

On the Validity of Commonly Used Covariance and Variogram Functions on the Sphere

By: Chunfeng Huang, [Haimeng Zhang](#), Scott M. Robeson

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Abstract:

Covariance and variogram functions have been extensively studied in Euclidean space. In this article, we investigate the validity of commonly used covariance and variogram functions on the sphere. In particular, we show that the spherical and exponential models, as well as power variograms with $0 < \alpha \leq 1$, are valid on the sphere. However, two Radon transforms of the exponential model, Cauchy model, the hole-effect model and power variograms with $1 < \alpha \leq 2$ are not valid on the sphere. A table that summarizes the validity of commonly used covariance and variogram functions on the sphere is provided.

Keywords: Power variogram | Spherical covariance | Stable model | Variogram models

Article:

1 Introduction

Global-scale processes and phenomena are of utmost importance in the geosciences. Data from global networks of in situ and satellite sensors are used to monitor a wide array of geophysical processes. Most methods and models in spatial statistics, however, are developed in Euclidean spaces n and these methods have not been investigated as intensively in spherical coordinate systems (Robeson 1997). Among the most commonly used covariance and variogram functions in the geosciences are the exponential, Gaussian, spherical, hole-effect, and power models (Kitandis 1997; Isaaks and Srivastava 1989; Webster and Oliver 2001). Haylock et al. (2008), for instance, compared these five models when developing a high-resolution data set of daily precipitation over Europe. Other geoscientists have used the exponential variogram model on the sphere to develop quantitative estimates of atmospheric carbon dioxide concentrations, global fire distributions, and oceanic mixed layer depths (Alkhaled et al. 2008; Carmona-Moreno et al. 2005; de Boyer Montégut et al. 2004). The Gaussian model on the sphere has been used to reconstruct paleoceanographic temperature (Schäfer-Neth et al. 2005) while Janis and Robeson (2004) used a power model with spherical distances to analyze errors in minimum temperature

data. Clearly, a wide range of geostatistical models are being used with databases that are coded in spherical coordinates. Before adapting Euclidean covariance and variogram models to the sphere, one must first evaluate their properties to ensure their validity.

A random process is stationary on the sphere if its covariance function depends solely on the spherical angle. To be valid, the covariance function must be positive definite on the sphere (Schoenberg 1942; Yaglom 1987). In practice, many applications also focus on intrinsically stationary processes and their variograms. While such processes have been well studied in Euclidean space (Cressie 1993; Chilès and Delfiner 1999), the extension to the sphere needs more investigation. In Sect. 2, we study the variogram of the intrinsically stationary process on the sphere, as well as the covariance function of the stationary process. Brownian motion on the sphere is presented as an example to demonstrate that an intrinsically stationary process may not be stationary. This answers some questions raised in Reguzzoni et al. (2005). In Sect. 3, several commonly used covariance and variogram models are checked for their validity on the sphere. In particular, we show that the spherical and exponential covariance models and power variograms with $0 < \alpha \leq 1$ are valid on the sphere. However, the Gaussian model, two Radon transforms of exponential model, Cauchy model, the hole-effect model and power variograms with $1 < \alpha \leq 2$ are not valid on the sphere. A summary of our results can be found in Table 1. A discussion of strictly positive (conditional negative) definiteness of the covariance (variogram) functions is presented in Sect. 4.

2 Covariance and Variogram Functions on the Sphere

Consider a random process $X(p)$, $p \in S^2$, where S^2 is a unit sphere in R^3 , and the location $p = (\varphi, \lambda)$ with latitude φ and longitude λ , $0 \leq \varphi \leq \pi$, $0 \leq \lambda < 2\pi$. The process is stationary if the covariance function $\text{cov}(X(p_1), X(p_2))$ depends solely on the spherical angle $\theta(p_1, p_2) \in [0, \pi]$, where

$$\cos(\theta(p_1, p_2)) = \sin\varphi_1 \sin\varphi_2 + \cos\varphi_1 \cos\varphi_2 \cos(\lambda_1 - \lambda_2).$$

A real continuous function $C(\cdot)$ is said to be a valid covariance function on the sphere if it is positive definite, namely,

$$\sum_{i=1}^m \sum_{j=1}^m C(\theta(p_i, p_j)) a_i a_j \geq 0$$

for any finite number of spatial locations $\{p_i, i = 1, \dots, m\}$ on S^2 and real numbers $\{a_i, i = 1, \dots, m\}$. The following theorem by Schoenberg (1942) provides the characterization of a valid covariance function on the sphere.

