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Construction of Correlation Functions in Two and Three Dimensions

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This document, Office Note 96-03R1, is the first revision of Office Note 96-03. The major revisions to Office Note 96-03 are listed below.

• The abstract and introduction were both modified to reflect revisions to Office Note 96-03.

• Section 2 was divided into four subsections. Much of the material differs only slightly from the original. The material in Section 2.2 significantly extends the development in Office Note 96-03.

• To maintain consistency with the notation used in the refereed publication related to this document, the subsection numbering was modified from that of Office Note 96-03. Theorem 3.1.5 (now Theorem 3.a.5) was strengthened. Consequently, the proof given is more involved than the original one. The proofs of Theorems 3.1.3 and 3.1.5, originally in Section 3 of Office Note 96-03, now appear in the Appendix. The detailed reduction of the integrals in the proof of Theorem 3.3.1, now appear in the Appendix. Several minor changes were made to several proofs to improve the clarity of presentation.

• The first three examples of Section 4 differ only slightly from those given in Office Note 96-03. The fourth example (Section 4.4) is new.

• An Appendix was added. Appendix A.1, A.2, and A.3 contain the proofs described above. Appendix A.4 is new.

• Four additional figures (Figures 9-12) were added. Sharper images of Figures 1-8 replace those given in Office Note 96-03.

Abstract

This article focuses on the construction, directly in physical space, of simply parameterized covariance functions for data assimilation applications. A self-contained, rigorous mathematical summary of relevant topics from correlation theory is provided as a foundation for this construction. Covariance and correlation functions are defined, and common notions of homogeneity and isotropy are clarified. Classical results are stated, and proven where instructive. Included are smoothness properties relevant to multivariate statistical analysis algorithms where wind/wind and wind/mass correlation models are obtained by differentiating the correlation model of a mass variable. The Convolution Theorem is introduced as the primary tool used to construct classes of covariance and cross-covariance functions on R^3. Among these are classes of compactly supported functions that restrict to covariance and cross-covariance functions on the unit sphere S^2, and that vanish identically on subsets of positive measure on S^2. It is shown that these covariance and cross-covariance functions on S^2, referred to as being *space-limited*, cannot be obtained using truncated spectral expansions. Compactly supported and space-limited covariance functions determine sparse covariance matrices when evaluated on a grid, thereby easing computational burdens in atmospheric data analysis algorithms.

Convolution integrals leading to practical examples of compactly supported covariance and cross-covariance functions on R^3 are reduced and evaluated. More specifically, suppose that g_i and g_j are radially symmetric functions defined on R^3 such that

$$g_i(\mathbf{x}) = 0 \quad \text{for} \quad \|\mathbf{x}\| > d_i \qquad \text{and} \qquad g_j(\mathbf{x}) = 0 \quad \text{for} \quad \|\mathbf{x}\| > d_j, \quad 0 < d_i, d_j \leq \infty,$$

where $\|\cdot\|$ denotes Euclidean distance in R^3. The parameters d_i and d_j are "cutoff" distances. Closed-form expressions are determined for classes of convolution cross-covariance functions

$$C_{ij}(\mathbf{x}, \mathbf{y}) := (g_i * g_j)(\mathbf{x} - \mathbf{y}), \qquad i \neq j,$$

and convolution covariance functions

$$C_{ii}(\mathbf{x}, \mathbf{y}) := (g_i * g_i)(\mathbf{x} - \mathbf{y}),$$

vanishing for $\|\mathbf{x} - \mathbf{y}\| > d_i + d_j$ and $\|\mathbf{x} - \mathbf{y}\| > 2d_i$, respectively. Additional covariance functions on R^3 are constructed using convolutions over R, rather than R^3. Families of compactly supported approximants to standard second- and third-order autoregressive functions are constructed as illustrative examples. Compactly supported covariance functions of the form

$$C(\mathbf{x}, \mathbf{y}) \quad := \quad C_0(\|\mathbf{x} - \mathbf{y}\|), \quad \mathbf{x}, \mathbf{y} \in R^3,$$

where the functions $C_0(r)$ for $r \in R$ are 5th-order piecewise rational functions, are also constructed. These functions are used to develop space-limited product covariance functions

$$B(\mathbf{x}, \mathbf{y})\, C(\mathbf{x}, \mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in S^2,$$

approximating given covariance functions $B(\mathbf{x}, \mathbf{y})$ supported on all of $S^2 \times S^2$.

Contents

1 Introduction

Operational atmospheric data assimilation systems have for many years required the specification of forecast and observation error covariances in two and three space dimensions using functions depending on a number of tunable parameters (Daley, 1991). There are many examples of simply parameterized covariance functions for statistical analysis of data in one dimension. Applications can be found, for instance, in signal analysis (Papoulis, 1984) and in time-series analysis (Priestley, 1981). Geophysical error fields, unlike one-dimensional error fields, are usually regarded as being distributed on all or part of a three-dimensional spherical annulus, and therefore can be conveniently modeled by random fields on subsets of R^3 (Christakos, 1992; Vanmarcke, 1983). In the current generation of spectral statistical analysis schemes for atmospheric data assimilation, for example, isotropic forecast error covariance or correlation functions are defined on spherical surfaces by means of truncated Legendre expansions (Parrish and Derber, 1992; Courtier *et al.*, 1998). In contrast to the one-dimensional setting, the development of correlation theory in higher dimensions has hardly been influenced by practical applications. Advanced data assimilation systems require flexible covariance models (Cohn *et al.*, 1998), and correlation theory tailored to data assimilation applications should aid the development of covariance models likely to improve analyses and forecasts in these systems.

This article represents an effort to develop basic theoretical and practical tools needed to construct flexible covariance functions for applications in data assimilation. We hope to achieve two major goals. The first is to expose, in a digestible format, mathematical theory relevant to the construction of simply parameterized covariance functions for data assimilation applications. The second is to provide the reader with algorithms for this construction, together with several illustrative examples. Since our covariance functions are constructed directly in physical space, their properties differ from those obtained through truncated Legendre expansions. One notable advantage is our ability to construct spatially limited covariance functions on the globe. This cannot be done using truncated Legendre expansions, as we show in Section 3.b. Approximations to such covariance functions have been developed at the European Centre for Medium-Range Weather Forecasts (Courtier *et al.*, 1998; Rabier *et al.*, 1998).

These spatially limited covariance functions are obtained by first constructing compactly supported covariance functions

$$C(\mathbf{x}, \mathbf{y}), \qquad \mathbf{x}, \mathbf{y} \in R^3,$$

depending on a tunable cutoff distance d such that $C(\mathbf{x}, \mathbf{y}) = 0$ whenever the Euclidean distance between $\mathbf{x}$ and $\mathbf{y}$ exceeds d. By then restricting $\mathbf{x}$ and $\mathbf{y}$ to the unit sphere S^2 and taking d less than the diameter of S^2, we obtain what we will call *space-limited* covariance functions on S^2. Space-limited covariance functions on S^2 and compactly supported covariance functions on R^3 determine *sparse* covariance matrices through grid evaluation, thereby reducing both storage and computational requirements, which are important considerations for the Physical-space Statistical Analysis System under development at the Data Assimilation Office (Cohn *et al.*, 1998). Compactly supported n-dimensional "spherical" covariance functions have already been used in geological applications (Armstrong and Diamond, 1984; Oliver, 1995). In interpolation theory, Wu (1995) obtained a class of compactly supported covariance functions on R^n in the form of "cutoff polynomials", using techniques different from those given in the present article. Compactly supported and/or space-limited assumptions are justifiable whenever covariances between points further apart than some cutoff distance are either known to be negligible (Hollingsworth and Lönnberg, 1986; Lönnberg and Hollingsworth, 1986), or are not known well enough to justify computational expense.

Because the terminology in correlation theory is not standard, we will provide formal definitions as needed throughout this article. A brief, informal exposition will suffice for now. A *correlation function* on a domain D (such as R^3 for instance) is a *covariance function* $C(\mathbf{x}, \mathbf{y})$ normalized through division by the standard deviations $C(\mathbf{x}, \mathbf{x})^{1/2}$ and $C(\mathbf{y}, \mathbf{y})^{1/2}$, where $\mathbf{x}$ and $\mathbf{y}$ are points in D. Covariance functions on D are those functions which determine *positive-semidefinite* matrices when evaluated on any grid over D. Thus in particular, the property of being a covariance function is *hereditary*: if C is a covariance function on D then it is also a covariance function on *every* subset of D. This article exploits the fact that covariance functions on S^2 can be obtained by restricting covariance functions on R^3 to S^2. The class of *autocorrelation* functions often used in electrical engineering is obtained through self-convolution of finite-energy signals defined on R (Papoulis, 1962), and is contained in the class of covariance functions on R. *Cross-covariance* and *cross-correlation* functions are defined for multivariate or multidimensional random fields. In geophysical applications, they are used to model covariances between different geophysical fields, or between different layers of the atmosphere, ocean, or solid earth, with the autocorrelation functions used to model covariances between points on each separate level. General definitions of cross-covariance functions are given in Christakos (1992) and Yaglom (1987, Ch. 4). Our definition uses cross-convolution, and is given in Section 3.c. This is the definition commonly used throughout the electrical engineering literature.

While correlation functions on a given domain D restrict to all subsets of D, these functions are not necessarily correlation functions on supersets of D. In Weber and Talkner (1993), for example, it was shown that standard time-series correlation functions which have commonly been used to model spatial correlations on so-called meteorologically significant spaces, such as S^2 and R^2, are not always valid correlation functions on these spaces. Special techniques are necessary to develop correlation functions on such spaces.

Two main themes from multidimensional/multivariate correlation theory are prominent in this article. The first is construction of homogeneous, isotropic correlation functions on R^3 using representing functions on R having monotonically decreasing one-dimensional Fourier transforms. Examples of parameterized correlation functions of this type abound in the time-series literature (*e.g.*, Papoulis, 1962, Example 12.2; Thiébaux and Pedder, 1987, p. 150). Correlation length scales are typical parameters. The primary advantage of this approach is the simplicity of the condition for determining valid correlation functions on R^3. However, it does not give a general procedure for construction of compactly supported correlation functions. The latter theme is constructive development of multivariate and multidimensional correlation functions through convolutions. Convolution is particularly effective for construction of both compactly supported and space-limited correlation functions. Thus the second theme complements the first.

Most correlation functions developed in this article are homogeneous and/or isotropic. Sample correlations of geophysical fields rarely have such special symmetries; however, there are many ways to construct nonhomogeneous and/or anisotropic correlation functions through transformations of homogeneous and/or isotropic correlation ones. One such transformation is illustrated by Example 2.6 below. Coordinate stretching is perhaps the most common technique used to construct anisotropic from isotropic correlation functions. This technique has been applied by Borgman and Chao (1994) to estimate the covariance function from data located irregularly in space, and by Derber and Rosati (1989) and Carton and Hackert (1990) for ocean data assimilation. A change of coordinates yielding flow-dependent anisotropic correlation functions has been described by Riishøjgaard (1998).

Background material for this article is summarized in Section 2. Covariance and correlation functions are defined, and common notions of homogeneity and isotropy are discussed. Classical results from correlation theory and from Fourier analysis are also introduced, including the Convolution Theorem. Section 3 contains theoretical results pertinent to correlation modeling on R^3 and S^2. Section 3.a develops properties of the convolution functions $g * g$ obtained by self-convolving radially symmetric functions g over R^3. Included are smoothness properties of $g * g$ relevant to multivariate statistical analysis algorithms where wind/wind and wind/mass correlation models are obtained by differentiating the correlation function of a mass variable (Daley, 1991, Ch. 5). The construction of correlation functions over R^3 using convolutions over R is also described. It is shown in Section 3.b that finite spectral expansions never determine space-limited isotropic correlation functions. Section 3.c gives a practical algorithm for evaluating the convolution integrals $g_i * g_j$, where g_i and g_j are both radially symmetric functions defined on R^3. Section 4 provides examples of convolution correlation functions. Families of compactly supported second-order autoregressive (SOAR)-like and compactly supported third-order autoregressive (TOAR)-like correlation functions are constructed. Compactly supported correlation functions of the form

$$C(\mathbf{x}, \mathbf{y}) \; := \; C_0(\|\mathbf{x} - \mathbf{y}\|), \quad \mathbf{x}, \mathbf{y} \in R^3,$$

where the functions $C_0(r)$ for $r \in R$ are 5th-order piecewise rational functions, are also constructed. These functions are used to develop space-limited product correlation functions

$$B(\mathbf{x}, \mathbf{y})\, C(\mathbf{x}, \mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in S^2,$$

approximating given correlation functions $B(\mathbf{x}, \mathbf{y})$ supported on all of $S^2 \times S^2$. Concluding remarks are given in Section 5. An Appendix contains detailed proofs of several results described in the text.

Although the development in this article is general, the results are slanted toward single-level univariate applications. The methodology extends readily to the nonseparable, multivariate setting, and results on this topic will be the subject of future articles. Covariance functions developed in this article have been successfully tuned to observed data using the maximum-likelihood estimation procedure developed by Dee (1995) and the generalized cross-validation technique of Wahba (1990, Ch. 4). These results are reported in Dee and da Silva (1998) and Dee *et al.* (1998).

2 Background Material

The purpose of this section is to summarize notation, definitions, and a variety of known results pertinent to correlation function modeling on R^3 and subsets of R^3. The general context of this summary is the correlation theory of *real-valued* (that is, scalar) random fields defined on a set W. The theory pertains primarily to the case where W is either Euclidean space R^n or the unit sphere S^{n-1}, however, emphasis is given to specialized results for R^3. It follows from Definition 2.2 below that correlation functions restrict to subsets, so that in particular, correlation functions on S^2 are readily obtained through restricting correlation functions on R^3 to S^2. This is the approach taken in this article, and it provides a simple and direct way of constructing a large class of correlation functions on S^2. In particular, this is a natural way to construct space-limited correlation functions.

The notation that follows abbreviates integrals over all R^n to integrals without limits where convenient:

$$\int f(\mathbf{x})\, d\mathbf{x} \quad \text{means} \quad \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(x_1, \ldots, x_n)\; dx_1 \ldots dx_n.$$

The space of integrable functions on R^n is denoted as $L^1(R^n)$, while the space of square-integrable functions on R^n is denoted by $L^2(R^n)$. The inner product of two (generally complex-valued) functions f_1 and f_2 in $L^2(R^n)$ is defined in the usual way:

$$(f_1, f_2) := \int f_1(\mathbf{x}) \overline{f_2(\mathbf{x})} \, d\mathbf{x}.$$

The notation $\mathbf{w} \cdot \mathbf{r}$ will denote the dot product of two vectors $\mathbf{w}$ and $\mathbf{r}$ in R^n.

2.1 Covariance and Correlation Functions: Definitions

Definition 2.1: *A function $B(\mathbf{x}, \mathbf{y})$ is the covariance function of a random field X defined on W if*

$$B(\mathbf{x}, \mathbf{y}) = \Big\langle (X(\mathbf{x}) - < X(\mathbf{x}) >) \, (X(\mathbf{y}) - < X(\mathbf{y}) >) \Big\rangle,$$

where $< \cdot >$ denotes mathematical expectation. □

It follows immediately that covariance functions are symmetric, that is,

$$B(\mathbf{x}, \mathbf{y}) = B(\mathbf{y}, \mathbf{x}). \tag{2.1}$$

Definition 2.1 provides a useful conceptual reference point, but actually using it to construct covariance functions $B(\mathbf{x}, \mathbf{y})$ would require knowledge of all multidimensional probability distribution functions of the underlying random field X. The following two alternative definitions provide a starting point for correlation function modeling in which no assumptions about the underlying probability distribution functions, other than existence of the expectation given in Definition 2.1, are required. Definition 2.2 is shown to be equivalent to Definition 2.1 in Loève (1963, pp. 466-467) or Wahba (1990, pp. 1-2), for example.

Definition 2.2: *A function $B(\mathbf{x}, \mathbf{y})$ is a covariance function on W if for each positive integer m, and for each choice of points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m$ in W, the matrix $\{B(\mathbf{x}_i, \mathbf{x}_j)\}$ is positive semidefinite.* □

The fact that covariance functions restrict to subsets of $W \times W$ follows from Definition 2.2: if $T \times T$ is any subset of $W \times W$ and the points $\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_m$ lie in T, then the fact that these points are also in W implies that the matrix $\{B(\mathbf{x}_i, \mathbf{x}_j)\}$ is positive semidefinite. That is, if $B(\mathbf{x}, \mathbf{y})$ is a covariance function on W, then it is also a covariance function on T. Example 2.6 below is one illustration of this principle.

If $B_1(\mathbf{x}, \mathbf{y})$ and $B_2(\mathbf{x}, \mathbf{y})$ are both covariance functions on W, then by the Schur product theorem (*cf.* Horn and Johnson, 1985, p. 458) and Definition 2.2, the product function

$$B_1(\mathbf{x}, \mathbf{y}) \, B_2(\mathbf{x}, \mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in W,$$

is also a covariance function on W. This property is used in Example 4.d.

Definition 2.2 is a *general* test for covariance functions on any set W. This definition is also useful as an experimental test for candidate covariance functions on a given, fixed grid.

Definition 2.3, as well as most of the results in the sequel, applies to correlation rather than covariance functions. A correlation function C is obtained from a covariance function B

through normalizing by the *standard deviations* $B(\mathbf{x},\mathbf{x})^{1/2}$ and $B(\mathbf{y},\mathbf{y})^{1/2}$:

$$C(\mathbf{x},\mathbf{y}) \;:=\; \frac{B(\mathbf{x},\mathbf{y})}{[B(\mathbf{x},\mathbf{x})\cdot B(\mathbf{y},\mathbf{y})]^{1/2}}. \tag{2.2}$$

Definition 2.2 implies that the *variance function* $B(\mathbf{x},\mathbf{x})$ is everywhere nonnegative, and in all that follows it will be assumed that $B(\mathbf{x},\mathbf{x})$ is in fact *strictly positive*, so that the correlation function (2.2) corresponding to a given covariance function is well-defined. From Definition 2.2 it follows that this correlation function is itself also a covariance function. In addition, Definition 2.3 applies only to correlation functions that lie in $L^2(R^n \times R^n)$. Since many classical results from correlation theory pertain only to such functions, Definition 2.3 will serve as the most convenient reference point for the general theoretical development in this article. The grid-independent nature of covariance functions is also clearly illustrated through this definition.

Applying the Cauchy-Schwartz inequality to the covariance function B in Definition 2.1 shows that C in Eq. (2.2) is bounded by one in absolute value. Note also that C assumes its maximum on the diagonal of $W \times W$, that is

$$C(\mathbf{x},\mathbf{x}) \;\equiv\; 1.$$

Because correlation functions are dimensionless, technical definitions and results that follow can be stated more simply than the corresponding statements for covariance functions. Nothing essential is lost in the transition between covariance and correlation functions. Only the standard deviations are necessary to recover the covariance function B from the correlation function C.

Definition 2.3: *Let the integral operator T be defined for real-valued functions f on $L^2(R^n)$ by*

$$Tf(\mathbf{x}) := \int C(\mathbf{x},\mathbf{y})f(\mathbf{y})\,d\mathbf{y}, \tag{2.3}$$

where the kernel C lies in $L^2(R^n \times R^n)$, is symmetric, that is, $C(\mathbf{x},\mathbf{y}) = C(\mathbf{y},\mathbf{x})$, is continuous, and satisfies $C(\mathbf{x},\mathbf{x}) = 1$. The operator T is called a correlation operator if it is non-negative, that is, if

$$(Tf,f) \;=\; \int\!\!\int C(\mathbf{x},\mathbf{y})\,f(\mathbf{x})\,f(\mathbf{y})\,d\mathbf{x}\,d\mathbf{y} \;\geq\; 0 \tag{2.4}$$

for every real-valued $f \in L^2(R^n)$. The kernel C of such an operator T is called a correlation function on R^n. □

Formula (2.3) is just an infinite-dimensional generalization of matrix-vector multiplication in finite dimensions, and (2.4) is the corresponding infinite-dimensional generalization of the finite-dimensional condition expressed by Definition 2.2.

An assumption that correlation functions are *continuous* appears in Definition 2.3, and is utilized throughout much of the sequel. The Fourier analysis applied to correlation function modeling in this article simplifies when the correlation functions are assumed continuous. Results can be established in this setting which otherwise would require more advanced mathematical tools to establish, or which would not be true under more general assumptions. In addition, self-convolution functions $B_1 * B_1$ over R^n are continuous whenever B_1 lies in $L^2(R^n)$ (*e.g.*, Stein and Weiss, 1971, p. 16). Theorems 2.13 and 2.14 below also illustrate that the continuity assumption is not unduly restrictive.

Definitions 2.1, 2.2, and 2.3 are equivalent whenever the kernel C satisfies the conditions of Definition 2.3. To see that Definition 2.1 implies Definition 2.3, let C be a continuous correlation function

$$C(\mathbf{x},\mathbf{y}) = \left\langle Y(\mathbf{x})\, Y(\mathbf{y}) \right\rangle$$

for some zero-mean random field $Y = X - < X >$. The linearity of the expectation operator implies that

$$\begin{aligned} &\int\int C(\mathbf{x},\mathbf{y})\, f(\mathbf{x})\, f(\mathbf{y})\, d\mathbf{x}\, d\mathbf{y} \\ &= \int\int \left\langle Y(\mathbf{x})\, Y(\mathbf{y}) \right\rangle f(\mathbf{x})\, f(\mathbf{y})\, d\mathbf{x}\, d\mathbf{y} \\ &= \left\langle \int Y(\mathbf{x}) f(\mathbf{x})\, d\mathbf{x} \int Y(\mathbf{y}) f(\mathbf{y})\, d\mathbf{y} \right\rangle \\ &= \left\langle \left| \int Y(\mathbf{z}) f(\mathbf{z})\, d\mathbf{z} \right|^2 \right\rangle \geq 0, \end{aligned}$$

which is Eq. (2.4). The proof that Definition 2.3 implies Definition 2.2 is a simple generalization of the one-dimensional argument found, for example, in Gelfand and Vilenkin (1964, pp. 152-157) or Horn and Johnson (1985, pp. 462-463).

