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Exploration of Spatio-Temporal Environmental Conditions: Harmonized Databases and Analytical Techniques

ECOST-DATA, Bari, Italy, July 3-4, 2025

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Editors

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Preface

This volume collects the scientific contributions presented at the Workshop “Exploration of Spatio-Temporal Environmental Conditions: Harmonized Databases and Analytical Techniques (ECoST-DATA)”, held at the University of Bari on July 3-4, 2025, as Satellite event of DUST 2025. It is a key result of the ECoST-DATA Project, funded by European Union – NextGenerationEU with the Cascade Open Calls published by ALMA MATER STUDIORUM – University of Bologna, inside the Project GRINS within the PNRR – Mission 4, Component 2, Investment 1.3 “Partnership extended to Universities, Research Centers, Firms and research projects funding”, D.D. 341 of 15/03/2022, CUP: J33C22002910001.

The contents are dedicated to advanced tools and techniques for analyzing and predicting environmental variables with a spatial or spatio-temporal structure. In particular, they include theoretical reviews on spatio-temporal covariance modelling as well as innovative approaches for assessing environmental quality and its effects on climate change by integrating georeferenced data from multiple sources.

Among the primary objectives of this collection, it is worth mentioning: transfer advanced analytic skills for the modelling, estimation, and prediction of spatial and spatio-temporal environmental variables; provide practical guidance on integrating heterogeneous georeferenced data while accounting for measurement error and spatial misalignment; support risk assessment by equipping practitioners with methods to quantify exposure and uncertainty relevant to human health; and inform sustainability planning through models that identify spatially and temporally targeted mitigation or adaptation strategies.

As a result, the contributions are intended for researchers and graduate students in spatial statistics, environmental science, and geosciences; data scientists and practitioners working on environmental monitoring, climate impacts, and public-health risk assessment; policy analysts interested in data-driven sustainability planning.

Regarding the outcomes, readers will gain both the theoretical grounding and the practical toolset necessary to build, validate, and deploy spatio-temporal models for environmental variables, produce reliable forecasts, and translate model outputs into actionable insights for health and sustainability interventions.

The volume is organized in three parts.

In the first one, *Random fields and Covariance modelling*, Posa clarifies the relationship between covariance functions and positive definite functions, emphasizing that Crum's theorem is the necessary generalization of Bochner's theorem. De Iaco discusses on some families of spatio-temporal complex covariance functions for vectorial data. It is also described how these functions can be generalized to the spatio-temporal setting, as well as how some other complex-valued covariance families can be constructed as positive mixtures of infinite components or as a convolution of the real part. Hristopulos presents the hybrid spectral approach for generating physically inspired, non-separable covariance kernels from stochastic ordinary differential equations. Pere et al. propose the stationary subspace analysis to decompose a random field into independent stationary and non-stationary subspaces.

In Part II, *Environmental control and integration*, Stein focuses on the use of modern deep learning methods for the analysis and management of large data volumes. His study explores the use of satellite imagery and time series to analyze air quality and monitor environmental changes. A further challenging approach is presented in Gómez-Hernández et al. to identify atmospheric dust sources, using the ensemble smoother with multiple data assimilation methodology. Capasso discusses the optimization of pollution control within an economic growth system, presenting a spatially structured model. This model analyzes an optimal control problem designed to maximize intertemporal utility while minimizing pollution, the disutility of taxation, and intervention costs. Additionally, the study by Dutillo and Di Battista explores the functional structure and variation of Italian carbon emissions from electricity using functional data analysis. Daily and monthly profiles are constructed using Fourier basis functions and analyzed at national and electricity market zone levels.

The volume concludes with Part III, *Environmental Analysis*, where Jalilian et al. apply a flexible generalized additive model framework for surface ozone prediction, using spatio-temporally varying coefficients to correct biases between satellite and in situ data. Gomes et al. investigate the geostatistical characterization of climate extremes dynamics, focusing on drought. A Random Forest-based short-term alert system is presented for predicting drought severity classes at a monthly scale, demonstrating strong predictive performance for local areas and offering a flexible tool for managing drought-related risks. For environmental quality assessment, the work by Masoumi et al. addresses a gap in biodiversity modelling in the Apulia region by comparing the performance of various machine learning models (Random Forests, Support Vector Machines, Extreme Gradient Boosting, Decision Trees,

and Linear Regression) for assessing the effects of environmental variables on the multilevel biodiversity index. Furthermore, in Cappello et al., spatio-temporal blind source separation model is reviewed and employed to model and predict ground-level ozone concentration in a complex multivariate spatio-temporal framework.

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Stationary Subspace Analysis for Spatiotemporal Data



Jaakko Pere, Sandra De Iaco, and Klaus Nordhausen

Abstract Multivariate spatiotemporal data, where multiple variables are measured over time and across space, present modeling challenges due to complex dependencies. Traditional approaches often rely on assumptions like stationarity and separability, which may be too restrictive. This work introduces a flexible alternative by decomposing the random field into two independent subspaces: one stationary and one nonstationary. The proposed method, spatiotemporal stationary subspace analysis (stSSA), identifies the subspaces by segmenting the space-time domain and comparing local and global means. This decomposition simplifies modeling and enhances interpretability. A simulation study assesses the method's sensitivity to segment construction, number of latent components and the choice of the covariance function.

