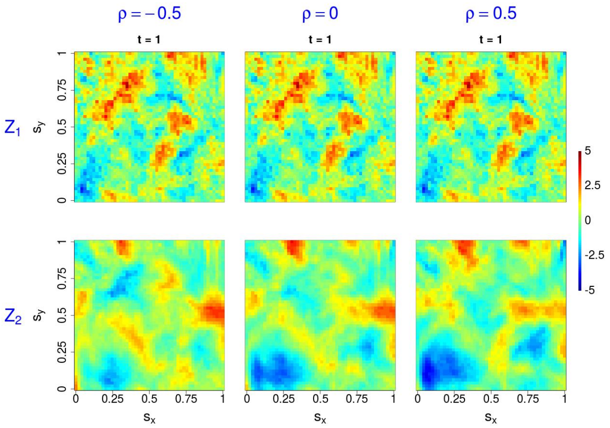

Fig. 12: Bivariate simulations on the unit square with $\mathbf{V} \sim \mathcal{N}_d(\boldsymbol{\mu}_\mathbf{V}, \boldsymbol{\Sigma}_\mathbf{V})$, $\boldsymbol{\mu}_\mathbf{V} = (0.1, 0.1)^\top$ and $\boldsymbol{\Sigma}_\mathbf{V} = 0.001 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ at different values of the correlation parameter ρ.

V. Multivariate Nonstationary Extension: Example 2

Multivariate Deformation Model

Theorem 3

If $\tilde{C}^S_{ij}(\mathbf{s}_1 - \mathbf{s}_2)$ *is a valid purely spatial stationary cross-covariance function on* $\mathbb{R}^d$*, then*

$$C^S_{ij}(\mathbf{s}_1, \mathbf{s}_2) = \tilde{C}^S_{ij}\left\{\|\mathbf{f}_i(\mathbf{s}_1) - \mathbf{f}_j(\mathbf{s}_2)\|\right\},$$

for $\mathbf{s}_1, \mathbf{s}_2 \in \mathbb{R}^d$*, where* $\mathbf{f}_i$*,* $i = 1, \ldots, p$*, represent deterministic non-linear smooth bijective functions of the geographical space onto the deformed space, is a valid purely spatial nonstationary cross-covariance function on* $\mathbb{R}^d$*.*

Multivariate Lagrangian Spatio-Temporal Deformation Model

$$C_{ij}(\mathbf{s}_1, \mathbf{s}_2; t_1, t_2) = \mathrm{E}_{\mathbf{V}}\left[\tilde{C}^S_{ij}\left\{\|\mathbf{f}_i(\mathbf{s}_1 - \mathbf{V}t_1) - \mathbf{f}_j(\mathbf{s}_2 - \mathbf{V}t_2)\|\right\}\right]$$

V. Multivariate Nonstationary Extension: Example 2

Bivariate Lagrangian Spatio-Temporal Deformation Model

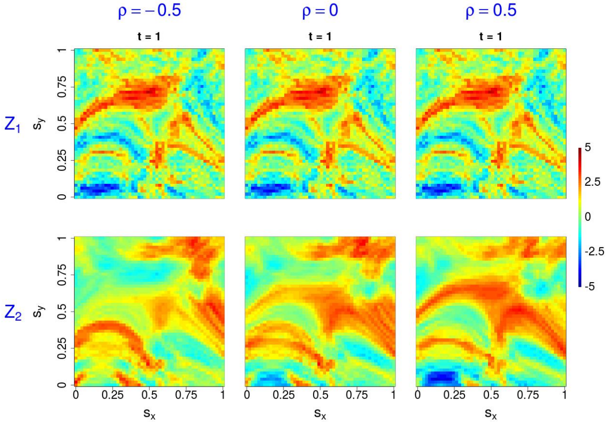

Fig. 13: Bivariate simulations on the unit square with $\mathbf{V} \sim \mathcal{N}_d(\boldsymbol{\mu}_\mathbf{V}, \boldsymbol{\Sigma}_\mathbf{V})$, $\boldsymbol{\mu}_\mathbf{V} = (0.1, 0.1)^\top$ and $\boldsymbol{\Sigma}_\mathbf{V} = 0.001 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ at different values of the correlation parameter ρ.