2.2 Homogeneity and Isotropy

Notions of homogeneity and isotropy for functions on $R^n \times R^n$ are defined below, and a notion of isotropy on $S^{n-1} \times S^{n-1}$ is also introduced. The general context for these definitions involves the action of a transitive group of motions on a homogeneous space, and belongs to the theory of Lie groups (*cf.* Yaglom, 1987, pp. 383-384; Warner, 1983, pp. 120-136). Although this context is not prerequisite to the material in this article, the reader should understand that different notions of homogeneity and isotropy exist due to the variety of homogeneous spaces and transitive group actions on these spaces. The terminology introduced below associates the notion of homogeneity with functions on $R^n \times R^n$ that are invariant under the translation group acting on R^n. The notion of isotropy is defined for functions on $R^n \times R^n$ and on $S^{n-1} \times S^{n-1}$ that are invariant under the orthogonal group acting on R^n. This naming convention is common throughout the correlation theory literature (*cf.* Yaglom, 1987, p. 323, p. 348; Yadrenko, 1983, p. 1).

Definition 2.4: *If a function $C(\mathbf{x},\mathbf{y})$ defined on $R^n \times R^n$ is componentwise invariant under all translations T of R^n, that is, if*

$$C(T(\mathbf{x}), T(\mathbf{y})) = C(\mathbf{x},\mathbf{y}), \tag{2.5}$$

then C is called homogeneous on R^n. □

Homogeneous functions defined on $R^n \times R^n$ can be represented by functions defined on R^n as follows. Given the homogeneous function $C(\mathbf{x},\mathbf{y})$, define

$$C_1(\mathbf{x}) \;:=\; C(\mathbf{x},\mathbf{0}). \tag{2.6}$$

If $T_{\mathbf{y}}$ is translation by $\mathbf{y}$:

$$T_{\mathbf{y}}(\mathbf{z}) \;=\; \mathbf{y} + \mathbf{z},$$

then

$$C_1(\mathbf{x} - \mathbf{y}) \;=\; C(\mathbf{x}-\mathbf{y},\mathbf{0}) \;=\; C(T_{\mathbf{y}}(\mathbf{x}-\mathbf{y}), T_{\mathbf{y}}(\mathbf{0})) \;=\; C(\mathbf{x},\mathbf{y}). \tag{2.7}$$

The function C_1 will be said to *represent* the homogeneous function C. Observe that formula (2.7) implies that $C_1(\mathbf{0}) = 1$ whenever C is a homogeneous *correlation* function. Further, in this case C_1 is also an *even* function with respect to each of its arguments, by virtue of the symmetry property (2.1) of correlation functions:

$$C_1(\text{-}\mathbf{y}) = C(\mathbf{0}, \mathbf{y}) = C(\mathbf{y}, \mathbf{0}) = C_1(\mathbf{y}). \tag{2.8}$$

Functions satisfying Eq. (2.8) will simply be referred to as even functions.

Definition 2.5: *If a function $C(\mathbf{x}, \mathbf{y})$ defined on $R^n \times R^n$ $(S^{n-1} \times S^{n-1})$ is componentwise invariant under all orthogonal transformations g of R^n, that is, if*

$$C(g(\mathbf{x}), g(\mathbf{y})) = C(\mathbf{x}, \mathbf{y}), \tag{2.9}$$

then C is called isotropic on R^n (S^{n-1}). □

A *rigid motion* of R^n is any map $\psi : R^n \to R^n$ (not necessarily linear) that preserves the Euclidean distance between any pair of points, *i.e.,*

$$\|\psi(\mathbf{x}) - \psi(\mathbf{y})\| = \|\mathbf{x} - \mathbf{y}\|, \qquad \mathbf{x}, \mathbf{y} \in R^n.$$

The orthogonal transformations g of R^n are rigid motions of R^n that are also linear transformations. If $g : R^n \to R^n$ is an orthogonal transformation, then

$$\|g(\mathbf{x} - \mathbf{y})\| = \|g(\mathbf{x}) - g(\mathbf{y})\| = \|\mathbf{x} - \mathbf{y}\|, \qquad \mathbf{x}, \mathbf{y} \in R^n,$$

where the first equality is due to the linearity of g, and the second is due to the fact that g is a rigid motion. Setting $\mathbf{y} = \mathbf{0}$ yields

$$\|g(\mathbf{x})\| = \|\mathbf{x}\|, \qquad \mathbf{x} \in R^n.$$

Thus, g is either a rotation of R^n, or a reflection of R^n.

Translations of R^n are also rigid motions of R^n, but all translations except the identity mapping are non-linear transformations. Given any $n-$vector $\mathbf{w}$, the translation

$$T_{\mathbf{w}}(\mathbf{z}) = \mathbf{w} + \mathbf{z}$$

is a rigid motion since

$$\|T_{\mathbf{w}}(\mathbf{x}) - T_{\mathbf{w}}(\mathbf{y})\| = \|\mathbf{w} + \mathbf{x} - (\mathbf{w} + \mathbf{y})\| = \|\mathbf{x} - \mathbf{y}\|, \qquad \mathbf{x}, \mathbf{y} \in R^n.$$

Observe that $T_{\mathbf{w}}(\mathbf{z})$ is a linear transformation if, and only if,

$$\mathbf{w} + \mathbf{x} + \mathbf{y} = T_{\mathbf{w}}(\mathbf{x} + \mathbf{y}) = T_{\mathbf{w}}(\mathbf{x}) + T_{\mathbf{w}}(\mathbf{y}) = \mathbf{w} + \mathbf{x} + \mathbf{w} + \mathbf{y},$$

which holds if, and only if, $\mathbf{w} = \mathbf{0}$. In other words, the identity mapping

$$T_{\mathbf{0}}(\mathbf{z}) = \mathbf{z}$$

is the only translation that is a linear transformation.

It is well known (*cf.* Thorpe, 1979, p. 210) that if ψ is any rigid motion of R^n, then there is a unique translation T of R^n, and a unique orthogonal transformation g of R^n, such that

$$\psi = T \circ g. \tag{2.10}$$

Using Eq. (2.10), it can be seen that the homogeneous and isotropic functions defined on $R^n \times R^n$ are those functions that are componentwise invariant under all rigid motions of R^n. Suppose that C is a homogeneous and isotropic function defined on $R^n \times R^n$. If ψ is any rigid motion of R^n, then by Eq. (2.10), $\psi = T \circ g$, where T is a translation acting on R^n and g is an orthogonal transformation acting on R^n. Thus we have that

$$C(\psi(\mathbf{x}), \psi(\mathbf{y})) = C(T \circ g(\mathbf{x}), T \circ g(\mathbf{y})) = C(g(\mathbf{x}), g(\mathbf{y})) = C(\mathbf{x}, \mathbf{y}), \qquad (2.11)$$

where the second equality is due to homogeneity, and the third due to isotropy: C is componentwise invariant under all rigid motions. On the other hand, since translations and orthogonal transformations are both rigid motions, any function C such that

$$C(\psi(\mathbf{x}), \psi(\mathbf{y})) = C(\mathbf{x}, \mathbf{y})$$

for each rigid motion ψ is both homogeneous and isotropic on R^n.

Suppose that C defined on $R^n \times R^n$ is both homogeneous and isotropic. Formulas (2.6), (2.9) and the linearity of the orthogonal transformation g together imply that

$$C_1(\mathbf{x}) = C(\mathbf{x}, \mathbf{0}) = C(g(\mathbf{x}), g(\mathbf{0})) = C(g(\mathbf{x}), \mathbf{0}) = C_1(g(\mathbf{x})), \qquad (2.12)$$

that is, $C_1 \circ g = C_1$ for each orthogonal transformation g of R^n. Furthermore, if $||\mathbf{x}|| = ||\mathbf{y}||$, there is an orthogonal transformation g_0 of R^n such that $g_0(\mathbf{x}) = \mathbf{y}$, and therefore

$$C_1(\mathbf{x}) = C_1(g_0(\mathbf{x})) = C_1(\mathbf{y});$$

such a function C_1 is called *radially symmetric.* Therefore $C_1(\mathbf{x} - \mathbf{y})$ for any $\mathbf{x}$ and $\mathbf{y}$ depends only on $||\mathbf{x}-\mathbf{y}||$, and there is an even function C_0 defined on R such that

$$C_0(||\mathbf{x} - \mathbf{y}||) := C_1(\mathbf{x} - \mathbf{y}) := C(\mathbf{x}, \mathbf{y}). \qquad (2.13)$$

The function C_0 will be said to *represent* the homogeneous and isotropic function C, and the radially symmetric function C_1.

Since the translation group on R^n does not act on S^{n-1}, the notion of homogeneity defined above does not carry over from R^n to S^{n-1}. The orthogonal group on R^n *does* act on S^{n-1}, however, since each orthogonal transformation g of R^n satisfies

$$||g(\mathbf{x})|| = ||\mathbf{x}|| = 1, \quad \mathbf{x} \in S^{n-1}.$$

Suppose that a function $C(\mathbf{x}, \mathbf{y})$ defined on $S^{n-1} \times S^{n-1}$ is isotropic on S^{n-1}. It is shown next that C depends only on $\mathbf{x}^T\mathbf{y}$. First observe that orthogonal transformations g of R^n preserve inner products, since

$$\mathbf{x}^T\mathbf{y} = \frac{1}{2}\left[||\mathbf{x}||^2 + ||\mathbf{y}||^2 - ||\mathbf{x} - \mathbf{y}||^2\right] = \frac{1}{2}\left[||g(\mathbf{x})||^2 + ||g(\mathbf{y})||^2 - ||g(\mathbf{x} - \mathbf{y})||^2\right]$$

$$= \frac{1}{2}\left[||g(\mathbf{x})||^2 + ||g(\mathbf{y})||^2 - ||g(\mathbf{x}) - g(\mathbf{y})||^2\right] = g(\mathbf{x})^T g(\mathbf{y}).$$

Suppose that

$$\mathbf{x}^T\mathbf{y} = \mathbf{w}^T\mathbf{z}, \qquad \mathbf{x}, \mathbf{y}, \mathbf{w}, \mathbf{z} \in S^{n-1}.$$

Let g_0 be an orthogonal transformation of R^n that takes $\mathbf{x}$ into $\mathbf{w}$, *i.e.*, $g_0(\mathbf{x}) = \mathbf{w}$. Introduce a local system of coordinates in which $\mathbf{w}$ is the $n-$vector

$$\mathbf{w} := [1, 0, 0, \ldots, 0]^T.$$

Since

$$\alpha := \mathbf{w}^T\mathbf{z} = \mathbf{x}^T\mathbf{y} = g_0(\mathbf{x})^T g_0(\mathbf{y}) = \mathbf{w}^T g_0(\mathbf{y}),$$

the leading component of both $\mathbf{z}$ and $g_0(\mathbf{y})$ is just α. Write $\mathbf{z}$ and $g_0(\mathbf{y})$ in component form in this coordinate system:

$$\mathbf{z} := [\alpha, u_2, u_3, \ldots, u_n]^T \quad \text{and} \quad g_0(\mathbf{y}) := [\alpha, v_2, v_3, \ldots, v_n]^T,$$

and denote

$$\mathbf{u} := [u_2, u_3, \ldots, u_n]^T \quad \text{and} \quad \mathbf{v} := [v_2, v_3, \ldots, v_n]^T.$$

Since

$$1 = \alpha^2 + \|\mathbf{u}\|^2 = \|\mathbf{z}\|^2 = \|g_0(\mathbf{y})\|^2 = \alpha^2 + \|\mathbf{v}\|^2,$$

it follows that

$$\sqrt{1-\alpha^2} = \|\mathbf{u}\| = \|\mathbf{v}\|.$$

Thus, there is an orthogonal transformation g_1 of R^n that fixes $\mathbf{w}$ and takes $g_0(\mathbf{y})$ into $\mathbf{z}$, *i.e.*,

$$g_1 \circ g_0(\mathbf{x}) = g_1(\mathbf{w}) = \mathbf{w} \quad \text{and} \quad g_1 \circ g_0(\mathbf{y}) = \mathbf{z};$$

one such orthogonal transformation fixes the first coordinate direction $\mathbf{w}$, and rotates the vector $\mathbf{v}$ into $\mathbf{u}$ about the axis coincident with $\mathbf{w}$. Since $g := g_1 \circ g_0$ is also an orthogonal transformation, Definition 2.5 and the above imply that

$$C(\mathbf{x},\mathbf{y}) = C(g(\mathbf{x}), g(\mathbf{y})) = C(\mathbf{w},\mathbf{z}).$$

Thus $C(\mathbf{x},\mathbf{y})$ depends only on $\mathbf{x}^T\mathbf{y}$.

Since $C(\mathbf{x},\mathbf{y})$ depends only on $\mathbf{x}^T\mathbf{y}$, there is a function R_0 on $[-1,1]$ given by

$$R_0(\mathbf{x}^T\mathbf{y}) := C(\mathbf{x},\mathbf{y}). \tag{2.14}$$

The function $R_0(x)$ for x in $[-1,1]$ will be said to *represent* the isotropic function C. Since

$$cos(\theta) = \mathbf{x}^T\mathbf{y} = \frac{1}{2}\left[2 - \|\mathbf{x}-\mathbf{y}\|^2\right], \qquad \mathbf{x},\mathbf{y} \in S^{n-1}, \tag{2.15}$$

where θ is the angle between $\mathbf{x}$ and $\mathbf{y}$, the isotropic functions $C(\mathbf{x},\mathbf{y})$ on S^{n-1} can be parameterized by θ:

$$R_0(cos(\theta)) = R_0(\mathbf{x}^T\mathbf{y}) = C(\mathbf{x},\mathbf{y}), \quad -\infty < \theta < \infty.$$

This parameterization is useful in theoretical work, since it provides a connection between correlation functions on S^1 and correlation functions on R; see the proof of Theorem 2.14 below. Since $R_0(cos(\theta))$ is an even function of θ, it suffices to parameterize by great circle (geodesic) distance:

$$R_0(cos(\theta)) = R_0(\mathbf{x}^T\mathbf{y}) = C(\mathbf{x},\mathbf{y}), \quad 0 \le \theta \le \pi.$$

By using Eqs. (2.14) and (2.15), the function $C(\mathbf{x},\mathbf{y})$ can also be parameterized by Euclidean distance in R^n (*cf.* Yadrenko, 1983, p. 71). This Euclidean distance is commonly known as *chordal distance*. Isotropic functions on S^{n-1} can be obtained, for example, by restricting isotropic functions on R^n to S^{n-1}. The argument following the proof of Theorem 2.12 illustrates this procedure.

Example 2.6 illustrates the application of Definition 2.2, and also clarifies the notions of homogeneity and isotropy introduced in this section.

Example 2.6: Given an $n \times n$ positive definite matrix A, define the so-called *covariance inner product* (*cf.* Tarantola, 1987, p. 214):

$$C(\mathbf{x},\mathbf{y}) \;:=\; \mathbf{x}^T A \mathbf{y} \;=\; (B\mathbf{x})^T (B\mathbf{y}), \qquad \mathbf{x},\mathbf{y} \in R^n, \tag{2.16}$$

where B is the (positive definite) square root of A, that is $B^2 = A$. Given any positive integer m, any choice of points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m$ in R^n, and any scalars $c_1, c_2, \ldots, c_m$, we have that

$$\sum_{i,j=1}^{m} (B\mathbf{x}_i)^T (B\mathbf{x}_j)\, c_i c_j \;=\; \|B(c_1\mathbf{x}_1 + c_2\mathbf{x}_2 + \cdots + c_m\mathbf{x}_m)\|^2 \;\geq\; 0,$$

so that by Definition 2.2, C is a covariance function on R^n. In general, C is neither homogeneous nor isotropic on R^n. The restriction of C to $S^{n-1} \times S^{n-1}$ is also a covariance function that is not isotropic, in general.

In the special case $A = I$, the covariance function defined by Eq. (2.16) reduces to the usual inner product on R^n. This function is isotropic on R^n, since orthogonal transformations g of R^n preserve the usual inner product. It is not homogeneous, since there are many vectors $\mathbf{z} \in R^n$ for which

$$(\mathbf{x}+\mathbf{z})^T(\mathbf{y}+\mathbf{z}) \;=\; \frac{1}{2}\left[\|\mathbf{x}+\mathbf{z}\|^2 + \|\mathbf{y}+\mathbf{z}\|^2 - \|\mathbf{x}-\mathbf{y}\|^2\right] \;\neq\; \frac{1}{2}\left[\|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 - \|\mathbf{x}-\mathbf{y}\|^2\right] \;=\; \mathbf{x}^T\mathbf{y}.$$

The restriction to S^{n-1} of the usual inner product on R^n yields Eq. (2.15), which is a correlation function on S^{n-1} by the argument above. The function $R_0(x) := x$ represents this correlation function:

$$R_0(cos(\theta)) \;=\; R_0(\mathbf{x}^T\mathbf{y}) \;=\; \mathbf{x}^T\mathbf{y}, \qquad \mathbf{x},\mathbf{y} \in S^{n-1}.$$

An example of a homogeneous correlation function on R^n that is not isotropic is given by

$$C(\mathbf{x},\mathbf{y}) \;:=\; exp(-|x_1 - y_1|)\, exp(-|x_2 - y_2|) \;\ldots\; exp(-|x_n - y_n|),$$

where $\mathbf{x} := [x_1, x_2, \ldots, x_n]^T$ and $\mathbf{y} := [y_1, y_2, \ldots, y_n]^T$ (Yaglom, 1987, p. 333). □

2.3 Characterization of Correlation Functions

The following definition of the Fourier transform for $L^1(R^n)$ functions, together with the Fourier inversion theorem, is found in Folland (1992, pp. 243-244).

Theorem 2.7: *The Fourier transform, or n-dimensional spectral density, of a function C_1 in $L^1(R^n)$ is defined by*

$$\hat{C}_1(\mathbf{w}) \;:=\; F[C_1](\mathbf{w}) = \int exp(-i\,\mathbf{w}\cdot\mathbf{r})\, C_1(\mathbf{r})\, d\mathbf{r}. \tag{2.17}$$

If C_1 is continuous and $\hat{C}_1$ is also in $L^1(R^n)$, then C_1 can be recovered from the inverse Fourier transform,

$$C_1(\mathbf{r}) \;:=\; \frac{1}{(2\pi)^n} \int exp(i\,\mathbf{w}\cdot\mathbf{r})\, \hat{C}_1(\mathbf{w})\, d\mathbf{w}. \tag{2.18}$$

□

If C_1 is a function lying in both $L^1(R^n)$ *and* $L^2(R^n)$, then it is known (see Theorem 2.8 below) that the $L^2(R^n)$ norms of C_1 and $\hat{C}_1$ are related through

$$\int C_1(\mathbf{r})^2 \, d\mathbf{r} \;=\; (C_1, C_1) = (2\pi)^{-n}(\hat{C}_1, \hat{C}_1) \;=\; \frac{1}{(2\pi)^n} \int \left|\hat{C}_1(\mathbf{w})\right|^2 d\mathbf{w}. \tag{2.19}$$

The mapping

$$\phi : L^1(R^n) \cap L^2(R^n) \rightarrow L^2(R^n), \qquad \phi(C_1) \;=\; \hat{C}_1,$$

is implied by Eq. (2.19). This mapping is known to extend to a mapping from $L^2(R^n)$ *onto* $L^2(R^n)$ through a limiting process described, for instance, in Stein and Weiss (1971, p. 17) and in Rudin (1987, pp. 185-186). The extension *defines* the Fourier transform of a function C_1 lying in $L^2(R^n)$. Plancherel's theorem (*e.g.*, Folland, 1992, p. 244), stated below as Theorem 2.8, is also obtained from the aforementioned limiting process.

Theorem 2.8: *If C_1 and C_2 are functions in $L^2(R^n)$, and if $\hat{C}_1$ and $\hat{C}_2$ are the $L^2(R^n)$ Fourier transforms of C_1 and C_2, then*

$$\int C_1(\mathbf{r})\, C_2(\mathbf{r})\, d\mathbf{r} \;=\; (C_1, C_2) = (2\pi)^{-n}(\hat{C}_1, \hat{C}_2) \;=\; \frac{1}{(2\pi)^n} \int \hat{C}_1(\mathbf{w})\, \overline{\hat{C}_2(\mathbf{w})}\, d\mathbf{w}. \tag{2.20}$$

□

Throughout most of this article, the Fourier transform will be applied to functions in $L^1(R^n) \cap L^2(R^n)$. Radially symmetric functions on R^n represented by piecewise continuous, compactly supported functions on R, used to construct correlation functions in this article, always lie in $L^1(R^n) \cap L^2(R^n)$. The $L^1(R^n)$ and $L^2(R^n)$ Fourier transforms agree in this case, and both the $L^1(R^n)$ and $L^2(R^n)$ Fourier theories apply. A standard result of the $L^1(R^n)$ theory is that the Fourier transform $\hat{C}_1$ of $C_1 \in L^1(R^n)$ is *continuous* (Stein and Weiss, 1971, p. 2), and this fact is exploited repeatedly in the sequel.

Theorem 2.9 is a form of the multidimensional Convolution Theorem (Stein and Weiss, 1971, Theorem 2.6, p. 18). Continuity of the convolution function follows from the argument given in Stein and Weiss (1971, Theorem 2.1, p. 16), while Eq. (2.22) below holds for every $\mathbf{w}$ by the continuity of the $L^1(R^n)$ Fourier transform. Theorem 2.9 serves as a foundation for most of the constructive theory developed in this article.