Keywords Blind source separation · Dimension reduction · Non-stationarity

1 Introduction

Increasingly, many variables are observed at different locations and regularly tracked over time, yielding so-called multivariate spatiotemporal data. Such data are challenging to model, as dependencies between the variables in space and time must be considered. The classical approach is to model such data using a p -variate random field $\mathbf{x} = \mathbf{x}(\mathbf{u}, t)$, where $(\mathbf{u}, t) \in \mathcal{U} \times \mathcal{T} \subset \mathbb{R}^{d+1}$, with $\mathbf{u} \in \mathcal{U} \subset \mathbb{R}^d$

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denoting the spatial domain (typically $d \in \{1, 2, 3\}$) and $\mathcal{T} \subset \mathbb{R}$ denoting the temporal domain.

Given the complex dependency structures in such data, it is common to make simplifying assumptions about the first two moments. A standard assumption is weak stationarity, which implies that $\mathbb{E}(\mathbf{x}(\mathbf{u}, t)) = \boldsymbol{\mu} \in \mathbb{R}^p$ for all $(\mathbf{u}, t) \in \mathcal{U} \times \mathcal{T}$, meaning that the expectation is constant across the entire domain and that the matrix-variate covariance function depends only on the spatial and temporal distances, i.e., the covariance can be expressed as $\text{Cov}(\mathbf{x}(\mathbf{u}, t), \mathbf{x}(\mathbf{u}', t')) = C(\mathbf{u} - \mathbf{u}', t - t')$, for some suitable function $C : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^{p \times p}$. Stronger assumptions are also possible, such as isotropy (in space) or separability of spatial and temporal dependencies [2, 9].

However, such simplifying assumptions often come at a cost, like inferior prediction performance. Hence, there has been growing interest in nonstationary approaches [1, 10, 12]. These nonstationary approaches, though flexible, are often complex and tend to scale poorly with increasing data dimension p . Additionally, they usually assume non-stationarity across all variables. Similarly, dimension reduction methods used as a preprocessing step often require either all components to be stationary [3, 8] or all to be nonstationary [11].

We are interested in a different form of dimension reduction for the field $\mathbf{x}$, namely, in one that decomposes it into stationary and nonstationary parts, which are independent of each other, after which the two independent random fields can be modeled separately. This dimension reduction approach is known in a time series context as stationary subspace analysis (SSA) [4], and we will refer to it here as spatiotemporal SSA (stSSA). Our focus will be on data where non-stationarity is present in the mean, while other forms of non-stationarity will be discussed in future work. Note that the approach considered here differs from the one where a random field is decomposed into a sum or product of stationary and nonstationary parts as discussed in [5].

The remainder of this chapter is organized as follows. Section 2 presents the assumptions of the stSSA model, and Sect. 3 describes the developed method for the estimation of the stationary and nonstationary subspaces. Section 4 gives a simulation study that demonstrates the method. Lastly, Sect. 5 concludes the paper by summarizing the contributions and offering future research directions.

2 Model Formulation

The idea of the stSSA model is that the underlying latent fields can be divided into stationary and nonstationary ones. Below, we present the stSSA model, which is an extension of the SSA model [4] to a spatiotemporal setting.

Definition 1 A p -variate random field $\mathbf{x} = \mathbf{x}(\mathbf{u}, t) = (x_1(\mathbf{u}, t), \dots, x_p(\mathbf{u}, t))^T$ on the domain $\mathcal{U} \times \mathcal{T} \subset \mathbb{R}^{d+1}$ follows the stSSA model if

$$\mathbf{x}(\mathbf{u}, t) = \mathbf{A}\mathbf{z}(\mathbf{u}, t) = [\mathbf{A}_s \mathbf{A}_n] \begin{pmatrix} \mathbf{s}(\mathbf{u}, t) \\ \mathbf{n}(\mathbf{u}, t) \end{pmatrix},$$

where $\mathbf{A} = [\mathbf{A}_s \mathbf{A}_n] \in \mathbb{R}^{p \times p}$ is full-rank not depending on location $\mathbf{u}$ or time t , $\mathbf{A}_s \in \mathbb{R}^{p \times (p-q)}$, $\mathbf{A}_n \in \mathbb{R}^{p \times q}$. Let $\mathbf{I}_r$ denote the $r \times r$ identity matrix, and let $\mathbf{D}_r^{(\mathbf{u}, t)}$ be an $r \times r$ diagonal matrix with positive diagonal elements, possibly depending on the location $\mathbf{u}$ and time t . The p -variate random field $\mathbf{z}$, consisting of $p - q$ -variate and q -variate random fields $\mathbf{s}$ and $\mathbf{n}$, satisfies the following assumptions:

- (A1) $\mathbb{E}(\mathbf{s}(\mathbf{u}, t)) = \mathbf{0}$ and $\text{Cov}(\mathbf{s}(\mathbf{u}, t)) = \mathbf{I}_{p-q}$ for all $(\mathbf{u}, t) \in \mathcal{U} \times \mathcal{T}$, and $\text{Cov}(\mathbf{s}(\mathbf{u}, t), \mathbf{s}(\mathbf{u}', t'))$ is finite and only a function of $\|\mathbf{u} - \mathbf{u}'\|$ and $\|t - t'\|$.
- (A2) $\mathbb{E}(\mathbf{n}(\mathbf{u}, t)) < \infty$ and $\text{Cov}(\mathbf{n}(\mathbf{u}, t)) = \mathbf{D}_q^{(\mathbf{u}, t)}$ for all $(\mathbf{u}, t) \in \mathcal{U} \times \mathcal{T}$, and $\text{Cov}(\mathbf{n}(\mathbf{u}, t), \mathbf{n}(\mathbf{u}', t'))$ is finite.
- (A3) The random fields $\mathbf{s}$ and $\mathbf{n}$ are independent, from which it follows that $\text{Cov}(\mathbf{s}(\mathbf{u}, t), \mathbf{n}(\mathbf{u}', t')) = \mathbf{0}$ for all $(\mathbf{u}, t), (\mathbf{u}', t') \in \mathcal{U} \times \mathcal{T}$.
- (A4) The dimension q is the smallest value that allows division of $\mathbf{x}$ such that Assumptions (A1)–(A3) hold.
- (A5) There exist $U_0 = \{\mathbf{u}_1, \dots, \mathbf{u}_{n_0}\} \subset \mathcal{U}$ and $[T] = \{1, \dots, T\} \subset \mathcal{T}$ such that $\sum_{(\mathbf{u}, t) \in U_0 \times [T]} \mathbb{E}(\mathbf{n}(\mathbf{u}, t)) = \mathbf{0}$ and $\sum_{(\mathbf{u}, t) \in U_0 \times [T]} \text{Cov}(\mathbf{n}(\mathbf{u}, t)) = \mathbf{I}_q$.

By Assumption (A1), the $(p - q)$ random fields in $\mathbf{s}$ are second-order stationary with finite second-order spatiotemporal dependence, and additionally, the location and covariance matrix of the stationary part are fixed for convenience. On the other hand, Assumption (A2) states that the q nonstationary components in $\mathbf{n}$ have finite first and second moments and are uncorrelated at $(\mathbf{u}, t)$ but can have arbitrary spatiotemporal second-order dependence for $(\mathbf{u}, t) \neq (\mathbf{u}', t')$. Assumption (A3) states that the nonstationary and stationary components are independent, and Assumption (A4) ensures that all the components of $\mathbf{n}$ are nonstationary.

Despite Assumptions (A1)–(A4) the model is not well defined. The stationary components are only specified up to a rotation by an orthogonal matrix. Furthermore, the nonstationary components can be marginally rescaled, shifted, and permuted. Thus, we have Assumption (A5) fixing the location and the scale of $\mathbf{n}$ based on a set of reference points $U_0 \times [T]$. Additionally, we will assume that the observed sample $\mathbf{x}(\mathbf{u}_i, t_j)$, $i \in \{1, \dots, n_s\}$, $j \in \{1, \dots, n_t\}$, can always be chosen to be the set of reference points such that Assumption (A5) is satisfied.

Throughout, we assume that the field $\mathbf{x}$ follows the stSSA model in Definition 1. The goal is to estimate the unmixing matrix $\mathbf{W}$ so that $\mathbf{W}\mathbf{x}(\mathbf{u}, t)$ can be partitioned into stationary and nonstationary fields. However, notice that the unmixing matrix is not uniquely defined since, for example, columns of $\mathbf{A}_s$ and $\mathbf{A}_n$ can be permuted. This has to be taken into account while measuring the performance of the estimation. Both the assumed model for $\mathbf{x}$ and the method for estimating $\mathbf{W}$ are called stSSA. It should be clear from the context if we refer to the model or the method of estimating $\mathbf{W}$.

3 The stSSA Method for the Mean

In the present chapter, we restrict to detecting non-stationarity in the mean. For example, the nonstationary components $n_i = n_i(\mathbf{u}, t)$ of $\mathbf{n} = (n_1, \dots, n_q)$ can exhibit trend, seasonality, or cyclicity.