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V. Multivariate Nonstationary Extension: Stationary Example

Lagrangian Spatio-Temporal Linear Model of Coregionalization

Theorem 4

Let $\mathbf{V}_r$, $r = 1, \ldots, R$, be random vectors on $\mathbb{R}^d$. If $\rho_r(\mathbf{h})$ is a valid univariate stationary correlation function on $\mathbb{R}^d$, then

$$\mathbf{C}(\mathbf{h}, u) = \sum_{r=1}^{R} \mathrm{E}_{\mathbf{V}_r} \{\rho_r(\mathbf{h} - \mathbf{V}_r u)\} \mathbf{T}_r$$

is a valid spatio-temporal matrix-valued stationary cross-covariance function on $\mathbb{R}^d \times \mathbb{R}$, for any $1 \leq R \leq p$ and $\mathbf{T}_r$, $r = 1, \ldots, R$, are positive semi-definite matrices.

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V. Multivariate Nonstationary Extension: Stationary Example

Lagrangian Spatio-Temporal Linear Model of Coregionalization

$$\mathbf{C}(\mathbf{h}, u) = \sum_{r=1}^{R} \mathrm{E}_{\mathbf{V}_r} \left\{\rho_r(\mathbf{h} - \mathbf{V}_r u)\right\} \mathbf{T}_r$$

The model above is the resulting Lagrangian spatio-temporal cross-covariance function of the multivariate spatio-temporal process:

$\mathbf{Z}(\mathbf{s}, t) = \mathbf{A}\mathbf{W}(\mathbf{s}, t) = \mathbf{A}[W_1(\mathbf{s}-\mathbf{V}_1 t), W_2(\mathbf{s}-\mathbf{V}_2 t), \ldots, W_R(\mathbf{s}-\mathbf{V}_R t)]^\top$,

where $\mathbf{A}$ is $p \times R$ matrix and the components of $\mathbf{W}(\mathbf{s}, t) \in \mathbb{R}^R$ are independent but not identically distributed. Each component W_r has a univariate Lagrangian spatio-temporal stationary correlation function $\rho_r(\mathbf{h} - \mathbf{V}_r u)$, $r = 1, \ldots, R$.

V. Multivariate Nonstationary Extension: Example 2

Lagrangian Spatio-Temporal Linear Model of Coregionalization

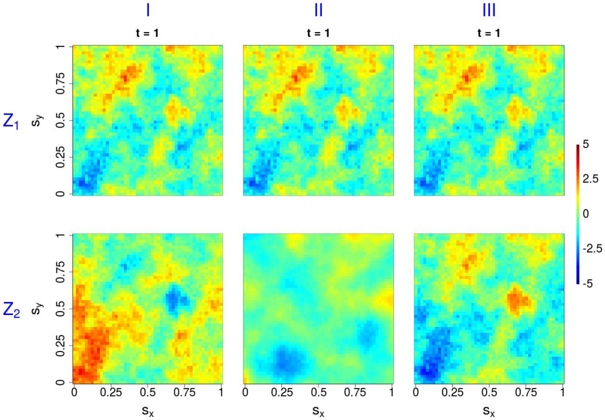

Fig. 14:
I: $Z_1(\mathbf{s},t) = 0.9W_1(\mathbf{s},t) - 0.1W_2(\mathbf{s},t)$ and $Z_2(\mathbf{s},t) = -0.6W_1(\mathbf{s},t) + 0.4W_2(\mathbf{s},t)$,
II: $Z_1(\mathbf{s},t) = W_1(\mathbf{s},t)$ and $Z_2(\mathbf{s},t) = W_2(\mathbf{s},t)$,
III: $Z_1(\mathbf{s},t) = 0.9W_1(\mathbf{s},t) + 0.1W_2(\mathbf{s},t)$ and $Z_2(\mathbf{s},t) = 0.6W_1(\mathbf{s},t) + 0.4W_2(\mathbf{s},t)$.
Here we have $\boldsymbol{\mu}_{\mathbf{W}_1} = (0.1, 0.1)^\top$ and $\boldsymbol{\mu}_{\mathbf{W}_2} = (-0.1, -0.1)^\top$.