Theorem 1 A real continuous function $C(\theta)$ is a valid covariance function on the sphere if and only if it is of the form

$$C(\theta) = \sum_{n=0}^{\infty} b_n P_n(\cos \theta), \quad \theta \in [0, \pi], \quad (1)$$

where $b_n \geq 0$, $\sum_{n=0}^{\infty} b_n < \infty$, are the Legendre polynomials.

By orthogonality of the Legendre polynomials (7.112.1 in Gradshteyn and Ryzhik 1994), the coefficients can be obtained by

$$b_n = \frac{2n+1}{2} \int_0^\pi C(\theta) P_n(\cos \theta) \sin \theta d\theta, \quad n = 0, 1, 2, \dots \quad (2)$$

Therefore, we can investigate the positive definiteness of a function $C(\cdot)$ by checking whether b_n is non-negative, and $\sum_n b_n < \infty$. In Sect. 3, the validity of commonly used covariance functions are studied.

Parallel to the intrinsically stationary process on R^n (Cressie 1993), we have the following.

Definition 1 Suppose $\{X(p) : p \in S_2\}$ satisfies $E(X(p)) = \mu$, for all $p \in S_2$, and $\text{var}(X(p_1) - X(p_2)) = 2\gamma(\theta(p_1, p_2))$, for all $p_1, p_2 \in S_2$; then $X(\cdot)$ is said to be intrinsically stationary. The quantity $2\gamma(\cdot)$ is called the variogram, and $\gamma(\cdot)$ is the semivariogram.

Proposition 1 The variogram $2\gamma(\cdot)$ is conditionally negative definite, namely

$$\sum_{i=1}^m \sum_{j=1}^m a_i a_j 2\gamma(\theta(p_i, p_j)) \leq 0$$

for any finite number of spatial locations $\{p_i, i = 1, \dots, m\}$ on S_2 and real numbers

$\{a_i, i = 1, \dots, m\}$ satisfying $\sum_{i=1}^m a_i = 0$.

To investigate whether a function is conditionally negative definite on the sphere, we have the following theorem.

Theorem 2 A continuous function $2\gamma(\cdot)$ satisfying $\gamma(0) = 0$ is conditionally negative definite if and only if $2\gamma(\cdot)$ is of the form

$$2\gamma(\theta) = \sum_{n=1}^{\infty} b_n (1 - P_n(\cos \theta)), \quad b_n \geq 0, \quad \sum_{n=1}^{\infty} b_n < \infty$$

and $P_n(\cdot)$ are the Legendre polynomials.

Remark 1 A general result can be found in Bochner (1941), Schoenberg (1942, note 12), Karpushev (1985) and Sasvari (1994). The proof of this theorem can be obtained by directly applying Theorem 3 of Bochner (1941).

Remark 2 Given a valid covariance function $C(\theta)$, one can always find a valid semivariogram $\gamma(\theta) = C(0) - C(\theta)$. The converse is not true in Euclidean space R^n . For example, the power variograms do not have counterpart covariance functions (Cressie 1993). However, when the space is the sphere S^2 , it is noted by Yaglom (1961) that the space of valid variograms coincides with the space of valid covariances. That is, for each valid variogram $2\gamma(\theta)$, $\theta \in [0, \pi]$, one can construct a covariance function $C(\theta) = c_0 - \gamma(\theta)$, for some $c_0 \geq \int_0^\pi \gamma(\theta) \sin\theta d\theta$.

Remark 3 If a function $C_0(h)$ is a valid covariance function in R^3 , then the function $C(\theta) = C_0(2\sin(\theta/2))$ is a valid covariance function on the unit sphere S^2 . In general, any function of the form $C(\theta) = \int_0^\infty \frac{\sin(2\omega(\sin(\theta/2)))}{2\omega \sin(\theta/2)} d\Phi(\omega)$, where $\Phi(\cdot)$ is a bounded non-decreasing function, is valid on a unit sphere S^2 (see Yadrenko 1983, p. 76; or Yaglom 1987, p. 389). Therefore, one can obtain a rich family of valid covariance functions on the sphere, see also Jun and Stein (2007) and Banerjee (2005).

