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Exploration of Spatio-Temporal Environmental Conditions: Harmonized Databases and Analytical Techniques

ECOST-DATA, Bari, Italy, July 3-4, 2025

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Sandra De Iaco • Monica Palma • Donato Posa
Editors

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Preface

This volume collects the scientific contributions presented at the Workshop “Exploration of Spatio-Temporal Environmental Conditions: Harmonized Databases and Analytical Techniques (ECoST-DATA)”, held at the University of Bari on July 3-4, 2025, as Satellite event of DUST 2025. It is a key result of the ECoST-DATA Project, funded by European Union – NextGenerationEU with the Cascade Open Calls published by ALMA MATER STUDIORUM – University of Bologna, inside the Project GRINS within the PNRR – Mission 4, Component 2, Investment 1.3 “Partnership extended to Universities, Research Centers, Firms and research projects funding”, D.D. 341 of 15/03/2022, CUP: J33C22002910001.

The contents are dedicated to advanced tools and techniques for analyzing and predicting environmental variables with a spatial or spatio-temporal structure. In particular, they include theoretical reviews on spatio-temporal covariance modelling as well as innovative approaches for assessing environmental quality and its effects on climate change by integrating georeferenced data from multiple sources.

Among the primary objectives of this collection, it is worth mentioning: transfer advanced analytic skills for the modelling, estimation, and prediction of spatial and spatio-temporal environmental variables; provide practical guidance on integrating heterogeneous georeferenced data while accounting for measurement error and spatial misalignment; support risk assessment by equipping practitioners with methods to quantify exposure and uncertainty relevant to human health; and inform sustainability planning through models that identify spatially and temporally targeted mitigation or adaptation strategies.

As a result, the contributions are intended for researchers and graduate students in spatial statistics, environmental science, and geosciences; data scientists and practitioners working on environmental monitoring, climate impacts, and public-health risk assessment; policy analysts interested in data-driven sustainability planning.

Regarding the outcomes, readers will gain both the theoretical grounding and the practical toolset necessary to build, validate, and deploy spatio-temporal models for environmental variables, produce reliable forecasts, and translate model outputs into actionable insights for health and sustainability interventions.

The volume is organized in three parts.

In the first one, *Random fields and Covariance modelling*, Posa clarifies the relationship between covariance functions and positive definite functions, emphasizing that Crum's theorem is the necessary generalization of Bochner's theorem. De Iaco discusses on some families of spatio-temporal complex covariance functions for vectorial data. It is also described how these functions can be generalized to the spatio-temporal setting, as well as how some other complex-valued covariance families can be constructed as positive mixtures of infinite components or as a convolution of the real part. Hristopulos presents the hybrid spectral approach for generating physically inspired, non-separable covariance kernels from stochastic ordinary differential equations. Pere et al. propose the stationary subspace analysis to decompose a random field into independent stationary and non-stationary subspaces.

In Part II, *Environmental control and integration*, Stein focuses on the use of modern deep learning methods for the analysis and management of large data volumes. His study explores the use of satellite imagery and time series to analyze air quality and monitor environmental changes. A further challenging approach is presented in Gómez-Hernández et al. to identify atmospheric dust sources, using the ensemble smoother with multiple data assimilation methodology. Capasso discusses the optimization of pollution control within an economic growth system, presenting a spatially structured model. This model analyzes an optimal control problem designed to maximize intertemporal utility while minimizing pollution, the disutility of taxation, and intervention costs. Additionally, the study by Dutillo and Di Battista explores the functional structure and variation of Italian carbon emissions from electricity using functional data analysis. Daily and monthly profiles are constructed using Fourier basis functions and analyzed at national and electricity market zone levels.

The volume concludes with Part III, *Environmental Analysis*, where Jalilian et al. apply a flexible generalized additive model framework for surface ozone prediction, using spatio-temporally varying coefficients to correct biases between satellite and in situ data. Gomes et al. investigate the geostatistical characterization of climate extremes dynamics, focusing on drought. A Random Forest-based short-term alert system is presented for predicting drought severity classes at a monthly scale, demonstrating strong predictive performance for local areas and offering a flexible tool for managing drought-related risks. For environmental quality assessment, the work by Masoumi et al. addresses a gap in biodiversity modelling in the Apulia region by comparing the performance of various machine learning models (Random Forests, Support Vector Machines, Extreme Gradient Boosting, Decision Trees,

and Linear Regression) for assessing the effects of environmental variables on the multilevel biodiversity index. Furthermore, in Cappello et al., spatio-temporal blind source separation model is reviewed and employed to model and predict ground-level ozone concentration in a complex multivariate spatio-temporal framework.