V. Multivariate Nonstationary Extension: Application

Regional Climate Model Output

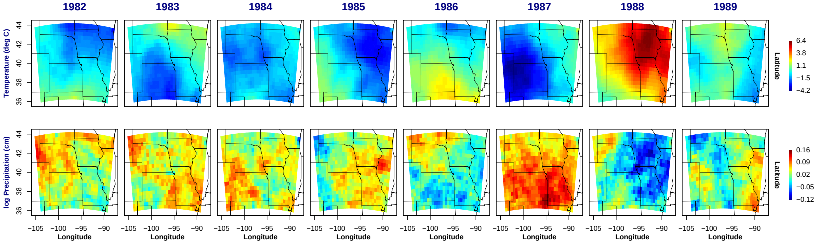

Fig. 15: Bivariate dataset of Genton and Kleiber (2015) with temporal resolution of 92 days (June to August), for the years 1982 – 1989.

V. Multivariate Nonstationary Extension: Results

Table 2: In-sample (log-likelihood, AIC, and BIC) and out-of-sample scores. The lower the AIC, BIC, and RMSE values, the better. The reverse is true for the log likelihood. The best scores are in bold. For concise comparison, we include the fit of three models in Genton and Kleiber (2015) and their corresponding out-of-sample prediction scores.

	Model	Log likelihood	AIC	BIC	Portion of Data Screened 5%	10%	15%	20%
Spatial	M1 (Nonstationary)	67,173	−134,218	−133,935	0.079	0.070	0.083	0.080
	Nonstationary Parsimonious Matérn in Genton and Kleiber (2015)	67,242	−134,476	−134,446	0.077	0.073	0.078	0.072
	Stationary Parsimonious Matérn in Genton and Kleiber (2015)	66,234	−132,456	−132,410	0.078	0.077	0.077	0.080
	Stationary LMC in Genton and Kleiber (2015)	65,611	−131,208	−131,155	0.074	0.078	0.079	0.078
Spatio-Temporal	M2 (Stationary)	67,564	−135,110	−135,042	0.034	0.047	0.048	0.059
	M3 (Nonstationary)	67,722	−135,508	−135,371	0.032	0.047	0.048	0.060
	M4 (Stationary)	68,771	−137,520	−137,436	0.028	0.032	0.042	0.049
	M5 (Nonstationary)	**68,952**	**−137,864**	**−137,712**	**0.027**	**0.032**	**0.041**	**0.049**
	M6 (Stationary)	67,435	−134,854	−134,793	0.034	0.047	0.048	0.059
	M7 (Nonstationary)	67,499	−134,674	−133,928	0.029	0.039	0.043	0.052
	M8 (Stationary)	67,563	−135,098	−134,992	0.030	0.042	0.055	0.068
	M9 (Nonstationary)	68,514	−136,826	−136,057	0.029	0.036	0.046	0.051

M5: Non-frozen Lagrangian spatio-temporal nonstationary LMC with multiple advection velocity vectors

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VI. The Multivariate Stationary with Multiple Advections Extension

VI. Multiple Advections Extension: Main Theorem

Theorem 5

Let $\mathbf{V}_{11}, \mathbf{V}_{22}, \ldots, \mathbf{V}_{pp}$ be random vectors on $\mathbb{R}^d$. If $\mathbf{C}^S(\mathbf{h})$ is a valid purely spatial matrix-valued stationary cross-covariance function on $\mathbb{R}^d$ then

$$\mathbf{C}(\mathbf{h}; t_1, t_2) = \mathrm{E}_{\mathscr{V}}\left[\{C_{ij}^S(\mathbf{h} - \mathbf{V}_{ii}t_1 + \mathbf{V}_{jj}t_2)\}_{i,j=1}^p\right],$$

where the expectation is taken with respect to the joint distribution of $\mathscr{V} = (\mathbf{V}_{11}^\top, \mathbf{V}_{22}^\top, \ldots, \mathbf{V}_{pp}^\top)^\top$, is a valid matrix-valued spatio-temporal cross-covariance function on $\mathbb{R}^d \times \mathbb{R}$ provided that the expectation exists.