Remark 4 When $C_1(\theta)$ and $C_2(\theta)$ are both valid on the sphere, so are $C_1(\theta)C_2(\theta)$ and $a_1C_1(\theta) + a_2C_2(\theta)$, $a_1, a_2 \geq 0$. For example, since both exponential and power models (see Table 1) are valid, their product $e^{-\theta}(\pi - \theta)$ is also valid.

Remark 5 In practice, one may use weighted least squares to estimate the parameters (Cressie 1985) for valid covariance and variogram models on the sphere.

It is clear that the stationary process is intrinsically stationary. However, the converse is not true even though the spaces of valid covariance functions and valid variogram functions coincide. For example, consider Brownian motion $X(p)$ on S^2 (Gangolli 1967) such that

$$\text{cov}(X(p_1), X(p_2)) = \frac{1}{2}(\theta(p_1, p_0) + \theta(p_2, p_0) - \theta(p_1, p_2)), \quad p_1, p_2 \in S^2$$

where p_0 is a fixed arbitrary point (for example, north pole). It is clear that this process is not stationary; however, the variance of $X(p_1) - X(p_2)$,

$$\text{var}(X(p_1) - X(p_2)) = \theta(p_1, p_2),$$

depends solely on $\theta(p_1, p_2)$. That is, the process $X(p)$ is intrinsically stationary, but not stationary. Note that this process has the power variogram $2\gamma(\theta) = \theta^\alpha$ with $\alpha = 1$, which is shown to be valid on the sphere in Sect. 3.

In this section, we check the validity of some commonly used covariance and variogram functions. A summary of all results is presented in Table 1.

Table 1 Validity (positive definiteness) of covariance functions on the sphere, $a > 0$, $\theta \in [0, \pi]$

Model	Covariance function	Validity
Spherical	$(1 - \frac{3\theta}{2a} + \frac{1}{2} \frac{\theta^3}{a^3}) \mathbf{1}_{(\theta \leq a)}$	Yes
Stable	$\exp(-(\frac{\theta}{a})^\alpha)$	Yes for $\alpha \in (0, 1]$ No for $\alpha \in (1, 2]$
Exponential	$\exp(-(\frac{\theta}{a}))$	Yes
Gaussian	$\exp[-(\frac{\theta}{a})^2]$	No
Power ^a	$c_0 - (\theta/a)^\alpha$	Yes for $\alpha \in (0, 1]$ No for $\alpha \in (1, 2]$
Radon transform of order 2	$e^{-\theta/a}(1 + \theta/a)$	No
Radon transform of order 4	$e^{-\theta/a}(1 + \theta/a + \theta^2/3a^2)$	No
Cauchy	$(1 + \theta^2/a^2)^{-1}$	No
Hole-effect	$\sin_{a\theta/\theta}$	No

^aWhen $\alpha \in (0, 1]$, power model is valid on the sphere for some $c_0 \geq \int_0^\pi (\theta/a)^\alpha \sin\theta d\theta$

3.1 Spherical Model

A spherical covariance function has the form

$$C(\theta) = \begin{cases} 1 - \frac{3\theta}{2a} + \frac{1}{2} \frac{\theta^3}{a^3}, & \text{if } \theta \leq a; \\ 0, & \text{if } \theta > a, \end{cases}$$

where $a > 0$ is a scale parameter. This model is valid in [eqnR]1, [eqnR]2 and [eqnR]3 (Cressie 1993). To check whether it is valid on the sphere, we compute the coefficients b_n in (2) through the following sine expansion of the Legendre polynomials (Hobson 1931, p. 20; also 8.826.1 in Gradshteyn and Ryzhik 1994):

$$\frac{\pi}{4} P_n(\cos\theta) = \frac{2 \cdot 4 \cdots 2n}{3 \cdot 5 \cdots (2n+1)} \left\{ \sin(n+1)\theta + \frac{1}{1} \frac{n+1}{(2n+3)} \sin(n+3)\theta + \cdots \right\}. \quad (3)$$

More compactly, $P_n(\cos\theta) = \sum_{k=0}^{\infty} D_{nk} \sin(n+2k+1)\theta$, for $0 < \theta < \pi$, where

$$D_{nk} = \frac{4}{\pi} \frac{2 \cdot 4 \cdots 2n}{3 \cdot 5 \cdots (2n+1)} \frac{1 \cdot 3 \cdots (2k-1) \cdot (n+1) \cdots (n+k)}{1 \cdot 2 \cdots k \cdot (2n+3) \cdots (2n+2k+1)} > 0. \quad (4)$$