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Part I
Random Fields and Covariance Modelling

Covariance Functions



Donato Posa

Abstract This chapter focuses on Bochner's theorem and its connection to positive definite functions and covariance functions. There exists a common misunderstanding among scientists regarding the precise relationships between these mathematical concepts. A key point is the limited scope of Bochner's theorem, as it only applies to continuous covariance functions. It will be emphasized the practical need for a generalization of the theorem, particularly for applications involving temporal, spatial, and spatiotemporal data analysis, where correlation models often exhibit discontinuity at the origin. Ultimately, the chapter aims to clarify and expand upon the theoretical understanding of these functions.

Keywords Covariance functions · Positive definite functions · Bochner's theorem

1 Introduction

Various areas of mathematics (Fourier analysis, complex analysis and probability, just to mention some of them) have to deal with the family of functions which are positive definite (*PD*) [29]. This last family of functions [20, 28] matches with the family of covariance functions: this relevant remark has been very often neglected in the literature or very frequently confused with the famous Bochner's theorem.

There is no need to recall any assumption of regularity or continuity to define the family of *PD* functions. Moreover, the subset of the continuous covariance functions is fully portrayed by the theorem of Bochner [2]. For this purpose, it will be underlined that any complex covariance function (*CF*), or equivalently any complex *PD* function, cannot be obtained from Bochner's theorem.

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The chapter clarifies the often confused relationships among *PD* functions, strictly positive definite (*SPD*) functions [21, 22] and *CFs*, noting that *CFs* are equivalent to *PD* functions. It highlights that Bochner's theorem only describes the subset of continuous *CFs*, while many real-world applications require models that are discontinuous at the origin. Crum's theorem will be introduced as a crucial generalization that accommodates these discontinuous functions, providing a more comprehensive understanding of correlation theory essential for temporal, spatial and spatiotemporal data analysis. The chapter supplies definitions and properties for each function type, emphasizing the distinctions and implications for various statistical applications.

Apart from the last remark which is essentially related to interpolation problems, the results given hereafter are not restricted to the applications which involve spatial and spatiotemporal analysis, in which several relevant contributions can be found in [5, 7, 9–11, 17, 19]; on the other hand, the same results regard the whole correlation theory and some properties, as well as, in general, all the fields related to *PD* functions.

The chapter outlines key aspects of *CFs*, particularly their properties as *PD* and *SPD* functions, independent of continuity assumptions. It discusses Bochner's theorem and its extensions, highlighting the connection between these function families. It is remarkable to note that Bochner's theorem is not applicable to certain *CF* models, specifically those exhibiting a discontinuity at the origin (known as *nugget effect*) or those that are almost everywhere zero, which are often encountered in time series and spatial analysis.

The present analysis just concerns the univariate case; some useful details regarding the multivariate case can be found in [15] and [30].

2 *CFs*, *PD* and *SPD* Functions

A brief overview on *PD* and *SPD* functions is given hereafter.

Consider the set $\mathbb{C}$ of complex numbers; then

$$C : \mathbb{R}^m \longrightarrow \mathbb{C}$$

is *PD* if, whatever they are $\mathbf{t}_1, \mathbf{t}_2, \dots, \mathbf{t}_n \in \mathbb{R}^m$ and any choice of $\lambda_k \in \mathbb{C}, k = 1, 2, \dots, n, \forall n \in \mathbb{N}_+$,

$$\sum_{k=1}^n \sum_{l=1}^n \lambda_k \bar{\lambda}_l C(\mathbf{t}_k - \mathbf{t}_l) \geq 0; \quad (1)$$

moreover, *C* is *SPD* on $\mathbb{R}^m$ if

$$\sum_{k=1}^n \sum_{l=1}^n \lambda_k \bar{\lambda}_l C(\mathbf{t}_k - \mathbf{t}_l) > 0, \quad (2)$$

for $\mathbf{t}_1, \mathbf{t}_2, \dots, \mathbf{t}_n, \mathbf{t}_k \neq \mathbf{t}_l, k \neq l, \forall n \in \mathbb{N}_+$ and $\lambda_k \in \mathbb{C}, k = 1, 2, \dots, n$, with at least one of them different from zero.