Suppose that the field $\mathbf{x}$ is observed at the locations $\{\mathbf{u}_i\}_{i=1}^{n_s}$ and time points $\{t_j\}_{j=1}^{n_t}$. The spatiotemporal locations $(\mathbf{u}_i, t_j)$ are divided into non-overlapping segments [11]. That is, firstly, the space-time domain $\mathcal{U} \times \mathcal{T}$ is divided into K parts by a partition $\mathcal{S}_1 = \mathcal{U}_1 \times \mathcal{T}_1, \dots, \mathcal{S}_K = \mathcal{U}_K \times \mathcal{T}_K$ such that $\mathcal{S}_i \cap \mathcal{S}_j = \emptyset$ for $1 \leq i \neq j \leq K$ and $\bigcup_{k \in K} \mathcal{S}_k = \mathcal{U} \times \mathcal{T}$. Secondly, an observation $\mathbf{x}(\mathbf{u}_i, t_j)$ is assigned to the segment $\mathbf{S}_k$ if $(\mathbf{u}_i, t_j) \in \mathcal{S}_k$, and let $|\mathbf{S}_k|$ denote the number of observations in $\mathbf{S}_k$. We denote $\mathbf{S} = \bigcup_{k \in K} \mathbf{S}_k$, and accordingly, $|\mathbf{S}|$ corresponds to the number of all realized space-time observations.

Based on the chosen space-time partition, the sample mean of each segment $\mathbf{S}_k$ is compared to the global sample mean. Denote the sample mean of a segment $\mathbf{S}_k$ by $\mathbf{m}_{\mathbf{S}_k}(\mathbf{x}) = |\mathbf{S}_k|^{-1} \sum_{(\mathbf{u}_i, t_j) \in \mathbf{S}_k} \mathbf{x}(\mathbf{u}_i, t_j)$. Hence, $\mathbf{m}_{\mathbf{S}}(\mathbf{x})$ denotes the global sample mean based on the whole sample of $\mathbf{x}$. Furthermore, we work with the whitened observations of the field $\mathbf{x}$, $\mathbf{x}^{st}(\mathbf{u}_i, t_j) = \mathbf{Q}(\mathbf{x})^{-1/2} (\mathbf{x}(\mathbf{u}_i, t_j) - \mathbf{m}_{\mathbf{S}}(\mathbf{x}))$, where $\mathbf{Q}_{\mathbf{S}}(\mathbf{x}) = |\mathbf{S}|^{-1} \sum_{(\mathbf{u}_i, t_j) \in \mathbf{S}} (\mathbf{x}(\mathbf{u}_i, t_j) - \mathbf{m}_{\mathbf{S}}(\mathbf{x})) (\mathbf{x}(\mathbf{u}_i, t_j) - \mathbf{m}_{\mathbf{S}}(\mathbf{x}))^\top$ is the sample covariance corresponding to the available sample of the field $\mathbf{x}$, and $\mathbf{A}^{-1/2}$ is the unique matrix corresponding to a symmetric positive definite matrix $\mathbf{A}$ such that $\mathbf{A}^{-1} = \mathbf{A}^{-1/2} \mathbf{A}^{-1/2}$. Now, for the whitened observations, segment sample means are compared to the global sample means by computing

$$\mathbf{M} = \sum_{k=1}^K \frac{|\mathbf{S}_k|}{|\mathbf{S}|} \mathbf{m}_{\mathbf{S}_k}(\mathbf{x}^{st}) \mathbf{m}_{\mathbf{S}_k}(\mathbf{x}^{st})^\top. \quad (1)$$

That is, $\mathbf{M} \in \mathbb{R}^{p \times p}$ is just the sample covariance matrix of sample means corresponding to different segments weighted by their number of observations.

The mean stationary components of the latent field $\mathbf{z}$ correspond to the eigenvalues of $\mathbf{M}$ that are close to zero. Likewise, the nonstationary components with respect to trend correspond to the nonzero eigenvalues of $\mathbf{M}$. Hence, the estimates for the stationary and nonstationary parts of the unmixing matrix

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}_s \\ \mathbf{W}_n \end{pmatrix}, \quad \mathbf{W}_s \in \mathbb{R}^{(p-q) \times p} \quad \text{and} \quad \mathbf{W}_n \in \mathbb{R}^{q \times p} \quad (2)$$

are obtained through the eigenvalue decomposition of $\mathbf{M}$. Below, we give the definitions for the estimators of $\mathbf{W}_s$ and $\mathbf{W}_n$.

Definition 2 Let $\mathbf{x}$ be a random field following the stSSA model of Definition 1. Write the eigenvalue decomposition of the matrix $\mathbf{M}$ from Eq. (1) as $\mathbf{M} = \mathbf{V} \mathbf{D} \mathbf{V}^\top$, where $\mathbf{D}$ is a diagonal matrix with eigenvalues ordered by $\lambda_1 \geq \dots \geq \lambda_p$, the i th column of $\mathbf{V} = [\mathbf{V}_n \ \mathbf{V}_s]$ is the eigenvector corresponding to the eigenvalue λ_i , $\mathbf{V}_s \in$

$\mathbb{R}^{p \times (p-q)}$, and $\mathbf{V}_n \in \mathbb{R}^{p \times q}$. The estimators for the stationary $\mathbf{W}_s$ and nonstationary $\mathbf{W}_n$ parts of the unmixing matrix from (2) are defined as $\widehat{\mathbf{W}}_s = \mathbf{V}_s^\top \mathbf{Q}_S(\mathbf{x})^{-1/2}$ and $\widehat{\mathbf{W}}_n = \mathbf{V}_n^\top \mathbf{Q}_S(\mathbf{x})^{-1/2}$, respectively.