The validity can be established by considering

$$\mathbf{Z}(\mathbf{s}, t) = \left\{\tilde{Z}_1(\mathbf{s} - \mathbf{V}_{11}t), \ldots, \tilde{Z}_p(\mathbf{s} - \mathbf{V}_{pp}t)\right\}^\top,$$

such that $\tilde{\mathbf{Z}}(\mathbf{s}) = \left\{\tilde{Z}_1(\mathbf{s}), \ldots, \tilde{Z}_p(\mathbf{s})\right\}^\top$ is a zero-mean multivariate purely spatial random field and every component is transported by different random advections $\mathbf{V}_{ii} \in \mathbb{R}^d, i = 1, \ldots, p$.

VI. Multiple Advections Extension: Explicit Form Example

Theorem 6

For $p>2$, let $\mathscr{V}=(\mathbf{V}_{11}^\top,\mathbf{V}_{22}^\top,\ldots,\mathbf{V}_{pp}^\top)^\top\sim\mathcal{N}_{pd}(\boldsymbol{\mu}_{\mathscr{V}},\boldsymbol{\Sigma}_{\mathscr{V}})$. If $\mathbf{C}^S(\mathbf{h})$ is a matrix-valued normal scale-mixture cross-covariance function, then

$$C_{ii}(\mathbf{h},u)=\frac{C_{ii}^S\{(\mathbf{h}-\mathbf{e}_{(di-1):(di)}^\top\boldsymbol{\mu}_{\mathscr{V}}u)^\top(\mathbf{I}_d+\mathbf{e}_{(di-1):(di)}^\top\boldsymbol{\Sigma}_{\mathscr{V}}u^2)^{-1}(\mathbf{h}-\mathbf{e}_{(di-1):(di)}^\top\boldsymbol{\mu}_{\mathscr{V}}u)\}}{|\mathbf{I}_d+\mathbf{e}_{(di-1):(di)}^\top\boldsymbol{\Sigma}_{\mathscr{V}}u^2|^{1/2}},$$

where $\mathbf{e}_{(di-1):(di)}$ is the sub-matrix of $\mathbf{I}_{pd}$, comprised of its $(di-1)$-th and (di)-th rows, for $i=1,\ldots,p$, and

$$C_{ij}(\mathbf{h};t_1,t_2)=\frac{C_{ij}^S((\mathbf{h}-\mathbf{T}\tilde{\mathbf{e}}^\top\boldsymbol{\mu}_{\mathscr{V}})^\top[\mathbf{I}_d-\mathbf{T}\{\mathbf{T}^\top\mathbf{T}+(\tilde{\mathbf{e}}^\top\boldsymbol{\Sigma}_{\mathscr{V}})^{-1}\}^{-1}\mathbf{T}^\top](\mathbf{h}-\mathbf{T}\tilde{\mathbf{e}}^\top\boldsymbol{\mu}_{\mathscr{V}}))}{|\mathbf{I}_{2d}+(\tilde{\mathbf{e}}^\top\boldsymbol{\Sigma}_{\mathscr{V}})\mathbf{T}^\top\mathbf{T}|^{1/2}},$$

where $\mathbf{T}=(t_1\mathbf{I}_d\ \ -t_2\mathbf{I}_d)$, $\tilde{\mathbf{e}}=\mathbf{e}_{\{(di-1):(di),(dj-1):(dj)\}}$, such that $\mathbf{e}_{\{(di-1):(di),(dj-1):(dj)\}}$ is the sub-matrix of $\mathbf{I}_{pd}$ comprised of its $(di-1)$-th, (di)-th, $(dj-1)$-th, and (dj)-th rows, for $i,j=1,\ldots,p$, $i\neq j$.

