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Reduction problems and deformation approaches to nonstationary covariance functions over spheres

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Abstract: The paper considers reduction problems and deformation approaches for nonstationary covariance functions on the $(d-1)$-dimensional spheres, $\mathbb{S}^{d-1}$, embedded in the d-dimensional Euclidean space. Given a covariance function C on $\mathbb{S}^{d-1}$, we chase a pair (R, Ψ), for a function $R : [-1, +1] \to \mathbb{R}$ and a smooth bijection Ψ, such that C can be reduced to a geodesically isotropic one: $C(\mathbf{x}, \mathbf{y}) = R(\langle \Psi(\mathbf{x}), \Psi(\mathbf{y}) \rangle)$, with $\langle \cdot, \cdot \rangle$ denoting the dot product.

The problem finds motivation in recent statistical literature devoted to the analysis of global phenomena, defined typically over the sphere of $\mathbb{R}^3$. The application domains considered in the manuscript makes the problem mathematically challenging. We show the uniqueness of the representation in the reduction problem. Then, under some regularity assumptions, we provide an inversion formula to recover the bijection Ψ, when it exists, for a given C. We also give sufficient conditions for reducibility.

Keywords and phrases: Covariance function, nonstationarity, reducibility problem, spheres.

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1. Introduction and statement of the problem

Positive definite functions are fundamental to mathematics, probability and statistics. Their use has become ubiquitous in many areas of applied sciences, and we refer the reader to Porcu et al. (2018) and Porcu et al. (2019) for recent overviews as well as for collections of open problems and statistical implications.

Recently, the advent of massive data sets distributed over the whole planet Earth has motivated several scientists to study modeling strategies for random fields defined over the sphere of $\mathbb{R}^3$ representing our planet. The natural metric on the sphere is the geodesic or great circle distance, which defines the length of the shortest arc joining any pair of points located over the sphere. The increasing interest in modeling stochastic processes over spheres or spheres cross time with an explicit covariance function is reflected in works in areas as diverse as mathematical analysis, spatial and space-time statistics, and we refer the reader to the recent reviews by Gneiting (2013), Jeong et al. (2017), Porcu et al. (2018) and Porcu et al. (2019) for a comprehensive account.

We recall that, for a non empty set X, a mapping $C : X \times X \to \mathbb{R}$ is called positive definite if, for any N-dimensional collection $\{a_i\}_{i=1}^N \subset \mathbb{R}$ and points $\{\boldsymbol{x}_i\}_{i=1}^N \subset X$, we have

$$\sum_{i=1}^{N} \sum_{j=1}^{N} a_i C(\boldsymbol{x}_i, \boldsymbol{x}_j) a_j \geq 0.$$

A well known fact is that $C : X \times X \to \mathbb{R}$ is a positive definite function if and only if C is the covariance function of a Gaussian random field Z on X.

This paper considers essentially the case $X = \mathbb{S}^{d-1} = \{\boldsymbol{x} \in \mathbb{R}^d \ : \ |\boldsymbol{x}| = 1\}$, that is, the unit sphere of $\mathbb{R}^d$ and where $|\cdot|$ is the Euclidean distance. Covariance functions on d-dimensional spheres are denoted C throughout. The covariance function $C : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R}$ is called geodesically isotropic (Porcu et al., 2018) if there exists a function $R : [-1, +1] \to \mathbb{R}$ such that

$$C(\boldsymbol{x}, \boldsymbol{y}) = R(\langle \boldsymbol{x}, \boldsymbol{y} \rangle), \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{S}^{d-1}, \tag{1.1}$$

where $\langle \cdot, \cdot \rangle$ denotes the dot product in $\mathbb{R}^d$. In view of the geodesic isotropy assumption, the function C in (1.1) depends exclusively on the geodesic (great circle) distance $d_{\mathrm{GC}}(\boldsymbol{x}, \boldsymbol{y}) = \mathrm{angle}[\boldsymbol{x}, \boldsymbol{y}] \in [0, \pi]$ between points. Thus, we have $C(\boldsymbol{x}, \boldsymbol{y}) = R\big(\cos(d_{\mathrm{GC}}(\boldsymbol{x}, \boldsymbol{y}))\big)$.

Characterization of covariance functions being geodesically isotropic on $\mathbb{S}^{d-1}$ has been available thanks to Schoenberg (1942). Recently, covariance functions became popular after the essays by Gneiting (2013) and Berg and Porcu (2017). Characterization of covariances of the type (1.1) has been proposed by Pinkus (2004) and the reader is referred to Menegatto (1994) and Guella and Menegatto (2016) for deep results in this direction. The following result of Schoenberg (1942) will illustrate some of our findings.

If C is geodesically isotropic on $\mathbb{S}^{d-1}$, then the function R in (1.1) admits the representation

$$R(u) = \sum_{n=0}^{\infty} b_{n,d-1} \frac{P_n^{(d-1)/2}(u)}{P_n^{(d-1)/2}(1)}, \qquad u \in [-1, +1], \tag{1.2}$$

where P_n^{λ} are the n-th Gegenbauer polynomials of order $\lambda \geq 0$, and $\{b_{n,d-1}\}_{n=0}^{\infty}$ is a sequence of nonnegative coefficients that additionally satisfy $\sum_{n=0}^{\infty} b_{n,d-1} = \sigma^2 < \infty$.

1.1. Motivation and statement of the problem

Recent applications regarding space or space-time data over the whole planet Earth have shown how global data typically exhibit nonstationarities over space, time, or both. This fact has been argued by several authors, and we refer the reader to Cressie et al. (2010); Kang et al. (2010); Castruccio and Guinness (2017) and Nguyen et al. (2014).

For random fields defined over small portions of the sphere and projected on the plane, the problem was noted by Sampson and Guttorp (1992), who suggested a space deformation approach: finding a pair (R, Φ), with R being a stationary covariance and Φ a bijection, such that a nonstationary covariance defined in $\mathbb{R}^d \times \mathbb{R}^d$ can be transformed into a stationary one. Solutions to this problem have been provided by Perrin and Senoussi (1999), Perrin and Senoussi (2000) and Genton and Perrin (2004). Thus, it becomes natural to adapt this problem to the case where the nonstationary covariance is defined over $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$. We state this formally for the convenience of the reader.

Problem 1. *Let $C : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R}$ be a differentiable covariance function. Chase, whenever it exists, a pair (R, Ψ), with a differentiable mapping $R : [-1, +1] \to \mathbb{R}$, and a diffeomorphism Ψ, such that*

$$C(\boldsymbol{x}, \boldsymbol{y}) = R\left(\langle \Psi(\boldsymbol{x}), \Psi(\boldsymbol{y})\rangle\right), \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{S}^{d-1}. \tag{1.3}$$

The covariance functions $C : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R}$ satisfying (1.3) for some pair (R, Φ) are called geodesically isotropic reducible thrughout. Apparenty, the geodesically isotropic case defined in Equation (1.1) is attained under the special case $\Psi = \mathbf{I}_d$, with $\mathbf{I}_d$ being the identity mapping. A collection of facts makes Problem 1 difficult. First, the set of positive definite functions on spheres is too large to be investigated if no regularity and/or smoothness conditions are assumed. Yet, even under such conditions, differential calculus on manifolds, such as spheres, is somewhat tricky.

Problem 1 can be simplified by consider an analogue within a more convenient domain extension: for any $\varepsilon \geq 0$, let us define the ε-extension of the sphere $\mathbb{S}^{d-1}$ by

$$\mathcal{D}^{\varepsilon} = \{\boldsymbol{x} \in \mathbb{R}^d \ : |\boldsymbol{x}| > \varepsilon\}. \tag{1.4}$$

Note that $\mathcal{D}^0 = \mathbb{R}^d_*$, the punctured space. Next, we call a positive definite function C^{ε}, defined on the product space $\mathcal{D}^{\varepsilon} \times \mathcal{D}^{\varepsilon}$, geodesically isotropic if there exists a mapping $R^{\varepsilon} : \mathbb{R} \to \mathbb{R}$ such that

$$C^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y}) = R^{\varepsilon}(\langle \boldsymbol{x}, \boldsymbol{y}\rangle) \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^{\varepsilon}.$$

This paper shows that solutions to a reducibility problem for covariance functions C^{ε} defined over $\mathcal{D}^{\varepsilon} \times \mathcal{D}^{\varepsilon}$ provide solutions to Problem 1. Clearly this implies that the functions C and C^{ε} must be related, and this fact is carefully explained in Section 3.

The rest of this section is devoted to two examples illustrating how nonstationarity can arise from some simple parametric spatial deformations. Section 2 provides the necessary mathematical background as well as some auxiliary results. Section 3 contains our main results, related to recovering all solutions to Problem 1 from the covariance function itself when it is geodesically isotropic reducible. Some examples will illustrate our findings. Section 4 provides sufficient conditions to the solution of Problem 1.

1.2. Examples of isotropic fields undergoing parametric deformations

We introduce a simple family of functions allowing for sphere deformations, specifically to model locations and forms of dilation/contraction at punctual nodes (*e.g.*, poles) and/or lines (*e.g.*, latitudes, longitudes) on the sphere surfaces.

Let $F_{\alpha,\beta}$ denote the beta probability distribution, defined as $F_{\alpha,\beta}(t) = \frac{1}{B(\alpha,\beta)}\int_0^t s^{\alpha-1}(1-s)^{\beta-1}\mathrm{d}s$, $t \in [0,1]$ for α and β being strictly positive. Let us define a smooth bijection of the interval $[-1,1]$ as follows (see the top-left graph of Figure 1):

$$\tilde{F}_{\alpha,\beta}(t) = \begin{cases} -F_{\alpha,\beta}(-t) & \text{if} \quad t \in \quad [-1,0], \\ F_{\alpha,\beta}(t) & \text{if} \quad t \in \quad (0,1]. \end{cases} \tag{1.5}$$

1.2.1. The case of the circle

Using the parametric representation $t \mapsto \boldsymbol{u}(t) = (\cos(\pi t), \sin(\pi t))^\top$, $t \in [-1,1)$ of $\mathbb{S}^1$, with $\top$ denoting transpose, we consider the transform $\boldsymbol{x} = \Psi^{-1}(\boldsymbol{u})$ given by the following parameterization (see top-right of Figure 1)

$$t \mapsto \boldsymbol{x}(t) = \boldsymbol{u}(\tilde{F}_{\alpha,\beta}(t)), \; t \in [-1,1), \tag{1.6}$$

so that the deformation can be written as $\Psi(\boldsymbol{x}(t)) = \boldsymbol{x}(\tilde{F}^{-1}_{\alpha,\beta}(t))$.

Regarding the choice of a geodesically isotropic covariance function on the circle, we make use of a truncated version of Schoenberg representation (Schoenberg, 1938), to define the covariance function:

$$R(u) = b_0 + b_1\cos(\pi u) + b_4\cos(4\pi u) + b_9\cos(9\pi u) + b_{50}\cos(50\pi u), \; u \in [-1,1]. \tag{1.7}$$

Figure 1 shows a simulated path of a geodesically isotropic Gaussian random field $Z(\boldsymbol{u}(t))$ on $\mathbb{S}^1$ and the same realization undergoing a spatial dilation at point $t = \pm 1$ and a contraction at the opposite point ($t = 0$), that is the path of $Z(\boldsymbol{x}(t))$.

1.2.2. The case of the sphere $\mathbb{S}^2$

We now propose a more elaborated transformation that intermingles coordinates, using a parameter change for the classical spherical coordinates:

$$(t_1,t_2) \mapsto \boldsymbol{u}^\top(t_1,t_2) = (\cos(2\pi t_1)\cos(\pi t_2), \sin(2\pi t_1)\cos(\pi t_2), \sin(\pi t_2)),$$

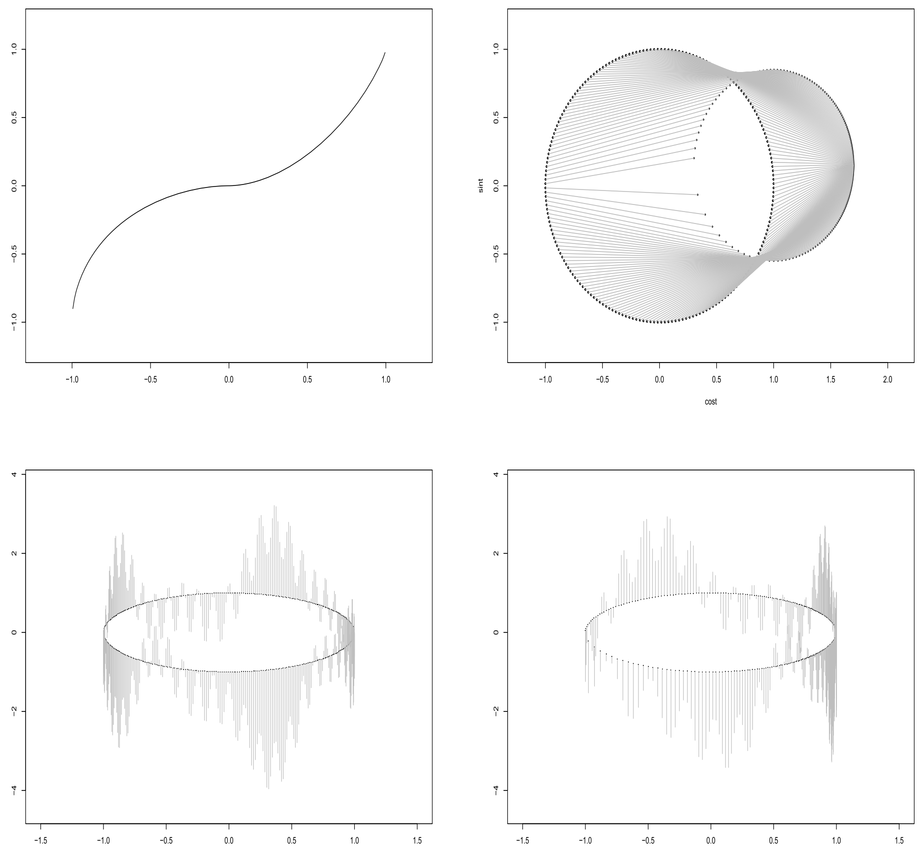

FIG 1. *Random field on the circle. Top-left: graph of the coordinate change* $\tilde{F}_{\alpha,\beta}$ *according to Equation (1.5) with* $\alpha = 3,\ \beta = 1$. *Right: representation of the corresponding circle bijection. Bottom-left: a path of a Gaussian geodesically isotropic field* $Z(\boldsymbol{u}(t))$ *with covariance function (1.7) defined by the coefficients* $b_0 = b_1 = b_4 = b_9 = b_{50} = 0.2$. *Right: The same path undergoing the space deformation* Ψ *given by Equation (1.6), that is the path of* $Z(\boldsymbol{x}(t))$ *transform.*

where $t_1, t_2 \in [-1, 1]$. To define the $\mathbb{S}^2$ deformation $\boldsymbol{x} = \Psi^{-1}(\boldsymbol{u})$, we first transform each coordinate t_i independently through the function $\tilde{F}_{\alpha_i,\beta_i}(t_i)$ in Equation (1.5), $i = 1, 2$ and then intermingle them via the following bijection (see top of Figure 2):

$$\begin{aligned}
\theta_1(t_1, t_2) &= \left(\tilde{F}_{\alpha_1,\beta_1}(t_1) + 1\right)\left(1 - \tfrac{(1-\tilde{F}_{\alpha_2,\beta_2}(t_2))\sqrt{1-\tilde{F}_{\alpha_1,\beta_1}(t_1))}}{2\sqrt{2}}\right) - 1,\\
\theta_2(t_1, t_2) &= \left(\tilde{F}_{\alpha_2,\beta_2}(t_2) + 1\right)\left(1 - \tfrac{(1-\tilde{F}_{\alpha_1,\beta_1}(t_1))\sqrt{1-\tilde{F}_{\alpha_2,\beta_2}(t_2)}}{2\sqrt{2}}\right) - 1.
\end{aligned} \tag{1.8}$$

