Chapter 4 A Simple Isotropic Correlation Family in \mathbb{R}^3 with Long-Range Dependence and Flexible Smoothness



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Abstract Most geostatistical applications use covariance functions that display short-range dependence, in part due to the wide variety and availability of these models in statistical packages, and in part due to spatial interpolation being the main goal of many analyses. But when the goal is spatial extrapolation or prediction based on sparsely located data, covariance functions that display long-range dependence may be more adequate. This paper constructs a new family of isotropic correlation functions whose members display long-range dependence and can also model different degrees of smoothness. This family is compared to a sub-family of the Matérn family commonly used in geostatistics, and two other recently proposed families of covariance functions with long-range dependence are discussed.

Keywords Fractal dimension · Geostatistics · Hurst coefficient · Mean square differentiability · Radial distribution

4.1 Introduction

Random fields are ubiquitous for the modeling of spatial data in most natural and earth sciences. When the main goal of the analysis is spatial prediction, an adequate specification of the correlation function of the random field is of utmost importance. In this paper, attention is restricted to correlation functions in \mathbb{R}^d with the properties of being *isotropic*, i.e., functions of the Euclidean distance which separates two locations that decrease monotonically to zero as distance increases without bound. These features are common in many spatial phenomena. A large number of parametric families of correlation functions with these properties have been proposed in the literature and used in applications; see, for instance, [2, 3]. Most of these families display *short-term* dependence, meaning that the correlation function decays to zero fast, usually exponentially fast, so spatial association between far-away observations is negligible. The Matérn family is a commonly used example. On the other hand,

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some spatial phenomena display *long-term* dependence, meaning that the correlation function decays to zero slowly, usually hyperbolically fast, so the spatial association between far-away observations is not negligible. An early example of this behavior was provided by [4] using data from agricultural uniformity trials, who empirically found that, for large distances r, the correlation function decays approximately as r^{-1} (a so-called power law). Similar behavior is commonly found in spatial geophysics and hydrology data; see [8] and the references therein. Fewer models have been proposed in the literature for phenomena that display this behavior.

Time series models displaying long-range dependence were discussed in [5] (discrete time) and [12] (continuous time). Spatial data models displaying long-range dependence were discussed in [10, 17] for the case when the index set is \mathbb{Z}^d (usually d = 2). Some families of correlation functions for random fields in \mathbb{R}^d that display long-range dependence were constructed by [21], and more recently [8, 13] developed new families in this class. In this paper, we construct what appears to be a new family using a correspondence between continuous isotropic correlation functions in \mathbb{R}^3 and probability density functions (pdfs) in \mathbb{R} with support $[0, \infty)$. In addition to displaying long-range dependence, the new family of correlation functions allows different degrees of smoothness, which is important for efficient spatial interpolation under infill asymptotics [20]. After describing its main properties, this family of correlation functions is contrasted with a sub-family of the Matérn family which also provides flexibility regarding smoothness, but displays short-range dependence. This paper ends with a discussion of two other families of correlations functions that also display long-range dependence.

4.1.1 A Spectral Representation

Let $K : [0, \infty) \to \mathbb{R}$ be the correlation function of a mean square continuous and isotropic random field $\{Z(\mathbf{s}) : \mathbf{s} \in D\}$, with $D \subset \mathbb{R}^d$ and $d \ge 1$, and let Φ_d denote the class of all such functions. A characterization of Φ_d is given in a classical result by [18], who showed that any $K \in \Phi_d$ can be written as

$$K(r) = \int_0^\infty \Lambda_d(rx) dF(x), \qquad r \ge 0,$$

where

$$\Lambda_d(t) = \left(\frac{2}{t}\right)^{\frac{d}{2}-1} \Gamma\left(\frac{d}{2}\right) J_{\frac{d}{2}-1}(t), \qquad t > 0,$$

 $\Gamma(\cdot)$ is the gamma function, $J_{\nu}(\cdot)$ is the Bessel function of the first kind and order ν , and $F(\cdot)$ is a cumulative distribution function on \mathbb{R} with support $[0, \infty)$. Such a function $K(\cdot)$ is also a radial positive definite function on \mathbb{R}^d , and can also be viewed as the *Hankel* transform of *F* of order $\frac{d}{2} - 1$. Any $K \in \Phi_d$ is continuous on $[0, \infty)$, and [(d - 1)/2]-times continuously differentiable on $(0, \infty)$, where [a] denotes the

integer part of a, and $\lim_{r\to\infty} K(r) = F(0) - F(0-)$; see [6, 15, 20, 22] for further properties of such functions.