Theorem 2.9: *Suppose that B_1 and B_2 are both in $L^1(R^n) \cap L^2(R^n)$. Let B_3 be the convolution of B_1 with B_2 over R^n (denoted by $B_3 := B_1 * B_2$), defined by*

$$B_3\,(\mathbf{x}) := \int B_1(\mathbf{y})\, B_2(\mathbf{x} - \mathbf{y})\, d\mathbf{y} = \int B_2(\mathbf{y})\, B_1(\mathbf{x} - \mathbf{y})\, d\mathbf{y}. \tag{2.21}$$

The function B_3 is continuous and lies in $L^1(R^n) \cap L^2(R^n)$. The n-dimensional Fourier transforms of B_1, B_2, and B_3 are related by

$$\hat{B}_3(\mathbf{w}) \;=\; \hat{B}_1(\mathbf{w})\, \hat{B}_2(\mathbf{w}). \tag{2.22}$$

□

Theorem 2.9, coupled with other results to follow, will be applied to construct covariance functions through *self*-convolution, $B_3 = B_1 * B_1$. Observe for now that if B_1 is compactly supported on the sphere of radius c centered at the origin in R^3, then B_3 is compactly supported on the sphere of radius $2c$ centered at the origin in R^3. Of primary importance in this article will be the case where B_1 is a radially symmetric function represented by a piecewise continuous and compactly supported function B_0 on R, and such functions are in $L^1(R^n) \cap L^2(R^n)$.

Theorem 2.10 combines a version of Bochner's original theorem (Bochner, 1934) with a classical result (Stein and Weiss, 1971, Corollary 1.26, p. 15), into a statement which is convenient for the development in this article. Theorem 2.11, due to Schoenberg (1942), completely characterizes the continuous isotropic correlation functions on spheres.

Theorem 2.10: *Let C_1 be any function defined on R^n which is continuous, lies in $L^1(R^n)$, and satisfies $C_1(\mathbf{0}) = 1$. Then the function*

$$C(\mathbf{x}, \mathbf{y}) := C_1(\mathbf{x} - \mathbf{y})$$

is a homogeneous correlation function on R^n if, and only if, the Fourier transform $\hat{C}_1$ of C_1 is everywhere nonnegative, that is, $\hat{C}_1(\mathbf{w}) \geq 0$ for each $\mathbf{w}$ in R^n. If C is a homogeneous correlation function, then $\hat{C}_1$ is in $L^1(R^n)$. In this case, C_1 is given by Eq. (2.18).

Proof: Since C_1 is continuous and lies in $L^1(R^n)$, C_1 also lies in $L^2(R^n)$. Let T be the correlation operator given by (2.3) with the kernel C represented by C_1. Given f in $L^1(R^n) \cap L^2(R^n)$, Theorem 2.9 implies that

$$F[Tf](\mathbf{w}) = \hat{C}_1(\mathbf{w})\, \hat{f}(\mathbf{w}). \tag{2.23}$$

Theorem 2.8 together with (2.23) imply that

$$(Tf, f) = (2\pi)^{-n}\, (F[Tf], \hat{f}) = (2\pi)^{-n}\, (\hat{C}_1, |\hat{f}|^2). \tag{2.24}$$

If $\hat{C}_1$ is everywhere nonnegative, then the operator T is nonnegative on $L^1(R^n) \cap L^2(R^n)$ by (2.24). Since $L^1(R^n) \cap L^2(R^n)$ is a dense subspace of $L^2(R^n)$, it follows that T is nonnegative on $L^2(R^n)$ as well. Definition 2.3 implies that C is a correlation function. Conversely, if $\hat{C}_1$ is negative at a single point in R^n, then by continuity of the $L^1(R^n)$ Fourier transform, it is negative in some neighborhood of this point. Let h be such that $\hat{h}$ is one on this neighborhood, and zero otherwise. Then (2.24) implies that (Th, h) is negative, so that the converse is established. The proof of the last assertion is given in Stein and Weiss (1971, Corollary 1.26, p. 15). □

Now let B_1 be an even function satisfying the hypothesis of Theorem 2.9 (it is evident from (2.8) that B_1 could, for instance, represent a homogeneous function on R^n). From Eq. (2.17) it follows that $\hat{B}_1(\mathbf{w})$ is real, and therefore if $B_3 := B_1 * B_1$, then Theorem 2.9 implies that $\hat{B}_3(\mathbf{w}) = \hat{B}_1(\mathbf{w})^2$, which is nonnegative. Further,

$$B_3(\mathbf{0}) = \int B_1(\mathbf{y})\, B_1(-\mathbf{y})\, d\mathbf{y} = \int B_1(\mathbf{y})^2\, d\mathbf{y} \tag{2.25}$$

is positive, assuming, for instance, that the support of B_1 has positive measure. Theorems 2.9 and 2.10 imply that $C_3(\mathbf{x}) := B_3(\mathbf{x}) \cdot [B_3(\mathbf{0})]^{-1}$ represents a homogeneous correlation function on R^n.

The following argument further clarifies the relation between Definition 2.3, Theorem 2.9, and Theorem 2.10. If the operator T is the convolution

$$Tf(\mathbf{x}) := \int B_1(\mathbf{x} - \mathbf{y}) f(\mathbf{y})\, d\mathbf{y} = (B_1 * f)(\mathbf{x}), \tag{2.26}$$

then the composition T^2 of T with itself is

$$T^2 f(\mathbf{x}) \;=\; T((B_1 * f)(\mathbf{x})) \;=\; (B_1 * B_1) * f(\mathbf{x}), \tag{2.27}$$

so that T^2 has the self-convolution function $B_1 * B_1$ as its kernel. If B_1 is even, then T^2 is a nonnegative operator, and since $B_3(\mathbf{0})$ is positive, the operator with kernel C_3 is also nonnegative, so that C_3 represents a homogeneous correlation function on R^n.

Theorem 2.11: *Let C be a continuous isotropic function on the $(n-1)$-dimensional unit sphere S^{n-1}, represented by the function $R_0(cos(\theta))$ defined by*

$$R_0(cos(\theta)) \;=\; R_0(\mathbf{x}^T\mathbf{y}) \;:=\; C(\mathbf{x},\mathbf{y}),$$

where $\theta \in R$ is the angle (**read:** *great circle distance if $0 \le \theta \le \pi$*) *between the two points $\mathbf{x}$ and $\mathbf{y}$ on S^{n-1}. Then C is a correlation function if, and only if, the function R_0 has the form*

$$R_0(cos(\theta)) \;=\; \sum_{m=0}^{\infty} a_m C_m^{\frac{n-2}{2}}(cos\,\theta), \tag{2.28}$$

where $C_m^{\frac{n-2}{2}}$ are Gegenbauer polynomials of degree m and order $\frac{n-2}{2}$, and where the coefficients a_m are all nonnegative and satisfy $\sum_{m=0}^{\infty} a_m C_m^{\frac{n-2}{2}}(1) \;=\; 1$. □

Remarks: *Gegenbauer polynomials, also known as ultraspherical polynomials, or as n-dimensional zonal surface harmonics, are defined in Folland (1992, p. 198), for instance. Using Eq. (2.15), Eq. (2.28) can also be parameterized by chordal distance. The condition $\sum_{m=0}^{\infty} a_m C_m^{\frac{n-2}{2}}(1) \;=\; 1$ arises from the fact that Theorem 2.11 is stated for correlation functions:*

$$\sum_{m=0}^{\infty} a_m C_m^{\frac{n-2}{2}}(1) \;=\; R_0(1) \;=\; 1.$$

□

The cases S^1 and S^2 in Theorem 2.11 are of primary interest here. All continuous isotropic correlation functions on the unit circle S^1 can be represented by *Fourier cosine expansions*

$$R_0(cos(\theta)) \;=\; \sum_{m=0}^{\infty} a_m \cos(m\theta)$$

with all Fourier coefficients a_m nonnegative, while all continuous isotropic correlation functions on the unit sphere S^2 can be represented by *Legendre expansions*

$$R_0(cos(\theta)) \;=\; \sum_{m=0}^{\infty} a_m P_m(cos\,\theta)$$

with all Legendre coefficients a_m nonnegative. Since S^1 is a subset of S^2, correlation functions on S^1 can also be obtained by restriction to S^1 of correlation functions on S^2, as remarked following Definition 2.2.

Theorem 2.11 characterizes completely the class of continuous isotropic correlation functions on S^{n-1}. It will be shown in Section 3.b that *space-limited* correlation functions on S^2 can *never* be obtained from *finite* Legendre expansions. Theorem 2.11 therefore cannot be applied directly in practice to construct space-limited correlation functions. Note, however, that space-limited correlation functions on S^2 may still be approximated by finite Legendre expansions with nonnegative coefficients. Such an approximation has been developed by Courtier *et al.* (1998).

If C is any homogeneous and isotropic function defined on $R \times R$, then the representing functions C_1 and C_0 in Eq. (2.13) are identical. Applied to R, Theorem 2.10 therefore shows that C is also a *correlation* function on R whenever C_0 has an everywhere nonnegative Fourier transform $\hat{C}_0$. Theorem 2.12 below shows that if $\hat{C}_0$ decreases monotonically as a function of positive wavenumber, then in fact $\hat{C}_0$ is everywhere nonnegative, and furthermore that C_0 represents a homogeneous and isotropic correlation function on R^3. Restricting such a correlation function on R^3 to S^2 gives an isotropic correlation function on S^2. Next to the convolution theorem, Theorem 2.12 is the most important basic result in this article for *construction* of correlation functions on R^3 and S^2. Yaglom (1987, p. 360) provides a different proof, valid for R^n.

Theorem 2.12: *Suppose that C is a homogeneous and isotropic function on R^3, represented by the radially symmetric function C_1 on R^3, and by the even function C_0 defined on R by*

$$C(\mathbf{x},\mathbf{y}) \;:=\; C_1(\mathbf{x}-\mathbf{y}) \;:=\; C_0(\|\mathbf{x}-\mathbf{y}\|),$$

where $\|\cdot\|$ denotes Euclidean distance in R^3. Suppose that C_1 is continuous, lies in $L^1(R^3)$, and satisfies $C_1(\mathbf{0}) = 1$. Then the one-dimensional Fourier transform $\hat{C}_0$ of C_0 is differentiable. The function C is a correlation function if, and only if, $\hat{C}_0$ is a monotonically decreasing function of wavenumber w for $w > 0$. If C is a correlation function, then $\hat{C}_0$ is everywhere nonnegative.

Proof: It is known (Folland, 1992, p. 246) that $\hat{C}_1$ is a radially symmetric function of three-dimensional wavenumber $\mathbf{w}$. Changing to spherical coordinates yields

$$\hat{C}_1(\mathbf{0}) = \int C_1(\mathbf{r})\, d\mathbf{r} = 4\pi \int_0^\infty C_0(r)\, r^2\, dr, \tag{2.29}$$

with the first equality in Eq. (2.29) obtained from Eq. (2.17). The fact that C_0 is even, together with Eq. (2.29), implies that $r^2 C_0(r)$ lies in $L^1(R)$. Since C_0 is also continuous, it follows that $rC_0(r)$ lies in $L^1(R)$. Thus $\hat{C}_0$ is differentiable, and

$$i\frac{d\hat{C}_0(w)}{dw} \;=\; F[rC_0](w) \;=\; -2i \int_0^\infty C_0(r)\, r\, sin(wr)\, dr, \tag{2.30}$$

the latter equality resulting from the fact that $rC_0(r)$ is an odd function; *cf.* Folland (1992, p. 214).

Applying the Hankel transform of C_0 yields (*e.g.*, Folland, 1992, p. 247):

$$\hat{C}_1(\mathbf{w}) \;=\; \frac{4\pi}{\|\mathbf{w}\|} \int_0^\infty C_0(r)\, r\, sin(\|\mathbf{w}\| r)\, dr, \qquad \|\mathbf{w}\| \neq 0. \tag{2.31}$$

Using (2.30) and (2.31), the relation

$$\hat{C}_1(\mathbf{w}) \;=\; -\frac{2\pi}{\|\mathbf{w}\|}\, \frac{d\hat{C}_0(\|\mathbf{w}\|)}{d\|\mathbf{w}\|} \tag{2.32}$$

holds for $\|\mathbf{w}\| \neq 0$, and implies that $\hat{C}_1(\mathbf{w})$ is nonnegative for $\|\mathbf{w}\| \neq 0$ if, and only if, $\hat{C}_0(w)$ is a monotonically decreasing function of wavenumber w for $w > 0$. If C is a correlation function, then Theorem 2.10 implies that $\hat{C}_1$ is everywhere nonnegative, so that $\hat{C}_0(w)$ is monotonically decreasing for $w > 0$. Conversely, if $\hat{C}_0(w)$ is monotonically decreasing for $w > 0$, then $\hat{C}_1(\mathbf{w})$ is nonnegative for $\|\mathbf{w}\| \neq 0$, and is nonnegative for $\mathbf{w} = \mathbf{0}$ by Eq. (2.29). Theorem 2.10 implies that C is a correlation function.

The proof of the last assertion uses the Riemann-Lebesgue lemma for C_0 to yield

$$\hat{C}_0(w) = -\int_w^\infty \frac{d\hat{C}_0(t)}{dt}\, dt,$$

implying that $\hat{C}_0(w)$ is nonnegative for $w \geq 0$. Because $\hat{C}_0(w)$ is an even function of w, $\hat{C}_0(w)$ is nonnegative for each $w \in R$. □

The homogeneous and isotropic correlation functions obtained using Theorem 2.12 depend only on Euclidean distance in R^3. These functions can in turn be restricted to isotropic correlation functions on S^2 (depending only on chordal distance on S^2). Chordal distance r on S^2 and great circle distance θ are in a one-to-one correspondence given by

$$r = r(\theta) = 2\,sin\left(\frac{\theta}{2}\right) = \sqrt{2(1 - cos(\theta))}, \qquad 0 \leq \theta \leq \pi. \tag{2.33}$$

By parameterizing r in this manner, isotropic correlation functions on S^2 are seen to depend only on $cos(\theta)$, or alternatively, only on great circle distance θ; *cf.* Eq. (2.15).

For example, consider the well-known second-order autoregressive function (SOAR; Daley, 1991, p. 117; Balgovind *et al.*, 1983, p. 714):

$$C_0(r) := \left(1 + \frac{|r|}{L}\right) \exp\left(-\frac{|r|}{L}\right), \tag{2.34}$$

where $|r|$ represents Euclidean distance in R^3. The hypotheses of Theorem 2.12 are readily verified for this function. The one-dimensional Fourier transform (Yaglom, 1987, p. 127) given by

$$\hat{C}_0(w) = \frac{4L}{(1 + w^2L^2)^2}, \tag{2.35}$$

is a monotonically decreasing function of w for $w > 0$, and is also everywhere nonnegative. According to Theorem 2.12, C_0 represents a homogeneous and isotropic correlation function on R^3, which in turn is restricted to S^2 using Eq. (2.33) (*e.g.*, Yaglom, 1987, p. 389; Weber and Talkner, 1993, p. 2614):

$$C_0(r(\theta)) = \left(1 + \frac{2\,sin(\theta/2)}{L}\right) \exp\left(-\frac{2\,sin(\theta/2)}{L}\right), \qquad 0 \leq \theta \leq \pi. \tag{2.36}$$

Equivalently, using the notation of Theorem 2.11,

$$R_0(cos(\theta)) = C_0(r(\theta)) = \left(1 + \frac{\sqrt{2\,(1 - cos(\theta))}}{L}\right) \exp\left(-\frac{\sqrt{2\,(1 - cos(\theta))}}{L}\right), \quad -\infty < \theta < \infty.$$

2.4 Smoothness Properties of Correlation Functions

Theorems 2.13 and 2.14 summarize well-known smoothness properties of homogeneous and isotropic correlation functions on R^n, and of isotropic correlation functions on S^n (Yaglom, 1987, pp. 64-66; Christakos, 1992, p. 62). These two theorems imply that the smoothness of such correlation functions is controlled by the smoothness of their representing functions at the origin.

Theorem 2.13: *Suppose that C is a homogeneous and isotropic correlation function on R^n, and let C_0 denote the even function on R representing C by*

$$C_0(\|\mathbf{x}-\mathbf{y}\|) \ := \ C(\mathbf{x},\mathbf{y}),$$

where $\|\cdot\|$ denotes Euclidean distance in R^n. If C_0 has a continuous derivative ${C_0}^{(2k)}$ of order $2k$ at zero for a given $k \geq 0$, then C_0 has a continuous derivative of order $2k$ at each point of R. In this case, each of the functions

$$\frac{(-1)^j {C_0}^{(2j)}(r)}{{C_0}^{(2j)}(0)}, \qquad j = 0, 1, 2, \ldots, k,$$

represents a correlation function on R (under Definition 2.1 or 2.2). □

Yaglom (1987, pp. 64-66) proves that even functions C_0 on R that are continuous at the origin and represent covariance functions on R, are in fact *everywhere* continuous on R; see also Christakos (1992, p. 62). He shows further that if such a function C_0 has two continuous derivatives at the origin, then $-{C_0}''$ represents a covariance function on R. Theorem 2.13 follows from these results and induction on k.

Theorem 2.14: *Suppose that C is an isotropic correlation function on S^n, and let $R_0(cos(\theta))$ be the function representing C:*

$$R_0(cos(\theta)) \ = \ R_0(\mathbf{x}^T\mathbf{y}) \ := \ C(\mathbf{x},\mathbf{y}),$$

where $\theta \in R$ is the angle (**read:** *great circle distance if $0 \leq \theta \leq \pi$) between $\mathbf{x}$ and $\mathbf{y}$. If $R_0(cos(\theta))$ has a continuous derivative ${R_0}^{(2k)}(cos(\theta))$ of order $2k$ at $\theta = 0$ for a given $k \geq 0$, then $R_0(cos(\theta))$ has a continuous derivative of order $2k$ at each point of R.*

Proof: The restriction of C to $S^1 \times S^1$ is an isotropic correlation function on S^1 which is also represented by $R_0(cos(\theta))$. According to Theorem 2.11, R_0 can be written as a Fourier cosine series

$$R_0(cos(\theta)) \ = \ \sum_{m=0}^{\infty} a_m \, cos\,(m\theta),$$

where $a_m \geq 0$ for each m. For each $m \geq 0$, $cos\,(m\theta)$ represents a correlation function on R (under Definition 2.1 or Definition 2.2); see Yaglom (1987, p. 120), for instance. Since $R_0(cos(\theta))$ is the sum of the functions $a_m\, cos\,(m\theta)$, $R_0(cos(\theta))$ represents a correlation function on R. Thus Theorem 2.13 implies Theorem 2.14. □

3 Correlation Modeling on R^3

This section is organized into three parts. Section 3.a provides results which show that homogeneous and isotropic correlation functions on R^3 can be obtained by self-convolution, and furthermore, that arbitrarily smooth correlation functions can be obtained in this manner. Section 3.b illustrates practical limitations of spectral correlation models obtained from finite Fourier or finite Legendre expansions. Results in Section 3.c aid in evaluation of self-convolution integrals over R^3. Applications of these results are given in Section 4.

3.1 Self-convolution Correlation Theory

Modeling correlation functions through convolutions is motivated by well-recognized physical ideas. Convolution typically has a broadening and smoothing effect. The broadening effect is witnessed by the well-known fact that the probability density function of the sum of two independent random variables is the convolution of the probability density functions of the two random variables (*e.g.*, Papoulis, 1984, pp. 134-135). When the variances are finite, the independence of the random variables implies that the variance of this sum is the sum of the variances, hence the convolution function is broader than the two functions being convolved. Theorem 3.a.3 illustrates the smoothing effect of self-convolution over R^3.

Convolution is the primary tool used for modeling correlations of one-dimensional time signals in electrical engineering. In fact, autocorrelation functions for finite-energy signals are *defined* by self-convolutions over R (Papoulis, 1984, pp. 241-242). The convolution approach to correlation modeling in two and three dimensions was used by Oliver (1995) to generate multidimensional Gaussian random fields.

This section provides comprehensive results concerning homogeneous and isotropic correlation functions on R^3 that are obtained by self-convolution. Theorem 3.a.3 asserts that homogeneous, isotropic correlation functions on R^3 can be constructed by self-convolution of compactly supported, radially symmetric functions on R^3, and establishes smoothness properties of these correlation functions. A proof of this theorem is given in the Appendix. Theorem 3.a.4 shows that correlation functions on R^3 can also be obtained through self-convolution over R, rather than R^3, of functions representing homogeneous and isotropic correlation functions on R^3. Theorem 3.a.5 provides a converse of Theorem 3.a.4.

The following result establishes that convolutions of radially symmetric functions are also radially symmetric.