Then,

$$b_n = \frac{2n+1}{2} \int_0^\pi C(\theta) \sum_{k=0}^{\infty} D_{nk} \sin(n+2k+1)\theta \sin\theta d\theta = \frac{2n+1}{2} \sum_{k=0}^{\infty} D_{nk} b_{nk}$$

Where, for integer $k \geq 0$, $b_{nk} = \int_0^\pi C(\theta) \sin(n+2k+1)\theta \sin\theta d\theta = \frac{1}{2}(g(n+2k) - (g(n+2k) - g(n+2k+2)))$. Here, we define, for $x > 0$, $g(x) = \int_0^a (1 - \frac{3\theta}{2a} + \frac{\theta^3}{2a^3}) \cos x\theta d\theta$. To show that $b_n \geq 0$ for all $n \geq 0$, it is sufficient to show that $b_{nk} \geq 0$. Evaluating the integral for $g(x)$ and then taking its first derivative leads to $g'(x) = -\frac{6}{x^5 a^3} (2 \sin \frac{ax}{2} - ax \cos \frac{ax}{2})^2 \leq 0$. This indicates that $g(x)$, $x > 0$, is non-increasing, implying that $b_{nk} = \frac{1}{2}[g(n+2k) - g(n+2k+2)] \geq 0$.

Next we show that $\sum_n b_n < \infty$. We first apply the mean value theorem to obtain $b_{nk} \leq \frac{C_1}{(n+2k)^3}$ for $k \geq 0$, where $C_1 > 0$ is a constant independent of n and k (for notational simplicity, the same C_1 will be used throughout this section, even if each instance of C_1 may not be the same). In addition, observing that

$$\frac{1 \cdot 3 \cdots (2k-1) \cdot (n+1) \cdots (n+k)}{1 \cdot 2 \cdots k \cdot (2n+1) \cdots (2n+2k+1)} < 1$$

and applying the Sterling's approximation to factorials for sufficiently large n , we have

$$D_{nk} \leq \frac{4}{\pi} \frac{2 \cdot 4 \cdots 2n}{3 \cdot 5 \cdots (2n+1)} = \frac{4}{\pi} \frac{(2^n n!) \cdot (2^n n!)}{(2n+1)!} \leq \frac{C_1}{\sqrt{n+1}}$$

Hence, for n large, $b_n \leq C_1(2n+1) \frac{1}{\sqrt{n+1}} \cdot \sum_{k=0}^{\infty} \frac{1}{(n+2k)^3} \leq \frac{C_1}{n^{3/2}}$, implying $\sum_n b_n < \infty$. Therefore, the spherical covariance function is valid on the sphere.

3.2 Stable Model and Power Model

In this subsection, we consider the stable covariance function (Chilès and Delfiner 1999)

$$C(\theta) = \exp\left\{-\left(\frac{\theta}{a}\right)^\alpha\right\}, \quad \theta \in [0, \pi], \quad a > 0, \quad \alpha \in (0, 2] \quad (5)$$

and the power variogram function (Cressie 1993)

$$\gamma(\theta) = \left(\frac{\theta}{a}\right)^\alpha, \quad a > 0, \quad \alpha \in (0, 2]. \quad (6)$$

Both functions are invalid when $\alpha > 2$ but valid when $\alpha \in (0, 2]$ in \mathbb{R}^n (Yaglom 1987). The exponential and Gaussian models are special cases of the stable model (5), corresponding to $\alpha =$

1 and $\alpha = 2$, respectively. Note that the function $\gamma(\cdot)$ is conditionally negative definite if and only if $e^{-\lambda\gamma(\cdot)}$ is positive definite for any $\lambda > 0$ (Schoenberg 1938). Therefore, it is equivalent to check the validity of the stable covariance function and the power variogram function. In addition, by Remark 2 in Sect. 2, it is also equivalent to check the power variogram function and the function

$$C(\theta) = c_0 - \left(\frac{\theta}{a}\right)^\alpha, \quad a > 0, \alpha \in (0, 2], \quad (7)$$

for some $c_0 \geq \int_0^\pi (\theta/a)^\alpha \sin \theta d\theta$. We term $C(\theta)$ in (7) the power covariance function. In summary, it is equivalent to check the validity among these three covariance and variogram functions.