The estimation method of Definition 2 is motivated by the sliced inverse regression (SIR), which is a supervised dimension reduction method [6]. In SIR one assumes to have a one-dimensional response y and a p -variate explanatory variable $\mathbf{x}$ such that $\mathbf{x}$ and y are conditionally independent given $\mathbf{U}\mathbf{x}$, where $\mathbf{U} \in \mathbb{R}^{k \times p}$ and $k < p$. That is, under the model, the dimension of the explanatory variable can be reduced from p to k dimensions. The matrix $\mathbf{U}$ spanning the lower dimensional subspace is estimated as follows. First, the whitened observations of the explanatory variable are divided into segments based on the values of the response variable. Then, the sample means corresponding to segments are used to compute a weighted covariance matrix similar to the matrix $\mathbf{M}$ of (1). Eigenvectors corresponding to the k largest eigenvalues of the weighted covariance matrix are used to acquire the estimate of $\mathbf{U}$. Thus, the method of Definition 2 is the SIR with a dummy response, which divides the spatiotemporal domain into segments.

We remark that in this work we restrict attention to non-stationarity in the mean. However, under the model specified in Definition 1, one could also consider cases where the component fields of $\mathbf{n}$ exhibit non-stationarity in the mean, variance, or autocorrelation. In such scenarios, as discussed in [4], one can compute different statistics—other than segment-wise means—and compare them to their global counterparts, formulating the task as a joint diagonalization problem. We will explore this extension in a follow-up paper.

4 Simulation Study

The finite sample performance of the stSSA method of Definition 2 is assessed with a simulation study. Throughout, we assume that the latent dimension q is known. For different choices of latent components and segmentation for the stSSA, we measure the method's performance in estimating the stationary $\mathbf{W}_s$ and nonstationary $\mathbf{W}_n$ parts of the unmixing matrix. However, as noted in Sect. 2, the unmixing matrix is not uniquely defined. Thus, the estimates $\widehat{\mathbf{W}}_s$ and $\widehat{\mathbf{W}}_n$ are not compared directly to $\mathbf{W}_s$ and $\mathbf{W}_n$, respectively. Instead, we compute the projection matrices $\mathbf{P}_s = \mathbf{W}_s^\top (\mathbf{W}_s \mathbf{W}_s^\top)^{-1} \mathbf{W}_s$ and $\mathbf{P}_n = \mathbf{W}_n^\top (\mathbf{W}_n \mathbf{W}_n^\top)^{-1} \mathbf{W}_n$ corresponding to the stationary and nonstationary subspaces. Similarly, let $\widehat{\mathbf{P}}_s$ and $\widehat{\mathbf{P}}_n$ be the projection matrices corresponding to $\widehat{\mathbf{W}}_s$ and $\widehat{\mathbf{W}}_n$. Then, as the performance measures for the stationary and nonstationary parts, we use the squared distances

$$s_{\text{perf}} = \frac{1}{2} \|\mathbf{P}_s - \widehat{\mathbf{P}}_s\|_F^2 \quad \text{and} \quad n_{\text{perf}} = \frac{1}{2} \|\mathbf{P}_n - \widehat{\mathbf{P}}_n\|_F^2, \quad (3)$$

where $\|\cdot\|_F$ is the Frobenius norm.

For a detailed treatment of the above performance measures, see [7]. The stSSA method is compared to a baseline method. In the baseline method, space-time segmentation is not used. Instead, we estimate the unmixing matrix with $\mathbf{W} = \mathbf{V}_{\text{rand}} \mathbf{Q} \mathbf{S}(\mathbf{x})^{-1/2}$, where $\mathbf{V}_{\text{rand}}$ is sampled from the uniform distribution (the Haar measure) on orthogonal matrices. With a sufficiently large sample size and a sufficiently good choice of segmentation, the stSSA should outperform the baseline method with respect to performance measures given in Eq. (3).

As the domain for each simulation setting, we choose $\mathcal{U} \times \mathcal{T} = [0, 1]^2 \times \{1, \dots, n_t\}$. Here, a *simulation setting* refers to a certain choice of latent components, and in total, we have seven different settings. In each setting, the i th component is of the form $z_i(\mathbf{u}, t) = \mu_i(\mathbf{u}, t) + \varepsilon_i(\mathbf{u}, t)$, where μ_i is a deterministic function giving the trend and ε_i is a zero-mean stationary field.