The symbol $\mathcal{P}$ will be utilized to represent the family of *PD* functions, whereas the symbol $\mathcal{P}^+$ will be utilized for the family of *SPD* functions, as a consequence $\mathcal{P}^+ \subset \mathcal{P}$.

It is required that a *CF* belongs to the class $\mathcal{P}^+$ to guarantee the invertibility of the kriging matrix for prediction.

2.1 PD Functions and Their Properties

In the following a brief overview concerning the properties of the family $\mathcal{P}$ of *PD* functions defined in (1) is given. Note that none of the hypotheses regarding continuity or regularity is needed.

1. $0 \leq C(\mathbf{0})$.
2. $C(\mathbf{t}) = \overline{C(-\mathbf{t})}, \quad \forall \mathbf{t} \in \mathbb{R}^m$.
3. $C(\mathbf{0}) \geq |C(\mathbf{t})|, \quad \forall \mathbf{t} \in \mathbb{R}^m$.
4. If $C_i, i = 1, \dots, n$, are *PD* on $\mathbb{R}^m$, then their product is *PD* on $\mathbb{R}^m$.
5. If $C_k, k = 1, \dots, n$, are *PD* on $\mathbb{R}^m$ with $a_k \geq 0, k = 1, \dots, n$, then $\sum_{k=1}^n a_k C_k(\mathbf{t})$ is *PD* on $\mathbb{R}^m$.
6. If C is *PD*, then C_{re} , i.e., the real component of C , is *PD*.
7. If $C_k, k \in \mathbb{N}$, are *PD* on $\mathbb{R}^m$, as a consequence

$$C(\mathbf{t}) = \lim_{i \rightarrow \infty} C_i(\mathbf{t})$$

is *PD* on $\mathbb{R}^m$, as long as the limit exists.

8. If $C(\cdot; \lambda)$ is *PD* on $\mathbb{R}^m \forall \lambda \in A \subseteq \mathbb{R}$, and $\sigma(d\lambda)$ is a measure on A , then

$$\int_A C(\mathbf{t}; \lambda) \sigma(d\lambda),$$

is *PD* on $\mathbb{R}^m$, provided that the integral exists $\forall \mathbf{t} \in \mathbb{R}^m$.

9. Suppose that a function be *PD* on $\mathbb{R}^n$; however nothing can be said about its positive definiteness on $\mathbb{R}^m, n < m$.
10. If C is *PD*, then for all $\mathbf{t}_1, \mathbf{t}_2 \in \mathbb{R}^m$

$$|C(\mathbf{t}_2) - C(\mathbf{t}_1)|^2 \leq 2C(\mathbf{0})Re[C(\mathbf{0}) - C(\mathbf{t}_2 - \mathbf{t}_1)],$$

where $Re[C(\mathbf{0}) - C(\mathbf{t}_2 - \mathbf{t}_1)]$ is the real component of $[C(\mathbf{0}) - C(\mathbf{t}_2 - \mathbf{t}_1)]$.

This last result is particularly useful since it distinguishes the class of the continuous *CFs*.

2.2 SPD Functions and Their Properties

A brief overview concerning the properties for the family $\mathcal{P}^+$ of *SPD* functions is given: even in this case, none of the hypotheses of continuity or regularity is needed.

1. If the function C is *SPD*, then $C(\mathbf{0}) > 0$; on the other hand, vice versa is not true. Indeed, there can be functions such that $C(\mathbf{0}) > 0$, however the same functions are not *SPD*; the cosine *CF* is a typical example.
2. Consider n functions which are *SPD* on the same space $\mathbb{R}^m$; then their sum, as well as their product, is a *SPD* function on the same space.
3. If C is *SPD* on $\mathbb{R}^m$, it could not be *SPD* on $\mathbb{R}^n$, with $n > m$.
4. The real component of a complex *SPD* is always *SPD*.
5. Consider n *PD* functions on $\mathbb{R}^m$. Suppose that there exists $C_k, k \in \{1, \dots, n\}$, which is *SPD*, with $\alpha_k > 0$, as a consequence

$$C(\mathbf{t}) = \sum_{i=1}^n \alpha_i C_i(\mathbf{t})$$

with $\alpha_i \geq 0, i = 1, \dots, n$, is *SPD* on $\mathbb{R}^m$.