Rephrased, Ψ^{-1} is obtained via the parameterization

$$(t_1, t_2) \mapsto \boldsymbol{x}^\top(t_1, t_2) = \Psi^{-1}(\boldsymbol{u}(t_1, t_2)) = \boldsymbol{u}^\top(\theta_1(t_1, t_2), \theta_2(t_1, t_2)). \tag{1.9}$$

To build a geodesically isotropic covariance function on $\mathbb{S}^2$, we invoke again a truncated version of Schoenberg representation for $d = 3$ (Schoenberg, 1938), choosing precisely the first four Legendre polynomials

$$R(u) = b_0 + b_1 u + b_2(3u^2 - 1)/2 + b_3(5u^3 - 3u)/2, \quad u \in [-1, 1], \tag{1.10}$$

with constraints $b_j \geq 0, j = 0, \ldots, 3$ and $\sum_0^3 b_j = 1$. The bottom-left of Figure 2 shows a sample path of a geodesically isotropic Gaussian field $Z(\boldsymbol{u}(t_1, t_2))$ on $\mathbb{S}^2$ and on the right, the same realization after the spatial deformation, that is a path realization of $Z(\boldsymbol{x}(t_1, t_2))$.

2. Notations and auxiliary results

2.1. Adapting differential tools to $\mathbb{S}^{d-1}$

We start with some notations concerning matrix and differential calculus. Let d be a positive integer. For a $d \times d$ matrix Γ we denote its jth row vector by $\Gamma_{j,\bullet}$ and its jth column vector by $\Gamma_{\bullet,j},\ j = 1, \ldots, d$.

A vector $\boldsymbol{x} = (x_1, \ldots, x_d)^\top$ of $\mathbb{R}^d$ is always assumed to be a column vector. In particular, $\boldsymbol{e}_j,\ j = 1, \ldots, d$ denotes the unit column vectors of a standard basis of $\mathbb{R}^d$. We equivalently use $\langle \boldsymbol{x}, \boldsymbol{y} \rangle$ or $\boldsymbol{x}^\top \boldsymbol{y}$ for the dot product. The differential (or gradient) of a real valued function $F : \mathcal{D} \to \mathbb{R}$, where $\mathcal{D}$ is an open domain of $\mathbb{R}^d$, is always assumed to be the row vector $D_{\boldsymbol{x}} F = (\partial_{x_1} F, \ldots, \partial_{x_d} F)$. For a univariate function R, the differential is denoted R'. For a differentiable real-valued function $G : \mathcal{D} \times \mathcal{D} \to \mathbb{R}$, the same row notations will hold for partial differentials:

$$DG(\boldsymbol{x}, \boldsymbol{y}) = D_{(\boldsymbol{x},\boldsymbol{y})} G(\boldsymbol{x}, \boldsymbol{y}) = (D_{\boldsymbol{x}} G(\boldsymbol{x}, \boldsymbol{y}), D_{\boldsymbol{y}} G(\boldsymbol{x}, \boldsymbol{y})), \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}.$$

Consistently, differentials are considered as linear forms, *e.g.*, for $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^d$,

$$DG(\boldsymbol{x}, \boldsymbol{y})(\boldsymbol{u}, \boldsymbol{v}) := D_{\boldsymbol{x}} G(\boldsymbol{x}, \boldsymbol{y})\, \boldsymbol{u} + D_{\boldsymbol{y}} G(\boldsymbol{x}, \boldsymbol{y})\, \boldsymbol{v}.$$

For a transformation $\Phi = (\phi_1, \ldots, \phi_d)^\top : \mathcal{D} \subset \mathbb{R}^d \to \mathbb{R}^d$, we will make large use of the following notations related to its Jacobian matrix $J_\Phi = [\partial_{x_j} \phi_i]_{i,j}(\boldsymbol{x})$, as well as to the inner product and projectors associated to Φ: *i.e.*, for $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}$,

$$\beta_\Phi(\boldsymbol{x}, \boldsymbol{y}) = \frac{\Phi^\top(\boldsymbol{x}) \Phi(\boldsymbol{y})}{|\Phi(\boldsymbol{x})||\Phi(\boldsymbol{y})|}, \qquad \text{and} \qquad P_{\Phi(\boldsymbol{x})} = \frac{\Phi(\boldsymbol{x}) \Phi^\top(\boldsymbol{x})}{|\Phi(\boldsymbol{x})||\Phi(\boldsymbol{x})|},$$

where $|\cdot|$ denotes the Euclidean norm.

When Φ is the identity function $\mathbf{I}_d$, we simply write $\beta(\boldsymbol{x}, \boldsymbol{y})$ and $P_{\boldsymbol{x}}$.

In this paper, the domain $\mathcal{D} \subset \mathbb{R}^d$ refers almost always to the ε-extension (1.4) of $\mathbb{S}^{d-1}$. The result below will be largely used in the sequel to convert differential calculus on spheres into calculus on $\mathbb{R}^d$.

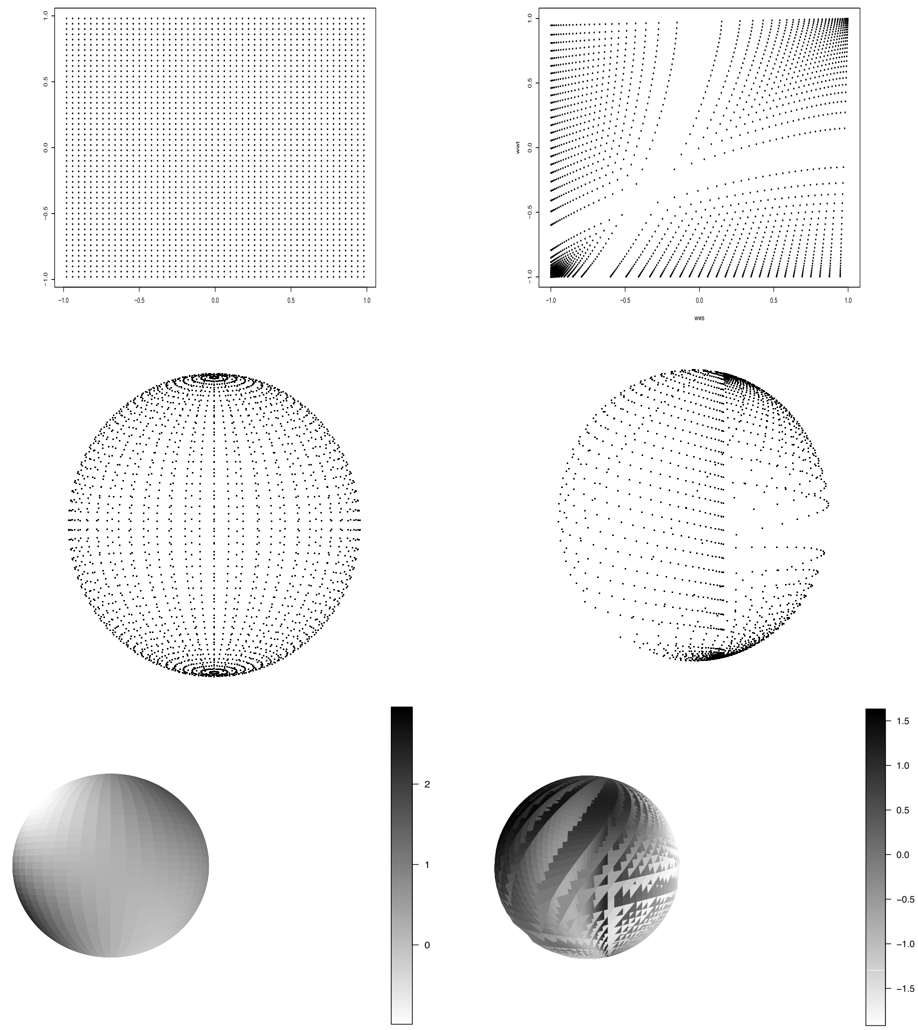

Fig 2. *Random fields on the unit sphere. Top-left: uniform grid of the square used for usual spherical coordinates. Right: the same square undergoing deformation $\theta(t_1, t_2)$ described by Equation (1.8) with parameters $\alpha_1 = 0.55, \beta_1 = 0.55, \alpha_2 = 1.5, \beta_2 = 1.5$. Middle: points of the sphere corresponding to the respective previous square grids on the top line. Bottom-left: a simulation of a geodesically isotropic Gaussian field $Z(\mathbf{u}(t_1, t_2))$ on $\mathbb{S}^2$, according to covariance function (1.10) with parameters $b_0 = 0.2, b_1 = 0.3, b_2 = 0.3, b_3 = 0.2$. Right: The same realization undergoing spatial deformation Ψ given by (1.9), that is the realization of $Z(\boldsymbol{x}(t_1, t_2))$.*

Proposition 1. *Let $\Phi : \mathcal{D}^{\varepsilon} \to \mathbb{R}^d$ be differentiable. Then,*

$$D_{\boldsymbol{x}} \beta_{\Phi}(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{|\Phi(\boldsymbol{x})|} \frac{\Phi^{\top}(\boldsymbol{y})}{|\Phi(\boldsymbol{y})|} \Big(\boldsymbol{I}_d - P_{\Phi(\boldsymbol{x})} \Big) J_{\Phi}(\boldsymbol{x}).$$

In particular, for Φ being the identity mapping, we have

$$D_{\boldsymbol{x}}\beta(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{|\boldsymbol{x}|}\frac{\boldsymbol{y}^\top}{|\boldsymbol{y}|}\Big(\boldsymbol{I}_d - P_{\boldsymbol{x}}\Big). \tag{2.1}$$

Proof. Apply the differential rules to the following function composition chain $(\boldsymbol{x},\boldsymbol{y}) \longmapsto (\boldsymbol{u} = \Phi(\boldsymbol{x}), \boldsymbol{v} = \Phi(\boldsymbol{y})) \longmapsto (\boldsymbol{w} = \boldsymbol{u}/|\boldsymbol{u}|, \boldsymbol{z} = \boldsymbol{v}/|\boldsymbol{v}|) \longmapsto \boldsymbol{w}^\top\boldsymbol{z}$, to obtain the corresponding results. □

2.2. Suitable diffeomorphism extensions

Let $\Psi : \mathbb{S}^{d-1} \to \mathbb{S}^{d-1}$ be a bijective and continuously differentiable deformation (*i.e.*, a manifold diffeomorphism) with differential (also termed Jacobian) $J_\Psi(\boldsymbol{x})$ acting on the tangent space at point $\boldsymbol{x}$. Clearly, Ψ^{-1} is also a diffeomorphism, with Jacobian $J_{\Psi^{-1}}$ satisfying $J_{\Psi^{-1}}(\boldsymbol{y}) = (J_\Psi(\boldsymbol{x}))^{-1} = J_\Psi^{-1}(\boldsymbol{x})$, where $\boldsymbol{x} = \Psi^{-1}(\boldsymbol{y})$.

There exist many ways of extending Ψ to domains of $\mathbb{R}^d$ containing $\mathbb{S}^{d-1}$. For our purpose, we can however restrict to domains $\mathcal{D}^\varepsilon$, $\varepsilon > 0$ and we consider candidates Φ extending the diffeomorphic mapping Ψ to $\mathcal{D}^\varepsilon$ in the following form

$$\Psi_\alpha^\varepsilon(\boldsymbol{x}) = |\boldsymbol{x}|^\alpha \Psi\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right), \ \alpha \geq 0. \tag{2.2}$$

A differentiable mapping $\Phi : \mathcal{D} \subset \mathbb{R}^d \to \mathbb{R}^d,\ \alpha \geq 0$, is called positively homogeneous of order α if $\Phi(\lambda\boldsymbol{x}) = \lambda^\alpha\Phi(\boldsymbol{x})$, for $\lambda \geq 0$ and such that $\boldsymbol{x}, \lambda\boldsymbol{x} \in \mathcal{D}$. Lemma 3 in Appendix B asserts that the condition

$$J_\Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{x}) = \alpha\boldsymbol{x}/|\boldsymbol{x}|^{2(1-\alpha)}$$

is necessary and sufficient to preserve norms and thus leaves spheres invariant.

Lemma 3 explains why caution is needed when differential calculus concerns space transformations of manifolds, such as $\mathbb{S}^{d-1}$, since transformations of $\mathbb{R}^d$ that coincide on $\mathbb{S}^{d-1}$ may have very different Jacobians on $\mathbb{S}^{d-1}$. For example, even if the common restriction of Ψ over $\mathbb{S}^{d-1}$ is a diffeomorphism, $J_{\Psi_0^\varepsilon}(\boldsymbol{x})$ is everywhere singular on $\mathbb{S}^{d-1}$ whereas $J_{\Psi_1^\varepsilon}(\boldsymbol{x})$ is not.