More precisely, the field ε_i is constructed by simulating two independent Gaussian fields $\varepsilon_i^{(1)} = \varepsilon_i^{(1)}(\mathbf{u})$ and $\varepsilon_i^{(2)} = \varepsilon_i^{(2)}(t)$. The covariance structure of the former field $\varepsilon_i^{(1)}$ is determined by the Matérn covariance function

$$C_{\nu, \phi}^{(1)}(\mathbf{u}_1, \mathbf{u}_2) = c_{\nu, \phi} \left(\frac{\|\mathbf{u}_2 - \mathbf{u}_1\|_2}{\phi} \right)^\nu K_\nu \left(\frac{\|\mathbf{u}_2 - \mathbf{u}_1\|_2}{\phi} \right),$$

where $c_{\nu, \phi}$ is a constant depending on ν and θ such that $\lim_{\mathbf{u}_1 \rightarrow \mathbf{u}_2} C_{\nu, \phi}^{(1)}(\mathbf{u}_1, \mathbf{u}_2) = 1$, K_ν is the modified Bessel function of the second kind, and $\|\cdot\|_2$ is the usual Euclidean norm. The covariance structure of the latter field $\varepsilon_i^{(2)}$ is determined by the exponential covariance function

$$C_\theta^{(2)}(t_1, t_2) = \exp \left(-\frac{|t_2 - t_1|}{\theta} \right).$$

Finally, the field ε_i is obtained by setting $\varepsilon_i(\mathbf{u}, t) = \varepsilon_i^{(1)}(\mathbf{u})\varepsilon_i^{(2)}(t)$.

For the trend function we consider the possibilities

$$\begin{aligned} \mu^{(1)}(\mathbf{u}, t) &= \begin{cases} 0, & \text{if } \mathbf{u} \in [0, 1] \times [0, 0.5] \\ 0.2, & \text{if } \mathbf{u} \in [0, 1] \times (0.5, 1] \end{cases}, \\ \mu^{(2)}(\mathbf{u}, t) &= \begin{cases} -1, & \text{if } t \leq n_t/2 \\ -1.2, & \text{if } t > n_t/2 \end{cases}, \\ \mu^{(3)}(\mathbf{u}, t) &= \begin{cases} 2, & \text{if } \mathbf{u} \in [0, 0.5] \times [0, 1] \\ 2.2, & \text{if } \mathbf{u} \in (0.5, 1] \times [0, 1] \end{cases}, \end{aligned}$$

$$\mu^{(5)}(\mathbf{u}, t) = \begin{cases} 5, & \text{if } \mathbf{u} \in [0, 0.5] \times [0, 0.5] \times [1, n_t/2] \\ 5, & \text{if } \mathbf{u} \in (0.5, 1] \times [0, 0.5] \times [1, n_t/2] \\ -5, & \text{if } \mathbf{u} \in [0, 0.5] \times (0.5, 1] \times [1, n_t/2] \\ -5, & \text{if } \mathbf{u} \in (0.5, 1] \times (0.5, 1] \times [1, n_t/2] \\ 5, & \text{if } \mathbf{u} \in [0, 0.5] \times [0, 0.5] \times (n_t/2, n_t] \\ 5, & \text{if } \mathbf{u} \in (0.5, 1] \times [0, 0.5] \times (n_t/2, n_t] \\ -5, & \text{if } \mathbf{u} \in [0, 0.5] \times (0.5, 1] \times (n_t/2, n_t] \\ -5, & \text{if } \mathbf{u} \in (0.5, 1] \times (0.5, 1] \times (n_t/2, n_t] \end{cases}, \quad (4)$$

and lastly, $\mu^{(4)}(\mathbf{u}, t)$ and $\mu^{(6)}(\mathbf{u}, t)$ are segmented similarly in space and time as $\mu^{(5)}(\mathbf{u}, t)$, but the values of the trend functions are different in the corresponding blocks. That is, the value of $\mu^{(4)}(\mathbf{u}, t)$ decreases from -2 to -2.2 monotonically, and the value of $\mu^{(6)}(\mathbf{u}, t)$ oscillates from 5 to -5 as one jumps from block to block from up to down in the order given by Eq. (4).

Now, we are ready to describe the latent components in the simulation settings in all of which we set $p = 2q$. For the stationary part we set $\mathbf{s} = (\varepsilon_1, \dots, \varepsilon_q)$, and for the nonstationary part we set $\mathbf{s} = (\mu^{(\pi(1))} + \varepsilon_{q+1}, \dots, \mu^{(\pi(q))} + \varepsilon_p)$ for some function $\pi : \{1, \dots, q\} \rightarrow \{1, \dots, 6\}$, where $\varepsilon_1 \dots \varepsilon_p$ are independent zero-mean Gaussian processes having dependence structure described by the parameters (ν, ϕ, θ) . That is, for a setting we select a trend function for each nonstationary component, and the parameters giving the dependence structure (ν, ϕ, θ) are the same for each component.