Theorem 3.a.1: *Suppose that B_1 and B_2 are radially symmetric functions in $L^1(R^n) \cap L^2(R^n)$. Let $C_1 := B_1 * B_2$ be the convolution of B_1 and B_2 over R^n. Then C_1 is a radially symmetric function that represents the homogeneous and isotropic function C on R^n given by*

$$C(\mathbf{x}, \mathbf{y}) \;:=\; C_1(\mathbf{x} - \mathbf{y}).$$

Proof: The function C_1 satisfies the following relation:

$$\begin{aligned} C_1(g(\mathbf{y})) &= \int B_1(\mathbf{x})\, B_2(g(\mathbf{y}) - \mathbf{x})\, d\mathbf{x} \\ &= \int B_1(g(\mathbf{v}))\, B_2(g(\mathbf{y}) - g(\mathbf{v}))\, d\mathbf{v} \\ &= \int B_1(g(\mathbf{v}))\, B_2(g(\mathbf{y} - \mathbf{v}))\, d\mathbf{v} \;=\; C_1(\mathbf{y}) \end{aligned} \qquad (3.a.1)$$

for each orthogonal transformation g of R^n and every $\mathbf{y} \in R^n$. The first equality in $(3.a.1)$ follows from Theorem 2.9, the second follows from the fact that $d\mathbf{x} = d\mathbf{v}$ because the orthogonal transformation $\mathbf{x} = g(\mathbf{v})$ is volume-preserving, the third follows because g is a linear transformation, and the fourth follows from the radial symmetry of B_1 and B_2. Equation $(3.a.1)$ establishes that C_1 is radially symmetric. The function C is homogeneous by definition, and is shown to be isotropic by applying $(3.a.1)$ with $\mathbf{y}$ replaced by $\mathbf{x}$-$\mathbf{y}$:

$$C(\mathbf{x}, \mathbf{y}) \;=\; C_1(\mathbf{x} - \mathbf{y}) \;=\; C_1(g(\mathbf{x}-\mathbf{y}))$$

$$= C_1(g(\mathbf{x}) - g(\mathbf{y})) = C(g(\mathbf{x}), g(\mathbf{y})).$$

□

Definition 3.a.2: *Suppose $-\infty < a < b < \infty$. The function f is piecewise continuous on $[a, b]$ provided that f is continuous there except at finitely many jump discontinuities. If, in addition, the derivative f' of f is piecewise continuous, then f is said to be piecewise smooth on $[a, b]$.* □

Theorem 3.a.3: *Let B_0 be the even function on R and let B_1 be the radially symmetric function in $L^1(R^3) \cap L^2(R^3)$, representing a homogeneous and isotropic function B on R^3 by*

$$B(\mathbf{x}, \mathbf{y}) := B_1(\mathbf{x} - \mathbf{y}) := B_0(\|\mathbf{x} - \mathbf{y}\|),$$

where $\|\cdot\|$ denotes Euclidean distance in R^3. Let C_1 denote the radially symmetric function on R^3 given by the self-convolution $C_1 := B_1 * B_1$ over R^3 (see Theorem 3.a.1). Then C_1 is continuous and lies in $L^1(R^3)$ (see Theorem 2.9). Suppose that B_0 is compactly supported with support $[-c, c]$. Let $h_1(r) := rB_0(r)$, and denote by $h_1{}^{(-1)}(r)$ the function defined on R by

$$h_1{}^{(-1)}(r) := \int_{-c}^{r} h_1(s)\, ds.$$

Suppose that $h_1{}^{(n)}$ is continuous and piecewise smooth for a given $n \geq -1$. Let C_0 be the even function on R given by

$$C_0(\|\mathbf{x} - \mathbf{y}\|) := C_1(\mathbf{x} - \mathbf{y}).$$

Then $C_0(r)$ is compactly supported with support $[-2c, 2c]$, has at least $2n + 3$ continuous derivatives everywhere on R except possibly at $r = 0$ and $r = \pm 2c$, and has at least $2n + 2$ continuous derivatives everywhere on R. Furthermore, if

$$C(\mathbf{x}, \mathbf{y}) := C_1(\mathbf{x} - \mathbf{y}),$$

then $C(\mathbf{x}, \mathbf{y})/C_0(0)$ is a continuous, homogeneous and isotropic correlation function on R^3.

Remark: *Since $h_1{}^{(-1)}$ is differentiable at each point of continuity of h_1 by the fundamental theorem of calculus, the hypothesis that $h_1{}^{(-1)}$ be continuous and piecewise smooth is the same as the hypothesis that $h_1(r) = rB_0(r)$ be piecewise continuous.* □

Theorem 3.a.3 gave smoothness properties of compactly supported, homogeneous and isotropic correlation functions on R^3 that are obtained through self-convolutions over R^3. Self-convolution correlation functions with these smoothness properties will actually be constructed in Sections 3.c and 4. Theorem 3.a.4 shows that if B_0 represents a homogeneous and isotropic correlation function on R^3, then the self-convolution

$$C_0(r) := B_0 * B_0(r) \cdot [B_0 * B_0(0)]^{-1}$$

over R represents yet another homogeneous and isotropic correlation function on R^3. Additional homogeneous and isotropic correlation functions on R^3 can be obtained by iterating this procedure. The function B_0 needed to initialize the procedure can be obtained through Theorem 3.a.3, for instance, as is illustrated by the examples in Section 4.

Theorem 3.a.4: *Let B_0 be the even function on R and let B_1 be the radially symmetric function in $L^1(R^3)$, representing a continuous, homogeneous and isotropic correlation function B on R^3 by*

$$B(\mathbf{x}, \mathbf{y}) := B_1(\mathbf{x} - \mathbf{y}) := B_0(\|\mathbf{x} - \mathbf{y}\|),$$

where $\|\cdot\|$ *denotes Euclidcan distance in* R^3. *Then the convolution function*

$$C_0(r) = B_0 * B_0(r) \cdot [B_0 * B_0(0)]^{-1}$$

over R *represents the continuous, homogeneous and isotropic correlation function* C *on* R^3 *defined by*

$$C(\mathbf{x}, \mathbf{y}) := C_0(\|\mathbf{x} - \mathbf{y}\|).$$

Proof: Since B_0 is continuous and lies in $L^1(R)$, B_0 also lies in $L^2(R)$. Theorem 2.9 implies that the convolution function C_0 is continuous, lies in $L^1(R) \cap L^2(R)$, and that

$$\hat{C}_0(w) = \hat{B}_0(w)^2 \cdot [B_0 * B_0(0)]^{-1}. \tag{3.a.2}$$

Since B and its representatives B_1 and B_0 satisfy the hypotheses of Theorem 2.12, $\hat{B}_0(w)$ is differentiable, so that by Eq. (3.a.2),

$$\frac{d\hat{C}_0(w)}{dw} = 2\,\hat{B}_0(w)\frac{d\hat{B}_0(w)}{dw}[B_0 * B_0(0)]^{-1}. \tag{3.a.3}$$

Combining Eq. (3.a.3), Eq. (2.32), and the restatement of Eq. (2.32) for B_0 and B_1:

$$\hat{B}_1(\mathbf{w}) = -\frac{2\pi}{\|\mathbf{w}\|}\frac{d\hat{B}_0(\|\mathbf{w}\|)}{d\|\mathbf{w}\|}, \quad \mathbf{w} \in R^3, \ \|\mathbf{w}\| \neq 0,$$

yields the relation

$$\hat{C}_1(\mathbf{w}) = 2\hat{B}_0(\|\mathbf{w}\|)\,\hat{B}_1(\mathbf{w})[B_0 * B_0(0)]^{-1}, \tag{3.a.4}$$

valid for $\|\mathbf{w}\| \neq 0$. Since both sides of Eq. (3.a.4) are continuous functions on R^3, this equality holds at $\mathbf{w} = \mathbf{0}$ as well. Since $\hat{B}_0(\|\mathbf{w}\|)$ and $\hat{B}_1(\mathbf{w})$ are everywhere nonnegative for each $\mathbf{w} \in R^3$ by Theorems 2.12 and 2.10 respectively, and since

$$B_0 * B_0(0) = \int B_0(r)^2\,dr > 0,$$

$\hat{C}_1(\mathbf{w})$ is everywhere nonnegative by Eq. (3.a.4). Thus, by Theorem 2.10, C is a correlation function. □

Remark: *Since the hypotheses on* B_0 *and* B_1 *are satisfied by* C_0 *and* C_1 *(see Theorem 2.9), the iterative procedure described before the statement of Theorem 3.a.4 is justified.* □

Theorem 3.a.5 shows that all continuous and integrable functions C_0 on R that also represent correlation functions are, in fact, self-convolutions over R. A proof of this theorem is given in the Appendix. Note that the most important case for this article is the one in Theorem 3.a.4 above, where C_0 represents a homogeneous and isotropic correlation function on R^3.

Theorem 3.a.5: *Let* C_0 *be any continuous even function in* $L^1(R)$ *such that* $C_0(0) = 1$ *and* $\hat{C}_0$ *is everywhere nonnegative. Then there is a square-integrable function* D_0 *defined on* R *so that* $C_0 = D_0 * D_0$. *If* C_0 *is also twice continuously differentiable and* C_0'' *lies in* $L^1(R)$, *then there is a continuous even function* F_0 *that lies in* $L^2(R)$ *and satisfies*

$$C_0 = F_0 * F_0. \tag{3.a.5}$$

Suppose it is known in addition that C_0 represents the homogeneous and isotropic correlation function C on R^3 and the radially symmetric function C_1 lying in $L^1(R^3)$ defined by

$$C(\mathbf{x},\mathbf{y}) \ := \ C_1(\mathbf{x} - \mathbf{y}) \ := \ C_0(\|\mathbf{x}-\mathbf{y}\|),$$

where $\|\cdot\|$ denotes Euclidean distance in R^3. Then $F_0(r)/F_0(0)$ also represents a homogeneous and isotropic correlation function on R^3.

3.2 Some Limitations of Spectral Covariance Modeling

Two results which illustrate practical limitations of spectral covariance modeling are proven in this section. The first result shows that compactly supported functions on R representing homogeneous and isotropic correlation functions on R^3 cannot be obtained through finite Fourier series. The second result shows that space-limited isotropic correlation functions on S^2 cannot be obtained through finite Legendre expansions.

Theorem 3.b.1: *Suppose that the continuous even function C_0 defined on R and compactly supported on $[-c, c]$ represents the homogeneous and isotropic correlation function C on R^3 by*

$$C(\mathbf{x},\mathbf{y}) \ := \ C_0(\|\mathbf{x}-\mathbf{y}\|),$$

where $\|\cdot\|$ denotes Euclidean distance in R^3. Then every coefficient of the Fourier series representation of C_0 on $[-c, c]$ is nonzero.

Proof: Since C_0 is continuous on R, it agrees with its Fourier series representation on $[-c, c]$, which is

$$C_0(r) = \sum_{-\infty}^{\infty} c_k\, exp\Big(\frac{k\pi r i}{c}\Big), \qquad |r| \le c, \tag{3.b.1}$$

where the Fourier coefficients are given by

$$c_k \ = \ \frac{1}{2c}\int_{-c}^{c} C_0(r)\, exp\Big(-\frac{k\pi r i}{c}\Big)\, dr \tag{3.b.2}$$

$$= \ \frac{1}{2c}\int_{-\infty}^{\infty} C_0(r)\, exp\Big(-\frac{k\pi r i}{c}\Big)\, dr \ = \ \frac{1}{2c}\hat{C}_0\Big(\frac{k\pi}{c}\Big).$$

Since C_0 is an even function on R,

$$C_0(r) = \frac{1}{2c}\hat{C}_0(0) + \frac{1}{c}\sum_{k=1}^{\infty}\hat{C}_0\Big(\frac{k\pi}{c}\Big)\cos\Big(\frac{k\pi r}{c}\Big), \quad |r| \le c. \tag{3.b.3}$$

Theorem 2.12 implies that $\hat{C}_0(w)$ is a monotonically decreasing function of wavenumber w for $w > 0$, as well as everywhere nonnegative. Therefore, if the Fourier coefficient $\hat{C}_0(j\pi/c)$ is zero, then $\hat{C}_0(w) = 0$ for each $w \ge (j\pi/c)$. In particular, the sum in (3.b.3) terminates at the $(j-1)$st term. This violates Heisenberg's inequality (Folland, 1992, p. 232), which implies that C_0 and $\hat{C}_0$ cannot both be compactly supported. □

Theorem 3.b.2: *Let $R_0(cos(\theta))$ be the continuous function defined on R which represents the space-limited isotropic correlation function C on the unit sphere S^2 by*

$$C(\mathbf{x},\mathbf{y}) \ := \ R_0(\mathbf{x}^T\mathbf{y}) \ = \ R_0(cos(\theta)), \qquad \mathbf{x},\mathbf{y} \in S^2,$$

where θ is the great circle distance between $\mathbf{x}$ *and* $\mathbf{y}$. *Then the Legendre expansion*

$$R_0(cos(\theta)) = \sum_{m=0}^{\infty} a_m P_m(cos\,\theta) \tag{3.b.4}$$

has infinitely many positive coefficients a_m.

Proof: Suppose that the expansion (3.*b*.4) terminates at $m = j$. Then the finite sum

$$R_0(cos(\theta)) = \sum_{m=0}^{j} a_m P_m(cos\,\theta), \tag{3.b.5}$$

where $a_m \geq 0$ for each m, $a_j > 0$, and $\sum_{m=0}^{j} a_m = 1$, is a polynomial in $cos\,\theta$ of exact degree j, since the Legendre polynomials P_m have degree m. The fundamental theorem of algebra implies that there are at most j roots of the polynomial

$$\sum_{m=0}^{j} a_m P_m(x), \qquad -1 \leq x \leq 1. \tag{3.b.6}$$

Since $cos\,\theta$ is injective for $0 \leq \theta \leq \pi$, the sum (3.*b*.5) vanishes for at most j different values of θ. Finite expansions of the form (3.*b*.5) therefore cannot represent space-limited functions. □

3.3 Calculation of Convolution Integrals for Radially Symmetric Functions

Given any m radially symmetric functions $B_1, B_2, \ldots, B_m$ in $L^1(R^3) \cap L^2(R^3)$, Theorem 3.a.1 implies that

$$C_{ij}(\mathbf{x}) := \frac{B_i * B_j(\mathbf{x})}{[B_i * B_i(\mathbf{0}) \cdot B_j * B_j(\mathbf{0})]^{1/2}} \tag{3.c.1}$$

are all radially symmetric on R^3. Theorem 3.a.3 implies that each C_{ii} represents a homogeneous and isotropic correlation function, under appropriate conditions on the functions B_i. Similarly, the C_{ij} for $i \neq j$ represent radially symmetric *cross-correlation* functions, in accordance with the terminology used in Papoulis (1962, pp. 244-245), for instance.

Theorem 3.c.1 exploits this radial symmetry to give expressions for the three-dimensional integrals $B_i * B_j(\mathbf{x})$, with the functions $C_{ij}(\mathbf{x})$ determined by Eq. (3.*c*.1). The triple integrals $B_i * B_j(\mathbf{x})$ are first reduced to two-dimensional integrals given by Eqs. (3.*c*.3) and (3.*c*.4). These integrals can be simplified analytically under appropriate conditions, as shown in the Appendix. If $c_i \neq c_j$, then the analytic expression given by Eq. (*A*.27) has five branches, and if $c_i = c_j$, then this expression collapses to two branches. The latter case is stated as Corollary 3.c.2, and illustrated by Examples 4.b and 4.c.

Although the formulas given in Theorem 3.c.1 and Corollary 3.c.2 apply when the functions B_i are infinitely supported, the case of primary interest in this article is where each function B_i is supported on a sphere of finite radius c_i. In this case, the functions C_{ij} are supported on spheres of radii $c_i + c_j$. The geometry involved in the reduction of the integrals is visualized by imagining the collision of two solid spheres of radii c_i and c_j, with the first point of contact when the centers are at distance $c_i + c_j$. The functions obtained by intersecting the C_{ij} with S^2 are space-limited isotropic functions; for each fixed $\mathbf{x} \in S^2$, the isolines of

$$C_{ij}(\mathbf{x}-\mathbf{y}), \quad \mathbf{y} \in S^2$$

are circles.

Theorem 3.c.1: *Suppose that B_i is a radially symmetric function in $L^1(R^3) \cap L^2(R^3)$ and supported on the sphere of radius c_i, $0 < c_i \leq \infty$, for $i = 1, 2, \ldots m$. Let ${B_i}^0$ and ${P_{ij}}^0$ denote the even representing functions on R given by*

$$ {B_i}^0(\|\mathbf{r}\|) := B_i(\mathbf{r}) \quad \text{and} \quad {P_{ij}}^0(\|\mathbf{r}\|) := P_{ij}(\mathbf{r}),$$

where P_{ij} is the function on R^3 defined by

$$P_{ij}(\mathbf{r}) := (B_i * B_j)(\mathbf{r}) = \int B_i(\mathbf{v})\, B_j(\mathbf{r} - \mathbf{v})\, d\mathbf{v}, \tag{3.c.2}$$

and where $\|\cdot\|$ denotes Euclidean distance. If $c_i \leq c_j$, then

$${P_{ij}}^0(z) = \frac{2\pi}{z} \int_0^{c_i} r\, {B_i}^0(r) \int_{|r-z|}^{r+z} s\, {B_j}^0(s)\, ds\, dr \tag{3.c.3}$$

for $z > 0$, while

$${P_{ij}}^0(0) = 4\pi \int_0^{c_i} r^2\, {B_i}^0(r)\, {B_j}^0(r)\, dr, \tag{3.c.4}$$

for $i, j = 1, 2, \ldots m$.

Proof: The convolution integral (3.c.2) can be written as

$${P_{ij}}^0(\|\mathbf{v}\|) = \int {B_i}^0(\|\mathbf{r}\|)\, {B_j}^0(\|\mathbf{v} - \mathbf{r}\|)\, d\mathbf{r}. \tag{3.c.5}$$

By choosing $\mathbf{v}$ along the positive z-axis, that is $\mathbf{v} = [0,0,z]^T$ where $z \geq 0$, the integral (3.c.5) can be written as

$${P_{ij}}^0(z) = \int {B_i}^0(\|\mathbf{r}\|)\, {B_j}^0(\|\mathbf{v} - \mathbf{r}\|)\, d\mathbf{r}. \tag{3.c.6}$$

Changing to the spherical coordinates (r, ϕ, θ), where ϕ and θ are longitude and latitude respectively, yields

$${P_{ij}}^0(z) = 2\pi \int_0^{c_i} r^2 {B_i}^0(r) \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} {B_j}^0\left((r^2 + z^2 - 2zr\sin\theta)^{1/2}\right) \cos\theta\, d\theta\, dr. \tag{3.c.7}$$

By substituting $z = 0$ into (3.c.7), the formula (3.c.4) for ${P_{ij}}^0(0)$ results.

Assume now that $z > 0$. Recall that the argument of ${B_j}^0$ in the θ integral of (3.c.7) is just $\|\mathbf{v} - \mathbf{r}\|$. This geometry motivates the change of variable $u = \sin\theta$ followed by $w = r^2 + z^2 - 2\,zru$, which reduces (3.c.7) to

$${P_{ij}}^0(z) = \frac{\pi}{z} \int_0^{c_i} r\, {B_i}^0(r) \int_{(r-z)^2}^{(r+z)^2} {B_j}^0(w^{1/2})\, dw\, dr. \tag{3.c.8}$$

Finally, the substitution $w = s^2$ yields Eq. (3.c.3). □

There is no loss of generality in the assumption that $c_i \leq c_j$ in the statement of Theorem 3.c.1; the formulas in case $c_j \leq c_i$ are obtained simply by interchanging the roles of c_i and c_j.

Corollary 3.c.2: *In Theorem 3.c.1 suppose that* $c := c_i = c_j$ *for some* i *and* j. *The formula* (3.c.3) *for the function* ${P_{ij}}^0(z)$ *simplifies to*

$$
{P_{ij}}^0(z) = \begin{cases} f_3(z) & 0 < z \leq c \\ f_5(z) & c \leq z \leq 2c \\ 0 & 2c \leq z \end{cases},
$$

where $f_3(z)$ and $f_5(z)$ are given in Eq. (A.27). □

4 Examples of Convolution Correlation Functions

The constructive development of convolution correlation functions is illustrated in this section. The first two examples show that the SOAR function (2.34) and the third-order autoregressive (TOAR) function are obtained by self-convolution over R and R^3, respectively, of the exponential function

$$
B_0(r) = exp\left(-\frac{|r|}{L}\right). \tag{4.1}
$$

The exponential, SOAR, and TOAR functions are the standard autoregressive functions associated with first-, second-, and third-order Gauss-Markov processes, respectively (Gelb, 1974, pp. 44-45).

Families of compactly supported SOAR- and TOAR-like functions are constructed in these two examples by self-convolving the discontinuous function

$$
B_0(r)I_c(r) = exp\left(-\frac{|r|}{L}\right) I_c(r), \tag{4.2}
$$

where I_c is the indicator function defined by

$$
I_c(x) := \begin{cases} 1 & -c \leq x \leq c \\ 0 & otherwise \end{cases},
$$

over R and R^3, respectively. These SOAR- and TOAR-like functions represent continuous, homogeneous and isotropic correlation functions on R and R^3, respectively. Cross-correlation functions for the TOAR-like model are also obtained. Another family of compactly supported TOAR-like functions is constructed by self-convolving the continuous function

$$
\left[exp\left(-\frac{|r|}{L}\right) - exp\left(-\frac{c}{L}\right)\right] I_c(r)
$$

over R^3, resulting in twice continuously differentiable, homogeneous and isotropic correlation functions on R^3.

Example 4.c provides a family of compactly supported 5th-order piecewise rational functions, each of which represents a twice continuously differentiable, homogeneous and isotropic correlation function on R^3. These functions, along with the TOAR-like functions, represent space-limited isotropic correlation functions on S^2 through the parameterization (2.33). Example 4.d describes a method of modifying correlation functions on S^2 that are not space-limited, to construct a class of space-limited correlation functions with properties similar to those of the non-space-limited class.

4.1 Compactly supported SOAR-like functions

The one-dimensional Fourier transform $\hat{B}_0(w)$ of the exponential function (4.1) is given by Yaglom (1987, p. 115):

$$\hat{B}_0(w) \;=\; \frac{2L}{1+w^2L^2}. \tag{4.3}$$

Recall that the SOAR function

$$C_0(r) := \left(1+\frac{|r|}{L}\right)\exp\left(-\frac{|r|}{L}\right) \tag{2.34}$$

has the one-dimensional Fourier transform

$$\hat{C}_0(w) = \frac{4L}{(1+w^2L^2)^2}. \tag{2.35}$$

The relation

$$\hat{C}_0(w) = \left[L^{-1/2}\hat{B}_0(w)\right]^2,$$

together with Theorem 2.9, demonstrate that $C_0(r)$ is the self-convolution of $L^{-1/2}\cdot B_0(r)$ over R.