Finally, as the differential calculus simplifies a bit with $\alpha = 1$, when referring to a diffeomorphism extension $\Phi = (\phi_1, \ldots, \phi_d)^\top$, we imply throughout

$$\Phi = \Psi_1^\varepsilon. \tag{2.3}$$

2.3. Orthogonal matrices

Some facts about the dot product operation $\boldsymbol{x}^\top\boldsymbol{y}$ in Euclidean space $\mathbb{R}^d$ are now needed. The dot product is not invariant under general space transformations. Actually, the unique set of transformations leaving the dot product invariant is the so-called orthogonal group within linear transformations. Let us recall the definition of orthogonal transformations while leaving to Appendix A their full characterization within the context of complex spaces $\mathbb{C}^d$ as well as examples.

An orthogonal transformation Φ is given via an invertible real valued matrix O such that $O^\top = O^{-1}$, and $\Phi(\boldsymbol{x}) = O\boldsymbol{x}$, so that $\Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{y}) = \boldsymbol{x}^\top\boldsymbol{y}$. The mostly used orthogonal transformations are rotations but other types, such as reflexions, are namely available. In this context we say that an invertible $d \times d$ matrix Γ is uniquely defined up to orthogonality if there exist an invertible matrix $d \times d$ matrix Γ_0, and an orthogonal matrix O, such that $\Gamma = O\Gamma_0$.

3. Restatement of Problem 1 within the space $\mathcal{D}^\varepsilon$

3.1. Extending C to $\mathcal{D}^\varepsilon$

Let $C : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{C}$ be positive definite. C can be used as a building block to construct positive definite functions over $\mathcal{D}^\varepsilon \times \mathcal{D}^\varepsilon$. For example,

$$C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = C\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}, \frac{\boldsymbol{y}}{|\boldsymbol{y}|}\right), \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon, \tag{3.1}$$

coincides with C on $\mathbb{S}^{d-1}$ and is clearly positive definite on $\mathcal{D}^\varepsilon \times \mathcal{D}^\varepsilon$. This extension has a straightforward interpretation in terms of any underlying random field $Z = \{Z(\boldsymbol{x}),\ \boldsymbol{x} \in \mathbb{S}^{d-1}\}$ with covariance function C. Indeed, direct inspection shows that the random field extension

$$Z^\varepsilon(\boldsymbol{x}) = Z\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right), \qquad \boldsymbol{x} \in \mathcal{D}^\varepsilon,$$

has covariance function C^ε.

A wealth of examples can be obtained. For instance, take a positive definite function $\widetilde{C}(\cdot,\cdot)$ on $\mathbb{R}_+ \times \mathbb{R}_+$ satisfying $\widetilde{C}(x,x) = 1$, and define the product kernel $C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = C\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}, \frac{\boldsymbol{y}}{|\boldsymbol{y}|}\right)\widetilde{C}(|\boldsymbol{x}|, |\boldsymbol{y}|)$. This model can also be physically related to another extension of the underlying random field Z on $\mathbb{S}^{d-1}$ by considering the product

$$Z^\varepsilon(\boldsymbol{x}) := Z\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right)\widetilde{Z}(|\boldsymbol{x}|), \qquad \boldsymbol{x} \in \mathcal{D}^\varepsilon,$$

where $\widetilde{Z}$ is any independent Gaussian field defined over $\mathbb{R}_+$ with covariance function $\widetilde{C}$.

Actually, Extension (3.1) (*i.e.*, constant on radii) is sufficient for our concern. The following technical result allows to takle properly the initial Problem 1 by working on $\mathcal{D}^\varepsilon$.

Proposition 2. *Let $C : \mathbb{S}^{d-1} \times \mathbb{S}^{d-1} \to \mathbb{R}$ be differentiable. Then,*

$$C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = C\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}, \frac{\boldsymbol{y}}{|\boldsymbol{y}|}\right), \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon,$$

if and only if

$$D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{x} = 0 \qquad \text{and} \qquad D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{y} = 0, \qquad \forall \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon.$$

The proof of Proposition 2 is a direct consequence of the following lemma.

Lemma 1. *Let F be a differentiable scalar function on $\mathcal{D}^\varepsilon$. Then,*

$$F(\boldsymbol{x}) = F\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right) \qquad \text{if and only if} \qquad D_{\boldsymbol{x}} F(\boldsymbol{x})\boldsymbol{x} = 0.$$

Proof. ($\Rightarrow$) We first note that

$$\partial_{x_j}\left(\frac{x_l}{|\boldsymbol{x}|}\right) = \frac{1}{|\boldsymbol{x}|}\left(\delta_{jl} - \frac{x_j x_l}{|\boldsymbol{x}|^2}\right),$$

with δ_{jl} denoting the Kronecker delta. Thus, $D_{\boldsymbol{x}} F(\boldsymbol{x}) = (1/|\boldsymbol{x}|) D_{\boldsymbol{x}} F(\boldsymbol{x}/|\boldsymbol{x}|) \times (\boldsymbol{I}_d - P_{\boldsymbol{x}})$. We thus get

$$(\boldsymbol{I}_d - P_{\boldsymbol{x}})\,\boldsymbol{x} = 0, \qquad \boldsymbol{x} \in \mathcal{D}^\varepsilon.$$

($\Leftarrow$) Consider the spherical coordinate system $\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{u})$, $\boldsymbol{u}(r, \theta_1, \ldots, \theta_{d-1})$ and define the function $\widetilde{F}(\boldsymbol{u}) = F(\boldsymbol{x}(\boldsymbol{u}))$. Differentiation with respect to the radius r gives $\partial_r x_l(\boldsymbol{u}) = x_l/r$. Thus, we get

$$\partial_r \widetilde{F} = \sum_l F(\boldsymbol{x}(\boldsymbol{u}))\partial_r x_l(\boldsymbol{u}) = \frac{1}{r} D_{\boldsymbol{x}} F(\boldsymbol{x}(\boldsymbol{u}))\boldsymbol{x}(\boldsymbol{u}) = 0.$$

The last equality implies that F does not depend on the radius r. The proof is completed. ◻

3.2. Rephrasing Problem 1 within the domain $\mathcal{D}^\varepsilon$

Problem 2. *Let $C^\varepsilon : \mathcal{D}^\varepsilon \times \mathcal{D}^\varepsilon \to \mathbb{R}$ be a differentiable covariance function that satisfies*

$$D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{x} = 0 \qquad \text{or} \qquad D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{y} = 0, \qquad \forall \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon.$$

Chase, if it exists, a pair (R, Φ), with Φ a diffeomorphism on $\mathcal{D}^\varepsilon$ satisfying

$$J_\Phi(\boldsymbol{x})\boldsymbol{x} = \Phi(\boldsymbol{x}) \quad \text{and} \quad J_\Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{x}) = \boldsymbol{x}, \qquad \boldsymbol{x} \in \mathcal{D}^\varepsilon,$$

and R a differentiable function on $[-1, +1]$ such that

$$C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = R\left(\beta_\Phi(\boldsymbol{x}, \boldsymbol{y})\right), \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon. \tag{3.2}$$

Proposition 3. *A solution (R, Ψ) to C in $\mathbb{S}^{d-1}$* (Problem 1) *exists if and only if a solution (R, Φ) to C^ε exists in $\mathcal{D}^\varepsilon$* (Problem 2).

Proof. ($\Rightarrow$) Taking the extensions $\Phi = \Psi_1^\varepsilon$ and C^ε of Ψ and C respectively defined by Equations (2.3) and (3.1), we get, for any $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon$,

$$\begin{aligned} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) &= C\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}, \frac{\boldsymbol{y}}{|\boldsymbol{y}|}\right) = R\left(\Psi^\top\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right)\Psi\left(\frac{\boldsymbol{y}}{|\boldsymbol{y}|}\right)\right) = R\left(\frac{\Phi^\top(\boldsymbol{x})}{|\boldsymbol{x}|}\frac{\Phi(\boldsymbol{y})}{|\boldsymbol{y}|}\right) \\ &= R\left(\frac{\Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{y})}{|\Phi(\boldsymbol{x})||\Phi(\boldsymbol{y})|}\right). \end{aligned}$$

($\Leftarrow$) Equation (3.2) clearly reduces to Equation (1.3) when $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{S}^{d-1}$. ◻

3.3. Uniqueness of the solution $(\boldsymbol{R}, \boldsymbol{\Phi})$

We first turn to the problem of uniqueness in the representation (3.2). Provided such a pair (R, Φ) exists, is it unique? Apparently, the answer is not: if the pair (R, Φ) is a solution to Problem 2, then any orthogonal matrix O will provide a new distinct solution $(R, O\Phi)$, since orthogonal matrices preserve norms and inner products. Consequently, if some uniqueness principle holds, it should be defined up to orthogonal transformations, and this will be actually the case under mild regularity conditions.

Since Φ can be defined up to an orthogonal transformation, and since it is a norm preserving and 1-order positively homogeneous diffeomorphisms, we are allowed to consider the following

Assumption 1. $\Phi(\boldsymbol{e}_1) = \boldsymbol{e}_1$ with inverse Jacobian $J_\Phi^{-1}(\boldsymbol{e}_1) = \Lambda$ satisfying $\boldsymbol{e}_1 = \Lambda \boldsymbol{e}_1 = \Lambda^\top \boldsymbol{e}_1$, i.e., $\Lambda_{1,\bullet} = \Lambda_{\bullet,1} = \boldsymbol{e}_1$.

Then, let us observe that the projector $(\boldsymbol{I}_d - P_{\Phi(\boldsymbol{e}_1)})$ and Λ can be written

$$\boldsymbol{I}_d - \boldsymbol{e}_1 \boldsymbol{e}_1^\top = \begin{bmatrix} 0 & \mathbf{0}_{d-1}^\top \\ \mathbf{0}_{d-1} & \boldsymbol{I}_{d-1} \end{bmatrix} \quad \text{and} \quad \boldsymbol{\Lambda} = \begin{bmatrix} 1 & \mathbf{0}_{d-1}^\top \\ \mathbf{0}_{d-1} & \tilde{\boldsymbol{\Lambda}} \end{bmatrix}. \tag{3.3}$$

Next result states what kind of uniqueness can be achieved within Problem 2.

Theorem 1. *For $i = 1, 2$, let Φ_i be norm preserving and positively homogeneous diffeomorphisms of order 1 on $\mathcal{D}^\varepsilon$. Let R_i be continuously differentiable real-valued functions on $\mathbb{R}$ with almost everywhere (a.e.) non vanishing derivatives, and such that*

$$R_1\big(\beta_{\Phi_1}(\boldsymbol{u}, \boldsymbol{v})\big) = R_2\big(\beta_{\Phi_2}(\boldsymbol{u}, \boldsymbol{v})\big), \qquad \boldsymbol{u}, \boldsymbol{v} \in \mathcal{D}^\varepsilon. \tag{3.4}$$

Then $R_1 = R_2$ and $\Phi_2 = O\Phi_1$, for some orthogonal matrix O.

Proof. Let $\Phi := \Phi_2 \circ \Phi_1^{-1}$. We note that Φ preserves norms, and that Φ is a positively homogeneous diffeomorphism of order 1. Then, setting $\boldsymbol{x} = \Phi_1(\boldsymbol{u})$ and $\boldsymbol{y} = \Phi_1(\boldsymbol{v})$ implies Equation (3.4) to be equivalent to

$$R_1\big(\beta(\boldsymbol{x}, \boldsymbol{y})\big) = R_2\big(\beta_\Phi(\boldsymbol{x}, \boldsymbol{y})\big), \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon. \tag{3.5}$$

Differentiation with respect to $\boldsymbol{x}$ yields

$$R_1'\big(\beta(\boldsymbol{x}, \boldsymbol{y})\big) \, \frac{1}{|\boldsymbol{x}|} \frac{\boldsymbol{y}^\top}{|\boldsymbol{y}|} \big(\boldsymbol{I}_d - P_{\boldsymbol{x}}\big) = R_2'\big(\beta_\Phi(\boldsymbol{x}, \boldsymbol{y})\big) \frac{1}{|\Phi(\boldsymbol{x})|} \frac{\Phi^\top(\boldsymbol{y})}{|\Phi(\boldsymbol{y})|} \Big(\boldsymbol{I}_d - P_{\Phi(\boldsymbol{x})}\Big) J_\Phi(\boldsymbol{x}),$$
$$\forall \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon.$$

Since $\beta(\boldsymbol{x}, \boldsymbol{y})$ and $\beta_\Phi(\boldsymbol{x}, \boldsymbol{y})$ are non constant functions, and since R_1', R_2' are *a.e.* non vanishing, we have, for almost all $\boldsymbol{x}$ and $\boldsymbol{y}$

$$\rho(\boldsymbol{x}, \boldsymbol{y}) = \frac{R_1'\big(\beta(\boldsymbol{x}, \boldsymbol{y})\big)}{R_2'\big(\beta_\Phi(\boldsymbol{x}, \boldsymbol{y})\big)} \neq 0.$$

Taking into account norm preservation, we get for almost all $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon$,

$$\left(\boldsymbol{I}_d - P_{\Phi(\boldsymbol{x})}\right)\Phi(\boldsymbol{y}) = \rho(\boldsymbol{x}, \boldsymbol{y}) \left(J_\Phi^{-1}\right)^\top (\boldsymbol{x})\left(\boldsymbol{I}_d - P_{\boldsymbol{x}}\right)\boldsymbol{y}. \tag{3.6}$$

We now use Assumption 1 and Equation (3.3) to write $\boldsymbol{y}$ and $\Phi(\boldsymbol{y}) \in \mathbb{R}^d$ as $\boldsymbol{y} = (y_1, \tilde{\boldsymbol{y}})$ and $\Phi(\boldsymbol{y}) = (\phi_1(\boldsymbol{y}), \tilde{\Phi}(\boldsymbol{y}))$ with $\tilde{\boldsymbol{y}},\ \tilde{\Phi}(\boldsymbol{y}) \in \mathbb{R}^{d-1}$, and set $\boldsymbol{x} = \boldsymbol{e}_1$ in Equation (3.6), to get

$$\tilde{\Phi}(\boldsymbol{y}) = \rho(\boldsymbol{e}_1, \boldsymbol{y})\tilde{\Lambda}^\top \tilde{\boldsymbol{y}}, \quad \text{with} \quad \rho(\boldsymbol{e}_1, \boldsymbol{y}) = \frac{R_1'\left(y_1/|\boldsymbol{y}|\right)}{R_2'\left(\phi_1/|\Phi(\boldsymbol{y})|\right)}. \tag{3.7}$$

The rest of the proof is structured into four steps:

1. We first show that $\rho(\boldsymbol{e}_1, \boldsymbol{y})$ actually depends only on $y_1/|\boldsymbol{y}|$.

Setting $\boldsymbol{x} = \boldsymbol{e}_1$ in Equation (3.5) yields $R_1\left(y_1/|\boldsymbol{y}|\right) = R_2\left(\phi_1/|\Phi(\boldsymbol{y})|\right)$. The fact that R_2 has a *a.e.* non vanishing derivative, implies the inverse R_2^{-1} to be *a.e.* well defined. Thus,

$$\phi_1/|\Phi(\boldsymbol{y})| = R_2^{-1} \circ R_1\left(y_1/|\boldsymbol{y}|\right) \equiv G\left(y_1/|\boldsymbol{y}|\right).$$

Consequently, we have

$$\rho(\boldsymbol{e}_1, \boldsymbol{y}) = R_1'\left(y_1/|\boldsymbol{y}|\right)/R_2'\left(G(y_1/|\boldsymbol{y}|)\right) \equiv H(y_1/|\boldsymbol{y}|).$$

2. We now prove that $\tilde{\Lambda}$ is, up to a scalar, an orthogonal matrix on $\mathbb{R}^{d-1}$.

Let us notice that $|\boldsymbol{y}|^2 = |\Phi(\boldsymbol{y})|^2 = \phi_1^2(\boldsymbol{y}) + \rho^2(\boldsymbol{e}_1, \boldsymbol{y})|\tilde{\Lambda}^\top \tilde{\boldsymbol{y}}|^2$ can be written as

$$1 = G^2\left(\frac{y_1}{|\boldsymbol{y}|}\right) + H^2\left(\frac{y_1}{|\boldsymbol{y}|}\right)\left|\tilde{\Lambda}^\top \frac{\tilde{\boldsymbol{y}}}{|\boldsymbol{y}|}\right|^2.$$

In other words, we have

$$\left|\tilde{\Lambda}^\top \frac{\tilde{\boldsymbol{y}}}{|\boldsymbol{y}|}\right|^2 = \frac{1 - G^2\left(\frac{y_1}{|\boldsymbol{y}|}\right)}{H^2\left(\frac{y_1}{|\boldsymbol{y}|}\right)} \equiv F^2\left(\frac{y_1}{|\boldsymbol{y}|}\right).$$

Next, for any $\boldsymbol{y}$ such that $y_1 = 0$, we have $|\tilde{\boldsymbol{y}}| = |\boldsymbol{y}|$ and therefore for any unit vector $\tilde{\boldsymbol{u}} = \tilde{\boldsymbol{y}}/|\tilde{\boldsymbol{y}}| \in \mathbb{R}^{d-1}$, we get $|\tilde{\Lambda}^\top \tilde{\boldsymbol{u}}|^2 \equiv F^2(0)$. This implies that the matrix $\tilde{\Lambda}^\top/F(0)$ preserves norms in $\mathbb{R}^{d-1}$. Therefore, it is orthogonal and thus satisfies $\tilde{\Lambda}^\top = F^2(0)\tilde{\Lambda}^{-1}$ with $|\det(\tilde{\Lambda})| = \pm F(0)$.

3. We now determine $\Phi_1(\boldsymbol{y})$.

We first determine the function F by setting $s = y_1/|\boldsymbol{y}|$. Since $\widetilde{\Lambda}^\top/F(0)$ is orthogonal, we get

$$F^2(0) = |\tilde{\Lambda}^\top \frac{\tilde{\boldsymbol{y}}}{|\tilde{\boldsymbol{y}}|}|^2 = \frac{|\boldsymbol{y}|^2}{|\tilde{\boldsymbol{y}}|^2}|\tilde{\Lambda}^\top \frac{\tilde{\boldsymbol{y}}}{|\boldsymbol{y}|}|^2 = \frac{|\boldsymbol{y}|^2}{|\tilde{\boldsymbol{y}}|^2}F^2(\frac{y_1}{|\boldsymbol{y}|}) = \frac{1}{1-s^2}F^2(s),$$

that is $F^2(s) = F^2(0)(1 - s^2)$.

On the other hand, one can easily prove that functions G and H satisfy *a.e.* $G'(s) = H(s),\ s \in [-1,1]$, and consequently we get

$$\frac{G'^2(s)}{1-G^2(s)} = \frac{1}{F^2(0)(1-s^2)}, \qquad \text{that is} \qquad \frac{G'(s)}{\sqrt{1-G^2(s)}} = \frac{1}{F(0)}\frac{1}{\sqrt{1-s^2}},$$
$$s \in [-1,1].$$

Since $G(1) = 1$, using the change of variable formula for integration over interval $[s,1]$, yields $\arccos(G(s)) = \arccos(s)/F(0)$. Since Φ is a diffeomorphism and $G(y_1/|\boldsymbol{y}|) = \phi_1(\boldsymbol{y})/|\Phi(\boldsymbol{y})|$, we have

$$\arccos(\phi_1(\boldsymbol{y})/|\Phi(\boldsymbol{y})|) = \arccos(y_1/|\boldsymbol{y}|))/F(0) \in [-\pi, 0]. \tag{3.8}$$

We now prove that $F(0) = \pm 1$.

Without loss of generality, let us assume that $F(0) \geq 0$ and consider the two cases.

If $F(0) < 1$, we can choose $\boldsymbol{y} = (-1, \mathbf{0_{d-1}})$ that is $s = -1$ and get $\arccos(G(-1)) = -\pi/F(0) < -\pi$. Similarly, if $F(0) > 1$, we can also choose $\boldsymbol{y}^*$, $|\boldsymbol{y}^*| = 1$ such that $\Phi(\boldsymbol{y^*}) = (-1, \mathbf{0_{d-1}})^\top$ that is $G(s) = -1$, and get $\arccos(y_1^*) = -\pi F(0) < -\pi$. Since both cases contraddict Equation (3.8), we necessarily have $F(0) = 1$, *i.e.*, $\Phi_1(\boldsymbol{y}) = y_1$, implying $\rho(\boldsymbol{e}_1, \boldsymbol{y}) = \pm 1$.

We have thus proved that $\Phi(\boldsymbol{y}) = \Phi_2 \circ \Phi_1^{-1}(\boldsymbol{y}) = \Lambda^\top \boldsymbol{y}$ with Λ orthogonal, and thus setting $\boldsymbol{y} = \Phi_1(\boldsymbol{v})$ yields $\Phi_1(\boldsymbol{v}) = \Lambda^{-1}\Phi_2(\boldsymbol{v})$. Actually, one can replace any orthogonal matrix O for the orthogonal matrix Λ.

4. To conclude the proof, we notice that $R_1 = R_2$ by Equation (3.4) since $\beta_{\Phi_1}(\boldsymbol{u}, \boldsymbol{v}) = \beta_{\Phi_2}(\boldsymbol{u}, \boldsymbol{v})$. ☐

3.4. Recovering R and Φ from C^ε (or C)

We now prove how one can recover, under mild identifiability conditions, a solution (R, Φ), provided it exists, from the knowledge of the covariance function and the inverse Jacobian at a single point of the sphere, say $\boldsymbol{e}_1$.

Theorem 2. *Let $C^\varepsilon : \mathcal{D}^\varepsilon \times \mathcal{D}^\varepsilon \to \mathbb{R}$ be a covariance function such that*

$$C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = R\big(\beta_{\hat{\Phi}}(\boldsymbol{x}, \boldsymbol{y})\big), \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon,$$

for some continuously differentiable function R on $[-1, +1]$ with a.e. non vanishing derivative, and for a positively homogeneous of order 1 and norm preserving diffeomorphism, $\hat{\Phi}$, on $\mathcal{D}^\varepsilon$. Then,

1. *the unique solution $\Phi = (\phi_1, \ldots, \phi_d)^\top$ satisfying Assumption 1 is given by:*

$$\phi_j(\boldsymbol{y}) = \begin{cases} |\boldsymbol{y}| \cos(\alpha(\boldsymbol{y})) & \textit{for} \quad j = 1 \\ |\boldsymbol{y}| \sin(\alpha(\boldsymbol{y})) \frac{D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y}) \Lambda_{\bullet, j}}{|D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y}) \Lambda|} & \textit{for} \quad 2 \leq j \leq d, \end{cases} \tag{3.9}$$

where

$$\alpha(\boldsymbol{y}) = -\left(\int_0^1 \frac{D_{\boldsymbol{y}} C^{\varepsilon}(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))}{|D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))\Lambda|} \mathrm{d}t\right)(\boldsymbol{y} - \boldsymbol{e}_1), \tag{3.10}$$

with

$$\gamma_{\boldsymbol{y}}(t) = (1-t)\boldsymbol{e}_1 + t\boldsymbol{y}, \qquad t \in [0,1]. \tag{3.11}$$

2. *R is uniquely defined by $R(u) = C(\boldsymbol{e}_1, \boldsymbol{y}(u))$, where $\boldsymbol{y}(u) = \Phi^{-1}(\boldsymbol{v}(u))$, $u \in [-1,1]$, and $\boldsymbol{v}^{\top}(u) = \left(u, \sqrt{1-u^2}, 0, \dots, 0\right) \in \mathbb{S}^{d-1}$.*

Proof. To favor neater exposition, we have divided the proof into four steps.

a. Differentiation with respect to $\boldsymbol{x}$ gives

$$D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y}) = R'\big(\beta_{\Phi}(\boldsymbol{x}, \boldsymbol{y})\big) \frac{1}{|\Phi(\boldsymbol{x})|} \frac{\Phi^{\top}(\boldsymbol{y})}{|\Phi(\boldsymbol{y})|} \big(\boldsymbol{I}_d - P_{\Phi(\boldsymbol{x})}\big) J_{\Phi}(\boldsymbol{x}).$$

By symmetry, we get $D_{\boldsymbol{y}} C^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y}) = D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{y}, \boldsymbol{x})$, that is

$$D_{\boldsymbol{y}} C^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y}) = R'\big(\beta_{\Phi}(\boldsymbol{x}, \boldsymbol{y})\big) \frac{1}{|\Phi(\boldsymbol{y})|} \frac{\Phi^{\top}(\boldsymbol{x})}{|\Phi(\boldsymbol{x})|} \big(\boldsymbol{I}_d - P_{\Phi(\boldsymbol{y})}\big) J_{\Phi}(\boldsymbol{y}).$$

As a consequence of Lemma 1, we notice that $C^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y})$ depends only on $\boldsymbol{x}/|\boldsymbol{x}|$ and $\boldsymbol{y}/|\boldsymbol{y}|$, since $D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{x} = D_{\boldsymbol{y}} C^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{y} = 0$. This is because Φ is positively homogeneous of order 1.

Using Assumption 1 and Equation (3.3), we obtain $\beta_{\Phi}(\boldsymbol{e}_1, \boldsymbol{y}) = \phi_1(\boldsymbol{y})/|\Phi(\boldsymbol{y})|$ and therefore

$$D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{e}_1, \boldsymbol{y})\Lambda = R'\left(\frac{\phi_1(\boldsymbol{y})}{|\Phi(\boldsymbol{y})|}\right) \frac{1}{|\Phi(\boldsymbol{y})|} \big(0, \phi_2(\boldsymbol{y}), \dots, \phi_d(\boldsymbol{y})\big).$$

For simplicity, put $\theta_j(\boldsymbol{y}) = \frac{\phi_j(\boldsymbol{y})}{|\Phi(\boldsymbol{y})|}$, $j = 1, \dots, d$. Since R' is continuous and *a.e.* non vanishing, the following relation holds *a.e.*:

$$\theta_j(\boldsymbol{y}) = \frac{D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{e}_1, \boldsymbol{y})\Lambda_{\bullet,j}}{R'\big(\theta_1(\boldsymbol{y})\big)}, \quad j = 2, \dots, d.$$

Then, taking into account that $\Sigma_{j=1}^d \theta_j^2(\boldsymbol{y}) = 1$, we get

$$\Big(R'\big(\theta_1(\boldsymbol{y})\big)\Big)^2 \Big(1 - \theta_1^2(\boldsymbol{y})\Big) = \Big|D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{e}_1, \boldsymbol{y})\Lambda\Big|^2,$$

that is

$$R'\big(\theta_1(\boldsymbol{y})\big) = \pm \frac{|D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{e}_1, \boldsymbol{y})\Lambda|}{\sqrt{1 - \theta_1^2(\boldsymbol{y})}}. \tag{3.12}$$

b. *Identification of* $\boldsymbol{\Phi}$. By a continuity argument, the $\pm$ sign in Equation (3.12) can be removed, so to get

$$\phi_j(\boldsymbol{y}) = \frac{D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{e}_1, \boldsymbol{y})\Lambda_{\bullet,j}}{|D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{e}_1, \boldsymbol{y})\Lambda|} \sqrt{|\Phi(\boldsymbol{y})|^2 - \phi_1^2(\boldsymbol{y})}, \quad j \geq 2. \tag{3.13}$$

Since $|\Phi(\boldsymbol{y})| = |\boldsymbol{y}|^2$, the components $\phi_j,\ j \geq 2$ are therefore determined by the differentials of C^ε as soon as ϕ_1 is known.

c. *Identification of* ϕ_1. Using Equation (3.2), we obtain

$$D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y}) = R'\big(\theta_1(\boldsymbol{y})\big) D_{\boldsymbol{y}}\theta_1(\boldsymbol{y}) = \frac{|D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y})\Lambda|}{\sqrt{1-\theta_1^2(\boldsymbol{y})}} D_{\boldsymbol{y}}\theta_1(\boldsymbol{y}).$$

Now, for $H(\boldsymbol{y}) = \arccos\big(\theta_1(\boldsymbol{y})\big)$, we have

$$D_{\boldsymbol{y}} H(\boldsymbol{y}) = -\frac{D_{\boldsymbol{y}}\theta_1(\boldsymbol{y})}{\sqrt{1-\theta_1^2(\boldsymbol{y})}}.$$

This implies that

$$D_{\boldsymbol{y}} H(\boldsymbol{y}) = -\frac{D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y})}{|D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y})\Lambda|}.$$

We can now determine H from C^ε: consider the segment $[\boldsymbol{e}_1, \boldsymbol{y}]$ in $\mathcal{D}^\varepsilon$ and the scalar function $h(t) = H(\gamma_{\boldsymbol{y}}(t))$, where $\gamma_{\boldsymbol{y}}(\cdot)$ has been defined in Equation (3.11). We have that h satisfies

$$h'(t) = D_{\boldsymbol{y}} H\big(\gamma_{\boldsymbol{y}}(t)\big)\gamma'_{\boldsymbol{y}}(t) = D_{\boldsymbol{y}} H\big(\gamma_{\boldsymbol{y}}(t)\big)\big(\boldsymbol{y}-\boldsymbol{e}_1\big) = -\frac{D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))}{|D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))\Lambda|}(\boldsymbol{y}-\boldsymbol{e}_1).$$