Settings 1–6 are quite similar, but the dependence structure and the latent dimension p change from setting to setting. For settings i and $i + 3$ we set $q = i + 1, i \in \{1, \dots, 3\}$, and as the trend functions we choose $\mu^{(1)}, \dots, \mu^{(q)}$ for the nonstationary components. That is, the latent dimension is 4, 6, or 8 depending on the setting. Furthermore, for Settings 1–3 and 4–6 we set $(\nu, \phi, \theta) = (0.5, 10, 0.5)$ and $(\nu, \phi, \theta) = (0.5, 1, 2)$, respectively. In the case $(\nu, \phi, \theta) = (0.5, 10, 0.5)$ we have short-range dependence, and in the case $(\nu, \phi, \theta) = (0.5, 1, 2)$ we have long-range dependence. For Setting 7 we set $q = 2$, and for the nonstationary latent components we choose the trend functions $\mu^{(5)}$ and $\mu^{(6)}$. We also set $(\nu, \phi, \theta) = (0.5, 10, 0.5)$. That is, in Setting 7, both nonstationary components have an “oscillating” trend in the space-time blocks given by Eq. (4).

For each simulation setting, with a chosen sample size (n_s, n_t) , simulation with either the baseline method or the stSSA with a chosen segmentation is repeated $m = 100$ times. In each round $j \in \{1, \dots, m\}$, the elements of $\mathbf{A}$ are generated from the uniform distribution on $[-1, 1]$. For Settings 1–6 we use the sample size $(n_s, n_t) = (50, 100)$, and for Setting 7 we use the sample size $(n_s, n_t) = (100, 300)$. For a setting the n_s spatial points are generated from a uniform distribution on $[0, 1]^2$; however, the spatial locations are fixed across the simulation rounds $j \in \{1, \dots, m\}$. That is, the value of the observed field $\mathbf{x}$ is recorded in time steps $\{1, \dots, n_t\}$ for fixed locations across simulation rounds. However, the mixing

matrix is different for each simulation round. The estimates $\widehat{\mathbf{W}}_s$ and $\widehat{\mathbf{W}}_n$ for the stationary part and the nonstationary part of the unmixing matrix are acquired with the stSSA or the baseline method. Simulation round j is finished by computing the performance measures of Eq. (3) for the stationary and nonstationary parts.

In total, we have seven segmentation options for the stSSA, which are labeled S1–S7. To describe the segmentations we refer to the first spatial coordinate, the second spatial coordinate, and time by first, second, and third coordinates. In segmentations S_i , $i \in \{1, 2, 3\}$, we do not segment the i th coordinate at all, but the two remaining coordinates are divided into two equally large segments. That is, in Segmentations S1–S3 one dimension is not segmented at all. In Segmentations S4–S7 all coordinates are divided into two, three, four, and ten equally large segments, respectively. For example, in Segmentation S5 the space-time is divided into 3^3 equally sized blocks. In Settings 1–6, all the segmentations are considered. However, in Setting 7 only Segmentations S1, S2, and S5 are used.

Table 1 shows the medians of the performance measures $\mathbf{s}_{\text{perf}}$ and $\mathbf{n}_{\text{perf}}$ computed from $m = 100$ simulation rounds for Settings 1–6 when the stSSA with Segmentations S1–S7 or alternatively, the baseline method (B) is used. For Settings 1–5 the median performances of both stationary and nonstationary parts corresponding to the best segmentation are bolded. For Settings 1–4 the best-performing segmentation corresponds to the true one. For example, in Setting 2 the trend is different in four blocks in space-time. Segmentation S4 matches the blocks in which the trends differ perfectly. Generally, Table 1 shows that as the dimension p increases and the short-range dependence $(\nu, \phi, \theta) = (0.5, 10, 0.5)$ is changed to the long-range dependence $(\nu, \phi, \theta) = (0.5, 1, 2)$, the performance of the stSSA deteriorates. This is most evident in Setting 6 where for any segmentation the stSSA performs almost equally poorly as the baseline method. Furthermore, in Setting 6 there is no unique segmentation for which the performance is the optimal for both stationary and nonstationary parts. Also, interestingly, for Setting 5, the best segmentation does not correspond to the theoretical one. This might be due to high dimension p and long-range dependence. Lastly, as the segmentation gets finer (from S4 to S7), the performance of the stSSA worsens due to the small sample size per segment $|\mathbf{S}_k|$.

Table 2 shows the simulation results for Setting 7. Similarly, as in Table 1, the median performance measures are shown for the stSSA with selected segmentations (S1, S2, and S5) and the baseline method. In addition, the average eigenvalues of the matrix $\mathbf{M}$ used in the stSSA for selected segmentations are given in the last four columns of the table. In this setting the trend changes only in space, not in time. Performance measures of Table 2 warn that it is not sufficient to choose any segmentation in space to acquire a sufficient performance. That is, because of the oscillating trend, if a wrong segmentation is chosen, the sample mean of some nonstationary latent component is close to zero in each segment. Eigenvalues corresponding to Segmentations S1 and S2 suggest that with both segmentations, the stSSA recognizes only one of the two nonstationary components.