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VI. Multiple Advections Extension: Examples with different distributional assumptions on $\mathscr{V}$

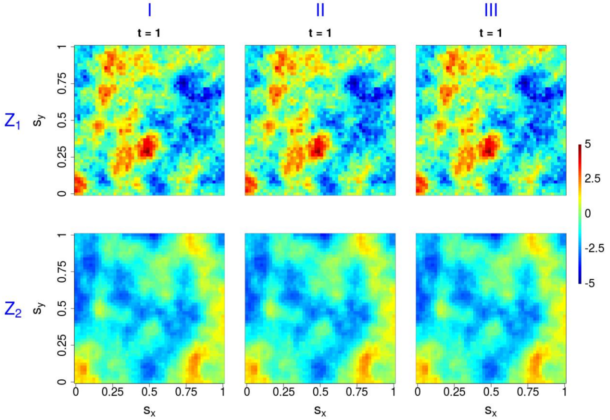

Fig. 16: Bivariate simulations on the unit square with I: $\mathbf{V}_{11} = -0.9\mathbf{V}_{22}$, II: $\mathbf{V}_{11}$ and $\mathbf{V}_{22}$ are independent, and III: $\mathbf{V}_{11} = 0.9\mathbf{V}_{22}$.

VI. Multiple Advections Extension: Simulation Study

- M1: Univariate Lagrangian spatio-temporal model, i.e.,

$$C_{ii}(\mathbf{h}, u) = \frac{\sigma_{ii}^2}{\sqrt{|\mathbf{I}_d + \boldsymbol{\Sigma}_{\mathbf{V}_{ii}} u^2|}} \mathcal{M}\{(\mathbf{h} - \boldsymbol{\mu}_{\mathbf{V}_{ii}} u)^\top (\mathbf{I}_d + \boldsymbol{\Sigma}_{\mathbf{V}_{ii}} u^2)^{-1} (\mathbf{h} - \boldsymbol{\mu}_{\mathbf{V}_{ii}} u); a_{ii}, \nu_{ii}\},$$

  where $\mathcal{M}(\mathbf{h}; a, \nu)$ is the univariate Matérn correlation with spatial scale and smoothness parameters a and ν, respectively;
- M2: Bivariate Lagrangian spatio-temporal model with single advection, i.e.,

$$C_{ij}(\mathbf{h}, u) = \frac{\rho\sigma_{ii}\sigma_{jj}}{\sqrt{|\mathbf{I}_d + \boldsymbol{\Sigma}_{\mathbf{V}} u^2|}} \mathcal{M}\{(\mathbf{h} - \boldsymbol{\mu}_{\mathbf{V}} u)^\top (\mathbf{I}_d + \boldsymbol{\Sigma}_{\mathbf{V}} u^2)^{-1} (\mathbf{h} - \boldsymbol{\mu}_{\mathbf{V}} u); a, \nu_{ij}\};$$

- M3: Bivariate Lagrangian spatio-temporal model with multiple advections in Theorem 6

VI. Multiple Advections Extension: Simulation Study

Experiment 1 – Data: M3
Models: M1 vs. M3

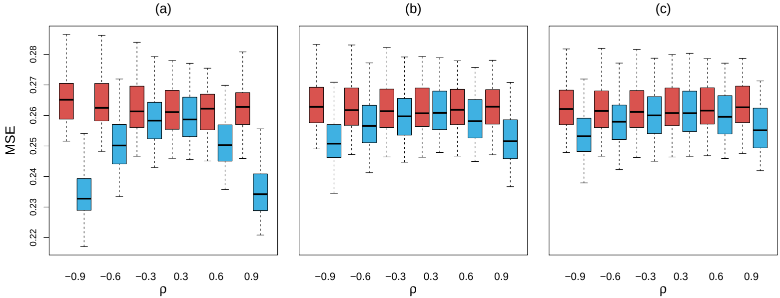

Fig. 17: Boxplots of the MSEs under different assumptions on the joint distribution of $\mathbf{V}_{11}$ and $\mathbf{V}_{22}$, namely, (a) $\mathbf{V}_{11} = 0.9\mathbf{V}_{22}$, (b) $\mathbf{V}_{11}$ and $\mathbf{V}_{22}$ are independent, and (c) $\mathbf{V}_{11} = -0.9\mathbf{V}_{22}$, when M1 (red) and M3 (blue) are fitted to data generated from M3 with different values of ρ.