Therefore, direct inspection shows that

$$\begin{aligned} H(\boldsymbol{y}) - H(\boldsymbol{e}_1) = h(1) - h(0) &= \int_0^1 h'(t)\mathrm{d}t \\ &= -\left(\int_0^1 \frac{D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))}{|D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))\Lambda|}\mathrm{d}t\right)(\boldsymbol{y}-\boldsymbol{e}_1). \end{aligned}$$

Since $\theta_1(\boldsymbol{e}_1) = 1,\ H(\boldsymbol{e}_1) = 0$ we get the solution

$$\theta_1(\boldsymbol{y}) = \cos\left(-\left(\int_0^1 \frac{D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))}{|D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))\Lambda|}\mathrm{d}t\right)(\boldsymbol{y}-\boldsymbol{e}_1)\right) = \cos\left(\alpha(\boldsymbol{y})\right).$$

Using the fact that $|\Phi(\boldsymbol{y})| = |\boldsymbol{y}|$, we have

$$\phi_1(\boldsymbol{y}) = |\boldsymbol{y}|\cos\left(\alpha(\boldsymbol{y})\right). \tag{3.14}$$

d. *Identification of* R. Let us consider on the "semi-circle" $\{\boldsymbol{v}(u) = (u, \sqrt{1-u^2}, 0, \ldots, 0),\ u \in [-1,1]\}$ whose preimage by the diffeomorphism Φ, is the curve $\{\boldsymbol{y}(u) = \Phi^{-1}(\boldsymbol{v}(u))\, u \in [-1,1]\}$. Since $\phi_1(\boldsymbol{y}(u)) = u$, we get $R(u) = R(\phi_1(\boldsymbol{y}(u))) = R\left(\Phi^\top(\boldsymbol{e}_1)\Phi(\boldsymbol{y}(u))\right) = C\left(\boldsymbol{e}_1, \boldsymbol{y}(u)\right)$, which implies that R is entirely determined by C and the knowledge of the inverse of Φ on a semi-circle. The proof is completed. $\square$

3.5. Some remarks

Remark 1. Let $d > 1$. We note that, for $\boldsymbol{x}$ and $\boldsymbol{y} \in \mathbb{S}^{d-1}$, β_Φ becomes

$$\beta_\Phi(\boldsymbol{x},\boldsymbol{y}) = \cos\big(\alpha(\boldsymbol{x})\big)\cos\big(\alpha(\boldsymbol{y})\big) + \sin\big(\alpha(\boldsymbol{x})\big)\sin\big(\alpha(\boldsymbol{y})\big)\frac{D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{x})\Lambda}{|D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{x})\Lambda|}\frac{\Big(D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{y})\Lambda\Big)^\top}{|D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{y})\Lambda|}.$$

This is actually the Viete formula called *Spherical Law of Cosines (resp. Sines)* in spherical trigonometry in $\mathbb{S}^2$. Since the points $\boldsymbol{e_1}$, $\Phi(\boldsymbol{x})$ and $\Phi(\boldsymbol{y})$ of $\mathbb{S}^{d-1}$ actually lie in a submanifold equivalent to $\mathbb{S}^2$, Viete law states that $\beta_\Phi(\boldsymbol{x},\boldsymbol{y}) = \cos(\text{angle}[\Phi(\boldsymbol{x}),\Phi(\boldsymbol{y})])$ is expressed via the cosine and sine of $\alpha(\boldsymbol{x}) = \text{angle}[\boldsymbol{e}_1,\Phi(\boldsymbol{x})]$ and $\alpha(\boldsymbol{y}) = \text{angle}[\boldsymbol{e}_1,\Phi(\boldsymbol{y})]$ and the cosine of the angle between the unit vectors $\tau(\boldsymbol{x})$ and $\tau(\boldsymbol{y})$ stemming at $\boldsymbol{e}_1 = \Phi(\boldsymbol{e}_1)$, and tangent to the great circles in $\mathbb{S}^2$ leading respectively to $\Phi(\boldsymbol{x})$ and $\Phi(\boldsymbol{y})$ with $\tau(\boldsymbol{w}) = D_{\boldsymbol{w}}C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{w})\Lambda/|D_{\boldsymbol{w}}C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{w})\Lambda|$.

Remark 2. Theorem 2 assumes the matrix $J_\Phi^{-1}(\boldsymbol{e}_1) = \Lambda$ (or rather $\tilde{\Lambda}$ in Equation (3.3), depending on $(d-1)^2$ parameters) as known, although this is not the case in general. To effectively determine $\tilde{\Lambda}$, we recall that it is defined up a $(d-1)$-dimensional orthogonal matrix $\tilde{\boldsymbol{O}}$ (see Appendix A) whose $(d-1)(d-2)/2$ parameters can be set arbitrarily. The remaining $(d-1)d/2$ unknown parameters have to be determined by imposing constraints that ensure the solution (3.9) to be a sphere diffeomorphism. Among other possibilities, one can make use of the different forms of the *Spherical Law of Cosines* on spheres (see Remark 1), or of other simpler constraints being specific to the case under study. Alternatively, one can use the following type of constraints involving a change of variable formula for moments of the Lebesgue measure over the unit ball $B_d(0,1) \subset \mathbb{R}^d$:

$$\alpha_{d,n} = \int_{B_d(0,1)} u_i^n \mathrm{d}\boldsymbol{u} = \int_{B_d(0,1)} |\Phi_i(\boldsymbol{y})|^n |\det(J_\Phi(\boldsymbol{y})|\ \mathrm{d}\boldsymbol{y},\ n \geq 0, \tag{3.15}$$

with

$$\alpha_{d,n} = \begin{cases} 0 & \text{if} \quad n \text{ odd}, \\ \frac{4}{n+2} W_n & \text{if} \quad n \text{ even and } d = 2, \\ \frac{2^{d+1}}{n+d}\frac{\Gamma((n+1)/2)\Gamma((d-1)/2)}{\Gamma((n+d)/2)} W_0 W_1 \ldots W_{d-3} & \text{if} \quad n \text{ even and } d \geq 3, \end{cases} \tag{3.16}$$

with $W_n = \int_0^{\pi/2} \sin^n(u)\mathrm{d}u$, $n \geq 0$ and $\Gamma(\cdot)$ is the Gamma function.

Note that the integrals $\alpha_{d,n}$ are independent of the index i of the coordinates. For example, in the case of $\mathbb{S}^1$ we may need the single constraint related to $\alpha_{2,0} = \pi$, while for $\mathbb{S}^2$, we may need $\alpha_{3,0} = 4\pi/3$, $\alpha_{3,1} = 0$ and $\alpha_{3,2} = 16\pi/15$. Of course, one can use as well integral formulas related to the mixed moments for higher dimensions.

Remark 3. If R is known and R' is almost everywhere non vanishing, R is locally monotonic. Thus, from the relation $C^{\varepsilon}(\boldsymbol{e}_1,\boldsymbol{y}) = R(\phi_1(\boldsymbol{y}))$ for $\boldsymbol{y} \in \mathbb{S}^{d-1}$, one can locally calculate $\phi_1(\boldsymbol{y}) = R^{-1}(C(\boldsymbol{e}_1,\boldsymbol{y}))$. Starting from equality $R(\phi_1(\boldsymbol{e}_1)) = R(1) = 1$, by a continuity argument we can therefore extend local identification to a global identification of ϕ_1 on $\mathbb{S}^{d-1}$. Thus, the knowledge of R can spare the computation of the integral (3.10).

Remark 4. Using the homogeneity property of C^{ε}, Equation (3.10) can be simplified, by replacing $(\gamma_{\boldsymbol{y}}(t) - \boldsymbol{e}_1)/t$ for $(\boldsymbol{y} - \boldsymbol{e}_1)$, so that

$$\alpha(\boldsymbol{y}) = -\int_0^1 \frac{\partial_{\boldsymbol{y}_1} C^{\varepsilon}(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))}{|D_{\boldsymbol{x}} C^{\varepsilon}(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))\Lambda|} \frac{\mathrm{d}t}{t}. \tag{3.17}$$

Remark 5. The assumption that R' is continuous and non vanishing *a.e.* is satisfied for many isotropic correlation functions (refer to Equation (1.2)). We start with a counterexample and then provide some examples:

1. $R(u) \equiv 1$ *i.e.*, $R'(u) \equiv 0$ does not satisfy our assumption. Of course, any deformation Φ of $\mathbb{S}^{d-1}$ is a solution for $C(\boldsymbol{x},\boldsymbol{y}) = R(\beta_{\Phi}(\boldsymbol{x},\boldsymbol{y}) \equiv 1$ on $\mathbb{S}^{d-1}$.
2. $R(u) = u$ gives $R'(u) \equiv 1$ and $R^{-1}(u) = u$.
3. $R(u) = b_{2,d-1} P_2^{(d-1)/2}(u)/P_2^{(d-1)/2}(1) = ((d+1)u^2 - 1)/d$ (see Equation (1.2)) yields $R'(u) = 2(d+1)/du$, that vanishes at $u = 0$. By continuity, we can determine which of the branch of $R^{-1}(u) = \pm\sqrt{(du+1)/(d+1)}$ is adapted for inversion.
4. Any truncation of order N in representation (1.2): $R(u) = \sum_{n=0}^{N} b_{n,d-1} P_n^{(d-1)/2}(u)/P_n^{(d-1)/2}(1)$ satisfies our assumption. This is because R is a polynomial of degree N and thus R' has at most $N-1$ distinct zeros by the fundamental theorem of algebra. Thus, R is locally invertible.

3.6. An example of reducibility in $\mathbb{S}^1$

We start by choosing a specific geodesically isotropic correlation function ρ on the circle. According to Theorem 1 of Gneiting (2013), taking $b_n = e^{-\nu}\nu^n/n!$, $n \geq 0$ we obtain $\rho(\theta) = \sum_{n\geq 0} b_n \cos^n(\theta) = \exp\left(\nu(\cos(\theta) - 1)\right)$, $\theta \in [-\pi,\pi]$, being positive definite on every d-dimensional sphere.

Equivalently, the Euclidean coordinate system $\boldsymbol{x} = (x_1,x_2)^{\top}$, $\boldsymbol{y} = (y_1,y_2)^{\top} \in \mathbb{S}^1$, provides the geodesically isotropic covariance function $C(\boldsymbol{x},\boldsymbol{y}) = \exp\left(\nu(\boldsymbol{x}^{\top}\boldsymbol{y} - 1)\right) = \exp\left(\nu(x_1y_1 + x_2y_2 - 1)\right)$, that can be written as $C(\boldsymbol{x},\boldsymbol{y}) = R(\boldsymbol{x}^{\top}\boldsymbol{y})$, with $R(u) = \exp(\nu(u-1))$ with positive derivative $R'(u) = \nu\exp(\nu(u-1))$, $u \in [-1,1]$.

Second, let us now define a circle diffeomorphism $\Psi : \mathbb{S}^1 \longrightarrow \mathbb{S}^1$ using the spherical coordinate system: $\boldsymbol{x} = \boldsymbol{x}(\theta) = (\cos(\theta),\sin(\theta))^{\top}$ and $\Psi(\boldsymbol{x}) = \Psi(\boldsymbol{x}(\theta)) = (\cos(\eta(\theta)),\sin(\eta(\theta))^{\top}$ where $\eta(\theta) = \pi/2\int_0^{\theta}|\cos(s)|\mathrm{d}s$. Since $\eta'(\theta) = \pi/2|\cos(\theta)|$ is nonnegative and continuous, η is a diffeomorphism of $[-\pi,\pi]$ with fixed points $\eta(0) = 0, \eta(\pi/2) = \pi/2, \eta(\pm\pi) = \pm\pi$, *i.e.*, Ψ preserves $e_1, -e_1, e_2$ and $-e_2$. Actually, $\eta(\theta)$ is a *linearly periodic* diffeomorphism on the whole real line.

Moreover, note that for $\theta \in (-\pi/2, \pi/2)$ and $\boldsymbol{x} \in \mathbb{S}^1$, we have

$$\eta(\theta) = \frac{\pi}{2}\sin(\theta) = \frac{\pi}{2}\sin\left(\arctan\left(x_2/x_1\right) \pm \tau\pi\right),$$

with $\tau = 0$ if $x_1 > 0$, $\tau = 1$ if $x_1 < 0, x_2 > 0$, and $\tau = -1$ if $x_1 < 0, x_2 < 0$. In other words, we have $\eta(\theta) = \mathrm{sign}(x_1)\pi x_2/2$, with inverse $\theta = \mathrm{sign}(x_1)\arctan\left(x_2/x_1\right)$. One can meticulously ensure that similar formulas hold for $\theta \in [-\pi, \pi]$, and therefore write the extension Φ of Ψ^ε to $\mathbb{R}^2$ as $\phi_1(\boldsymbol{x}) = |\boldsymbol{x}|\cos\left(\pi x_2/(2|\boldsymbol{x}|)\right)$, $\phi_2(\boldsymbol{x}) = \mathrm{sign}(x_1)|\boldsymbol{x}|\sin\left(\pi x_2/(2|\boldsymbol{x}|)\right)$, so that

$$\beta_\Phi(\boldsymbol{x}, \boldsymbol{y}) = \frac{\Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{y})}{|\Phi(\boldsymbol{x})||\Phi(\boldsymbol{y})|} = \cos\left(\frac{\pi}{2}\left(\frac{x_2}{|\boldsymbol{x}|} - \frac{y_2}{|\boldsymbol{y}|}\right)\right).$$

Third, let us finally consider the non-geodesically isotropic correlation function

$$C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = R(\Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{y})) = e^{\nu\left(\cos\left(\frac{\pi}{2}\left(\frac{x_2}{|\boldsymbol{x}|} - \frac{y_2}{|\boldsymbol{y}|}\right)\right) - 1\right)}, \tag{3.18}$$

and show how to recover R and Ψ.

According to Theorem 2, let us set $J_\Phi^{-1}(\boldsymbol{e}_1) = \Lambda = \begin{bmatrix} 1 & 0 \\ 0 & \lambda_{2,2} \end{bmatrix}$, where according to Remark 2, the parameter $\lambda_{2,2}$ has to be determined according to one of the constraints (3.15).