6. If C is *SPD* on $\mathbb{R}^m$, then $C(\mathbf{t}) \neq C(\mathbf{0}), \forall \mathbf{t} \neq \mathbf{0}$.
7. Furthermore, if C is *PD* and there exists $\mathbf{t}$ such that $C(\mathbf{t}) = C(\mathbf{0})$, with $C(\mathbf{0}) > 0$, it comes out that C is not *SPD*.
8. Let $C_1, \dots, C_n$ be not identically zero *PD* on $\mathbb{R}^m$ [8]. Then,

$$C(\mathbf{t}) = \prod_{i=1}^n C_i(\mathbf{t})$$

is *SPD* on $\mathbb{R}^m$ if $\exists i \in \{1, \dots, n\}$ such that C_i is *SPD*.

Consider the *nugget effect* function [18]

$$C(\mathbf{t}) = \begin{cases} C_0 & \mathbf{t} = \mathbf{0} \\ 0 & \mathbf{t} \neq \mathbf{0}, \end{cases} \quad (3)$$

with $\mathbf{t} \in \mathbb{R}^m, C_0 > 0$; this last function presents a discontinuity at the origin and it can be easily proved that it is *SPD*.

2.3 CFs

Consider the complex random function $Z : \mathbb{R}^m \longrightarrow \mathbb{C}$:

$$Z(\mathbf{w}) = Z_1(\mathbf{w}) + i Z_2(\mathbf{w}), \quad \mathbf{w} \in \mathbb{R}^m, \quad (4)$$

with Z_1 and Z_2 real random functions and suppose that (4) is stationary of the second order; as a consequence, the corresponding CF is defined as follows:

$$C(\mathbf{t}) = E[(Z(\mathbf{w}) - m)\overline{(Z(\mathbf{w} + \mathbf{t}) - m)}],$$

with $\mathbf{w} \in \mathbb{R}^m$ and $(\mathbf{w} + \mathbf{t}) \in \mathbb{R}^m$, m is the expected value of (4), supposed to be constant. Equivalently, the CF can be represented as follows:

$$C(\mathbf{t}) = C_{re}(\mathbf{t}) + iC_{im}(\mathbf{t}),$$

where the sum of C_{Z_1} and C_{Z_2} (the CF s of Z_1 and Z_2 , respectively) corresponds to the real component C_{re} , whereas the difference of the cross-covariances $C_{Z_2Z_1}$ and $C_{Z_1Z_2}$ is the imaginary part, i.e.,

$$C_{re}(\mathbf{t}) = C_{Z_1}(\mathbf{t}) + C_{Z_2}(\mathbf{t}), \quad C_{im}(\mathbf{t}) = C_{Z_2Z_1}(\mathbf{t}) - C_{Z_1Z_2}(\mathbf{t}). \quad (5)$$

Note that C_{re} is a real CF ; on the other hand C_{im} cannot be a CF , and this last satisfies the property related to cross- CF s, i.e.,

$$C_{Z_1Z_2}(-\mathbf{t}) = C_{Z_2Z_1}(\mathbf{t}).$$

The symbol $\mathcal{C}$ will be used to define the family of CF s.

Remarks

- It can be easily established that the class of CF s coincides with the class of PD functions [25], hence $\mathcal{P} \equiv \mathcal{C}$.
- Taking into account the previous item, the above two classes follow the same properties already established in the previous section. A discussion on some characteristics can also be found in [14, 16].
- By definition, a covariance is a complex function, although several case studies utilize the subclass of the real CF s.

3 Bochner's Theorem and the Corresponding Generalization

Theorem 1 [Bochner [2]] *A function ϕ on $\mathbb{R}^m$ is candidate to be a continuous CF if and only if it can be expressed as follows:*

$$\phi(\mathbf{t}) = \int_{\mathbb{R}^m} \exp(i\mathbf{t}^T \boldsymbol{\tau}) dF(\boldsymbol{\tau}), \quad (6)$$

where the measure F is bounded and it is usually called spectral distribution function.