For all $d \ge 1$, $\Lambda_d(t)$ is itself a continuous isotropic correlation function in \mathbb{R}^d (so $\Lambda_d(0) = 1$), which can be written in terms of elementary functions when *d* is an odd integer. For instance, for d = 1, 2, 3 it holds that

$$\Lambda_1(t) = \cos(t), \quad \Lambda_2(t) = J_0(t), \quad \Lambda_3(t) = \frac{\sin(t)}{t},$$

and $\Lambda_{\infty}(t) := \lim_{d \to \infty} \Lambda_d(t) = e^{-t^2}$. In particular, any isotropic correlation function in \mathbb{R}^3 admits the representation

$$K(r) = \int_0^\infty \frac{\sin(rx)}{rx} dF(x), \qquad r \ge 0,$$

and any such function is also an isotropic correlation function in \mathbb{R}^2 and \mathbb{R}^1 , since the classes of functions Φ_d are decreasing in *d*. If $F(\cdot)$ is absolutely continuous, with pdf $f(\cdot)$ say, then

$$K(r) = \int_0^\infty \frac{\sin(rx)}{rx} f(x) dx, \qquad r \ge 0; \tag{4.1}$$

the functions *F* and *f* are also called, respectively, the *radial distribution* and *radial pdf* functions of the random field $Z(\cdot)$ [15]. Therefore, (4.1) establishes a bijection between the class of continuous isotropic correlation functions in \mathbb{R}^3 and the class of pdfs in \mathbb{R} (w.r.t. Lebesgue measure) having support $[0, \infty)$. Consequently, choosing a continuous isotropic correlation function $K(\cdot)$ amounts to choosing a pdf $f(\cdot)$ with support in $[0, \infty)$.

4.2 A New Correlation Family

In this section, we use (4.1) with a particular family of radial pdfs to construct what appears to be a new family of correlation functions in \mathbb{R}^3 whose members display long-range dependence and various degrees of smoothness. For $\sigma > 0$ and $m \in \mathbb{N}_0$, let $f_{\sigma,m}(x)$ be the pdf of the $t_{2m+1}(0, \sigma^2)$ distribution¹ truncated to $[0, \infty)$, i.e.,

¹ The symbol $t_{\nu}(\mu, \sigma^2)$ denotes the *t* distribution with ν degrees of freedom, location parameter μ and scale parameter σ .

$$f_{\sigma,m}(x) = \frac{2\Gamma(m+1)}{\sigma\sqrt{\pi(2m+1)}\Gamma(\frac{2m+1}{2})} \left(1 + \frac{1}{2m+1}\left(\frac{x}{\sigma}\right)^2\right)^{-(m+1)} \mathbf{1}_{(0,\infty)}(x)$$
$$= \frac{2\Gamma(m+1)}{\sigma\sqrt{\pi(2m+1)}\Gamma(\frac{2m+1}{2})} \left((2m+1)\sigma^2\right)^{m+1} \left((2m+1)\sigma^2 + x^2\right)^{-(m+1)},$$

when x > 0. Then from (4.1), the correlation function in \mathbb{R}^3 that corresponds to this radial pdf is

$$K_{\sigma,m}(r) = \frac{2\Gamma(m+1)\big((2m+1)\sigma^2\big)^{m+1}}{\sigma\sqrt{\pi(2m+1)}\Gamma(\frac{2m+1}{2})r} \int_0^\infty \frac{\sin(rx)}{x\big((2m+1)\sigma^2 + x^2\big)^{m+1}} dx$$

