Non-stationary Global Models

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Abstract

Building computationally feasible spatial models for large data sets is a challenging problem. In this work, a new flexible class of spatial models is introduced. The models can be used for data in $\mathbb{R}^d$ or on the sphere, and can easily be made non-stationary. Results are illustrated with global total column ozone data.

1. Spatial Differential Models

The Matérn family of covariance functions is a popular choice for modeling spatial data. As noticed by [1], a random process on $\mathbb{R}^d$ with a Matérn covariance function can be viewed as the solution to the stochastic differential equation

$$(\kappa^2 - \Delta)^{\frac{\alpha}{2}} X(s) = W(s), \tag{1}$$

where $W(s)$ is Gaussian white noise. Here, we are interested in building models for data on 2-manifolds, such as $\mathbb{R}^2$ or the sphere, and we can then take the solution to (1) as the definition of a Matérn field. A natural generalization of (1) is the system of stochastic differential equations

$$\begin{aligned} \mathcal{L}_1 X_0(s) &= W(s), \\ X(s) &= \mathcal{L}_2 X_0(s), \end{aligned} \tag{2}$$

where $\mathcal{L}_1$ and $\mathcal{L}_2$ are some differential operators. The system generates a quite general class of random fields, even if we restrict operators $\mathcal{L}_1$ and $\mathcal{L}_2$ to operators closely related to (1). We restrict $\mathcal{L}_1$ to the form

$$\mathcal{L}_1 = \prod_{i=1}^{n_1} (1 - \nabla^\top A_i \nabla)^{\frac{\alpha_i}{2}}$$

for some symmetric positive semi definite matrices A_i, and $\alpha_i \in \mathbb{N}$. We further restrict $\mathcal{L}_2$ to the form

$$\mathcal{L}_2 = \prod_{i=1}^{n_2} (b_i + B_i^\top \nabla)$$

for some $b_i \in \mathbb{R}$ and some vector B_i. For the solutions X to exist in the usual sense, the order of the operator $\mathcal{L}_2$ must be smaller than that of $\mathcal{L}_1$. Non-stationarity is easily introduced in these models by allowing the parameters in the differential operators to depend on location. This approach will be used in Section 3.

Many different types of covariance functions can be obtained from the model (2). We can obtain standard Matérn fields by letting $\mathcal{L}_2$ be the identity operator and $\mathcal{L}_1 = (\kappa^2 - \Delta)^{\frac{\alpha}{2}}$. But also different types of oscillating covariance functions can be obtained. Some examples are shown in Figure 1.

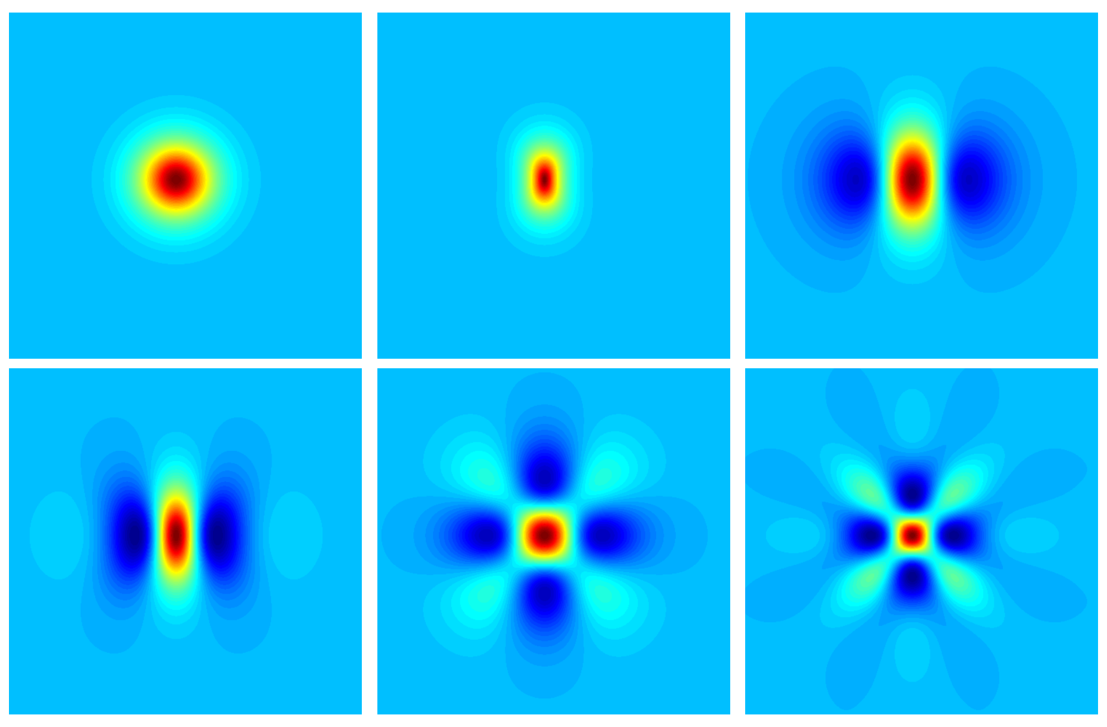

Figure 1: *Some examples of covariance functions of random fields obtained from* (2) *with different parameters.*

2. Efficient Computations

In order to apply these models on large data sets, we use the computationally efficient Markov approximations obtained by the method introduced in [2]. The method is based on a Finite Element approach, and utilizes sparse matrices to reduce the computational cost for many operations, typically from $O(m^3)$ to $O(n^{\frac{3}{2}})$, where m is the number of observations, and n is the number of basis functions used in the Finite Element model.