In the peculiar case the distribution function F is absolutely continuous; then there exists a nonnegative function f which allows to formulate (6) as follows:

$$\phi(\mathbf{t}) = \int_{\mathbb{R}^m} \exp(i\mathbf{t}^T \boldsymbol{\tau}) f(\boldsymbol{\tau}) d\boldsymbol{\tau}, \quad (7)$$

where $f \in L^1(\mathbb{R}^m)$. The function f is named *spectral density* and it is not necessarily a continuous function; however, ϕ satisfies the following asymptotic condition:

$$\lim_{\|\mathbf{t}\| \rightarrow \infty} \phi(\mathbf{t}) = 0. \quad (8)$$

On the other hand, the function ϕ could not be integrable; if ϕ is integrable, then

$$f(\boldsymbol{\tau}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^m} \exp(-i\boldsymbol{\tau}^T \mathbf{t}) \phi(\mathbf{t}) d\mathbf{t}, \quad (9)$$

in addition f is continuous.

From (9) it follows that if the Fourier transform of a function ϕ is nonnegative, then the same function ϕ is the *CF* of a random field.

The symbol $\mathcal{B}$ will be utilized to denote the class of the continuous *CFs*, already defined through expression (1); as a consequence, $\mathcal{B} \subset \mathcal{P}$. On the other hand, the set of the family of *PD* functions contains the set of the family of functions that are *SPD* ($\mathcal{P}^+ \subset \mathcal{P}$); however, the family of functions which are *SPD* cannot be a subset of $\mathcal{B}$.

Remark The chapter discusses the nature of *CFs*, explaining that they can be either complex or real. This distinction hinges on the properties of the function F . Specifically, if F is asymmetric around the origin or the spectral density f is not an even function, the resulting *CF* will be complex. Conversely, a symmetric F , or an even spectral density f , will yield a real *CF*. The chapter aims to provide a thorough characterization for these continuous *CFs*, building upon prior work.

Corollary 1 *A complex covariance is a continuous function if and only if its real component is continuous at the origin.*

From the previous corollary, it comes out that any *CF* can be represented through relation (6) if and only if it is continuous at the origin. As a consequence, the entire class of *PD* functions (or *CFs*) can be split into two sets, which are disjoint: the family of continuous *PD* (or continuous *CFs*), which can be expressed by Bochner's theorem, and the family of *PDs* (or *CFs*) which present a discontinuity at the origin. Several details concerning the techniques to construct extensive family of continuous complex *CFs* can be found in [23].

It is not ensured that the difference between *CFs* can be an admissible covariance: details to obtain admissible *CFs* starting from such a difference have been discussed in [24].

3.1 SPD Functions and Bochner's Theorem

In the present section some results concerning the class $\mathcal{B}$ of continuous CF s, which satisfy Bochner's theorem, will be provided.

Some peculiar properties stemming from Bochner's theorem and concerning SPD functions are detailed hereafter.

1. Let f be integrable, nonnegative, continuous and not identically zero; then

$$\phi(\mathbf{t}) = \int_{\mathbb{R}^m} \exp(i\mathbf{t}^T \boldsymbol{\tau}) f(\boldsymbol{\tau}) d\boldsymbol{\tau} \quad (10)$$

is SPD and continuous on $\mathbb{R}^m$.

2. Consider n CF s $\phi_1, \dots, \phi_n$ which are continuous on $\mathbb{R}^m$. Then

$$\phi(\mathbf{t}) = \sum_{i=1}^n \alpha_i \phi_i(\mathbf{t}),$$

with $\alpha_i \geq 0, i = 1, \dots, n$, is SPD and continuous on $\mathbb{R}^m$, if and only if there exists $k \in \{1, \dots, n\}$ with ϕ_k SPD on $\mathbb{R}^m, \alpha_k > 0$ [8, 12, 13].

3. Suppose that the support of the measure F in (6) contains an open subset; then ϕ is SPD and continuous.

3.2 Crum's Theorem: A Generalization of Bochner's Result

Taking into account all the results of the previous sections, it comes out that any PD function (or equivalently any CF) cannot be expressed through Bochner's theorem. Unfortunately, this relevant aspect has generated a lot of misunderstanding, as well as confusion, as can be detected through some statements collected from important books on the subject.