We focus our discussion on validity of these functions when $\alpha \in (0, 2]$. Wood (1995) and Gneiting (1998) show that the stable covariance function is not valid on the circle when $\alpha \in (1, 2]$. Therefore, the stable covariance function is not valid on the sphere, since a valid covariance function on the sphere will always be valid on the circle (Schoenberg 1942). When $\alpha \in (0, 1]$, in Appendix we show that the power covariance function (7) is valid on the sphere.

Our findings are summarized in Table 1. The stable covariance function and power variogram are valid when $\alpha \in (0, 1]$, but not valid when $\alpha \in (1, 2]$. In particular, the exponential covariance function $\exp\{-\theta/a\}$ is valid, and equivalently the power variogram $2\gamma(\theta) = \theta/a$ is also valid. However, the Gaussian covariance function $\exp\{-(\theta/a)^2\}$ is not valid (see also Gneiting 1999). Note that power models with $\alpha > 1$ are not uncommon in practice. Janis and Robeson (2004) estimated over 300 period-of-record variograms using the power model, with approximately 26% having $\alpha > 1$.

3.3 Other Models

In this subsection, we check the validity of the following covariance functions: Radon transforms of exponential model (orders 2 and 4), Cauchy model, and hole-effect model. The computations are carried out by directly checking some of the coefficients b_n in (2).

3.3.1 Radon Transforms of Exponential Model

The following two Radon transforms of exponential model (orders 2 and 4) can be found in Chilès and Delfiner (1999, p. 85) and Gneiting (1999)

$$C_1(\theta) = e^{-\theta/a}(1 + \theta/a), \quad \text{and} \quad C_2(\theta) = e^{-\theta/a}(1 + \theta/a + \theta^2/3a^2)$$

By direct computation, we found that $b_6 < 0$ for $C_1(\theta)$, and $b_2 < 0$ for $C_2(\theta)$, when $a = 1$. Therefore, neither is a valid covariance function on the sphere.

3.3.2 Cauchy Model

The Cauchy model has the form (Chilès and Delfiner 1999, p. 86)

$$C(\theta) = (1 + \theta^2/a^2)^{-1}.$$

It is also termed “rational quadratic model” in Cressie (1993). It is valid on R^n (Yaglom 1987, p. 365). A direct computation yields $b_{14} < 0$, when $a = 0.5$. Therefore, the Cauchy model is not valid on the sphere.

3.3.3 Hole-Effect Model

The hole-effect model has the form

$$C(\theta) = c_0 \frac{\sin a\theta}{\theta}$$

for some $c_0 > 0$ and scale parameter $a > 0$. A direct computation shows that $b_3 < 0$ with $a = 2$. Therefore, it is not a valid covariance function on the sphere.

The Matérn class model has the form (Sect. 22 in Yaglom 1987):

$$C(\theta) = c_0(a\theta)^\nu K_\nu(a\theta),$$

where $c_0 > 0$, $a > 0$, and $K_\nu(\cdot)$, $\nu \geq 0$ is the modified Bessel function of the second kind of order ν . It appears that the validity of the Matérn class on the sphere depends on the smoothing parameter ν . For example, the case $\nu = 12$ corresponds to the exponential model, a valid model on the sphere. When $\nu = 32, 52$ and ∞ , the corresponding models are the Radon transforms of exponential family with order 2, order 4, and the Gaussian model, respectively, all being shown to be invalid on the sphere. Direct computation shows that the Matérn models are not valid when $\nu = 2, 3, \dots, 10$. In view of the connection between the stable and the Matérn models (Stein 1999, p. 50), it is likely that the Matérn models are not valid when $\nu > 1/2$, which needs further investigation.

Discussion of Strictly Positive Definiteness

In this section, we discuss the strictly positive (conditional negative) definiteness of covariance (variogram) functions in Sect. 3. A real continuous function $C(\cdot)$ is said to be strictly positive definite on S^2 if

$$\sum_{i=1}^m \sum_{j=1}^m C(\theta(p_i, p_j)) a_i a_j > 0$$

for any finite number of distinct spatial locations $\{p_i, i = 1, \dots, m\}$ on S_2 and real numbers $\{a_i, i = 1, \dots, m\}$. A parallel definition for strictly conditional negative definiteness can be given as well.

There is a rich discussion in the literature about the strictly positive (conditional negative) definiteness of a continuous function on the sphere (e.g. the sufficient conditions in Xu and Cheney 1992 and Schreiner 1997, and the necessary conditions in Chen et al. 2003). Here, we summarize our findings as the following.