First, we show that

$$\frac{D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y})\Lambda_{\bullet,2}}{|D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y})\Lambda|} = \pm 1. \tag{3.19}$$

Set $\theta_{\boldsymbol{x},\boldsymbol{y}} = \frac{\pi}{2}\left(\frac{x_2}{|\boldsymbol{x}|} - \frac{y_2}{|\boldsymbol{y}|}\right)$ and observe that

$$D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = \frac{\nu\pi}{2|\boldsymbol{x}|^3}C^\varepsilon(\boldsymbol{x}, \boldsymbol{y})\sin(\theta_{\boldsymbol{x},\boldsymbol{y}})\left(x_1x_2, -x_1^2\right); \tag{3.20}$$

$$D_{\boldsymbol{y}}C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = \frac{\nu\pi}{2|\boldsymbol{y}|^3}C^\varepsilon(\boldsymbol{x}, \boldsymbol{y})\sin(\theta_{\boldsymbol{x},\boldsymbol{y}})\left(-y_1y_2, y_1^2\right). \tag{3.21}$$

In particular,

$$D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y}) = \frac{\nu\pi}{2}C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y})\sin(\theta_{\boldsymbol{e}_1,\boldsymbol{y}})\left(0, -1\right),$$

so that $D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y})\Lambda_{\bullet,1} = 0$, and $D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y})\Lambda_{\bullet,2} = -\lambda_{2,2}\nu\pi 2C^\varepsilon/(\boldsymbol{e}_1, \boldsymbol{y})\sin(\theta_{\boldsymbol{e}_1,\boldsymbol{y}})$, which clearly imply Equation (3.19).

Let us now establish the analytic form of the integral $\alpha(\boldsymbol{y})$ of Equation (3.10), for any given $\boldsymbol{y}$.

Here, $\gamma_{\boldsymbol{y}}(t) = (1-t)\boldsymbol{e}_1 + t\boldsymbol{y}$ with derivative $\gamma'_{\boldsymbol{y}}(t) = \boldsymbol{y} - \boldsymbol{e}_1$, and norm $|\gamma_{\boldsymbol{y}}(t)| = \sqrt{(1-t(1-y_1))^2 + t^2y_2^2}$ satisfying

$$|D_{\boldsymbol{x}}C^\varepsilon(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))\Lambda| = |\frac{\lambda_{2,2}\nu\pi}{2}\ C^\varepsilon(\boldsymbol{e}_1, \gamma_{\boldsymbol{y}}(t))\sin(\theta_{\boldsymbol{e}_1,\gamma_{\boldsymbol{y}}(t)})|.$$

Similarly, we obtain

$$D_{\boldsymbol{y}}C^{\varepsilon}(\boldsymbol{e}_1,\gamma_{\boldsymbol{y}}(t))(\boldsymbol{y}-\boldsymbol{e}_1)=\frac{\nu\pi}{2}C^{\varepsilon}(\boldsymbol{e}_1,\gamma_{\boldsymbol{y}}(t))\sin(\theta_{\boldsymbol{e}_1,\gamma_{\boldsymbol{y}}(t)})\frac{y_2(1+t(y_1-1))}{|\gamma_{\boldsymbol{y}}(t)|^3}, \tag{3.22}$$

and then

$$\begin{aligned}\alpha(\boldsymbol{y})&=-\left(\int_0^1\frac{D_{\boldsymbol{y}}C_{\varepsilon}(\boldsymbol{e}_1,\gamma_{\boldsymbol{y}}(t))}{|D_{\boldsymbol{x}}C_{\varepsilon}(\boldsymbol{e}_1,\gamma_{\boldsymbol{y}}(t))\Lambda|}\mathrm{d}t\right)(\boldsymbol{y}-\boldsymbol{e}_1)\\&=\pm\frac{1}{\lambda_{2,2}}\int_0^1\frac{y_2(1+t(y_1-1)}{(1-t(1-y_1))^2+t^2y_2^2)^{3/2}}\mathrm{d}t.\end{aligned}$$

We notice that $H(t)=ty_2/\sqrt{(1+t(y_1-1)))^2+t^2y_2^2}$ has derivative $\frac{y_2(1+t(y_1-1)}{(1-t(1-y_1))^2+t^2y_2^2)^{3/2}}$. Thus, $\alpha(\boldsymbol{y})=\pm\frac{1}{\lambda_{2,2}}(H(1)-H(0))=\pm\frac{1}{\lambda_{2,2}}\frac{y_2}{|\boldsymbol{y}|}$, implying

$$\phi_1(\boldsymbol{y})=|\boldsymbol{y}|\cos\left(\frac{1}{\lambda_{2,2}}\frac{y_2}{|\boldsymbol{y}|}\right)\qquad\text{and}\qquad\phi_2(\boldsymbol{y})=\pm|\boldsymbol{y}|\sin\left(\frac{1}{\lambda_{2,2}}\frac{y_2}{|\boldsymbol{y}|}\right).$$

The Jacobian satisfies $\det(J_{\Phi}(\boldsymbol{y}))=y_1/\lambda_{2,2}|\boldsymbol{y}|$.

Next, if we take the single 0-order moment constraint (3.15), we get $\lambda_{2,2}=2/\pi$, since

$$\alpha_{2,0}=\pi=\int_{B_d(0,1)}|\det(J_{\Phi}(\boldsymbol{y})|\;\mathrm{d}\boldsymbol{y}=\frac{1}{\lambda_{2,2}}\int_0^1 r\mathrm{d}r\int_0^{2\pi}|\cos(v)|\mathrm{d}v=\frac{2}{\lambda_{2,2}},$$

which indeed leads to the *hidden* transformation Ψ.

The isotropic correlation function is finally given by Theorem 2: since $\boldsymbol{y}(u)=\Phi^{-1}((u,\sqrt{1-u^2}))$ is a unit vector with component $y_2(u)=\frac{2}{\pi}\arccos(u)$, we have

$$R(u)=C(\boldsymbol{e}_1,\boldsymbol{y}(u))=e^{\nu(cos(\frac{\pi}{2}y_2(u))-1)}=e^{\nu(u-1)}.$$

3.7. *An example of reducibility in* $\mathbb{S}^2$

Even if more sophisticated models can be handled by Theorem 1, Theorem 2 and Remark 2 with more tedious calculus, we only show here how the machinery of uniqueness and identification can be carried out in $\mathbb{S}^2$, taking the simple example of an *ellipsoidal* diffeomorphism $\Psi(\boldsymbol{x})=\Omega\boldsymbol{x}/|\Omega\boldsymbol{x}|$ with $\Omega=\mathrm{diag}(\omega_1,\omega_2,\omega_3)$ and $\boldsymbol{x}\in\mathbb{S}^2$. Regarding the geodesically isotropic correlation function, we take $R(u)=au^2+b$ where $a=(d+1)/d$ and $b=-1/d$ (see Gneiting, 2013). In other words, we have to show the reducibility of the correlation function

$$C^{\varepsilon}(\boldsymbol{x},\boldsymbol{y})=a\frac{(\sum_{i=1}^3\omega_i^2x_iy_i)^2}{(\sum_{i=1}^3\omega_i^2x_i^2)(\sum_{i=1}^3\omega_i^2y_i^2)}+b,\qquad\boldsymbol{x},\boldsymbol{y}\in\mathbb{R}^3.$$

1. First, let $\Lambda=J_{\Phi}^{-1}(\boldsymbol{e}_1)$, or rather $\tilde{\Lambda}$ as in (3.3), $\boldsymbol{y}^{\top}=(y_1,\tilde{\boldsymbol{y}}^{\top})$ with $\tilde{\boldsymbol{y}}^{\top}=(y_2,y_3)$, and $\tilde{\Omega}=\mathrm{diag}(\omega_2,\omega_3)$. The matrix $\tilde{\Lambda}=\left(\lambda_{i,j}\right)_{2\le i,j\le 3}$ has 4 unknowns entries, but since it is defined up to a 2×2 orthogonal matrix defined by a single parameter ν, we can assume without loss of generality that $\lambda_{3,2}=0$.

Indeed, for any 2×2 invertible matrix $\tilde{\mathbf{M}} = \big(m_{i,j}\big)_{2\le i,j\le 3}$, if we choose the 2×2 orthogonal matrix

$$\tilde{\mathbf{O}} = \begin{pmatrix} \nu & -\sqrt{1-\nu^2} \\ \sqrt{1-\nu^2} & \nu \end{pmatrix},$$

with $\nu = m_{2,2}/\sqrt{m_{2,2}^2 + m_{3,2}^2}$, then $\tilde{\Lambda} = \tilde{\mathbf{O}}\tilde{\mathbf{M}}$ satisfies $\lambda_{3,2} = 0$.

The remaining 3 parameters are to be determined through C^ε itself.

2. Equation (2.1) yields

$$D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{x},\boldsymbol{y}) = 2a \frac{\boldsymbol{x}^\top \Omega^\top}{|\Omega \boldsymbol{x}|} \frac{\Omega \boldsymbol{y}}{|\Omega \boldsymbol{y}|} \frac{\boldsymbol{y}^\top \Omega^\top}{|\Omega \boldsymbol{y}|} \Big(\boldsymbol{I}_d - \frac{\Omega \boldsymbol{x}}{|\Omega \boldsymbol{x}|} \frac{\boldsymbol{x}^\top \Omega^\top}{|\Omega \boldsymbol{x}|} \Big) \frac{\Omega}{|\Omega \boldsymbol{x}|}.$$

A symmetric relation holds as well for $D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{x},\boldsymbol{y})$, and we get the following:

$$D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{y}) = \pm 2a \frac{y_1}{\sum_{i=1}^3 \omega_i^2 y_i^2} \Big(0, \tilde{\boldsymbol{y}}^\top \tilde{\Omega}^\top \tilde{\Omega}\Big),$$

$$D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{y})\Lambda = \pm 2a \frac{y_1}{\sum_{i=1}^3 \omega_i^2 y_i^2} \Big(0, \tilde{\boldsymbol{y}}^\top \tilde{\Omega}^\top \tilde{\Omega}\tilde{\Lambda}\Big),$$

which imply

$$\frac{D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{y})\Lambda_{\bullet,j}}{|D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1,\boldsymbol{y})\Lambda|} = \pm \frac{\tilde{\boldsymbol{y}}^\top \tilde{\Omega}^\top \tilde{\Omega}\tilde{\Lambda}_{\bullet,j}}{|\tilde{\boldsymbol{y}}^\top \tilde{\Omega}^\top \tilde{\Omega}\tilde{\Lambda}|},\ j = 2,3. \tag{3.23}$$

3. Next, to calculate $\alpha(\boldsymbol{y})$, let us observe that $\gamma_{\boldsymbol{y}}(t) = (1-t)\boldsymbol{e}_1 + t\boldsymbol{y} = \big(\gamma_{\boldsymbol{y},1}(t), \tilde{\gamma}_{\boldsymbol{y}}(t)\big)^T$ has components $\gamma_{\boldsymbol{y},1}(t) = 1 + t(y_1 - 1)$ and $\tilde{\gamma}_{\boldsymbol{y}}(t) = t\tilde{\boldsymbol{y}}$, so that we obtain

$$D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{e}_1,\gamma_{\boldsymbol{y}}(t))\Lambda = 2a \frac{\gamma_{\boldsymbol{y},1}(t)}{|\Omega \gamma_{\boldsymbol{y}}(t)|^2} \Big(0, t\tilde{\boldsymbol{y}}^\top \tilde{\Omega}^\top \tilde{\Omega}\tilde{\Lambda}\Big).$$

Similar calculations, using equality $\boldsymbol{y} - \boldsymbol{e}_1 = (\gamma_{\boldsymbol{y}}(t) - \boldsymbol{e}_1)/t$, lead to

$$D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{e}_1,\gamma_{\boldsymbol{y}}(t))\Big(\boldsymbol{y} - \boldsymbol{e}_1\Big) = -2ta \frac{\omega_1^2 \gamma_{\boldsymbol{y},1}(t)}{|\Omega \gamma_{\boldsymbol{y}}(t)|^2} \frac{|\tilde{\Omega}\tilde{\boldsymbol{y}}|^2}{|\Omega \gamma_{\boldsymbol{y}}(t)|^2},$$

and imply

$$\alpha(\boldsymbol{y}) = \pm \frac{|\tilde{\Omega}\tilde{\boldsymbol{y}}|}{|\tilde{\boldsymbol{y}}^\top \tilde{\Omega}^\top \tilde{\Omega}\tilde{\Lambda}|} \int_0^1 \frac{\omega_1^2 |\tilde{\Omega}\tilde{\boldsymbol{y}}|\,\mathrm{d}t}{\omega_1^2(1 - t(1-y_1))^2 + t^2 |\tilde{\Omega}\tilde{\boldsymbol{y}}|^2}.$$

The change of variable $v(t) = A/(B-t)$ with $A = |\tilde{\Omega}\tilde{\boldsymbol{y}}|/\left(|\omega_1|C^2\right)$, $B = (1-y_1)/C^2$, and $C^2 = \Big(\omega_1^2(1-y_1)^2 + |\tilde{\Omega}\tilde{\boldsymbol{y}}|^2\Big)/|\omega_1|^2$, and the use of the identity $\arctan(v_1) - \arctan(v_0) = \arctan\left((v_1 - v_0)/(1 + v_1 v_0)\right)$, yield

$$\alpha(\boldsymbol{y}) = \pm \frac{\omega_1 |\tilde{\Omega}\tilde{\boldsymbol{y}}|}{|\tilde{\boldsymbol{y}}^\top \tilde{\Omega}^\top \tilde{\Omega}\tilde{\Lambda}|} \arctan\left(\frac{|\tilde{\Omega}\tilde{\boldsymbol{y}}|}{\omega_1 y_1}\right).$$

4. We now prove that $\cos(\alpha(\boldsymbol{y})) = \omega_1 y_1/|\Omega \boldsymbol{y}|$. Since $\arctan\left(|\tilde{\Omega}\tilde{\boldsymbol{y}}|/\omega_1 y_1\right) = \arccos\left(\omega_1 y_1/|\Omega \boldsymbol{y}|\right)$, we only need to prove that $\omega_1 |\tilde{\Omega}\tilde{\boldsymbol{y}}| = |\tilde{\boldsymbol{y}}^\top \tilde{\Omega}^\top \tilde{\Omega}\tilde{\Lambda}|$.

