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Isotropic covariance functions on spheres: Some properties and modeling considerations

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ABSTRACT

Introducing flexible covariance functions is critical for interpolating spatial data since the properties of interpolated surfaces depend on the covariance function used for Kriging. An extensive literature is devoted to covariance functions on Euclidean spaces, where the Matérn covariance family is a valid and flexible parametric family capable of controlling the smoothness of corresponding stochastic processes. Many applications in environmental statistics involve data located on spheres, where less is known about properties of covariance functions, and where the Matérn is not generally a valid model with great circle distance metric. In this paper, we advance the understanding of covariance functions on spheres by defining the notion of and proving a characterization theorem for m times mean square differentiable processes on d-dimensional spheres. Stochastic processes on spheres are commonly constructed by restricting processes on Euclidean spaces to spheres of lower dimension. We prove that the resulting sphere-restricted process retains its differentiability properties, which has the important implication that the Matérn family retains its full range of smoothness when applied to spheres so long as Euclidean distance is used. The restriction operation has been questioned for using Euclidean instead of great circle distance. To address this question, we construct several new covariance functions and compare them to the Matérn with Euclidean distance on the task of interpolating smooth and non-smooth datasets. The Matérn with Euclidean distance is not outperformed by the new covariance functions or the existing covariance functions, so we recommend using the Matérn with Euclidean distance due to the ease with which it can be computed.

1. Introduction

When modeling dependent spatial data, the covariance function used is crucial for producing accurate predictions and estimating prediction uncertainties. Statistical theory [24,28] shows that when the goal is interpolation of highly dependent data packed tightly on a compact domain, it is of utmost importance to correctly specify the local properties of the process, which are determined by the behavior of the covariance function near the origin. In recent years the Matérn family of covariance functions has gained widespread popularity in spatial statistics [8] due partly to its ability to control the local behavior of the process. Specifically, let $Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{R}^d$, be a random field. The isotropic Matérn covariance function is given by

$$M(\|\boldsymbol{h}\|) = \mathrm{Cov}(Z(\boldsymbol{x}), Z(\boldsymbol{x}+\boldsymbol{h})) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)}\mathcal{K}_\nu(\alpha\|\boldsymbol{h}\|)(\alpha\|\boldsymbol{h}\|)^\nu, \tag{1}$$

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where $\sigma^2, \alpha, \nu > 0$, and $\mathcal{K}_\nu$ is the modified Bessel function of the second kind. The popularity of the Matérn is also due partly to this representation, which allows the function to be computed by way of rapidly converging series expansions for the Bessel function [5, Chapter 10]. We say that M is isotropic because it depends on the locations $\boldsymbol{x}$ and $\boldsymbol{x}+\boldsymbol{h}$ only through the Euclidean distance $\|\boldsymbol{h}\|$ between them. The parameter of interest here is ν, which controls the smoothness of the process, defined in terms of its mean square differentiability: a process on a Euclidean space that has covariance function M has m mean square derivatives if and only if $\nu > m$.

In environmental statistics, we often encounter data associated with locations on the surface of the Earth, for example observations from satellites or output from climate models, and in astronomy and cosmology, the observations are often associated with an azimuth and altitude in the sky, so it is important to introduce flexible classes of covariance functions that are valid on spheres. Marinucci and Peccati [19] provide a broad overview of the theory of random fields on spheres. The question of validity of covariance functions on spheres has been studied extensively by Huang et al. [12] and further by Gneiting [7], who proved that many of the commonly used covariance functions on Euclidean spaces are valid on spheres when Euclidean distance is replaced by great circle distance—the more natural distance metric on a sphere. However, the Matérn is positive definite with great circle distance only if $\nu \leq 1/2$. The fact that the validity of the Matérn on spheres is tied to the value of the smoothness parameter handcuffs its usefulness for modeling a wide range of smooth and non-smooth spatial data. Recently there have been efforts to introduce new covariance functions on spheres. Ma [17], Du et al. [6], and Ma [18] provide closed-form covariance functions and variogram functions for vector-valued processes on spheres, and Heaton et al. [9] defines covariance functions on spheres in terms of kernel convolutions. However, none of the functions any of these authors studied possess the flexibility to specify the smoothness of the process like the Matérn does. An exception is Jeong and Jun [13], who introduce a "Matérn-like" covariance function on spheres but this covariance function must be approximated and does not outperform much simpler alternatives.