Both $B_0(r)$ and $C_0(r)$ represent correlation functions on R according to Theorem 2.10, and also represent correlation functions on R^3 according to Theorem 2.12. A compactly supported approximant of $C_0(r)$, which will be denoted by $f(r,L,c)$, is obtained by self-convolving the function

$$D_0(r,L,c) \;:=\; \left(L\left[1-exp\left(-\frac{2c}{L}\right)\right]\right)^{-1/2} exp\left(-\frac{|r|}{L}\right)\, I_c(r)$$

over R. The function $f(r,L,c)$ is given on its support by

$$f(r,L,c) \,=\, (D_0{*}D_0)(r,L,c) \,=\, \left[1-exp\left(-\frac{2c}{L}\right)\right]^{-1}\cdot\left[C_0(r)-exp\left(\frac{|r|-2c}{L}\right)\right],\;\; 0\le|r|\le c,$$

$$=\left[1-exp\left(-\frac{2c}{L}\right)\right]^{-1}\cdot\left(\frac{2c-|r|}{L}\right)exp\left(-\frac{|r|}{L}\right),\;\; c\le|r|\le 2c. \tag{4.4}$$

The function $D_0(r,L,c)$ is continuous at $r=0$, yet discontinuous at $r=c$. It therefore follows from Theorems 2.10 and 2.13 that $\hat{D}_0(w)$ crosses the w-axis. In fact, direct calculation shows that $\hat{D}_0(w)$ decays like a damped-sinusoid, intersecting the w-axis a countably infinite number of times (*cf.*, Papoulis, 1962, p. 30). The Fourier transform of $f(r,L,c)$, given by

$$\hat{f}(w) \;=\; \hat{D}_0(w)^2,$$

is everywhere nonnegative, but also has a countable infinity of zeros along the w-axis. By Theorem 2.10, $f(r, L, c)$ represents a correlation function on R. It is evident however, that $\hat{f}(w)$ does not decrease monotonically for $w > 0$, so that by Theorem 2.12, $f(r, L, c)$ does not represent a homogeneous and isotropic correlation function on R^3. As c tends to infinity, the oscillations of $\hat{f}(w, L, c)$ disappear, and $f(r, L, c)$ tends to the SOAR function $C_0(r)$, which *does* represent a homogeneous and isotropic correlation function on R^3. Figure 1 is a graph of $f(r, L, c)$ for $c = 1500\,km$ and $c = 3000\,km$, with $L = 600\,km$, along with the SOAR function with $L = 600\,km$.

4.2 Compactly supported TOAR-like functions

Given the m radially symmetric functions $B_1, B_2, \ldots, B_m$ on R^3 represented by

$$B_i^0(r) = exp\left(-\frac{|r|}{L_i}\right) I_{c_i}(r), \tag{4.5}$$

the two-dimensional integrals in Eq. (3.c.3) can be evaluated analytically through formula (A.27). The resulting expressions for $P_{ij}^0(z)$ are rather complicated when $c_i \neq c_j$ or $L_i \neq L_j$, and are not given here. Instead, the functions

$$C_{ij}^0(z) := \frac{P_{ij}^0(z)}{\left[P_{ii}^0(0) \cdot P_{jj}^0(0)\right]^{1/2}} \tag{4.6}$$

representing $C_{ij}(\mathbf{x})$ [see Eq. (3.c.1)] are plotted in Figures 2 and 3 for $c_i = c_j = 3000\,km$ and for several values of L_i and L_j. The general formulas simplify considerably when $c := c_i = c_j$ and $L := L_i = L_j$, and in this case

$$\begin{aligned} P_{ii}^0(z) &= \frac{2\pi L z(z+3L)}{6} exp\left(-\frac{z}{L}\right) + \frac{2\pi L^2(c+L)^2}{z} exp\left(-\frac{2c}{L}\right)\left[1 - \left(1 - \frac{z}{c+L}\right) exp\left(\frac{z}{L}\right)\right] \\ &\quad + \pi L^3 \left[exp\left(-\frac{z}{L}\right) - exp\left(\frac{z-2c}{L}\right)\right], \qquad 0 < z \leq c, \\ &= \frac{2\pi L}{z} exp\left(-\frac{z}{L}\right)\left[\frac{z(z+L)(2c-z)}{2} + \frac{(z-c)^3 - c^3}{3} - L(c+L)(z-c+L) \right. \\ &\quad \left. + L(c+L)^2 exp\left(\frac{z-2c}{L}\right)\right], \qquad c \leq z \leq 2c, \end{aligned}$$

with the formula for $P_{ii}^0(0)$ obtained using (3.c.4):

$$P_{ii}^0(0) = \pi L^3\left[1 - exp\left(-\frac{2c}{L}\right)\right] - 2\pi c L\left(c+L\right) exp\left(-\frac{2c}{L}\right). \tag{4.7}$$

The functions $C_{ii}^0(z)$ represent continuous, homogeneous and isotropic correlation functions on R^3 according to Theorem 3.a.3.

The third-order autoregressive (TOAR) function

$$C_0(z) = \left(1 + \frac{|z|}{L} + \frac{z^2}{3L^2}\right) exp\left(-\frac{|z|}{L}\right). \qquad (4.8)$$

is obtained by taking the limit of $C_{ii}{}^0(z)$ as c tends to infinity. While $C_0(z)$ in Eq. (4.8) is four times continuously differentiable, the compactly supported TOAR-like function $C_{ii}{}^0(z)$ obtained from $P_{ii}{}^0(z)$ is not even once differentiable at $z = 0$. However, both one-sided derivatives exist at the origin, with the derivative from the right given by

$$\frac{dC_{ii}{}^0(0+)}{dz} = -\frac{1}{c}\left(\frac{c}{L}\right)^3 \left[exp\left(\frac{2c}{L}\right) - 1 - \frac{2c}{L} - \frac{1}{2}\left(\frac{2c}{L}\right)^2\right]^{-1}. \qquad (4.9)$$

A smoother TOAR-like function can be obtained by starting with the *continuous* functions

$$B_i{}^0(r) \;=\; \left[exp\left(-\frac{|r|}{L_i}\right) - exp\left(-\frac{c_i}{L_i}\right)\right] I_{c_i}(r),$$

instead of with (4.5). The representing functions obtained in this case will be denoted by $S_{ij}{}^0(z)$, and are defined analogously to the $C_{ij}{}^0(z)$ of Eq. (4.6). Theorem 3.a.3 guarantees that the $S_{ii}{}^0(z)$ are at least twice continuously differentiable on R, and represent homogeneous and isotropic correlation functions on R^3. Like $C_{ii}{}^0(z)$, $S_{ii}{}^0(z)$ tends to the TOAR function (4.8) as c_i tends to infinity, and is close to $C_{ii}{}^0(z)$ when $L_i << c_i$. Plots of $S_{ii}{}^0(z)$, the TOAR function, and $C_{ii}{}^0(z)$ are given in Figures 4 and 5.

4.3 Compactly supported 5th-order piecewise rational functions

A two-parameter 5th-order piecewise rational function is obtained by self-convolving the continuous, piecewise linear function

$$B_0(r,a,c) \;=\; \begin{cases} 2(a-1)|r|/c + 1 & 0 \le |r| \le c/2 \\ 2a(1 - |r|/c) & c/2 \le |r| \le c \\ 0 & c \le |r| \end{cases},$$

over R^3. Theorem 3.a.3 guarantees that the self-convolution function $C_0(z,a,c)$ is at least twice continuously differentiable on R, and represents a homogeneous and isotropic correlation function on R^3.

The function $C_0(z,a,c)$ has a large number of terms, but simplifies considerably in several cases. If $a = 0$ or $a = 1/2$, B_0 is a triangular function. It is well known that self-convolution over R of a triangular function yields a cubic B-spline (Strang, 1986, p. 327). Self-convolution of the triangular function

$$B_0(r,1/2,c) = \left(1 - \frac{|r|}{c}\right) I_c(r)$$

over R^3 yields the 5th-order piecewise rational function

$$C_0(z,1/2,c) \;=\; \begin{cases} f_1(z/c) & 0 \le |z| \le c \\ f_2(z/c) & c \le |z| \le 2c \\ 0 & 2c \le |z| \end{cases},$$

where the even functions f_1 and f_2 are given for $z \geq 0$ by

$$f_1(z) = -\frac{z^5}{4} + \frac{z^4}{2} + \frac{5z^3}{8} - \frac{5z^2}{3} + 1, \quad 0 \leq z \leq 1,$$

and

$$f_2(z) = \frac{z^5}{12} - \frac{z^4}{2} + \frac{5z^3}{8} + \frac{5z^2}{3} - 5z + 4 - \frac{2}{3z}, \quad 1 \leq z \leq 2. \tag{4.10}$$

The function $C_0(z, \infty, c)$ obtained by taking the limit of $C_0(z, a, c)$ as a tends to $\pm\infty$ is given by

$$C_0(z, \infty, c) = \begin{cases} f_1(z/c) & 0 \leq |z| \leq c/2 \\ f_2(z/c) & c/2 \leq |z| \leq c \\ f_3(z/c) & c \leq |z| \leq 3c/2 \\ f_4(z/c) & 3c/2 \leq |z| \leq 2c \\ 0 & 2c \leq |z| \end{cases},$$

where the even functions $f_1, \ldots, f_4$ are given for $z \geq 0$ by

$$f_1(z) = -\frac{28z^5}{33} + \frac{8z^4}{11} + \frac{20z^3}{11} - \frac{80z^2}{33} + 1, \quad 0 \leq z \leq 1/2,$$

$$f_2(z) = \frac{20z^5}{33} - \frac{16z^4}{11} + \frac{100z^2}{33} - \frac{45z}{11} + \frac{51}{22} - \frac{7}{44z}, \quad 1/2 \leq z \leq 1,$$

$$f_3(z) = -\frac{4z^5}{11} + \frac{16z^4}{11} - \frac{10z^3}{11} - \frac{100z^2}{33} + 5z - \frac{61}{22} + \frac{115}{132z}, \quad 1 \leq z \leq 3/2,$$

and

$$f_4(z) = \frac{4z^5}{33} - \frac{8z^4}{11} + \frac{10z^3}{11} + \frac{80z^2}{33} - \frac{80z}{11} + \frac{64}{11} - \frac{32}{33z}, \quad 3/2 \leq z \leq 2. \tag{4.11}$$

The function $C_0(z, \infty, c)$ is three times continuously differentiable on R.

The function $C_0(z, a, c)$ and the Gaussian function

$$G_0(z, L) = exp\left(-\frac{z^2}{2L^2}\right) \tag{4.12}$$

represent homogeneous and isotropic correlation functions on R^3. The functions $C_0(z, 1/2, c)$ and $G_0(z, L)$ are similar for selected parameter values, as is illustrated in Figure 6 by matching the length scales of these two functions (as defined below in Eq. (4.16)) for $c = 1500\,km$. Here both $G_0(z, L)$ and $C_0(z, 1/2, c)$ where $L = c\sqrt{.3}$ have length scale $L \approx 822\,km$. Figures 7 and 8 are graphs of $C_0(z, a, c)$ for $c = 1000\,km$ and various values of a.

4.4 Compactly supported product correlation functions

It is widely accepted that sample single-level short-term geopotential height forecast error correlations essentially vanish beyond distances of a few thousand *km* in the troposphere (Hollingsworth and Lönnberg, 1986; Lönnberg and Hollingsworth, 1986; Bartello and Mitchell, 1992; Courtier *et al.*, 1998). For both computational and scientific reasons, it is desirable in the Physical-space Statistical Analysis System (PSAS) under development at the Data Assimilation Office (Cohn *et al.*, 1998) to reflect this property by developing a space-limited horizontal correlation model that retains the essential features of the geopotential height forecast error correlation model used in the predecessor GEOS-1 optimal interpolation system (Pfaendtner *et al.*, 1995). A general method for constructing space-limited approximants of a given single-level univariate correlation model is described and illustrated in this example.

The function used in the GEOS-1 optimal interpolation system for single-level geopotential height forecast error correlations is modeled after the so-called *powerlaw* function

$$B_0(z, L) \ := \ \frac{1}{1 + .5(z/L)^2}. \tag{4.13}$$

The one-dimensional Fourier transform of B_0,

$$\hat{B}_0(w, L) \ = \ \pi L\sqrt{2}\ exp\Big(-L\sqrt{2}\,|w|\Big), \tag{4.14}$$

is everywhere nonnegative. By Theorem 2.10, B_0 represents a correlation function on R. Let B_1 denote the radially symmetric function given by

$$B_1(\mathbf{x}) \ := \ B_0(\|\mathbf{x}\|), \quad \mathbf{x} \in R^3.$$

Since $z^2 B_0(z, L)$ does *not* lie in $L^1(R)$, B_1 does not lie in $L^1(R^3)$ – see Eq. (2.29) – implying that the $L^1(R^3)$ Fourier transform of B_1 (Theorem 2.7) is not defined. Thus, although $\hat{B}_0(w, L)$ decreases monotonically for $w > 0$, Theorems 2.10 and 2.12 cannot be applied here. Reparameterize z in $B_0(z, L)$ by great circle distance, as in Eq. (2.33):

$$z \ = \ z(\theta) \ = \ 2\,sin\left(\frac{\theta}{2}\right) \ = \ \sqrt{2(1 - cos(\theta))}, \qquad 0 \le \theta \le \pi,$$

and define

$$B(\mathbf{x}, \mathbf{y}) \ := \ B_0(z(\theta), L) \ = \ \frac{1}{1 + .5(z(\theta)/L)^2} \ = \ \frac{1}{1 + (1 - cos(\theta))/L^2}, \quad \mathbf{x}, \mathbf{y} \in S^2,$$

where θ is the great circle distance between $\mathbf{x}$ and $\mathbf{y}$ on S^2. In the Appendix, it is shown that each Legendre coefficient

$$a_m \ = \ \frac{2m + 1}{2} \int_0^\pi B_0(z(\theta), L)\, P_m(cos(\theta))\, sin(\theta)\, d\theta, \qquad m \ge 0,$$

of

$$B_0(z(\theta), L) \ = \ \sum_{m=0}^{\infty} a_m P_m(cos\,\theta),$$

is nonnegative, so that by Theorem 2.11, $B(\mathbf{x}, \mathbf{y})$ is an isotropic correlation function on S^2. Note, however, that B is not space-limited.

Recall from the discussion following Definition 2.2 that the product function

$$D(\mathbf{x}, \mathbf{y}) \ := \ B(\mathbf{x}, \mathbf{y})\, C(\mathbf{x}, \mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in S^2, \tag{4.15}$$

is a covariance function on S^2 whenever both B and C are covariance functions on S^2. If C is space-limited, vanishing identically for pairs of points on S^2 beyond distance $d < 2$:

$$C(\mathbf{x}, \mathbf{y}) \ = \ 0, \quad \|\mathbf{x} - \mathbf{y}\| > d,$$

then since B is everywhere positive, D vanishes exactly where C does, *i.e.*, for $\|\mathbf{x}-\mathbf{y}\| > d$. If C is isotropic, then D is isotropic by Definition 2.5.

In the case of the powerlaw, the choice

$$C(\mathbf{x},\mathbf{y}) \;:=\; C_0(\|\mathbf{x}-\mathbf{y}\|, 1/2, c), \quad \mathbf{x},\mathbf{y} \in R^3$$

in Eq. (4.15), where C_0 is as in Eq. (4.10), yields a space-limited, isotropic correlation function

$$D(\mathbf{x},\mathbf{y}) \;:=\; D_0(z(\theta), L, c) \;:=\; B_0(z(\theta), L)\, C_0(z(\theta), 1/2, c), \quad 0 \leq \theta \leq \pi, \quad \mathbf{x},\mathbf{y} \in S^2,$$

where θ is the great circle distance between $\mathbf{x}$ and $\mathbf{y}$ on S^2. The function D, vanishing for $|z(\theta)| > 2c$, provides a reasonable approximation to the powerlaw, as is demonstrated below.

Given any twice differentiable function f that is concave in an interval containing zero, define a length scale L_f in the usual way (Daley, 1991, p. 110):

$$L_f \;:=\; \frac{1}{\sqrt{-f''(0)}}. \tag{4.16}$$

Using lowercase letters to simplify notation, *e.g.*,

$$L_{b_0} \;:=\; \frac{1}{\sqrt{-B_0''(0)}},$$

it can be verified that $L_{b_0} = L$ in Eq. (4.13), and that the length scale of $C_0(z, 1/2, c)$ is given by $L_{c_0} = c\sqrt{.3}$. The product rule for differentiation together with the fact that $B_0(0) = C_0(0) = 1$ and $B_0'(0) = C_0'(0) = 0$ imply that

$$\frac{1}{{L_{d_0}}^2} \;=\; \frac{1}{{L_{b_0}}^2} + \frac{1}{{L_{c_0}}^2} \;=\; \frac{1}{L^2} + \frac{10}{3c^2}. \tag{4.17}$$

If L_0 is the parameter obtained by solving for L in Eq. (4.17):

$$L_0 \;=\; \sqrt{\frac{{L_{c_0}}^2 {L_{d_0}}^2}{{L_{c_0}}^2 - {L_{d_0}}^2}} \;=\; \sqrt{\frac{3c^2 {L_{d_0}}^2}{3c^2 - 10{L_{d_0}}^2}}, \qquad L_{c_0} > L_{d_0}, \tag{4.18}$$

then $D_0(z, L_0, c)$ has length scale L_{d_0}.

In Figures 9-12, c is held fixed at $c = 3000\,km$. Figure 9 is a graph of $D_0(z, L_0, c)$ and $B_0(z, L_{d_0})$ for $L_{d_0} = 600\,km$ and $L_{d_0} = 1200\,km$. Note that both functions $D_0(z, L_0, c)$ and $B_0(z, L_{d_0})$ have the length scale L_{d_0}. The compactly supported function $D_0(z, L_0, c)$ agrees well with $B_0(z, L_{d_0})$ for $0 \leq z \leq L_{d_0}$. However, $D_0(z, L_0, c)$ falls off to zero more rapidly than $B_0(z, L_{d_0})$, especially for larger values of L_{d_0}, as indeed it must.

The wind/height and wind/wind correlation models derived under the geostrophic assumption from either $D_0(z, L_0, c)$ or $B_0(z, L_{d_0})$ are similar whenever the first two derivatives of $D_0(z, L_0, c)$ and $B_0(z, L_{d_0})$ are similar (*cf.* Daley, 1991, Sec. 5.2). Figure 10 is a graph of

$$\frac{dD_0(z, L_0, c)}{dz} \quad \text{and} \quad \frac{dB_0(z, L_{d_0})}{dz}, \qquad z \geq 0, \tag{4.19}$$

for $L_{d_0} = 600\,km$ and $L_{d_0} = 1200\,km$, while Figure 11 is a graph of

$$\frac{d^2 D_0(z, L_0, c)}{dz^2} \quad \text{and} \quad \frac{d^2 B_0(z, L_{d_0})}{dz^2}, \qquad z \geq 0,$$

for $L_{d_0} = 600\,km$ and $L_{d_0} = 1200\,km$. The graphs illustrate the degree of similarity of the wind/height and wind/wind correlation models derived from $D_0(z, L_0, c)$ and $B_0(z, L_{d_0})$.

The Legendre coefficients of $D_0(z, L_0, c)$ and $B_0(z, L_{d_0})$ are plotted in Figure 12 for $L_{d_0} = 600\,km$ and $L_{d_0} = 1200\,km$. Compare with Figures 3a and 6 of Rabier *et al.* (1998). For each L_{d_0}, there is less power at large spatial scales for $D_0(z, L_0, c)$ than for $B_0(z, L_{d_0})$. The Legendre spectra of both functions begin to exhibit an oscillation at smaller spatial scales, even though the one-dimensional Fourier spectrum (4.14) of B_0 decreases monotonically with positive wavenumber.

5 Concluding Remarks

The recent development of truly global atmospheric data analysis systems (*e.g.*, Parrish and Derber, 1992; Cohn *et al.*, 1998; Courtier *et al.*, 1998; Rabier *et al.*, 1998) requires the concomitant development of correlation models that are legitimate correlation functions on the sphere. This article provides a comprehensive summary of mathematical theory pertinent to correlation modeling on the sphere, and establishes several techniques for the actual construction of legitimate correlation functions on the sphere. These functions typically depend on a small number of tunable parameters. Special emphasis has been placed on the construction of space-limited correlation functions, in which one parameter determines a distance beyond which the correlation function vanishes identically. Correlation models of this type are especially important for data analysis systems that operate directly in physical space (Cohn *et al.*, 1998). Several examples have been included to illustrate the practical application of both the constructive techniques and the basic mathematical theory developed in this article.

Although the theory and constructive techniques are general, the results given here are slanted toward the single-level, univariate case. Extension of these results to the nonseparable, multi-level, multivariate case will be the subject of future articles.