For that purpose, let us apply the *Spherical Law of Sines* for the three unit vectors $\boldsymbol{e}_1, \boldsymbol{v} = \Omega\boldsymbol{y}/|\Omega\boldsymbol{y}|$, and $\boldsymbol{w} = \Gamma\boldsymbol{y}/|\Gamma\boldsymbol{y}|$ of $\mathbb{S}^2$, where $\Gamma = \Lambda^T\Omega^T\Omega$. Again let us denote $\boldsymbol{v} = \big(v_1, \tilde{\boldsymbol{v}}\big)$, $\boldsymbol{w} = \big(w_1, \tilde{\boldsymbol{w}}\big)$, so that we have $v_1 = \omega_1 y_1/|\Omega\boldsymbol{y}|$, $w_1 = \omega_1^2 y_1/|\Gamma\boldsymbol{y}|$, $\tilde{\boldsymbol{v}} = \tilde{\Omega}\tilde{\boldsymbol{y}}/|\Omega\boldsymbol{y}|$, and $\tilde{\boldsymbol{w}} = \tilde{\Gamma}\tilde{\boldsymbol{y}}/|\Gamma\boldsymbol{y}|$, with $\tilde{\Gamma} = \tilde{\Lambda}^T\tilde{\Omega}^T\tilde{\Omega}$.

We note that $a = |\boldsymbol{w} - \boldsymbol{e}_1| = \sqrt{2}\sqrt{1-v_1}$, and $b = |\boldsymbol{v} - \boldsymbol{e}_1| = \sqrt{2}\sqrt{1-w_1}$. Considering the angles A (resp. B) between $\boldsymbol{e}_1$ and $\boldsymbol{v}$ (resp. between $\boldsymbol{e}_1$ and $\boldsymbol{w}$) satisfying $\sin(A) = |\tilde{\boldsymbol{v}}|$ (resp. $\sin(B) = |\tilde{\boldsymbol{w}}|$), according to the sine law we have $\sin(B) = \frac{b}{a}\sin(A)$:

$$\frac{|\tilde{\Omega}\tilde{\boldsymbol{y}}|}{|\tilde{\Gamma}\tilde{\boldsymbol{y}}|} = \sqrt{\frac{|\Omega\boldsymbol{y}|}{|\Gamma\boldsymbol{y}|}}\sqrt{\frac{|\Omega\boldsymbol{y}| - \omega_1 y_1}{|\Gamma\boldsymbol{y}| - \omega_1^2 y_1}}. \tag{3.24}$$

Then, using the equality $U_1/V_1 = U_2/V_2 = (U_1 - U_2)/(V_1 - V_2)$, we get

$$\begin{aligned}\left(\frac{|\tilde{\Omega}\tilde{\boldsymbol{y}}|}{|\tilde{\Gamma}\tilde{\boldsymbol{y}}|}\right)^2 &= \frac{|\tilde{\Omega}\tilde{\boldsymbol{y}}|^2 + (\omega_1 y_1)^2 - \omega_1 y_1|\Omega\boldsymbol{y}|}{|\tilde{\Gamma}\tilde{\boldsymbol{y}}|^2 + (\omega_1^2 y_1)^2 - \omega_1^2 y_1|\Gamma\boldsymbol{y}|} = \frac{(\omega_1 y_1)^2 - \omega_1 y_1|\Omega\boldsymbol{y}|}{(\omega_1^2 y_1)^2 - \omega_1^2 y_1|\Gamma\boldsymbol{y}|}\\ &= \frac{1}{\omega_1}\frac{\omega_1 y_1 - |\Omega\boldsymbol{y}|}{\omega_1^2 y_1 - |\Gamma\boldsymbol{y}|},\end{aligned}$$

that is

$$\frac{|\tilde{\Omega}\tilde{\boldsymbol{y}}|}{|\tilde{\Gamma}\tilde{\boldsymbol{y}}|} = \frac{1}{\sqrt{\omega_1}}\sqrt{\frac{|\Omega\boldsymbol{y}| - \omega_1 y_1}{|\Gamma\boldsymbol{y}| - \omega_1^2 y_1}}. \tag{3.25}$$

Equations (3.24) and (3.25) therefore yield,

$$\omega_1|\Omega\boldsymbol{y}| = |\Gamma\boldsymbol{y}|, \text{ and } \omega_1|\tilde{\Omega}\tilde{\boldsymbol{y}}| = |\tilde{\Gamma}\tilde{\boldsymbol{y}}| = |\tilde{\boldsymbol{y}}^\top\tilde{\Omega}^\top\tilde{\Omega}\tilde{\Lambda}|. \tag{3.26}$$

5. We now identify the transformation $\Phi(\boldsymbol{y})$ and the isotropic correlation function, R.

Since Equation (3.23) can be written as

$$\frac{D_{\boldsymbol{x}}C^{\varepsilon}(\boldsymbol{e}_1, \boldsymbol{y})\Lambda}{|D_{\boldsymbol{x}}C^{\varepsilon}(\boldsymbol{e}_1, \boldsymbol{y})\Lambda|} = \left(0, \frac{\tilde{\Gamma}\tilde{\boldsymbol{y}}}{|\tilde{\Gamma}\tilde{\boldsymbol{y}}|}\right),$$

using previous findings and Equation (3.9), we finally obtain

$$\phi_1(\boldsymbol{y}) = |\boldsymbol{y}|\frac{\omega_1 y_1}{|\Omega\boldsymbol{y}|} = |\boldsymbol{y}|\frac{\omega_1^2 y_1}{|\Gamma\boldsymbol{y}|}, \quad \text{and } \tilde{\Phi}(\boldsymbol{y}) = |\boldsymbol{y}|\frac{|\tilde{\Omega}\tilde{\boldsymbol{y}}|}{|\Omega\boldsymbol{y}|}\frac{\tilde{\Gamma}\tilde{\boldsymbol{y}}}{|\tilde{\Gamma}\tilde{\boldsymbol{y}}|} = |\boldsymbol{y}|\frac{\tilde{\Gamma}\tilde{\boldsymbol{y}}}{|\Gamma\boldsymbol{y}|}.$$

Rephrased, we have

$$\Phi(y) = |\boldsymbol{y}|\frac{\Gamma\boldsymbol{y}}{|\Gamma\boldsymbol{y}|}, \text{ with } \Gamma = \begin{pmatrix}\omega_1^2 & 0 & 0\\ 0 & \lambda_{2,2}\omega_2^2, & 0\\ 0 & \lambda_{2,3}\omega_2^2 & \lambda_{3,3}\omega_3^2\end{pmatrix}.$$

To identify Λ, instead of using the moment constraints given in Remark 2 involving the Jacobian

$$J_\Phi(\boldsymbol{y}) = \frac{\Gamma\boldsymbol{y}}{|\Gamma\boldsymbol{y}|}\frac{\boldsymbol{y}^\top}{|\boldsymbol{y}|} + |\boldsymbol{y}|\left(\mathbf{I} - \frac{\Gamma\boldsymbol{y}}{|\Gamma\boldsymbol{y}|}\frac{\boldsymbol{y}^\top\Gamma^\top}{|\Gamma\boldsymbol{y}|}\right)\frac{\Gamma}{|\Gamma\boldsymbol{y}|},$$

Equation (3.26) is apparently more efficient. Indeed, (3.26) corresponds to the equality of the two quadratic functions, namely

$$\omega_1^4 y_1^2 + \omega_1^2\omega_2^2 y_2^2 + \omega_1^2\omega_3^2 y_3^2 = \omega_1^4 y_1^2 + \big(\lambda_{2,2}^2 + \lambda_{2,3}^2\big)\omega_2^4 y_2^2 + \lambda_{3,3}^2\omega_3^4 y_3^2 \\ + 2\lambda_{2,3}\lambda_{3,3}\omega_2^2\omega_3^2 y_2 y_3,$$

which implies that

$$\lambda_{2,2} = \pm\omega_1/|\omega_2|, \ \ \lambda_{2,3} = 0, \ \ \lambda_{3,3} = \pm\omega_1/|\omega_3|,$$

and leads to the *hidden* ellipsoidal transformation Ψ.

Without loss of generality, one can remove the $\pm$ sign everywhere, as reversing axis direction corresponds to particular orthogonal transformations that do not change the form of C^ε, and then obtain

$$\Gamma = \omega_1\Omega \text{ and } \Lambda = \operatorname{diag}\left(1, \frac{\omega_2}{\omega_1}, \frac{\omega_3}{\omega_1}\right).$$

To conclude our illustration, it sufficient to observe that $\Phi^{-1}(\boldsymbol{u}) = |\boldsymbol{u}|\Omega^{-1}\boldsymbol{u}/|\Omega^{-1}\boldsymbol{u}|$, so that according to Theorem 2, for $u \in]-1,1[$, $\ \boldsymbol{u}^\top = (u, \sqrt{1-u^2}, 0)$ and $\boldsymbol{y}(u) = \Phi^{-1}(\boldsymbol{u})$, we obtain

$$R(u) = C^\varepsilon(\boldsymbol{e}_1, \boldsymbol{y}(t))) = au^2 + b.$$

4. Sufficient conditions for local reducibility

Given a covariance function C on $\mathbb{S}^{d-1} \times \mathbb{S}^{d-1}$, one may ask for sufficient conditions on C to be reducible to geodesic isotropy. If C is regular and smooth enough, sufficient conditions are to be sought in terms of C and of its differentials. In any case, previous findings show that it is equivalent and much easier to seek for a set of sufficient conditions on its extension C^ε.

Theorem 3. *Let $C^\varepsilon : \mathcal{D}^\varepsilon \times \mathcal{D}^\varepsilon \to \mathbb{R}$, be a continuously differentiable covariance function such that the following assumptions hold:*

H1- $D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y})\boldsymbol{x} \equiv 0, \quad \forall \boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon$.

H2- $D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y})$ *is non vanishing for almost all* $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{D}^\varepsilon$.

H3- The vector function $\Phi = (\phi_1, \ldots, \phi_d)^\top$, defined by Equations (3.9)–(3.10), through the C^ε differentials, is a diffeomorphism on $\mathcal{D}^\varepsilon$ for some invertible matrix Λ satisfying (3.3).

H4- The scalar function $R(u) = C^\varepsilon\big(\boldsymbol{e}_1, \boldsymbol{y}(u)\big)$, where $\boldsymbol{y}(u) = \Phi^{-1}(\boldsymbol{u})$, $\boldsymbol{u} = (u, \sqrt{1-u^2}, \boldsymbol{0}) \in \mathbb{S}^{d-1}$, with $u \in [-1,1]$, has a continuous and almost everywhere non vanishing derivative.

Then, $C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = R(\beta_\Phi(\boldsymbol{x}, \boldsymbol{y})) + \kappa$ with some constant $\kappa \in \mathbb{R}$, if

$$|\boldsymbol{x}||\boldsymbol{y}| \ D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = R'\big(\beta_\Phi(\boldsymbol{x}, \boldsymbol{y})\big) \ \Phi^\top(\boldsymbol{y}) \ \big(\boldsymbol{I}_d - P_{\Phi(\boldsymbol{x})}\big) J_\Phi(\boldsymbol{x}). \tag{4.1}$$

Proof. Again we divide the proof into three steps to favor a neater exposition. We first notice that, since C^ε is symmetric, we have $D_{\boldsymbol{y}} C^\varepsilon(\boldsymbol{x}, \boldsymbol{y}) = D_{\boldsymbol{x}} C^\varepsilon(\boldsymbol{y}, \boldsymbol{x})$

and thus Assumptions *H1* and *H2* hold as well for $D_{\boldsymbol{y}}C^{\varepsilon}(\boldsymbol{x},\boldsymbol{y})$, and also entail that $\kappa(\boldsymbol{x}) = C^{\varepsilon}(\boldsymbol{x},\boldsymbol{x})$ is a constant function.

1. In concert with Proposition 2, *H3* implies that C^{ε} is positively homogeneous of order 0 with respect to $\boldsymbol{x}$ and $\boldsymbol{y}$. Thus it is entirely defined by its values on $\mathbb{S}^{d-1}$.

2. The function $\alpha(\boldsymbol{y})$, given by Equation (3.10) is well defined in virtue of assumption *H3*, and thus it is positively homogeneous of order 0. Indeed, since C^{ε} is homogeneous of order 0, its differentials $D_{\boldsymbol{x}}C^{\varepsilon}$ and $D_{\boldsymbol{y}}C^{\varepsilon}$ are positively homogeneous of order 1. Thus, the integral $\alpha(\cdot)$ in Equation (3.10) is positively homogeneous of order 0. This also means that Φ is positively homogeneous of order 1.

Next, using orthogonal transformations, one may assume under *H2* that $D_{\boldsymbol{x}}C^{\varepsilon}(\boldsymbol{e}_1,\boldsymbol{y}) \neq 0$. Therefore, $D_{\boldsymbol{x}}C^{\varepsilon}(\boldsymbol{e}_1,\boldsymbol{y})\Lambda \neq 0$, and $D_{\boldsymbol{x}}C^{\varepsilon}(\boldsymbol{e}_1,\boldsymbol{y})\Lambda_{\bullet,1} = 0$. Thus, $|D_{\boldsymbol{x}}C^{\varepsilon}(\boldsymbol{e}_1,\boldsymbol{y})\Gamma|^2 = \sum_{j\geq 2}\big(D_{\boldsymbol{x}}C^{\varepsilon}(\boldsymbol{e}_1,\boldsymbol{y})\Lambda_{\bullet,j}\big)^2$, that is $|\Phi(\boldsymbol{y})|^2 = |\boldsymbol{y}|^2\big(\cos^2(\alpha(\boldsymbol{y}))+\sin^2(\alpha(\boldsymbol{y}))\big) = |\boldsymbol{y}|^2$. This means that the transformation Φ preserves norms.

Next, according to Proposition 1, Equation (4.1) can be written as

$$D_{\boldsymbol{x}}C^{\varepsilon}(\boldsymbol{x},\boldsymbol{y}) = R'\big(\beta_\Phi(\boldsymbol{x},\boldsymbol{y})\big)D_{\boldsymbol{x}}\beta_\Phi(\boldsymbol{x},\boldsymbol{y}).$$

Since a similar result holds for $D_{\boldsymbol{y}}C^{\varepsilon}(\boldsymbol{x},\boldsymbol{y})$, setting $\boldsymbol{w} = (\boldsymbol{x},\boldsymbol{y}) \in \mathbb{S}^{d-1}\times\mathbb{S}^{d-1}$, one can summarize these latter equations into

$$D_{\boldsymbol{w}}C^{\varepsilon}(\boldsymbol{w}) = R'\big(\beta_\Phi(\boldsymbol{w})\big)D_{\boldsymbol{w}}\beta_\Phi(\boldsymbol{w}). \tag{4.2}$$

3. For a small ε, there exists, for any couple $\boldsymbol{w} = (\boldsymbol{x},\boldsymbol{y})$ of $\mathbb{S}^{d-1}$, at least an unit vector $\boldsymbol{z} \in \mathbb{S}^{d-1}$ such that, the segment $\gamma_{\boldsymbol{w}}(t) = (1-t)\boldsymbol{w}_0 + t\boldsymbol{w} \in \mathcal{D}^{\varepsilon}\times\mathcal{D}^{\varepsilon}$ for all $t\in[0,1]$, where $\boldsymbol{w}_0 = (\boldsymbol{z},\boldsymbol{z})$. One can take for example $\boldsymbol{z} = (\boldsymbol{x}+\boldsymbol{y})/|\boldsymbol{x}+\boldsymbol{y}|$ if $\boldsymbol{y}\neq -\boldsymbol{x}$, and $\boldsymbol{z}$ being any unit vector orthogonal to $\boldsymbol{x}$ otherwise.