The sufficient condition for strictly positive definite functions on a sphere is that b_n in the expansion (1) should be positive with a finite number of them being zero (e.g. Xu and Cheney 1992; Schreiner 1997). By inspecting the coefficients b_n for the power model in Appendix, one can conclude that all the coefficients b_n are positive when $0 < \alpha < 1$, which leads to the strictly positive definiteness. In parallel, the spherical covariance function is also strictly positive definite on the sphere.

The case of $\alpha = 1$ in the power model yields the coefficients ((8) in Appendix) to be zero for all even terms and positive for all odd terms, which does not satisfy the necessary condition in Chen et al. (2003). Therefore, it is not strictly positive definite on the sphere, even though it is positive definite. Consequently, the power variogram $\gamma(\theta) = \theta$ is not strictly conditionally negative definite. As an example, we consider such an intrinsic stationary process $X(p)$, $p \in S_2$, at four locations: north pole (pN), south pole (pS) and two points on the equator, pE and pW , such that $\theta(pE, pW) = \pi$. It is clear that $\text{var}(X(pN) + X(pS) - X(pE) - X(pW)) = 0$.

The stable model $\exp(-(\theta/a)\alpha)$, $0 < \alpha < 1$, $a > 0$, is strictly positive definite on the sphere. The case of $\alpha = 1$, corresponding to the exponential covariance function $C(\theta) = \exp(-\theta/a)$, $a > 0$, is also strictly positive definite, since the coefficients $b_n = \frac{2n+1}{2} \sum_{k=0}^{\infty} D_{nk} b_{nk} > 0$ for all n , where b_{nk} can be shown to be

$$b_{nk} = \begin{cases} \frac{a(1-e^{-\pi/a})}{2} \left(\frac{1}{1+(n+2k)^2 a^2} - \frac{1}{1+(n+2k+2)^2 a^2} \right) > 0, & n \text{ even;} \\ \frac{a(1+e^{-\pi/a})}{2} \left(\frac{1}{1+(n+2k)^2 a^2} - \frac{1}{1+(n+2k+2)^2 a^2} \right) > 0, & n \text{ odd.} \end{cases}$$

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Appendix: Validity of Power Covariance Functions

In this Appendix, we show that the power covariance function $C(\theta)$ is valid when $\alpha \in (0, 1]$, where

$$C(\theta) = c_0 - \left(\frac{\theta}{a}\right)^\alpha, \quad \theta \in [0, \pi]$$

for some $c_0 \geq \int_0^\pi (\theta/a)^\alpha \sin \theta d\theta$. We explore (2) to show that $b_n \geq 0$ for all $n \geq 0$. First, we present the following result. Lemma 1 Let $k \geq 1$ be an integer. If $g(\theta)$ is a non-negative and non-increasing function on $[0, k\pi]$, then $\int_0^{k\pi} g(\theta) \sin \theta d\theta \geq 0$.

The proof of Lemma 1 is trivial, but the result will be extensively used in the calculation below. Note that this lemma was also used in Gneiting (1998). First, notice that $P_0(\cdot) = 1$.

$$b_0 = \frac{1}{2} \int_0^\pi (c_0 - (\theta/a)^\alpha) P_0(\cos \theta) \sin \theta d\theta = \frac{1}{2} \int_0^\pi (c_0 - (\theta/a)^\alpha) \sin \theta d\theta \geq 0.$$

Next, if $n \geq 1$, by the orthogonality of $P_n(\cos \theta)$ and $\sin \theta$,

$$\begin{aligned} b_n &= \frac{2n+1}{2} \int_0^\pi (c_0 - (\theta/a)^\alpha) P_n(\cos \theta) \sin \theta d\theta \\ &= -\frac{2n+1}{2a^\alpha} \int_0^\pi \theta^\alpha P_n(\cos \theta) \sin \theta d\theta. \end{aligned}$$

It is clear that the selection of a scale parameter a does not affect the sign of b_n , and consequently the validity of $C(\theta)$. Without loss of generality, we assume $a = 1$ throughout the rest of the Appendix.