$$= \frac{2\Gamma(m+1)\big((2m+1)\sigma^2\big)^{m+1}}{\sigma\sqrt{\pi(2m+1)}\Gamma(\frac{2m+1}{2})r}$$
$$\times \frac{\pi}{2\big((2m+1)\sigma^2\big)^{m+1}} \Big(1 - \frac{e^{-\sigma\sqrt{2m+1}r}}{2^m m!} P_m\big(\sigma\sqrt{2m+1}r\big)\Big)$$

$$= \frac{\sqrt{\pi}\Gamma(m+1)}{\sigma\sqrt{(2m+1)}\Gamma(\frac{2m+1}{2})r} \Big(1 - \frac{e^{-\sigma\sqrt{2m+1}r}}{2^m m!} P_m\big(\sigma\sqrt{2m+1}r\big)\Big), \quad (4.2)$$

where the second equality follows from [9, 3.737.3], and $P_m(\cdot)$ is the polynomial of degree *m* obtained by the recursion

$$P_m(x) = (x + 2m)P_{m-1}(x) - xP'_{m-1}(x), \quad m \ge 1, \text{ with } P_0(x) = 1.$$

For instance, for m = 1, 2, 3 we have

$$P_1(x) = x + 2$$
, $P_2(x) = x^2 + 5x + 8$, $P_3(x) = x^3 + 9x^2 + 33x + 48$.

Reparametrizing (4.2) with $\theta := (\sigma \sqrt{2m+1})^{-1}$, we obtain the following twoparameter family of continuous isotropic correlation functions in \mathbb{R}^3

$$\mathcal{D} = \left\{ K_{\theta,m}(r) := c_m \frac{\theta}{r} \left(1 - \frac{e^{-\frac{r}{\theta}}}{2^m m!} P_m\left(\frac{r}{\theta}\right) \right) : \theta > 0, m \in \mathbb{N}_0 \right\},\tag{4.3}$$

with²

$$c_m = \frac{\sqrt{\pi}\,\Gamma(m+1)}{\Gamma(\frac{2m+1}{2})}.$$

For instance, for $r \ge 0$ and m = 0, 1, 2 we have

² The fact $K_{\theta,m}(0) = 1$ follows by continuity.



$$\begin{split} K_{\theta,0}(r) &= \frac{\theta}{r} \Big(1 - e^{-\frac{r}{\theta}} \Big), \\ K_{\theta,1}(r) &= \frac{\theta}{r} \Big(2 - e^{-\frac{r}{\theta}} \Big(\frac{r}{\theta} + 2 \Big) \Big), \\ K_{\theta,2}(r) &= \frac{\theta}{3r} \Big(8 - e^{-\frac{r}{\theta}} \Big(\Big(\frac{r}{\theta} \Big)^2 + 5\frac{r}{\theta} + 8 \Big) \Big) \end{split}$$

4.3 Properties

In this section, we describe some of the properties of the new family of correlation functions. First, any of the correlation functions in (4.3) displays long-range dependence, as it decays slowly with increasing distance *r*. Specifically, for any $\theta > 0$ and $m \in \mathbb{N}_0$ it holds that $K_{\theta,m}(r) \to 0$ and $K_{\theta,m}(r) = O(1/r)$ as $r \to \infty$, so

$$\int_{0}^{\infty} r^{d-1} K_{\theta,m}(r) dr \text{ diverges } (d = 1, 2, 3).$$
 (4.4)

For isotropic correlation functions, the above property defines long-range dependence. Second, the interpretation of the parameters is the following. The parameter θ is a *range* parameter that controls how fast the correlation function decays with distance *r*. This is illustrated in Fig. 4.1 where plots $K_{\theta,m}(r)$ are displayed for m = 1 and three values of θ . On the other hand, *m* is a *smoothness* parameter that controls the mean square differentiability of the random field $Z(\cdot)$, as stated by the following result.