The unknown variance and differentiation parameters, ψ, in the model can be estimated by numerical optimization of the marginal likelihood $\pi(\boldsymbol{\psi}|Y)$, where Y is the measured data. Uncertainty estimates can then be obtained by the methods developed in [3].

3. Application: Ozone Data

On October 24, 1978, NASA launched the near-polar, Sun-synchronous orbiting satellite Nimbus-7. The satellite carried a Total Ozone Mapping Spectrometer (TOMS) with the purpose of obtaining daily high-resolution global maps of atmospheric ozone. Once the data is received by the satellite, it is calibrated and preprocessed into spatially and temporally irregular Total Column Ozone (TCO) measurements following the satellite orbit. In what follows, we will analyze TCO from October 1st, 1988.

3.1 Statistical Model

We assume the following model for the ozone X:

$$\begin{aligned} &\left(\kappa^2 - \Delta\right)^{\frac{\alpha}{2}} X_0(s) = W(s) \\ &X(s) = \mu(s) + \phi(s)\left(1 + B(s)^\top \nabla\right) X_0(s). \end{aligned}$$

In other words, we assume that the ozone can be modeled as a Gaussian field $X(s)$ with some mean value $\mu(s)$ and a covariance structure that is obtained by applying the differential operator $\phi(s)\left(1 + B(s)^\top \nabla\right)$ to a stationary Matérn field. We model $\mu(s)$, $\phi(s)$, and $B(s)$ using basis functions,

$$\begin{aligned} \mu(s) &= \textstyle\sum_{k,m} \mu_{k,m} Y_{k,m}(s), \\ B(s) &= \textstyle\sum_{k} \beta_k F_k(s), \\ \phi(s) &= \exp\left(\textstyle\sum_{k,m} \phi_{k,m} Y_{k,m}(s)\right), \end{aligned}$$

where $Y_{k,m}$ is the spherical harmonic of order k and mode m, and the functions F_k are chosen as a basis for a vector field on the sphere. The data, $Y(s)$, is assumed to be observations of the latent field $X(s)$ under Gaussian measurement noise $\mathcal{E}(s)$ with a constant variance σ:

$$Y(s) = X(s) + \mathcal{E}(s).$$

3.2 Results

Using the first four spherical harmonics as basis functions for the mean, the first nine for the variance, and 11 basis functions for the vector field B, the model contains 26 parameters in total. Using a basis of 9002 piecewise linear functions induced by a triangulation of the Earth, we use the approximation procedure in Section 2 and estimate the parameters through numerical optimization. Figure 2 shows the resulting TCO estimate (left) and the Kriging standard errors (right). The results are based on 87035 data points, and took approximately 39 minutes to compute using Matlab on a dual CPU (2×2.1 GHz) personal computer.

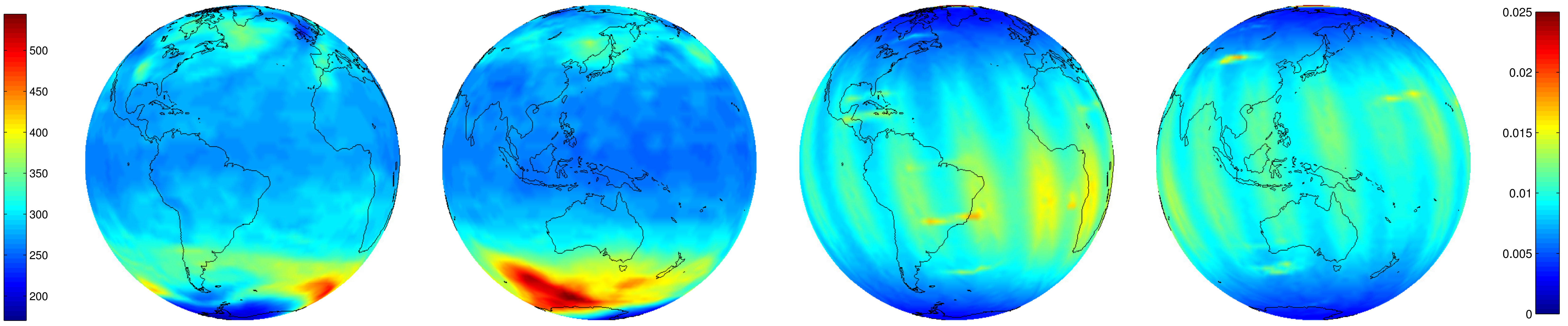

Figure 2: *Ozone estimate (left) and Kriging standard errors (right) in Dobson units*

References

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