When $\alpha = 1$, by 7.249.1 in Gradshteyn and Ryzhik (1994), we have

$$\begin{aligned} b_n &= -\frac{2n+1}{2} \int_0^\pi \theta P_n(\cos \theta) \sin \theta d\theta \\ &= \begin{cases} 0, & n = 2m \text{ even;} \\ \frac{(2n+1)\pi}{2} \left\{ \frac{(n-2)!!}{2^{(n+1)/2} (\frac{n+1}{2}!) } \right\}^2, & n = 2m + 1 \text{ odd.} \end{cases} \end{aligned} \quad (8)$$

Therefore, $b_n \geq 0$, $n = 0, 1, \dots$. To show that $\sum_n b_n < \infty$, we first note that $n = 2m+1$:

$$\frac{(n-2)!!}{2^{(n+1)/2} (\frac{n+1}{2}!) } = \frac{(2m+1)!}{2^{2m+1} m!(m+1)!} = \frac{1}{2^{2m+1}} \binom{2m+1}{m}.$$

Applying Stirling's approximation to factorials, we have

$$b_{2m+1} \leq C_1 \frac{4m+3}{2} \pi \left(\frac{1}{\sqrt{m\pi}(2m+1)} \right)^2 \leq C_1 \frac{m}{m(2m+1)^2} \leq \frac{C_1}{m^2},$$

for some constant $C_1 > 0$ independent of m (each appearance of C_1 above may not be the same). Hence, $\sum_n b_n < \infty$, implying that $C(\theta) = c_0 - \theta$ is a valid covariance function for some $c_0 \geq \int_0^\pi (\theta/a)^\alpha \sin \theta d\theta = \pi$. Consequently, the exponential covariance function $\exp\{-\theta\}$ is valid, so is the power variogram $2\gamma(\theta) = \theta$.

When $0 < \alpha < 1$, based on the sine expansion (3) of $P_n(\cos \theta)$, we can write

$$b_n = -\frac{2n+1}{2} \sum_{k=0}^{\infty} D_{nk} b_{nk},$$

where $D_{nk} > 0$ is given by (4), and

$$b_{nk} = \int_0^\pi \theta^\alpha \sin(n+2k+1)\theta \sin \theta d\theta, \quad k = 0, 1, \dots$$

First, the proof of $\sum_n b_n < \infty$ can be followed along the same lines with those for the spherical covariance function with $D_{nk} \leq \frac{C_1}{\sqrt{k}\sqrt{n+k}}$, for large n and k . Therefore, to prove the validity of $C(\theta)$, it is sufficient to show that $b_n \geq 0$, or in turn, that $b_{nk} \leq 0$ for all $k \geq 0$.

Now for any $n \geq 1, k \geq 0$, by the trigonometry identity and integration by parts,

$$\begin{aligned} 2b_{nk} &= \int_0^\pi \theta^\alpha \cos(n+2k)\theta d\theta - \int_0^\pi \theta^\alpha \cos(n+2k+2)\theta d\theta \\ &= \frac{1}{(n+2k)^{\alpha+1}} \int_0^{(n+2k)\pi} \theta^\alpha \cos \theta d\theta \\ &\quad - \frac{1}{(n+2k+2)^{\alpha+1}} \int_0^{(n+2k+2)\pi} \theta^\alpha \cos \theta d\theta \\ &= -\alpha \left(\frac{1}{(n+2k)^{\alpha+1}} - \frac{1}{(n+2k+2)^{\alpha+1}} \right) \int_0^{(n+2k)\pi} \theta^{\alpha-1} \sin \theta d\theta \\ &\quad + \alpha \left(\frac{1}{(n+2k+2)^{\alpha+1}} \right) \int_{(n+2k)\pi}^{(n+2k+2)\pi} \theta^{\alpha-1} \sin \theta d\theta. \end{aligned} \quad (9)$$

From Lemma 1, the first term in (9) is non-positive for any $n \geq 1, k \geq 0$. To prove that the second term is non-positive, we explore the cases of $n+2k$ being odd or even.

When $n + 2k$ is odd, by substitution $u = \theta - (n + 2k)\pi$, the integral of second term in (9) becomes

$$\int_{(n+2k)\pi}^{(n+2k+2)\pi} \theta^{\alpha-1} \sin \theta \, d\theta = - \int_0^{2\pi} (u + (n + 2k)\pi)^{\alpha-1} \sin(u) \, du < 0,$$

implying that $bnk < 0$ by Lemma 1.