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VI. Multiple Advections Extension: Simulation Study

Experiment 2 – Data: M3
Models: M2 vs. M3

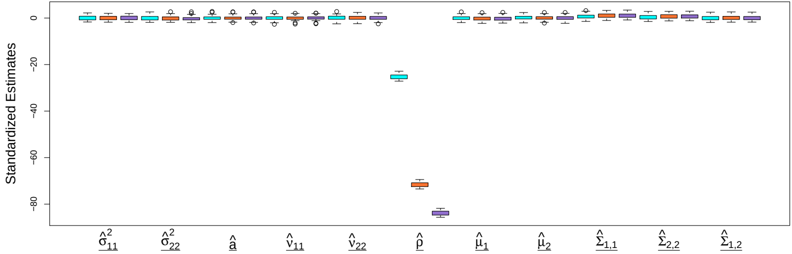

Fig. 18: Boxplots of the centered and scaled MLEs of the parameters of M2 when it is fitted to data generated from M3 under scenarios (d), in cyan, (e), in orange, and (f), in purple, when $\rho = 0.6$. Scenarios (d) and (f) represent the highly positive and negative dependence between the corresponding components of $\mathbf{V}_{11}$ and $\mathbf{V}_{22}$, respectively, while (e) establishes that $\mathbf{V}_{11}$ and $\mathbf{V}_{22}$ are independent.

VI. Multiple Advections Extension: Simulation Study

Experiment 2 – Data: M3
Models: M2 vs. M3

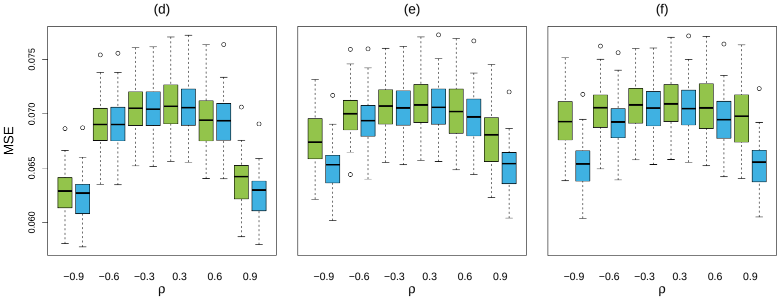

Fig. 19: Boxplots of the MSEs under scenarios (d)-(f) when M2 (green) and M3 (blue) are fitted to data generated from M3 at different values of ρ.

VI. Multiple Advections Extension: Application

Modern-Era Retrospective Analysis for Research and Applications, version 2 (MERRA-2) reanalysis
log PM2.5 residuals

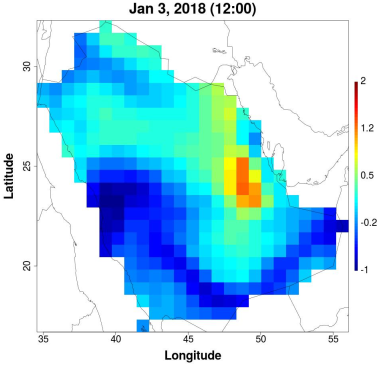

Fig. 20: 880 hPa

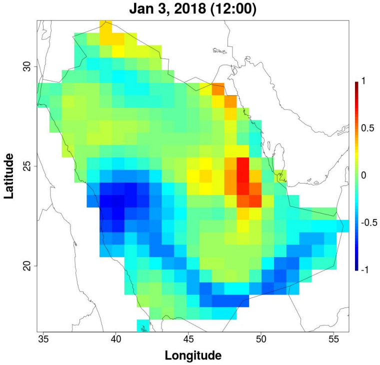

Fig. 21: 985 hPa

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VI. Multiple Advections Extension: Application

We fit six different spatio-temporal cross-covariance functions, namely, M1-M3, and