Fig. 4.2 Plots of the even extension of $K_{\theta,m}(r)$ (left) and corresponding realizations of zero-mean Gaussian random fields with these correlation functions (right). In all $\theta = 0.25$ and m = 0 (top), 1 (middle) and 2 (bottom)

Proposition 4.1 Let $\{Z(\mathbf{s}) : \mathbf{s} \in D\}$, with $D \subset \mathbb{R}^d$ and $d \leq 3$, be an isotropic mean square continuous random field with correlation function $K_{\theta,m}(r)$ from the family (4.3). Then $Z(\cdot)$ is m-times mean square differentiable.

Proof For any $k \in \mathbb{N}_0$, an isotropic random field $Z(\cdot)$ is *k*-times mean square differentiable if and only if its correlation function is 2k-times differentiable at zero³ [20]. In addition, for any radial positive definite function in \mathbb{R}^d , K(r) say, $K^{(2k)}(0)$ exists if and only if the radial pdf f in the representation (4.1) has a finite moment of order 2k [6, Lemma 3]. Since the radial distribution associated with $K_{\theta,m}(r)$ is the $t_{2m+1}(0, \sigma^2)$ distribution truncated to $[0, \infty)$ and this has finite moments up to order 2m, the above results imply that a random field with correlation function $K_{\theta,m}(r)$ is exactly *m*-times mean square differentiable.

To illustrate the above result, Fig. 4.2 plots the even extension of $K_{\theta,m}(r)$ (left) and corresponding realizations of zero-mean Gaussian random fields in the real line with these correlation functions (right), where $\theta = 0.25$ and m = 0 (top), 1 (middle),

³ Differentiability of $K(\cdot)$ at zero refers to differentiability of its even extension over the real line, defined as $K^{e}(r) := K(|r|), r \in \mathbb{R}$. Also, the phrase ' $Z(\cdot)$ is 0-times mean square differentiable' is used if $Z(\cdot)$ is mean square continuous.

and 2 (bottom). The plots show the smoothness of $K_{\theta,m}(r)$ at the origin increasing with *m*, and its corresponding effect on the smoothness of the realizations. The three realizations were obtained from the same seed. Together, Figs. 4.1 and 4.2 suggest that \mathcal{D} is a flexible family of correlation functions capable of describing different degrees of spatial association and smoothness in random fields that display long-range dependence.

4.4 Comparison With a Matérn Sub-family

The Matérn family of correlation functions [15, 20] is a two-parameter family of correlation functions in \mathbb{R}^d for all $d \ge 1$ that is commonly used in geostatistical applications. It is given by

$$M_{\theta,\nu}(r) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\frac{r}{\theta}\right)^{\nu} \mathcal{K}_{\nu}\left(\frac{r}{\theta}\right), \qquad (4.5)$$

where θ , $\nu > 0$ and $\mathcal{K}_{\nu}(.)$ is the modified Bessel function of second kind and order ν ; see [9, 8.40] for details on the behavior of this special function. This family contains the exponential correlation function $e^{-r/\theta}$ (obtained when $\nu = 0.5$), and the squared exponential correlation function $e^{-(r/\vartheta)^2}$ is a limit case (obtained when $\theta = \vartheta/2\sqrt{\nu}$ and $\nu \to \infty$). We consider here the following sub-family:

$$\mathcal{M} = \{ M_{\theta, m+0.5}(r) : \theta > 0, m \in \mathbb{N}_0 \}.$$
(4.6)

Like the family \mathcal{D} in (4.3), θ is a *range* parameter that controls how fast the correlation function decreases with distance r, and m is a *smoothness* parameter that controls the mean square differentiability of the random field $Z(\cdot)$. It was shown by [20] that a random field $Z(\cdot)$ with correlation function $M_{\theta,m+0.5}(r)$ is exactly m-times mean square differentiable. Additionally, $M_{\theta,m+0.5}(r)$ can be written as $e^{-r/\theta}$ times a polynomial in r of degree m [9, 8.468]. For instance, for $r \ge 0$ and m = 0, 1, 2 we have

$$M_{\theta,0.5}(r) = e^{-\frac{r}{\theta}},$$

$$M_{\theta,1.5}(r) = e^{-\frac{r}{\theta}} \left(\frac{r}{\theta} + 1\right),$$

$$M_{\theta,2.5}(r) = e^{-\frac{r}{\theta}} \left(\frac{1}{3} \left(\frac{r}{\theta}\right)^2 + \frac{r}{\theta} + 1\right).$$