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A Appendix

A.1 Proof of Theorem 3.a.3

The fact that $rB_0(r)$ and $rC_0(r)$ are both compactly supported and piecewise continuous (C_0 is in fact continuous by Theorem 2.9) implies that they both lie in $L^1(R)$. Thus, if $h_2(r) := rC_0(r)$, then [see Eq. (2.30)]:

$$
\begin{aligned}
i\frac{d\hat{B}_0(w)}{dw} &= F[rB_0](w) = \hat{h}_1(w) \quad \text{and} \\
i\frac{d\hat{C}_0(w)}{dw} &= F[rC_0](w) = \hat{h}_2(w). \qquad (A.1)
\end{aligned}
$$

Theorem 2.9 together with (2.32) imply that

$$
-\frac{2\pi}{\|\mathbf{w}\|}\frac{d\hat{C}_0(\|\mathbf{w}\|)}{d\|\mathbf{w}\|} = \hat{C}_1(\mathbf{w}) = \hat{B}_1(\mathbf{w})^2 = \left[-\frac{2\pi}{\|\mathbf{w}\|}\frac{d\hat{B}_0(\|\mathbf{w}\|)}{d\|\mathbf{w}\|}\right]^2. \qquad (A.2)
$$

Note that $\hat{B}_0$ and $\hat{C}_0$ are real since B_0 and C_0 are both even functions by hypothesis, so that (A.2) implies that

$$
\frac{d\hat{C}_0(w)}{dw} \leq 0 \qquad \text{for} \quad w > 0. \qquad (A.3)
$$

Combining $(A.1)$ and $(A.2)$ yields

$$
\hat{h}_2(w) = \frac{2\pi i}{w}\left[\hat{h}_1(w)\right]^2. \qquad (A.4)
$$

Now, the fact that B_0 is compactly supported implies that each derivative of B_0 that exists is also compactly supported. The function ${h_1}^{(n+1)}$ is piecewise continuous by hypothesis, and is given by

$$
{h_1}^{(n+1)}(r) = (n+1){B_0}^{(n)}(r) + r{B_0}^{(n+1)}(r). \qquad (A.5)
$$

Therefore, ${h_1}^{(n+1)}$ is both compactly supported and piecewise continuous, so that in particular, ${h_1}^{(n+1)}$ lies in $L^1(R)$. It is known (Folland, 1992, p. 214) that the facts that ${h_1}^{(n)}$ is continuous and piecewise smooth and that ${h_1}^{(n+1)}$ lies in $L^1(R)$ imply that the Fourier transform of ${h_1}^{(n+1)}$ is related to $\hat{h}_1$ by

$$
(iw)^{n+1}\hat{h}_1(w) = F[{h_1}^{(n+1)}](w). \qquad (A.6)
$$

Further, because ${h_1}^{(n+1)}$ is compactly supported and piecewise continuous, the argument used in Folland (1992, p. 217) and in Bochner and Chandrasekharan (1949, Theorem 1, p. 4) to establish the Riemann-Lebesgue lemma implies that

$$
F[{h_1}^{(n+1)}](w) = O\left(\frac{1}{w}\right), \qquad (A.7)
$$

where $O(1/w)$ means that the expression on the left is bounded by K/w in absolute value for sufficiently large w, K being some fixed constant independent of w. Combining $(A.1)$, $(A.4)$, $(A.6)$, and $(A.7)$ yields the relation

$$
i\frac{d\hat{C}_0(w)}{dw} = \hat{h}_2(w) = O\left(\frac{1}{w^{2n+5}}\right). \qquad (A.8)
$$

Since B_0 is compactly supported on $[-c, c]$, C_0 and $h_2(r) = rC_0(r)$ are also compactly supported, with support $[-2c, 2c]$. Write the Fourier series of h_2 on $[-2c, 2c]$ as

$$h_2(r) = \sum_{-\infty}^{\infty} c_k \, exp\Big(\frac{k\pi ri}{2c}\Big), \qquad |r| \leq 2c. \tag{A.9}$$

The compact support of h_2 implies the following relation between the Fourier coefficients c_k of the (odd) 4c-periodic extension of h_2, and the Fourier transform $\hat{h}_2$ of h_2:

$$\begin{aligned} c_k &= \frac{1}{4c}\int_{-2c}^{2c} h_2(r)\, exp\Big(-\frac{k\pi ri}{2c}\Big)\, dr \\ = \frac{1}{4c}\int_{-\infty}^{\infty} h_2(r)\, exp\Big(-\frac{k\pi ri}{2c}\Big)\, dr &= \frac{1}{4c}\hat{h}_2\Big(\frac{k\pi}{2c}\Big). \end{aligned} \tag{A.10}$$

Formulas $(A.8)$ and $(A.10)$ together imply that

$$c_k = \frac{1}{4c}\hat{h}_2\Big(\frac{k\pi}{2c}\Big) = O\left(\frac{1}{k^{2n+5}}\right). \tag{A.11}$$

It is well-known (Folland, 1992, p. 41) that formula $(A.11)$ implies that the 4c-periodic extension of h_2 is at least $2n+3$ times continuously differentiable on R, hence h_2 is at least $2n+3$ times continuously differentiable on $(-2c, 2c)$. All derivatives of h_2 outside $[-2c, 2c]$ vanish because h_2 is compactly supported, so that h_2 is at least $2n+3$ times continuously differentiable except possibly when $r = \pm 2c$. Since C_0 is the quotient

$$C_0(r) = \frac{h_2(r)}{r}, \qquad r \neq 0, \tag{A.12}$$

it follows that C_0 is at least $2n+3$ times continuously differentiable, except possibly at $r = 0$ and at $r = \pm 2c$.

The Riemann-Lebesgue lemma for C_0 together with $(A.8)$ imply the relation

$$\hat{C}_0(w) = -\int_w^{\infty} \frac{d\hat{C}_0(t)}{dt}\, dt. \tag{A.13}$$

Formulas $(A.8)$ and $(A.13)$ imply that

$$\hat{C}_0(w) = O\left(\frac{1}{w^{2n+4}}\right),$$

so that the Fourier coefficients of C_0 have the property that

$$\frac{1}{4c}\hat{C}_0\Big(\frac{k\pi}{2c}\Big) = O\left(\frac{1}{k^{2n+4}}\right). \tag{A.14}$$

Formula $(A.14)$ implies that C_0 is at least $2n+2$ times continuously differentiable on $(-2c, 2c)$.

Theorem 2.9 implies in particular that C_1 is continuous and lies in $L^1(R^3)$. It follows from Eq. $(A.3)$ and Theorem 2.12 that $C(\mathbf{x}, \mathbf{y})/C_0(0)$ is a continuous, homogeneous and isotropic correlation function on R^3. Since C_0 is at least $2n+2$ times continuously differentiable on $(-2c, 2c)$, ${C_0}^{(2n+2)}(r)$ is continuous at $r = 0$ in particular, and Theorem 2.13 implies that ${C_0}^{(2n+2)}$ is continuously differentiable on all of R. □

A.2 Proof of Theorem 3.a.5

The Fourier transform $\hat{C}_0$ lies in $L^1(R)$ by Theorem 2.10 and is also continuous. Thus the function ϕ defined on R by

$$\phi(w) := \sqrt{\hat{C}_0(w)} \tag{A.15}$$

lies in $L^2(R)$ and is continuous. The Fourier transform on $L^2(R)$ (*cf.* Stein and Weiss, 1971, Theorem 2.3, p. 17; Rudin, 1987, Theorem 9.13c, p. 186) associates with ϕ, a function D_0 in $L^2(R)$ such that, for almost all w in R,

$$\phi(w) = \hat{D}_0(w). \tag{A.16}$$

Combining $(A.15)$ and $(A.16)$ yields the relation

$$\hat{C}_0(w) = \hat{D}_0(w)^2, \tag{A.17}$$

valid for almost all w in R. Since $\hat{C}_0$ is continuous and lies in $L^1(R)$, $\hat{C}_0$ also lies in $L^2(R)$. The convolution theorem for $L^2(R)$ functions (Weidmann, 1980, p. 295) therefore implies that $(A.17)$ can be inverted to yield $C_0 = D_0 * D_0$.

Suppose now that C_0 is twice continuously differentiable and that $C_0{''}$ lies in $L^1(R)$. It follows that $C_0{'}$ lies in $L^1(R)$ (Bochner and Chandrasekharan, 1949, Theorem 17, p. 29), since C_0 lies in $L^1(R)$. Thus

$$F[-C_0{''}](w) = w^2 \hat{C}_0(w) \tag{A.18}$$

follows (*e.g.*, Folland, 1992, p. 214). Therefore, $w^2\hat{C}_0(w)$ lies in $L^1(R)$ (*e.g.*, Stein and Weiss, 1971, Corollary 1.26, p. 15), so that by $(A.17)$, $w\hat{D}_0(w)$ lies in $L^2(R)$. Let $h(w)$ be the function on R which is zero on $[-1,1]$ and equal to $1/w$ otherwise. The product of $h(w)$ and $w\hat{D}_0(w)$ gives $\hat{D}_0(w)$ for w outside $[-1,1]$. Since $h(w)$ and $w\hat{D}_0(w)$ both lie in $L^2(R)$, $\hat{D}_0(w)$ is integrable outside $[-1,1]$. Since $\hat{D}_0(w)$ is square-integrable over $[-1,1]$, $\hat{D}_0$ is integrable over $[-1,1]$ as well. Thus $\hat{D}_0$ also lies in $L^1(R)$. Since $\hat{D}_0$ lies in $L^1(R)$, the function

$$F_0(r) := \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{D}_0(w)\, exp(iwr)\, dw \tag{A.19}$$

can be defined. Applying the argument used in Rudin (1987, Theorem 9.6, p. 182) shows that F_0 is continuous (and also vanishes at infinity). It is also true that D_0 and F_0 agree almost everywhere (Rudin, 1987, Theorem 9.14, p. 187), so that F_0 lies in $L^2(R)$ and $(3.a.5)$ holds.

Suppose that C_0 represents the radially symmetric function C_1 lying in $L^1(R^3)$ and the homogeneous and isotropic correlation function C. Using Eqs. $(A.15)$, $(A.16)$, and $(A.19)$ yields:

$$\begin{aligned} F_0(r) &:= \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{D}_0(w)\, exp(iwr)\, dw = \frac{1}{2\pi} \int_{-\infty}^{\infty} \phi(w)\, exp(iwr)\, dw \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \phi(w)\, exp(-iwr)\, dw, \end{aligned} \tag{A.20}$$

where the last inequality in Eq. (A.20) holds since $\phi(w)$ is an even function. The fact that $\phi(w)$ is even also implies that $F_0(r)$ is an even function. Equation (A.20) shows that $F_0(r)$ is the Fourier transform of the continuous function $\phi(w)/2\pi$. According to Folland (1992, p. 224, Exercise 7), F_0 lies in $L^1(R)$ if $\phi(w)$ also lies in $L^2(R)$, $\phi(w)$ is piecewise smooth, and $d\phi(w)/dw$ lies in $L^2(R)$. It was shown above that $\phi(w)$ lies in $L^2(R)$. Below it is shown that the other two conditions also hold, so that in fact F_0 does lie in $L^1(R)$.

Changing to spherical coordinates yields

$$\hat{C}_1(\mathbf{0}) = \int C_1(\mathbf{r})\, d\mathbf{r} = 4\pi \int_0^\infty C_0(r)\, r^2\, dr.$$

Thus $rC_0(r)$ and $r^2C_0(r)$ both lie in $L^1(R)$ – see the proof of Theorem 2.12. Since $r^2C_0(r)$ lies in $L^1(R)$, applying Folland (1992, p. 223, Formula 6) twice yields

$$-\frac{d^2\hat{C}_0(w)}{dw^2} = \int_{-\infty}^{\infty} r^2 C_0(r) exp(-iwr)\, dr,$$

i.e., $\hat{C}_0$ is twice differentiable. Since C is a homogeneous and isotropic correlation function, Theorem 2.12 implies that $\hat{C}_0$ decreases monotonically for $w > 0$. Since $\hat{C}_0$ is even, continuous, everywhere nonnegative, and decreases monotonically for $w > 0$, $\hat{C}_0$ is either everywhere positive, or there is a constant $w_0 > 0$ so that $\hat{C}_0$ is positive on $(-w_0, w_0)$ and vanishes identically outside $(-w_0, w_0)$. In either case, $\phi(w)$ is piecewise smooth. In the case where $\hat{C}_0$ vanishes identically outside $(-w_0, w_0)$, $d\phi(w)/dw$ clearly lies in $L^2(R)$. If $\hat{C}_0$ is everywhere positive, then $\phi(w)$ is twice differentiable everywhere. In addition,

$$\frac{d\phi(w)}{dw} = \frac{1}{2\sqrt{\hat{C}_0(w)}} \frac{d\hat{C}_0(w)}{dw} \tag{A.21}$$

is nonpositive for each $w > 0$, implying that $\phi(w)$ decreases monotonically for each $w > 0$. Applying the Fundamental Theorem of Calculus yields

$$\int_0^b \frac{d\phi(w)}{dw}\, dw = \phi(b) - \phi(0), \qquad b > 0. \tag{A.22}$$

Since $\phi(w)$ vanishes at infinity by the Riemann-Lebesgue Lemma, letting b tend to infinity in Eq. (A.22) yields

$$\int_0^\infty \left|\frac{d\phi(w)}{dw}\right| dw = -\int_0^\infty \frac{d\phi(w)}{dw}\, dw = \phi(0), \tag{A.23}$$

where the first inequality in Eq. (A.23) holds due to the monotonicity property established in Eq. (A.21). Using Eq. (A.23) and the fact that $|d\phi(w)/dw|$ is an even function shows that $d\phi(w)/dw$ lies in $L^1(R)$. Since this function is also continuous, it lies in $L^2(R)$. Thus F_0 lies in $L^1(R)$, as asserted above.

Since F_0 lies in $L^1(R)$, the Fourier transform of F_0 (given by Eq. (2.17)),

$$\hat{F}_0(w) = \int_{-\infty}^{\infty} F_0(r)\, exp(-iwr)\, dr, \tag{A.24}$$

exists, is a continuous function, and furthermore

$$\hat{F}_0(w) \;=\; \phi(w) \qquad (A.25)$$

holds for *each* w in R. In particular, $\hat{F}_0(w)$ decreases monotonically for each $w > 0$. Let F_1 be the radially symmetric function on R^3, and let F be the homogeneous and isotropic function defined by

$$F(\mathbf{x},\mathbf{y}) \;:=\; F_1(\mathbf{x} - \mathbf{y}) \;:=\; F_0(\|\mathbf{x}-\mathbf{y}\|), \quad \mathbf{x},\mathbf{y} \in R^3.$$

Since $\hat{F}_0(w)$ (see Eq. (A.25)) was shown above to be twice differentiable for $w \in (-w_0, w_0)$, evaluating the second derivative at zero yields

$$-\frac{d^2\hat{F}_0(0)}{dw^2} \;=\; \int_{-\infty}^{\infty} r^2 F_0(r)\,dr \;=\; 2\int_0^{\infty} r^2 F_0(r)\,dr \;=\; \frac{1}{2\pi}\int F_1(\mathbf{r})\,d\mathbf{r};$$

the first inequality follows from Folland (1992, p. 223, Formula 6), the second since $r^2F_0(r)$ is an even function of r, and the third by changing to spherical coordinates. Thus F_1 lies in $L^1(R^3)$. Recall from the argument following Eq. (A.19) that F_0 is a continuous function, implying that F_1 is also continuous. It follows from Theorem 2.12 that $F(\mathbf{x},\mathbf{y})/F_0(0)$ is a correlation function. □

A.3 Detailed reduction of the convolution integral in Theorem 3.c.1

Theorem: *Same hypotheses as Theorem 3.c.1. Assume now that each* $rB_i{}^0(r)$ *is continuous on* $[-c_i, c_i]$. *Define* $G_j(s)$ *for* $s \geq 0$ *to be the antiderivative*

$$G_j(s) := \int_0^s t\,B_j{}^0(t)\,dt$$

of $sB_j{}^0(s)$. *For fixed* z, *let* $H_{ij}(r,z)$ *and* $R_{ij}(r,z)$ *be antiderivatives of*

$$r\,B_i{}^0(r)\,G_j(r+z), \quad r \geq 0, \quad r+z \geq 0,$$

and

$$r\,B_i{}^0(r)\,G_j(z-r), \quad r \geq 0, \quad z-r \geq 0,$$

respectively, so that

$$H_{ij}(b,z) - H_{ij}(a,z) = \int_a^b r\,B_i{}^0(r)\,G_j(r+z)\,dr, \quad a+z \geq 0,$$

and

$$R_{ij}(b,z) - R_{ij}(a,z) = \int_a^b r\,B_i{}^0(r)\,G_j(z-r)\,dr, \quad z-b \geq 0,$$

hold for $b \geq a \geq 0$. *If* $z > 0$ *and* $c_i \leq c_j$, *then*

$$P_{ij}{}^0(z) \;=\; \begin{cases} f_1(z) & 0 < z \leq min(c_i, c_j - c_i) \\ f_2(z) & c_i \leq z \leq c_j - c_i \\ f_3(z) & c_j - c_i \leq z \leq c_i \\ f_4(z) & max(c_i, c_j - c_i) \leq z \leq c_j \\ f_5(z) & c_j \leq z \leq c_i + c_j \\ 0 & c_i + c_j \leq z \end{cases},$$

for $i, j = 1, 2, \ldots, m$, *where* $f_1, \ldots, f_5$ *are given by:*

$$f_1(z) = \frac{2\pi}{z}\Big[H_{ij}(c_i, z) - H_{ij}(0, z) - R_{ij}(z, z)$$
$$+R_{ij}(0, z) - H_{ij}(c_i, -z) + H_{ij}(z, -z)\Big],$$

$$f_2(z) = \frac{2\pi}{z}\Big[H_{ij}(c_i, z) - H_{ij}(0, z) - R_{ij}(c_i, z) + R_{ij}(0, z)\Big],$$

$$f_3(z) = \frac{2\pi}{z}\Big[H_{ij}(c_j - z, z) - H_{ij}(0, z) + G_j(c_j)[G_i(c_i) - G_i(c_j - z)]$$
$$-R_{ij}(z, z) + R_{ij}(0, z) - H_{ij}(c_i, -z) + H_{ij}(z, -z)\Big],$$

$$f_4(z) = \frac{2\pi}{z}\Big[H_{ij}(c_j - z, z) - H_{ij}(0, z)$$
$$+G_j(c_j)[G_i(c_i) - G_i(c_j - z)] - R_{ij}(c_i, z) + R_{ij}(0, z)\Big],$$

$$f_5(z) = \frac{2\pi}{z}\Big[R_{ij}(z - c_j, z) - R_{ij}(c_i, z) + G_j(c_j)[G_i(c_i) - G_i(z - c_j)]\Big]. \qquad (A.27)$$

Proof: The reduction of formula (3.*c*.3) to integrals over the support of the integrand $rB_i{}^0(r)sB_j{}^0(s)$ yields three integrals which will be denoted by I_1, I_2 and I_3, respectively:

$$I_1(z) := \frac{2\pi}{z}\int_0^{c_i} r\,B_i{}^0(r)\int_{|r-z|}^{r+z} s\,B_j{}^0(s)\,ds\,dr, \;\; 0 < z \le c_j - c_i,$$

$$I_2(z) := \frac{2\pi}{z}\int_0^{c_j - z} r\,B_i{}^0(r)\int_{|r-z|}^{r+z} sB_j{}^0(s)\,ds\,dr$$
$$+\frac{2\pi}{z}\int_{c_j - z}^{c_i} r\,B_i{}^0(r)\int_{|r-z|}^{c_j} s\,B_j{}^0(s)\,ds\,dr, \;\; c_j - c_i \le z \le c_j,$$

$$I_3(z) := \frac{2\pi}{z}\int_{z-c_j}^{c_i} r\,B_i{}^0(r)\int_{z-r}^{c_j} sB_j{}^0(s)\,ds\,dr, \;\; c_j \le z \le c_i + c_j. \qquad (A.28)$$

The integral $I_1(z)$ can be written as

$$I_1(z) \;=\; \frac{2\pi}{z}\int_0^{c_i} r\,B_i{}^0(r)\Big[G_j(r+z) - G_j(|r-z|)\Big]\,dr. \qquad (A.29)$$

If $c_i \le z \le c_j - c_i$, then $|r - z| = z - r$ everywhere over the interval $[0, c_i]$ of integration in $(A.29)$, and $I_1(z)$ reduces to $f_2(z)$. If $0 < z \le \min(c_i, c_j - c_i)$, then $(A.29)$ reduces to $f_1(z)$:

$$I_1(z) = \frac{2\pi}{z}\Big[H_{ij}(c_i, z) - H_{ij}(0, z) - \int_0^z r\, B_i^0(r)\, G_j(z - r)\, dr$$

$$- \int_z^{c_i} r\, B_i^0(r)\, G_j(r - z)\, dr\Big]$$

$$= \frac{2\pi}{z}\Big[H_{ij}(c_i, z) - H_{ij}(0, z) - R_{ij}(z, z) + R_{ij}(0, z) - H_{ij}(c_i, -z) + H_{ij}(z, -z)\Big].$$

The formulas for f_3 and f_4 are obtained from I_2:

$$I_2(z) = \frac{2\pi}{z} \int_0^{c_j - z} r\, B_i^0(r)\Big[G_j(r+z) - G_j(|r-z|)\Big]\, dr + \frac{2\pi}{z} \int_{c_j - z}^{c_i} r\, B_i^0(r)\Big[G_j(c_j) - G_j(|r-z|)\Big]\, dr$$

$$= \frac{2\pi}{z} \int_0^{c_j - z} r\, B_i^0(r) G_j(r + z)\, dr \;+\; \frac{2\pi G_j(c_j)}{z}\Big[G_i(c_i) - G_i(c_j - z)\Big]$$

$$- \frac{2\pi}{z} \int_0^{c_i} r\, B_i^0(r)\, G_j(|r - z|)\, dr. \qquad (A.30)$$

If $\max(c_i, c_j - c_i) \le z \le c_j$, then $|r - z| = z - r$ everywhere over the interval $[0, c_i]$ of integration in the last term of $(A.30)$, and $I_2(z)$ reduces to $f_4(z)$. If $c_j - c_i \le z \le c_i$, then $(A.30)$ reduces to $f_3(z)$ in a manner similar to the way that $(A.29)$ was reduced to $f_1(z)$.