- M4: Bivariate Lagrangian spatio-temporal model with variable specific multiple advections, i.e.,

$$C_{ij}\{(\mathbf{h},\mathbf{h}'_{ij});t_1,t_2\} = \mathrm{E}_{\tilde{\mathscr{V}}}\{C^S_{ij}(\mathbf{h}-\mathbf{V}_{ii}t_1+\mathbf{V}_{jj}t_2,\mathbf{h}'_{ij}-\mathbf{V}'_{ii}t_1+\mathbf{V}'_{jj}t_2)\},$$

  where $\mathbf{h}'_{ij}=\mathbf{s}'_{ii}-\mathbf{s}'_{jj}$, for $\mathbf{s}'_{ii},\mathbf{s}'_{jj}\in\mathbb{R}^{d'}$, and the expectation is taken with respect to the joint distribution of $\tilde{\mathscr{V}}=\{(\mathbf{V}_{11}^\top,\mathbf{V}_{11}'^\top),(\mathbf{V}_{22}^\top,\mathbf{V}_{22}'^\top))\}^\top$;
- M5: Bivariate Lagrangian spatio-temporal LMC;
- M6: Bivariate non-Lagrangian fully symmetric Gneiting-Matérn, i.e.,

$$C_{ij}(\mathbf{h},u) = \frac{\rho\sigma_{ii}\sigma_{jj}}{\alpha|u|^{2\xi}+1}\mathscr{M}\left\{\frac{\mathbf{h}}{(\alpha|u|^{2\xi}+1)^{b/2}};a,\nu_{ij}\right\},$$

  where $\alpha>0$, $\xi\in(0,1]$, and $b\in[0,1]$ are the temporal range and smoothness, and space-time nonseparability parameters, respectively.

VI. Multiple Advections Extension: Results

Table 3: In-sample (log-likelihood, AIC*, and BIC*) and out-of-sample (MSE) scores. The lower the values, the better. The best scores are given in bold.

	In-Sample			Out-of-Sample		Computation
Model	log-likelihood	AIC*	BIC*	MSE	NumParams	Time (secs)
M1	461,825	−923,614	−923,439	0.0521	18	10,857
M2	479,159	−958,290	−958,156	0.0546	14	13,446
M3	484,070	−968,094	**−967,873**	0.0516	23	68,784
M4	**484,150**	**−968,210**	−967,777	**0.0514**	45	227,444
M5	470,852	−941,658	−941,437	0.1602	23	15,059
M6	477,480	−954,936	−954,821	0.0601	12	8,391

M4: Bivariate Lagrangian spatio-temporal model with variable specific multiple advections

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VI. Multiple Advections Extension: Results

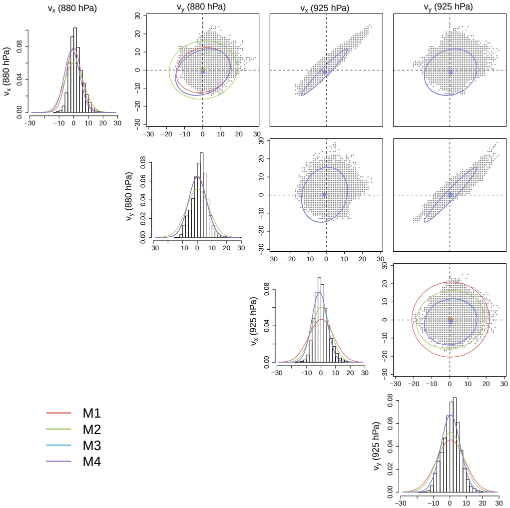

Fig. 22: Empirical and fitted bivariate distributions of the MERRA-2 simulated wind vectors (in m/s).

VII. Summary

VII. Summary

- Developed the multivariate, nonstationary, and multiple advections extensions of the covariance functions under the Lagrangian framework
- Proposed three main theorems that provide more flexibility and features designed to cover a wider range of transport scenarios
- Proposed appropriate estimation procedures for models of this class
- Demonstrated, through real and simulated datasets, the merits of the proposed models
- Other avenues for research: Taylor's hypothesis for non-frozen nonstationary spatio-temporal random fields, high performance implementation of the Lagrangian spatio-temporal models in ExaGeoStat, and stochastic partial differential equations (SPDEs) extension

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Questions?