When $n+2k = 2m$ is an even number for some $m \geq 1$, substituting $n+2k+2 = 2m+2$ and $n+2k = 2m$ into (9), we have

$$\begin{aligned} 2b_{nk} &= - \left(\frac{\alpha}{(2m)^{\alpha+1}} - \frac{\alpha}{(2m+2)^{\alpha+1}} \right) \sum_{j=0}^{m-1} \int_{2j\pi}^{(2j+2)\pi} \theta^{\alpha-1} \sin \theta \, d\theta \\ &\quad + \int_{2m\pi}^{(2m+2)\pi} \frac{\alpha \theta^{\alpha-1} \sin \theta \, d\theta}{(2m+2)^{\alpha+1}} \\ &= - \left(\frac{\alpha}{(2m)^{\alpha+1}} - \frac{\alpha}{(2m+2)^{\alpha+1}} \right) \sum_{j=0}^{m-1} \int_0^{2\pi} (\theta + 2j\pi)^{\alpha-1} \sin \theta \, d\theta \\ &\quad + \int_0^{2\pi} \frac{\alpha(\theta + 2m\pi)^{\alpha-1} \sin \theta \, d\theta}{(2m+2)^{\alpha+1}} \\ &= -\alpha \int_0^{2\pi} \left\{ \left(\frac{1}{(2m)^{\alpha+1}} - \frac{1}{(2m+2)^{\alpha+1}} \right) \sum_{j=0}^{m-1} (\theta + 2j\pi)^{\alpha-1} \right. \\ &\quad \left. - \frac{(\theta + 2m\pi)^{\alpha-1}}{(2m+2)^{\alpha+1}} \right\} \sin \theta \, d\theta \\ &= -\alpha \int_0^{2\pi} g(\theta) \sin \theta \, d\theta, \end{aligned}$$

where

$$\begin{aligned} g(\theta) &= \left(\frac{1}{(2m)^{\alpha+1}} - \frac{1}{(2m+2)^{\alpha+1}} \right) \sum_{j=0}^{m-1} (\theta + 2j\pi)^{\alpha-1} \\ &\quad - \frac{1}{(2m+2)^{\alpha+1}} (\theta + 2m\pi)^{\alpha-1}, \quad 0 < \theta < 2\pi. \end{aligned}$$

From Lemma 1, to prove $bnk < 0$ and hence conclude the whole proof, it is now sufficient to show that $g(\theta)$ is non-negative and non-increasing.

To show that $g(\theta) \geq 0$, we recall that for $0 < \alpha < 1$, $\theta^{\alpha-1}$ is a decreasing function

$$\begin{aligned}
g(\theta) &\geq \left(\frac{1}{(2m)^{\alpha+1}} - \frac{1}{(2m+2)^{\alpha+1}} \right) \sum_{j=0}^{m-1} (\theta + 2m\pi)^{\alpha-1} \\
&\quad - \frac{1}{(2m+2)^{\alpha+1}} (\theta + 2m\pi)^{\alpha-1} \\
&= \left(\frac{m}{(2m)^{\alpha+1}} - \frac{m+1}{(2m+2)^{\alpha+1}} \right) (\theta + 2m\pi)^{\alpha-1} \geq 0.
\end{aligned}$$

To show that $g(\theta)$ is non-increasing, we take the first derivative of $g(\theta)$ with respect to θ , and note that $\alpha - 1 < 0$

$$\begin{aligned}
\frac{dg(\theta)}{d\theta} &= (\alpha - 1) \left\{ \left(\frac{1}{(2m)^{\alpha+1}} - \frac{1}{(2m+2)^{\alpha+1}} \right) \sum_{j=0}^{m-1} (\theta + 2j\pi)^{\alpha-2} \right. \\
&\quad \left. - \frac{1}{(2m+2)^{\alpha+1}} (\theta + 2m\pi)^{\alpha-2} \right\} \\
&\leq (\alpha - 1) \left\{ \left(\frac{1}{(2m)^{\alpha+1}} - \frac{1}{(2m+2)^{\alpha+1}} \right) \sum_{j=0}^{m-1} (\theta + 2m\pi)^{\alpha-2} \right. \\
&\quad \left. - \frac{1}{(2m+2)^{\alpha+1}} (\theta + 2m\pi)^{\alpha-2} \right\} \\
&= \frac{\alpha - 1}{2^{\alpha+1}} \left(\frac{1}{m^\alpha} - \frac{1}{(m+1)^\alpha} \right) (\theta + 2m\pi)^{\alpha-2} \leq 0.
\end{aligned}$$

Therefore, $g(\theta)$ is non-increasing, concluding the proof.

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