1. Statistics for spatial data [4, p. 84]
2. The geometry of random fields [1, p. 25]
3. Correlation theory of stationary and related random functions [31, p. 93]
4. Geostatistics: modeling spatial uncertainty [3, p. 64]

The above sentences underline a common misconception regarding CF s and Bochner's theorem: there appears to be a direct correlation between PD functions and continuous CF s that adhere to Bochner's theorem; this is not universally true. Indeed, the entire category of CF s exhibiting discontinuity at the origin cannot be represented by the conditions of Bochner's theorem. A key illustration of this aspect is the nugget effect, which represents a typical example of such a discontinuous function. Hence, it is relevant to differentiate the types of CF s, highlighting those

that fall outside the scope of traditional Bochner's theorem applications due to their inherent discontinuities.

A first generalization of Bochner's theorem was given by Riesz [27]; a further upgrade was obtained by Crum [6], through the result given hereafter.

Theorem 2 (Crum's Theorem) *A measurable and PD complex function C , defined on $\mathbb{R}^m$, can always be written as follows:*

$$C(\mathbf{t}) = \phi(\mathbf{t}) + \psi(\mathbf{t}), \quad (11)$$

where

$$\phi(\mathbf{t}) = \int_{\mathbb{R}^m} \exp(i\mathbf{t}^T \boldsymbol{\tau}) dF(\boldsymbol{\tau}),$$

and ψ is PD; moreover $\psi = 0$ almost everywhere.

In the special case $C(\mathbf{t}) = C(\|\mathbf{t}\|)$ (i.e., C is isotropic) and $m > 1$; then $\psi(\mathbf{t}) = 0$, for $\mathbf{t} \neq \mathbf{0}$.

Unfortunately, the previous result is rarely referred to in the literature, although it is widely utilized in most of the case studies, as underlined hereafter.

In Fig. 1 the relationship among CFs, PD and SPD functions has been properly represented.

3.3 Crum's Theorem in the Applications

It is well acknowledged the importance of the theory of correlation in any context regarding temporal and spatial data analysis, as summarized hereafter.

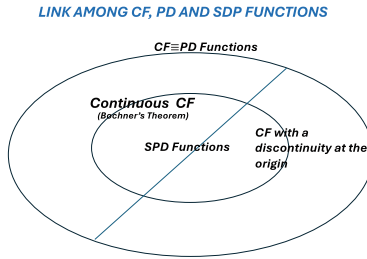


Fig. 1 Relationship among CFs, PD and SPD functions. The set of CFs coincides with the set of PD functions. The whole family of the CF can be partitioned into two subsets: the subset of the continuous CF and the subset of the CF which presents a discontinuity at the origin. The subset of SPD functions is not a subset of the family of continuous CFs, neither of the family of the CFs which are not continuous at the origin

- In discrete time series analysis [26] stationary models take up a dominant role. At this purpose, the autocorrelation function related to autoregressive, moving average, as well as autoregressive moving average models is zero almost everywhere. In this case, expression (11) shrinks as follows:

$$C(\mathbf{t}) = \psi(\mathbf{t}).$$

For the following autoregressive process:

$$z_t = \varphi_1 z_{t-1} + a_t, \quad -1 < \varphi_1 < 1,$$

the autocorrelation function

$$\rho(k) = \varphi^k, \quad k = 0, 1, 2, \dots,$$

is nil almost everywhere; then because of (11), $\phi = 0$ and $\psi \equiv \rho$.

- In geostatistics, expression (11) is usually employed; in other terms, the resulting models consist of a linear combination of a nugget effect, described by the function ψ , with a continuous correlation model, described by the function ϕ . On the other hand, Bochner's theorem can be invoked in all the situations corresponding to correlation models which are continuous at the origin.

4 Conclusions

This chapter clarifies the interconnectedness of *PD* functions, *CFs* and continuous *CFs*, addressing prior confusion in the literature. It highlights how Crum's result expands upon Bochner's theorem, further illuminating the relationship between *PD* functions (which are equivalent to *CFs*) and continuous *CFs*. It has been also emphasized the significance of *SPD* functions. Essentially, the work aims to precisely define and distinguish these related mathematical concepts, which are crucial in various analytical applications.

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