The reduction of I_3 to f_5 is straightforward:

$$I_3(z) = \frac{2\pi}{z} \int_{z - c_j}^{c_i} r\, B_i^0(r)\Big[G_j(c_j) - G_j(z - r)\Big]\, dr$$

$$= \frac{2\pi}{z}\Big[G_j(c_j)[G_i(c_i) - G_i(z - c_j)] - R_{ij}(c_i, z) + R_{ij}(z - c_j, z)\Big].$$

□

A.4 Proof that the powerlaw represents a correlation function on the sphere

To show that the powerlaw

$$B_0(z(\theta), L) = \frac{1}{1 + (1 - cos(\theta))/L^2}, \qquad 0 \le \theta \le \pi,$$

represents a correlation function $B(\mathbf{x}, \mathbf{y})$ on S^2, it suffices to show (Theorem 2.11) that each Legendre coefficient

$$a_m \;=\; \frac{2m+1}{2} \int_0^{\pi} B_0(z(\theta), L)\, P_m(cos(\theta))\, sin(\theta)\, d\theta, \qquad m \geq 0, \tag{A.31}$$

of

$$B_0(z(\theta), L) \;=\; \sum_{m=0}^{\infty} a_m P_m(cos\,\theta),$$

is nonnegative. Put $b := 1/L^2$ for now, and change the integration variable in $(A.31)$ to $x = cos(\theta)$:

$$a_m \;=\; \frac{2m+1}{2} \int_{-1}^{1} \frac{P_m(x)}{1+b-bx}\, dx \;=\; \frac{2m+1}{2(1+b)} \int_{-1}^{1} \frac{P_m(x)}{1\,-\,bx/(1+b)}\, dx. \tag{A.32}$$

Since $|x| \leq 1$ over the interval of integration in $(A.32)$, the geometric series formula

$$\frac{1}{1\,-\,bx/(1+b)} \;=\; \sum_{k=0}^{\infty} \left(\frac{bx}{1+b}\right)^k, \qquad \left|\frac{bx}{1+b}\right| \leq \frac{b}{b+1} < 1, \tag{A.33}$$

can be applied. By substituting $(A.33)$ into $(A.32)$, it follows that

$$\begin{aligned} a_m \;&=\; \frac{2m+1}{2(1+b)} \sum_{k=0}^{\infty} \left(\frac{b}{1+b}\right)^k \int_{-1}^{1} P_m(x)\, x^k\, dx \\ &=\; \frac{(2m+1)L^2}{2(1+L^2)} \sum_{k=0}^{\infty} \frac{1}{(1+L^2)^k} \int_{-1}^{1} P_m(x)\, x^k\, dx; \end{aligned} \tag{A.34}$$

the order of summation and integration is justified, since the integrand in $(A.32)$ is continuous on the compact set $[-1, 1]$, and hence also bounded on $[-1, 1]$.

To complete the proof, it suffices to show that

$$c(m, k) \;:=\; \int_{-1}^{1} P_m(x)\, x^k\, dx, \qquad m, k \geq 0,$$

is nonnegative for each $m, k \geq 0$. Multiplying both sides of the recurrence relation (*e.g.*, Folland, 1992, p. 173, Exercise 5)

$$(2m+1)xP_m(x) \;=\; (m+1)P_{m+1}(x) + mP_{m-1}(x), \quad m \geq 1,$$

by x^{k-1} and then integrating over $[-1, 1]$ yields

$$(2m+1)\, c(m, k) \;=\; (m+1)\, c(m+1, k-1) + m\, c(m-1, k-1), \quad m, k \geq 1. \tag{A.35}$$

Using the recurrence Eq. $(A.35)$, $c(m, k)$ can be determined for *each* $m, k \geq 1$ from the initial conditions

$$c(m, 0) \quad \text{and} \quad c(0, k), \quad m, k \geq 0. \tag{A.36}$$

Since $c(m, k)$ is nonnegative whenever $c(m+1, k-1)$ and $c(m-1, k-1)$ are both nonnegative, the proof will be complete if it is shown that the initial conditions in $(A.36)$ are all nonnegative. If $k < m$, then since the first m Legendre polynomials

$$P_0(x), P_1(x), \ldots, P_{m-1}(x)$$

are a basis for the polynomials of degree less than m, there are coefficients α_j such that

$$x^k = \alpha_0 P_0(x) + \alpha_1 P_1(x) + \cdots + \alpha_{m-1} P_{m-1}(x), \qquad -1 \le x \le 1. \tag{A.36}$$

Using Eq. $(A.36)$ together with the orthogonality relation

$$\int_{-1}^{1} P_m(x) P_j(x)\, dx, \quad j \neq m,$$

it follows that

$$c(m,k) = 0, \qquad m > k, \tag{A.37}$$

so that in particular,

$$c(m,0) = 0, \qquad m \ge 1. \tag{A.38}$$

Observe that $P_m(x)x^k$ is an odd function for $m+k$ odd and an even function if $m+k$ is even. Thus

$$c(m,k) = 0, \qquad m+k \quad \text{odd}, \quad m,k \ge 0, \tag{A.39}$$

and

$$c(m,k) = 2\int_0^1 P_m(x)\, x^k\, dx, \quad m+k \quad \text{even}, \quad m,k \ge 0.$$

It follows from

$$c(0,2j) = 2\int_0^1 P_0(x) x^{2j}\, dx = 2\int_0^1 x^{2j}\, dx = \frac{2}{2j+1}, \quad j \ge 0,$$

and Eqs. $(A.38)$ and $(A.39)$, that the initial conditions in $(A.36)$ are all nonnegative, thus completing the proof. □

Remark: Using Eqs. $(A.35)$, $(A.38)$, and $(A.39)$, the nonzero $c(m,k)$ can be generated using the initial conditions

$$c(j,j) \quad \text{and} \quad c(0,2j), \quad j \ge 0$$

where

$$c(j+1,j+1) = \frac{j+1}{2j+3}\, c(j,j), \quad j \ge 0.$$

REFERENCES

Armstrong, M., and Diamond, P., 1984, Testing variograms for positive-definitiness: Math. Geology, v. 16, no. 4, pp. 407–421.

Balgovind, R., Dalcher, A., Ghil, M., and Kalnay, E., 1983, A stochastic-dynamic model for the spectral structure of forecast errors: Mon. Wea. Rev., v. 111, pp. 701–721.

Bartello, P. and Mitchell, H. L., 1992, A continuous three-dimensional model of short-range forecast error covariances: Tellus, 44A, pp. 217–235.

Bochner, S., 1934, A theorem on Fourier-Stieltjes integrals: Bull. Amer. Math. Soc., v. 40, pp. 271–276.

Bochner, S. and Chandrasekharan, K., 1949, *Fourier Transforms:* Princeton University Press, Princeton, 219 pp.

Borgman, L. and Chao, L., 1994, Estimation of a multidimensional covariance function in case of anisotropy: Math. Geology, v. 26, no. 2, pp. 161-179.

Carton, J. A. and Hackert, E. C., 1990, Data assimilation applied to the temperature and circulation in the tropical Atlantic, 1983-84: Journal of Physical Oceanography, v. 20, pp. 1150–1165.

Christakos, G., 1992, *Random Field Models in Earth Sciences:* Academic Press, San Diego, 474 pp.

Cohn, S. E., da Silva, A., Guo, J., Sienkiewicz, M., and Lamich, D., 1998, Assessing the effects of data selection with the DAO Physical-space Statistical Analysis System: Mon. Wea. Rev., in press, *DAO Office Note 97-08*, Data Assimilation Office, Goddard Space Flight Center, Greenbelt, MD 20771. Available on-line from **http://dao.gsfc.nasa.gov/subpages/office-notes.html**

Courtier, P., Andersson, E., Heckley, W., Pailleux, J., Vasiljević, D., Hamrud, M., Hollingsworth, A., Rabier, F., and Fisher, M., 1998, The ECMWF implementation of three dimensional variational assimilation (3D-Var). Part I: Formulation: Submitted to Quarterly Journal of the Royal Meteorological Society.

Daley, R., 1991, *Atmospheric Data Analysis:* Cambridge University Press, New York, 457 pp.

Dee, D. P., 1995, On-line estimation of error covariance parameters for atmospheric data assimilation: Mon. Wea. Rev., v. 123, pp. 1128–1145.

Dee, D. P., and da Silva, A. M., 1998, Maximum-likelihood estimation of forecast and observation error covariance parameters. Part I: Methodology: Submitted to Mon. Wea. Rev. Available on-line from **http://dao.gsfc.nasa.gov/DAO_people/dee/dee.html**

Dee. D. P., Gaspari, G., Redder, C., Rukhovets, L., and da Silva, A. M., 1998, Maximum-likelihood estimation of forecast and observation error covariance parameters. Part II: Applications: Submitted to Mon. Wea. Rev. Available on-line from **http://dao.gsfc.nasa.gov/DAO_people/dee/dee.html**

Derber, J. and Rosati, A., 1989, A global oceanic data assimilation system: Journal of Physical Oceanography, v. 19, pp. 1333–1347.

Folland, G. B., 1992, *Fourier Analysis and its Applications:* Wadsworth & Brooks, Pacific-Grove, CA., 433 pp.

Gelb, A., 1974, *Applied Optimal Estimation:* MIT Press, Cambridge, MA., 374 pp.

Gelfand, I. M. and Vilenkin, N. Ya., 1964, *Generalized Functions: Applications of Harmonic Analysis, Vol. 4,* Academic Press, New York.

Hollingsworth, A. and Lönnberg, P., 1986, The statistical structure of short-range forecast errors as determined from radiosonde data. Part I: The wind field: Tellus, v. 38A, pp. 111–136.

Horn, R. A. and Johnson, C. R., 1985, *Matrix Analysis:* Cambridge University Press, New York, 561 pp.

Loève, M., 1963, *Probability Theory, 3rd ed.:* Van Nostrand, Princeton, 685 pp.

Lönnberg, P. and Hollingsworth, A., 1986, The statistical structure of short-range forecast errors as determined from radiosonde data, Part II: The covariance of height and wind errors: Tellus, v. 38A, pp. 137–161.

Oliver, D., 1995, Moving averages for Gaussian simulation in two and three dimensions: Math. Geology, v. 27, no. 8, pp. 939-960.

Parrish, D. F. and Derber, J. C., 1992, The National Meteorological Center's spectral statistical-interpolation analysis system: Mon. Wea. Rev., v. 120, pp. 1747–1763.

Papoulis, A, 1962, *The Fourier Integral and its Applications:* Mc-Graw Hill, New York, 318 pp.

Papoulis, A., 1984, *Probability, Random Variables, and Stochastic Processes:* Mc-Graw Hill, New York, 576 pp.

Pfaendtner, J., Bloom, S., Lamich, D., Seablom, M., Sienkiewicz, M., Stobie, J., and da Silva, A., 1995, Documentation of the Goddard Earth Observing System (GEOS) Data Assimilation System–Version 1. NASA Tech. Memo. No. 104606, Vol. 4, NASA Goddard Space Flight Center, Greenbelt, MD 20771. Available on-line from **http://dao.gsfc.nasa.gov/subpages/tech-reports.html**

Priestley, M., 1981, *Spectral Analysis and Time Series: Vols. 1 and 2:* Academic Press, London, 890 pp.

Rabier, F., Mc Nally, A., Andersson, E., Courtier, P, Undén, P., Eyre, J., Hollingsworth, A., and Bouttier, F., 1998, The ECMWF implementation of three dimensional variational assimilation (3D-Var). Part II: Structure functions: Submitted to Quarterly Journal of the Royal Meteorological Society.

Riishøjgaard, L. P., 1998, A direct way of specifying flow-dependent background error correlations for meteorological analysis systems: Tellus, v. 50A, pp. 42–57.

Rudin, W., 1987, *Real and Complex Analysis, 3rd ed.:* McGraw-Hill, New York, 416 pp.

Schoenberg, I. J., 1942, Positive definite functions on spheres: Duke Math. J., v. 9, pp. 96-108.

Stein, E. M. and Weiss, G., 1971, *Introduction to Fourier Analysis on Euclidean Spaces:* Princeton University Press, Princeton, 297 pp.

Strang, G., 1986, *An Introduction to Applied Mathematics:* Wellesley-Cambridge Press, Wellesley, MA, 758 pp.

Tarantola, A., 1987, *Inverse Problem Theory: Methods for Data Fitting and Model Parameter Estimation:* Elsevier, Amsterdam, 613 pp.

Thiébaux, H. J. and Pedder, M. A., 1987, *Spatial Objective Analysis:* Academic Press, New York, 299 pp.

Thorpe, J. A., 1979, *Elementary Topics in Differential Geometry:* Springer-Verlag, New York, 253 pp.

Vanmarcke, E., 1983, *Random Fields: Analysis and Synthesis:* MIT Press, Cambridge, MA., 382 pp.

Wahba, G., 1990, *Spline Models for Observational Data:* CBMS-NSF Regional Conference Series in Applied Mathematics, Philadelphia, 169 pp.

Warner, F. W., 1983, *Foundations of Differentiable Manifolds and Lie Groups:* Springer-Verlag, New York, 272 pp.

Weber, R. O. and Talkner, P., 1993, Some remarks on spatial correlation function models: Mon. Wea. Rev., v. 121, pp. 2611–2617.

Weidmann, J., 1980, *Linear Operators in Hilbert Spaces:* Springer-Verlag, New York, 402 pp.

Wu, Z., 1995, Compactly supported positive definite radial functions: Advances in Computational Mathematics, v. 4, pp. 283–292.

Yadrenko, M. I., 1983, *Spectral Theory of Random Fields:* Optimization Software, Inc., New York, 259 pp.

Yaglom, A. M., 1987, *Correlation Theory of Stationary and Related Random Functions, Vol. I: Basic Results:* Springer-Verlag, New York, 526 pp.

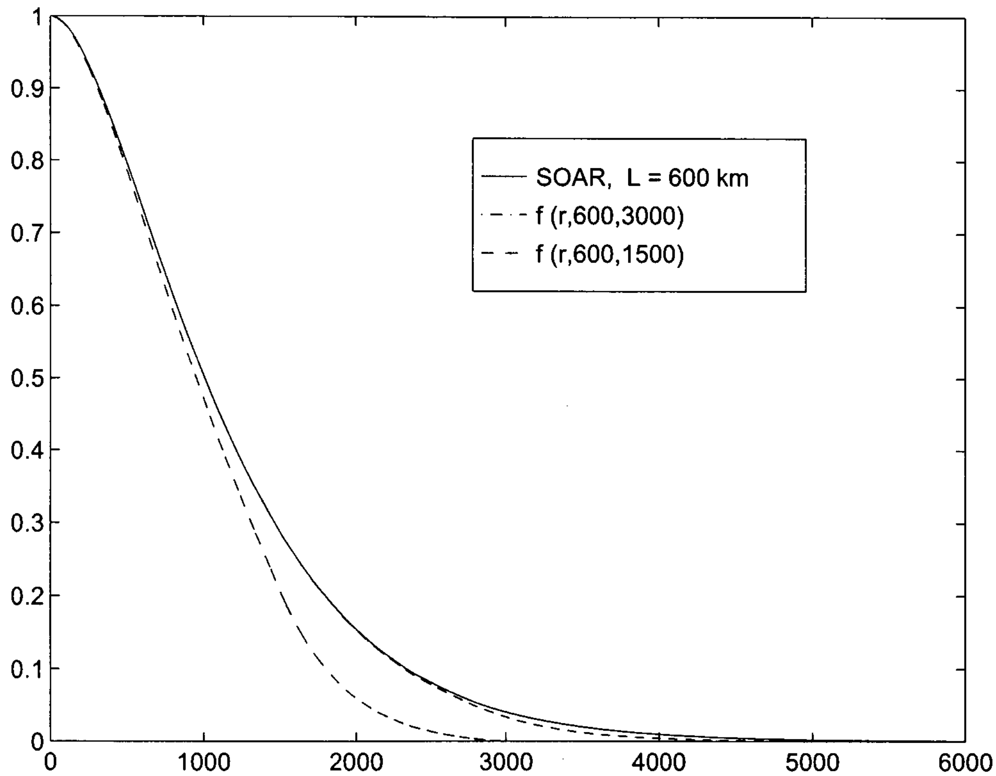

Figure 1: The compactly supported function $f(r, L, c)$ in Eq. (4.4) for $c = 1500\,km$ and $c = 3000\,km$, with $L = 600\,km$, along with the SOAR function in Eq. (2.34), with $L = 600\,km$.

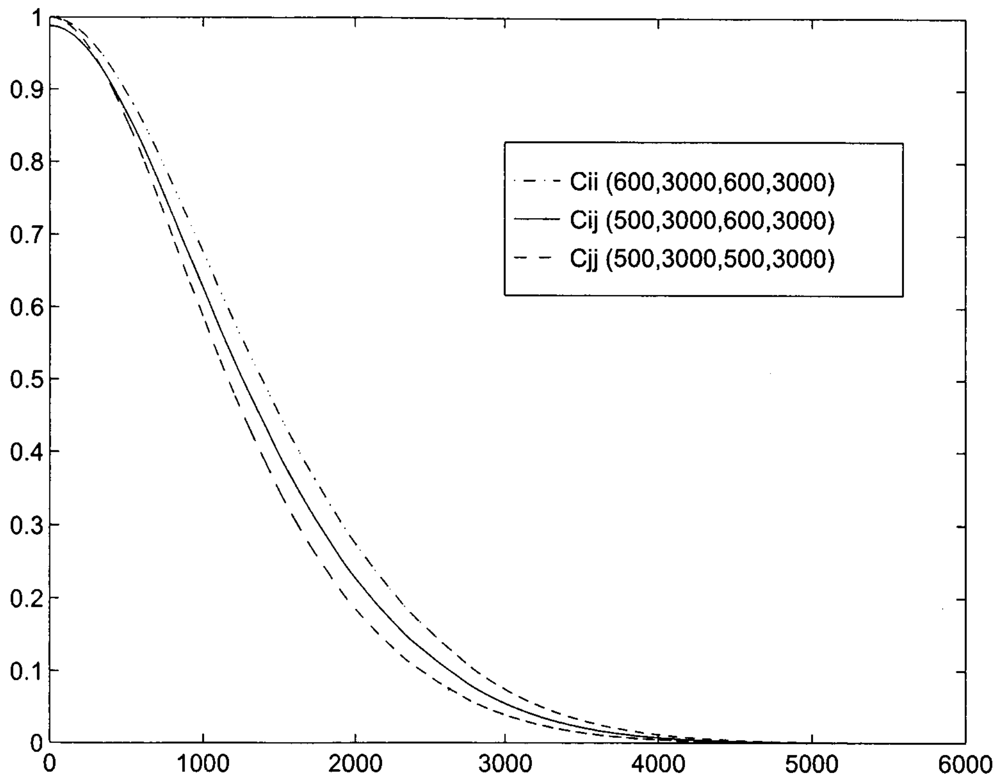

Figure 2: The functions ${C_{ii}}^0$, ${C_{ij}}^0$, and ${C_{jj}}^0$ of Example 4.b, with the legend indicating the length scales and cutoffs (in km) in the format $C_{ij}(L_i, c_i, L_j, c_j)$.

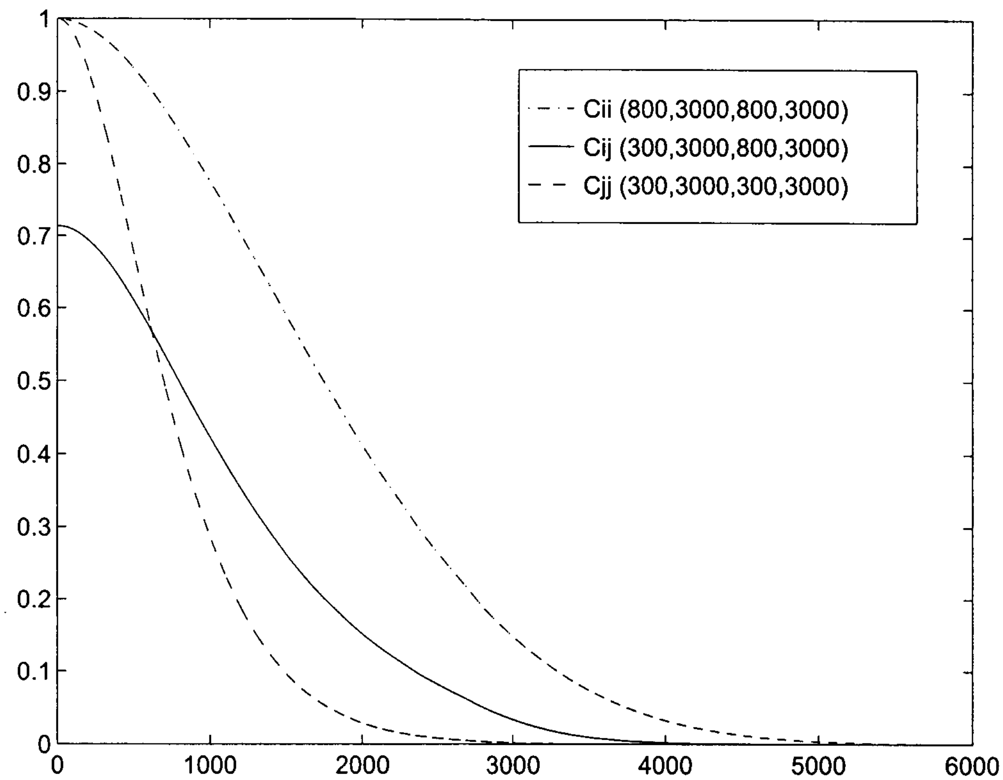

Figure 3: As in Figure 2, but for different length scales.