Spheres are subsets of Euclidean spaces, so a covariance function that is valid on a Euclidean space – such as the Matérn– can be applied to a sphere of lower dimension if the Euclidean distance is used. More formally, for $d \geq 1$, define the d-sphere as $\mathbb{S}^d = \{\boldsymbol{x} \in \mathbb{R}^{d+1} : \|\boldsymbol{x}\| = 1\}$ and the great circle distance metric as $\theta(\boldsymbol{x}, \boldsymbol{y}) = \arccos(\langle \boldsymbol{x}, \boldsymbol{y} \rangle)$ for $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{S}^d$, where $\langle \cdot, \cdot \rangle$ denotes the usual inner product on $\mathbb{R}^d$. The Euclidean distance between two points on a sphere, which is also known as the chordal distance, can be expressed in terms of great circle distance as $\|\boldsymbol{x} - \boldsymbol{y}\| = 2\sin(\theta(\boldsymbol{x}, \boldsymbol{y})/2)$, so if K is a valid isotropic covariance function on $\mathbb{R}^{d+1}$, then $\psi(\theta) = K(2\sin(\theta/2))$ is a valid covariance function on $\mathbb{S}^d$ [26,27]. Stated more simply, this approach starts with a valid process on $\mathbb{R}^{d+1}$ and restricts it to the sphere $\mathbb{S}^d$, so while the process on $\mathbb{S}^d$ is trivially valid, we must use the chordal distance in calculations of the covariance. In what follows, we refer to the Matérn with chordal distance, $\varphi(\theta) = M(2\sin(\theta/2))$, as the chordal Matérn covariance function.

Our work is concerned with understanding the properties of covariance functions on spheres, specifically with respect to mean square differentiability, and exploring the modeling capabilities of the chordal Matérn with real data. In Section 2, we define the notion of a mean square differentiable process on a sphere and provide a concise theorem characterizing m times mean square differentiable processes in terms of their covariance functions and Fourier series. Since it is common to use the restriction construction to define valid covariance functions on spheres, we prove a corollary stating that the process restricted to a sphere retains the differentiability properties of the original process. This result has the important implication that the chordal Matérn retains the full flexibility that the Matérn does, in terms of smoothness.

While the restriction operation is convenient due to the abundance of flexible models on Euclidean spaces, such as the Matérn, Gneiting [7] argued that this "may result in physically unrealistic distortions". It is important to understand the implications of defining a covariance function in terms of chordal distance and whether such covariance functions will poorly model data observed over large regions on a sphere. There have been some efforts to compare the two distance metrics, most notably Banerjee [2], who fits parametric spatial covariance functions to data observed at locations on the Earth. The results there suggested that using the chordal versus great circle distance may produce slightly different model estimates. However, the observation region for those data was quite small compared to the entire globe – less than $5^\circ \times 5^\circ$ latitude $\times$ longitude – and the study considered the Matérn with great circle distance, which is not generally a positive definite function on a sphere, so a more thorough investigation is warranted.

To provide insight into the appropriateness of the chordal Matérn for data observed on spheres, we compare its ability to model and interpolate smooth and non-smooth datasets to that of a number of existing and new covariance functions that we introduce in Section 3. The existing covariance functions were introduced in [12,7] and consist of covariance functions that are valid on Euclidean spaces that remain valid on spheres when Euclidean distance is replaced by great circle distance. In Section 3, we introduce several new families of covariance functions capable of modeling smooth and nonsmooth processes and whose constructions respect circular and spherical geometry. Using existing theoretical results and our new theoretical results we outline the differentiability properties of the new covariance functions. We also discuss computational considerations and provide closed forms for the covariance functions in some cases, one of which corresponds to the characteristic function of an integer-valued version of the t-distribution.

The covariance functions are compared in Section 4 on two datasets of different degrees of smoothness, both of which span large distances around the Earth. We find that for the problem of dense interpolation, the chordal Matérn is not outperformed by any of the new or existing covariance functions, and it is sometimes a substantial improvement in terms of loglikelihood and predictive performance over existing covariance functions that take great circle distance as the argument. Finally, we conclude in Section 5 with a discussion of our work and practical recommendations for choosing covariance functions to model data observed on spheres.