Table 1 Simulation results for Settings 1–6. For each simulation setting, we use the stSSA with the chosen segmentation (S1–S7) or the baseline method (B). In each simulation round $j \in \{1, \dots, m\}$, a random mixing matrix is used, but the sample size $(n_s, n_t) = (50, 100)$ is fixed. Each cell corresponds to the median computed from $m = 100$ performance measures for the estimator of the stationary or nonstationary part of the mixing matrix. For all settings, except for Setting 6, the medians corresponding to the best-performing segmentation are bolded. Abbreviations seg. and sub. stand for segmentation and subspace, respectively

Seg.	Sub.	$(\nu, \phi, \theta) = (0.5, 10, 0.5)$					
		$(q, p) = (2, 4)$	$(q, p) = (3, 6)$	$(q, p) = (4, 8)$	$(q, p) = (2, 4)$	$(q, p) = (3, 6)$	$(q, p) = (4, 8)$
S1	S _{perf}	0.10	0.79	1.12	0.40	0.95	1.30
	n _{perf}	0.12	0.65	1.11	0.43	0.90	1.40
S2	S _{perf}	0.62	0.73	1.02	0.69	0.97	1.24
	n _{perf}	0.62	0.63	1.10	0.66	0.93	1.26
S3	S _{perf}	0.53	0.79	1.12	0.47	0.83	1.14
	n _{perf}	0.59	0.77	1.17	0.68	0.88	1.26
S4	S _{perf}	0.11	0.41	0.92	0.44	0.85	1.19
	n _{perf}	0.12	0.34	0.97	0.49	0.91	1.21
S5	S _{perf}	0.43	0.85	1.09	0.62	1.00	1.34
	n _{perf}	0.49	0.86	1.11	0.72	0.89	1.32
S6	S _{perf}	0.45	0.87	1.13	0.64	0.96	1.28
	n _{perf}	0.43	0.80	1.21	0.66	0.95	1.38
S7	S _{perf}	0.69	0.96	1.25	0.72	0.95	1.29
	n _{perf}	0.75	0.96	1.24	0.76	0.91	1.28
B	S _{perf}	0.66	0.98	1.32	0.65	1.00	1.30
	n _{perf}	0.69	0.99	1.33	0.73	1.00	1.33
		Setting 1	Setting 2	Setting 3	Setting 4	Setting 5	Setting 6

Table 2 Simulation results for Setting 7. For each simulation setting, we use the stSSA with the chosen segmentation (S1, S2, or S5) or the baseline method (B). In each simulation round $j \in \{1, \dots, m\}$, a random mixing matrix is used, but the sample size $(n_s, n_t) = (100, 300)$ is fixed. Each cell in the first two columns corresponds to the median computed from $m = 100$ performance measures for the estimator of the stationary or nonstationary part of the mixing matrix. Cells of the remaining four columns give the average eigenvalues of the matrix $\mathbf{M}$ used in the stSSA computed from $m = 100$ simulation rounds. The average eigenvalues are ordered from the largest to the smallest $\lambda_1 \geq \dots \geq \lambda_4$. Abbreviations seg. and sub. stand for segmentation and subspace, respectively

Seg.	Sub.		Eigenvalues			
	$\mathbf{s}_{\text{perf}}$	$\mathbf{n}_{\text{perf}}$	λ_1	λ_2	λ_3	λ_4
S1	0.64	0.80	9.6×10^{-1}	7.5×10^{-4}	3.9×10^{-5}	8.9×10^{-20}
S2	0.69	0.72	9.6×10^{-1}	8.1×10^{-4}	6.0×10^{-5}	5.1×10^{-18}
S5	1.0×10^{-5}	1.5×10^{-3}	6.8×10^{-1}	5.6×10^{-1}	5.5×10^{-3}	1.6×10^{-3}
B	0.083	0.95	—	—	—	—

For reproducibility, the simulation codes are provided in <https://github.com/perej1/sim-temporal-spatial-ssa/releases/tag/v1.1>. Also, related to simulation scenarios of Tables 1 and 2, boxplots illustrating the scatter of the performance measures are provided in the GitHub repository.

5 Conclusions

We developed a statistical method for separating the stationary and nonstationary latent subspaces spanned by the matrices $\mathbf{A}_s$ and $\mathbf{A}_n$ from Definition 1, respectively. The practicality of the method is illustrated with a simulation study. The simulation study suggests that, for a fixed sample size, the performance of the method suffers in the presence of long-range dependence or if the latent dimension is high. Furthermore, Simulation Setting 7 indicates that, in some cases, the segmentation has to be chosen carefully to acquire satisfactory results. Thus, it is advisable to perform the method with multiple segmentations. Nonetheless, if the segmentation is too fine, the method might fail due to an insufficient sample size per segment.

Throughout the simulations, we assume that the dimension of the nonstationary subspace q is known. However, in practical settings, one usually does not know the value of q . Thus, methods for estimating q are crucial. As Table 2 shows, for a sufficiently large sample size and a reasonable segmentation, exactly the q largest eigenvalues of the matrix $\mathbf{M}$ from (1) differ significantly from zero. Thus, the magnitudes of the eigenvalues of $\mathbf{M}$, or the scree plot, can be used to guess the dimension q . Furthermore, in the context of spatiotemporal data, detecting combined non-stationarity in mean, variance, and covariance is a topic of future research. Also under additional assumptions the actual latent components might be fully identifiable following considerations of [8, 11].

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