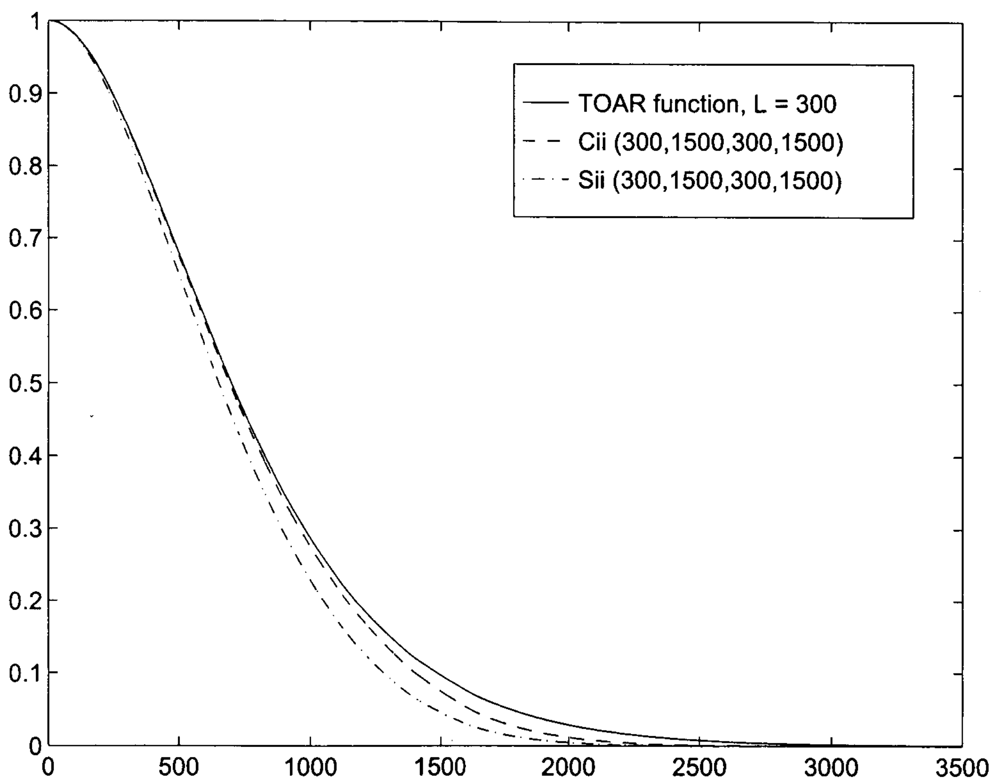

Figure 4: The TOAR function (4.8), the compactly supported TOAR-like function ${C_{ii}}^0$, and the compactly supported and twice continuously differentiable TOAR-like function ${S_{ii}}^0$ of Example 4.b, with the legend indicating the length scales and cutoffs. The format for reading length scales and cutoffs is the same as for Fig. 2.

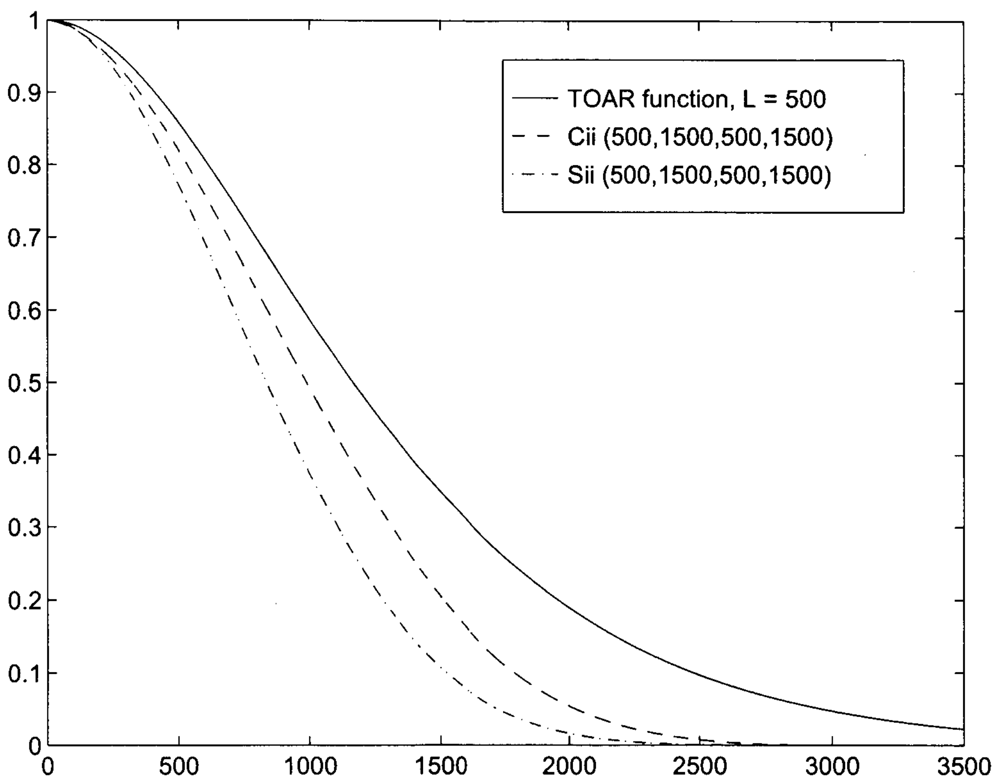

Figure 5: As in Figure 4, but for different length scales.

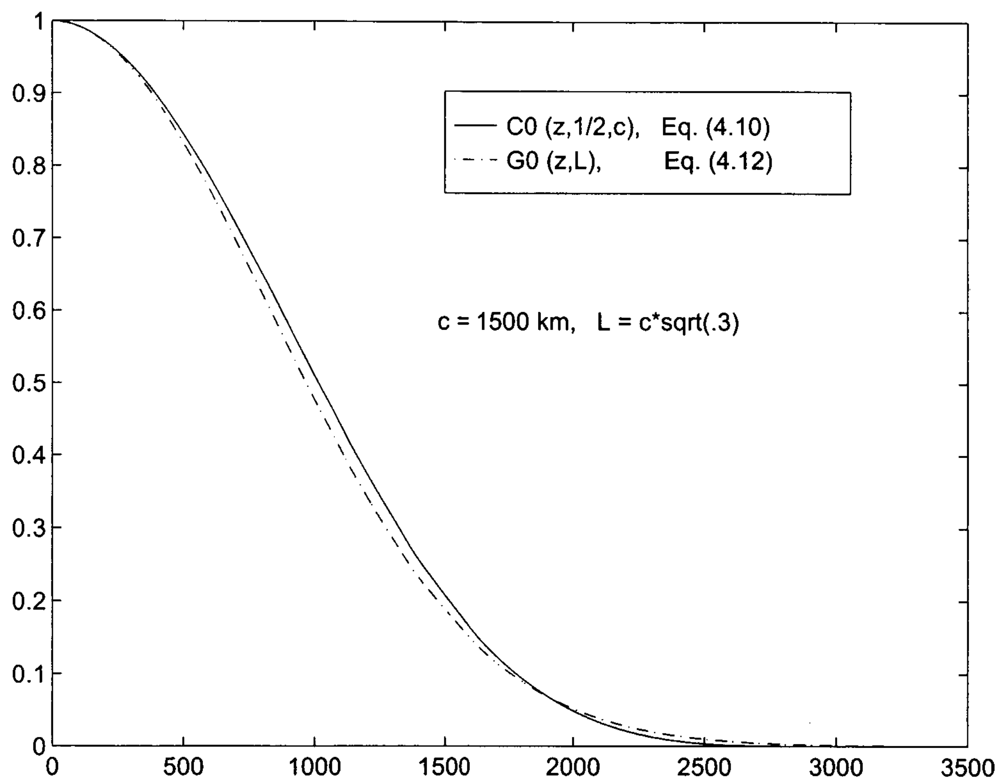

Figure 6: The piecewise rational function $C_0(z, 1/2, c)$ of Example 4.c and the Gaussian function $G_0(z, L)$ in Eq. (4.12), for $c = 1500\,km$ and $L = c\sqrt{.3}\,km$.

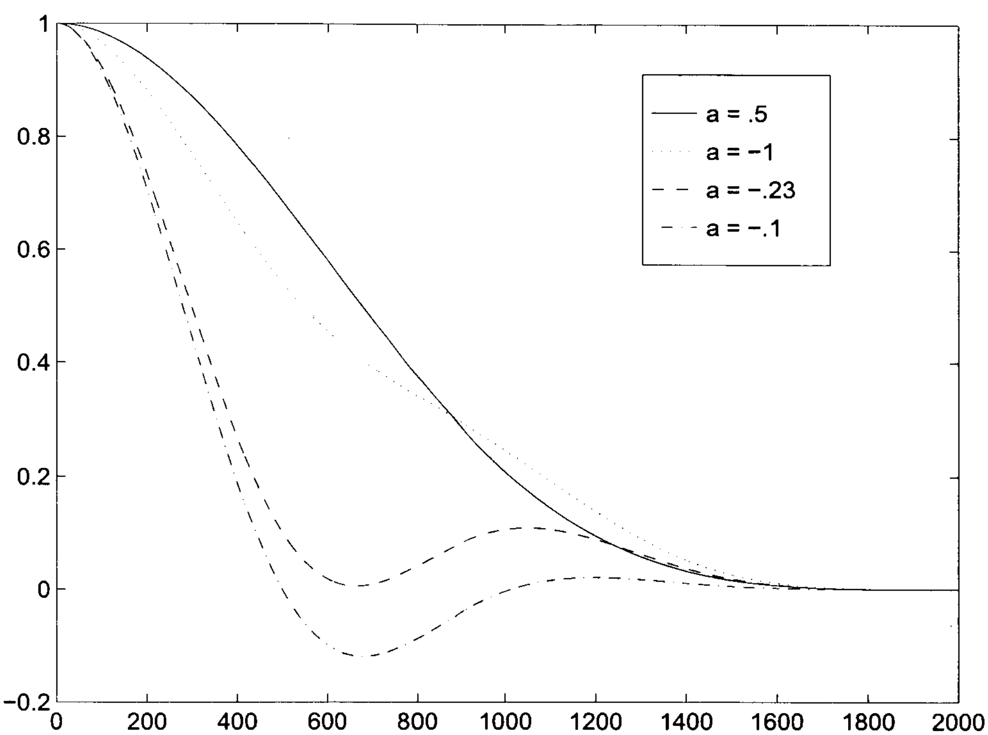

Figure 7: The function $C_0(z, a, c)$ of Example 4.c for $c = 1000\,km$ and various values of a.

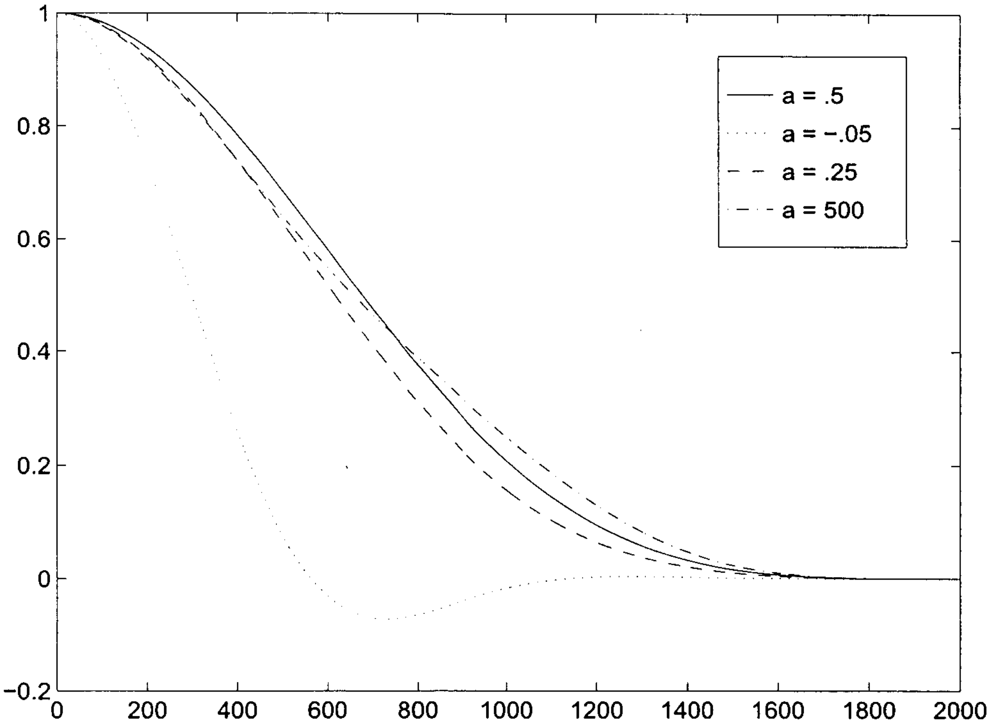

Figure 8: As in Fig. 7.

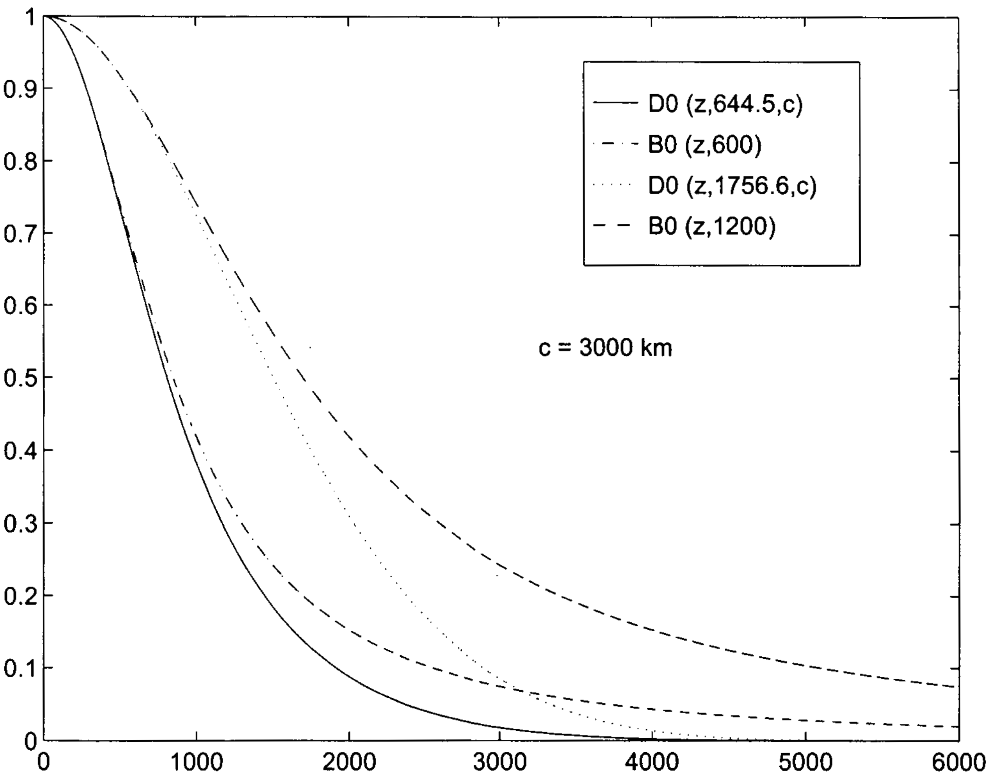

Figure 9: The functions $D_0(z, L_0, c)$ and $B_0(z, L_{d_0})$ of Example 4.d, for $L_{d_0} = 600\,km$ and $L_{d_0} = 1200\,km$, with L_0 defined by Eq. (4.18).

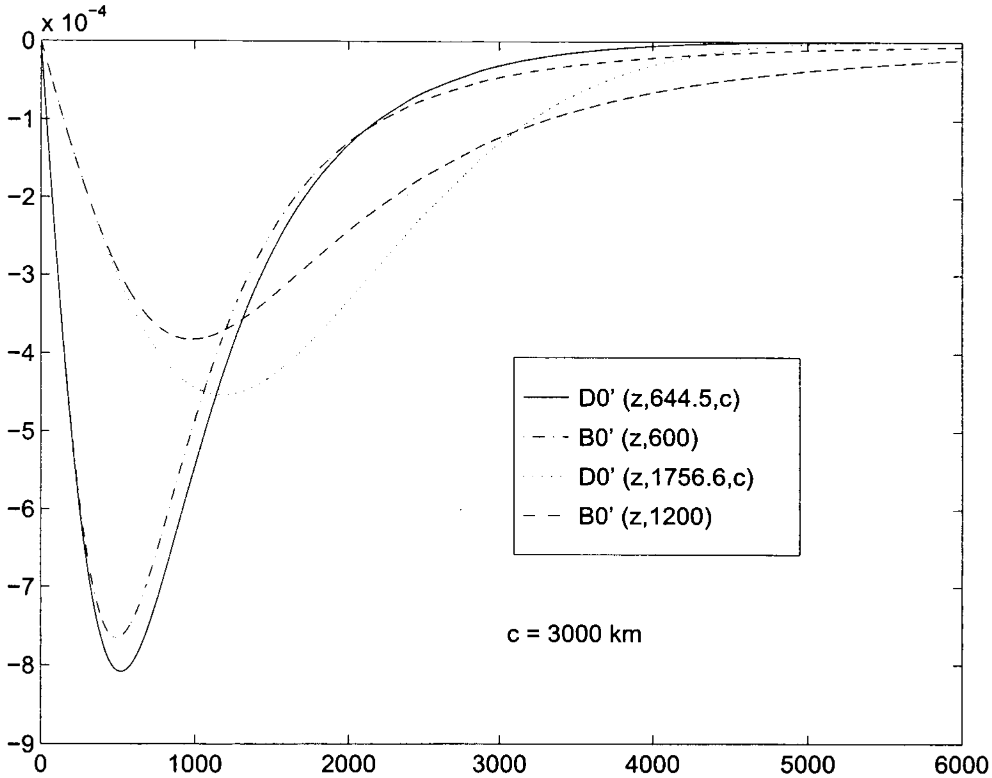

Figure 10: The first derivatives of the functions in Fig. 9. The parameters L_{d_0}, L_0, and c are as in Fig. 9.

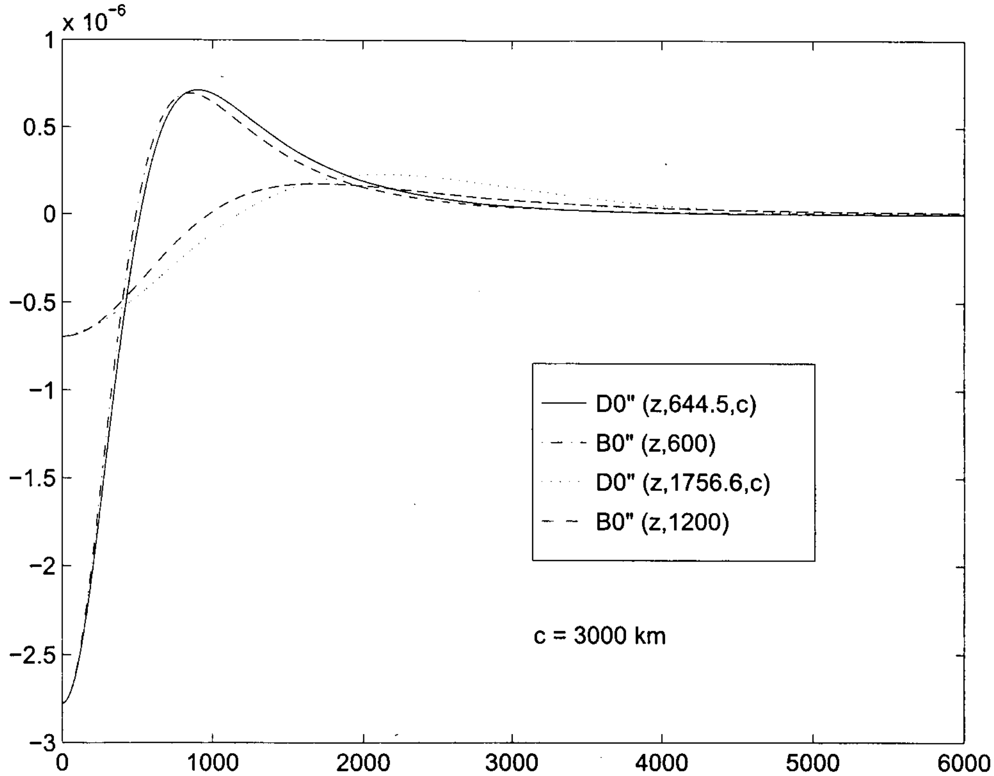

Figure 11: The second derivatives of the functions in Fig. 9. The parameters L_{d_0}, L_0, and c are as in Fig. 9.

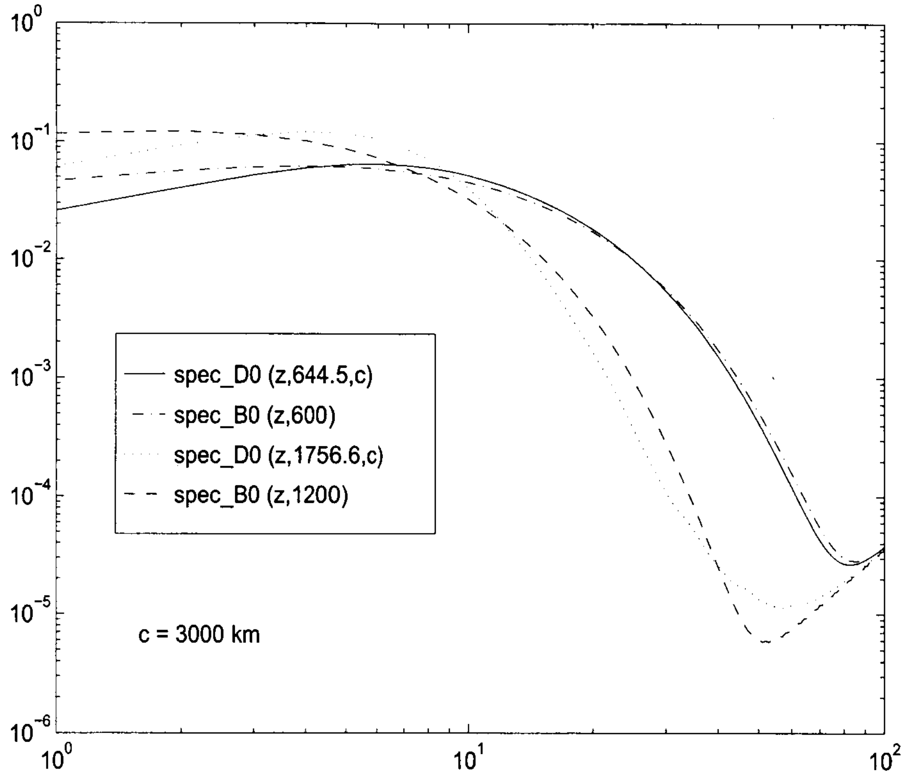

Figure 12: The Legendre coefficients of the functions in Fig. 9. The parameters L_{d_0}, L_0, and c are as in Fig. 9. The prefix "spec" in the legend abbreviates "spectrum".