Next, let us observe that the functions $c(t) = C^{\varepsilon}(\gamma_{\boldsymbol{w}}(t))$ and $p(t) = R\big(\beta_\Phi\big(\gamma_{\boldsymbol{w}}(t)\big)\big)$ satisfy

$$c'(t) = D_{\boldsymbol{w}}C^{\varepsilon}(\gamma_{\boldsymbol{w}}(t))\gamma_{\boldsymbol{w}}'(t) \text{ and } p'(t) = R'(\beta_\Phi(\gamma_{\boldsymbol{w}}(t))D_{\boldsymbol{w}}\beta_\Phi(\gamma_{\boldsymbol{w}}(t))\gamma_{\boldsymbol{w}}'(t).$$

Then, using Equation (4.2), we obtain

$$\begin{aligned} C^{\epsilon}(\boldsymbol{w}) - C^{\epsilon}(\boldsymbol{w}_0) &= \int_0^1 c'(s)\mathrm{d}s = \int_0^1 R'\big(\beta_\Phi(\gamma_{\boldsymbol{w}}(s))\big)D_{\boldsymbol{w}}\beta_\Phi(\gamma_{\boldsymbol{w}}(s))\gamma_{\boldsymbol{w}}'(s)\mathrm{d}s \\ &= \int_0^1 p'(s)\mathrm{d}s = p(1)-p(0) = R\big(\beta_\Phi(\boldsymbol{w})\big) - R\big(\beta_\Phi(\boldsymbol{w}_0)\big), \end{aligned}$$

that is $C^{\varepsilon}(\boldsymbol{x},\boldsymbol{y}) = R\big(\beta_\Phi(\boldsymbol{x},\boldsymbol{y})\big) + \big[C^{\varepsilon}(\boldsymbol{z},\boldsymbol{z}) - R\big(\beta_\Phi(\boldsymbol{z},\boldsymbol{z})\big)\big] = R\big(\beta_\Phi(\boldsymbol{x},\boldsymbol{y})\big)+\kappa$, since $C^{\varepsilon}(\boldsymbol{z},\boldsymbol{z})$ is constant and $\beta_\Phi(\boldsymbol{z},\boldsymbol{z}) = 1$. □

Remark 6. The attentive reader might argue on whether the assumptions in Theorem 3 are sharp. For example, the covariance function $C(\boldsymbol{x},\boldsymbol{y}) \equiv 1$ can be reduced to isotropy with any diffeomorphism Φ although *H2* is not satisfied. One can also notice that Assumption *H4* (related to R) is subordinate to *H3* (related to Φ) and thus can be partially redundant. This can be seen through

Equation (4.2): if R' vanishes on a whole segment of $[-1, 1]$, then $D_{\boldsymbol{w}} C^{\varepsilon}$ vanishes as well and Φ can not be well defined at all by Equations (3.9)–(3.10). Our set of assumptions is however not far from the optimal ones ensuring the reducibility of C for smooth and regular covariance functions as it can be seen through the results of Theorem 2.

Further, since the differentials are local indicators, one can rely on local $\mathbb{S}^{d-1}$ diffeomorphisms and thus weaken this set of assumptions.

Last but not least, this work does not deapen into differentiability of covariance functions on spheres, for which detailed results can be found in Ziegel (2014) and Trübner and Ziegel (2017).

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Appendix A: Characterization of orthogonal matrices

Since uniqueness of the diffeomorphism is only defined up to orthogonal transformations, we give here for sake of completeness, some existing results regarding their characterization and parametrization issues. A full characterization of orthogonal transformations can be provided only within complex spaces, and for that purpose, let us recall that the adjoint of a complex matrix A is the conjugate transpose $A^* = \overline{A}^\top$.

A complex (or real) valued matrix A is called *unitary* if $A^* = A^{-1}$. Apparently, real-valued orthogonal matrices are unitary. Thus, the concept of real orthogonal matrices extends naturally to a complex unitary matrix A via the property $(A\boldsymbol{x})^* A\boldsymbol{y} = \boldsymbol{x}^* A^* A\boldsymbol{y} = \boldsymbol{x}^*\boldsymbol{y}$ for any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{C}^d$.

We similarly need the extension of the notion of antisymmetry. A matrix B is called *antihermitian* if $B^* = -B$. Rephrased, an antihermitian matrix B has the form:

$$B = \begin{bmatrix} b_{1,1} & b_{1,2} & \dots & b_{1,d} \\ -\overline{b}_{1,2} & \ddots & & \vdots \\ \vdots & & & b_{d-1,d} \\ -\overline{b}_{1,d} & \dots & -\overline{b}_{d-1,d} & b_{d,d} \end{bmatrix}.$$

Note that the diagonal coefficients $b_{j,j},\ j = 1, \dots, d$ are therefore vanishing or pure imaginary numbers. Finally, let us recall that the *exponential matrix* A of any matrix B is defined through the series:

$$A = e^B = \sum_{k=0}^{\infty} \frac{B^k}{k!}.$$

A useful fact is that B antisymmetric implies e^B orthogonal. This is due to the fact that $B^\top = -B$, so that $A^{-1} = e^{-B} = e^{B^\top} = (e^B)^\top = A$. However, the converse proposition is only true in the complex context. The following result will turn to be the useful one for parametrization purpose.

Lemma 2. *A complex valued matrix A is unitary if and only if there exists an antihermitian matrix B such that $A = e^B$.*

Proof. The proof of the if part is analogous to the real case. Le B be antihermitian. If $A = e^B$, then $A^* = e^{B^*} = e^{-B} = A^{-1}$. To show the necessary part of the assertion, notice that any unitary matrix A is invertible and diogonalizable, so that $A = U\Lambda U^*$, with U unitary and $\Lambda = \mathrm{diag}(\lambda_j)$ with $\lambda_j\overline{\lambda}_j = 1$, $j = 1, \dots, d$ (Gantmacher, 1960). The last equalities imply that Λ is also unitary. Invertibility implies that there exists possibly many matrices B such $A = e^B$. Thus, we only need prove that we can always choose a matrix B that is antihermitian. Among solutions B of equation $A = e^B$, we can choose $B = U\log(\Lambda)U^*$, where $\log(\Lambda) = \mathrm{diag}(\log(\lambda_j))$. Now, we notice that $(\log(\Lambda))^* = -\log(\Lambda)$ because $\lambda_j\overline{\lambda}_j = 1$, for all j. Consequently, $B^* = -U\log(\Lambda)U^* = -B$. $\square$

Remark 7. Lemma 2 describes how the set of $d \times d$ unitary matrices is in bijection with $(\imath\mathbb{R})^d \times \mathbb{C}^{d(d-1)/2}$. Thus, $d + 2d(d-1)/2 = d^2$ real parameters are needed to uniquely define a unitary matrix. However, for $A = e^B$ to be real valued when B is antihermitian (complex valued in general), the components b_{ij} of B are necessarily real or complex conjugates Gantmacher (1960) so that a real orthogonal matrix A can be identified by $d(d-1)/2$ parameters at most.

Remark 8. The group of orthogonal transformations includes the classical set of space rotations, but also other useful transformations, such the space reflexions.

Appendix B: Positively homogeneous transformations leaving spheres invariant

A part of the lemma below was used to establish the results obtained in this paper. The other part, of potential interest, is given for sake of completeness as we think that parallel approaches can be taken as well to shed new light on the issue.

Lemma 3. *Let $\alpha \geq 0$, and let $\Phi : \mathcal{D} \subset \mathbb{R}^d \to \mathbb{R}^d$ be any differentiable and positively homogeneous of order α. Then, for $\boldsymbol{x} \in \mathcal{D}$,* *1.-* $|\Phi(\boldsymbol{x}/|\boldsymbol{x}|)| = 1$ *if and only if* $J_\Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{x}) = \alpha\boldsymbol{x}/|\boldsymbol{x}|^{2(1-\alpha)}$*;*

2.- In particular, if Φ_A *is of order* 0 *and* Φ_B *of order 1, then*

2.1.- $J_{\Phi_A}^\top(\boldsymbol{x})\Phi_A(\boldsymbol{x}) = 0$ *and* $J_{\Phi_B}^\top(\boldsymbol{x})\Phi_B(\boldsymbol{x}) = \boldsymbol{x}$*;*

2.2.- If $\Phi_A \equiv \Phi_B$ *on* $\mathbb{S}^{d-1}$*, then for* $\boldsymbol{x} \neq 0$*,*
$J_{\Phi_B}(\boldsymbol{x}) = |\boldsymbol{x}|J_{\Phi_A}(\boldsymbol{x}) + \frac{1}{|\boldsymbol{x}|}\Phi_A(\boldsymbol{x})\boldsymbol{x}^\top$ *and* $J_{\Phi_A}(\boldsymbol{x}) = \frac{1}{|\boldsymbol{x}|}\Big(J_{\Phi_B}(\boldsymbol{x}) + \frac{1}{|\boldsymbol{x}|^2}\Phi_B(\boldsymbol{x})\boldsymbol{x}^\top\Big)$.

Proof. Let $\boldsymbol{x} \in \mathcal{D}^\varepsilon$. Let Φ be a positively homogeneous function of order α. Thus, we have

$$|\Phi(\boldsymbol{x})| = \left|\Phi\left(|\boldsymbol{x}| \cdot \frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right)\right| = |\boldsymbol{x}|^\alpha \left|\Phi\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|}\right)\right|.$$

To prove Assertion *1.*, we call $\rho(\boldsymbol{x}) = \sum_{i=1}^d \phi_i^2(\boldsymbol{x}) - (\sum_{i=1}^d x_i^2)^\alpha$ and we note that $\partial_{x_j}\rho(\boldsymbol{x}) = \sum_{i=1}^d \big(2\partial_{x_j}\phi_i(\boldsymbol{x})\phi_i(\boldsymbol{x})\big) - 2\alpha x_j(\sum_{i=1}^d x_i^2)^{\alpha-1}$. This in turn implies that, if $|\Phi(\boldsymbol{x}/|\boldsymbol{x}|)| = 1$, then $|\Phi(\boldsymbol{x})| = |\boldsymbol{x}|^\alpha$. Thus, $\rho(\boldsymbol{x}) = 0$. Consequently, $\partial_{x_j}\rho(\boldsymbol{x}) = 0$, $j = 1, \dots, d$, and $J_\Phi^\top(\boldsymbol{x})\Phi(\boldsymbol{x}) = \boldsymbol{x}$. The sufficient part of the assertion is proved. To prove the necessary part, let $r \geq 0$ and define, for $\boldsymbol{u} = (r, \theta_1, \dots, \theta_{d-1})$, the usual spherical coordinates $\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{u})$, so that $|\boldsymbol{x}(\boldsymbol{u})| = r$; we have $x_1(\boldsymbol{u}) = r\cos(\theta_1), \dots, x_{d-1}(\boldsymbol{u}) = r\sin(\theta_1)\sin(\theta_2)\cdots\sin(\theta_{d-1})$. Then, consider the function $\widetilde{\rho}(\boldsymbol{u}) = \sum_{i=1}^d \phi_i^2(\boldsymbol{x}(\boldsymbol{u}))$. The partial derivatives with respect to θ_j, $j = 1, \dots, d-1$, yield

$$\partial_{\theta_j}\widetilde{\rho}(\boldsymbol{u}) = 2\sum_{l=1}^d \left(\sum_{i=1}^d \partial_{x_l}\phi_i(\boldsymbol{x}(\boldsymbol{u}))\phi_i(\boldsymbol{x}(\boldsymbol{u}))\right)\partial_{\theta_j}x_l(\boldsymbol{u}),$$

which can be rewritten as

$$\sum_{i=1}^d \partial_{x_l}\phi_i(\boldsymbol{x}(\boldsymbol{u}))\phi_i(\boldsymbol{x}(\boldsymbol{u})) \quad = \quad \alpha x_l(\boldsymbol{u})r^{2(\alpha-1)},$$

since $\partial_{\theta_j}\widetilde{\rho}(\boldsymbol{u}) = \sum_{l=1}^d 2\partial_{\theta_j}x_l(\boldsymbol{u})\alpha x_l(\boldsymbol{u})r^{2(\alpha-1)}$. Thus, we also have that

$$\partial_{\theta_j}\left(\sum_{l=1}^d x_l^2(\boldsymbol{u})\right)\alpha r^{2(\alpha-1)} = \partial_{\theta_j}(r^2)\alpha r^{2(\alpha-1)} = 0,$$

because r and θ_j are independent variables. Consequently, $\widetilde{\rho}$ is independent of each θ_j. Thus, we can use to abuse of notation $\widetilde{\rho}(\boldsymbol{u}) = \widetilde{\rho}(r)$. Next, a similar calculus shows that $\partial_r\widetilde{\rho}(\boldsymbol{u}) = \partial_r(r^2)\alpha r^{2(\alpha-1)} = \partial_r(r^{2\alpha})$ and this proves that $|\Phi(\boldsymbol{x})| = |\boldsymbol{x}|^\alpha$.

Assertion *2.1.* can be easily proved on the basis of previous arguments.

As for Assertion *2.2.*, it is equivalent to prove that $\Phi_B(\boldsymbol{x}) = |\boldsymbol{x}|\Phi_A(\boldsymbol{x})$. By noticing that $D_{\boldsymbol{x}}(|\boldsymbol{x}|) = \boldsymbol{x}/|\boldsymbol{x}|$, we get

$$\partial_{x_j}\phi_{B,i}(\boldsymbol{x}) = \frac{x_j}{|\boldsymbol{x}|}\phi_{A,i}(\boldsymbol{x}) + |\boldsymbol{x}|\partial_{x_j}\phi_{A,i}(\boldsymbol{x}).$$

The proof is complete. □