But unlike the family \mathcal{D} , the correlation functions in (4.6) display short-range dependence, since for any $\theta > 0$ and $m \in \mathbb{N}_0$

$$M_{\theta,m+0.5}(r) \sim ar^{m-\frac{1}{2}}e^{-\frac{r}{\theta}}, \quad \text{as } r \to \infty,$$



Fig. 4.3 Plots of $K_{0.25,1}(r)$ and $M_{1.285,1.5}(r)$ (left) and corresponding realizations of zero-mean Gaussian random fields with these correlation functions (right)

for some a > 0 [1, 9.7.2]. So $M_{\theta,m+0.5}(r)$ decreases to zero exponentially fast as $r \to \infty$, and consequently $\int_0^\infty r^{d-1} M_{\theta,m}(r) dr$ converges. To illustrate the different behaviors of correlation functions in the families \mathcal{D} and \mathcal{M} with the same smoothness and similar rates of decay, Fig. 4.3 plots $K_{0.25,1}(r)$ and $M_{1,285,1,5}(r)$ (left) and corresponding realizations of zero-mean Gaussian random fields in the real line with these correlations functions (right); the two realizations were obtained from the same seed. Both correlation functions correspond to random fields that are 1-time mean square differentiable, and their range parameters are such that their correlations at distance r = 5 is 0.1. Note that $M_{1,285,1.5}(r)$ has larger correlations than $K_{0,25,1}(r)$ for small distances, but the opposite holds for large distances. As a result, the realization of the random field with correlation function $K_{0.25,1}(r)$ displays more 'oscillatory' behavior for small distances, but process values for large distances are more 'alike' than process values of the realization of the random field with correlation function $M_{1,285,1,5}(r)$. Therefore, the families of correlations \mathcal{D} and \mathcal{M} appear equally flexible in terms of describing different degrees of spatial association and smoothness, but are complementary in terms of the range of dependence, as one displays long-range dependence while the other short-range dependence.

4.5 Other Correlation Families With Long-Range Dependence

4.5.1 The Generalized Cauchy Family

The generalized Cauchy family [8, 11] is a three-parameter family of isotropic correlation functions in \mathbb{R}^d , for all $d \ge 1$, given by

$$C_{\alpha,\beta,\theta}(r) = \left(1 + \left(\frac{r}{\theta}\right)^{\alpha}\right)^{-\beta/\alpha}$$

where $\alpha \in (0, 2], \beta > 0$ and $\theta > 0$. As in the previous families, θ is a range parameter. The main virtue of this family is that it allows for independent choices of *fractal dimension* and *Hurst coefficient*, where the former is a measure of the 'roughness' of realizations of random fields with this correlation function, and the latter is a measure of 'persistence' or long-range dependence [7]. Specifically, realizations of a random field in \mathbb{R}^d with correlation function $C_{\alpha,\beta,\theta}(r)$ have fractal dimension [11]

$$D = d + 1 - \alpha/2 \in [d, d + 1),$$

with D = d (D > d) when the random field is (is not) mean square differentiable; the larger D is, the rougher the realizations. So this property is entirely controlled by the parameter α .

Additionally, $C_{\alpha,\beta,\theta}(r) \sim r^{-\beta}$ as $r \to \infty$, so it satisfies (4.4) when $\beta \in (0, d]$, and the random field has long-range dependence with Hurst coefficient [11, 16]

$$H = \frac{d+\beta}{2} \in (d/2, d];$$

the closer *H* is to d/2, the stronger the persistence. So this property is entirely controlled by the parameter $\beta \in (0, d]$. The random field has short-range dependence when $\beta > d$. Hence, *D* and *H* can vary independently of each other, and they can take any value in their respective ranges of possible values [8]. This property is in sharp contrast with that of self-affine processes often used to model long-range dependence [14] where the fractal dimension and Hurst coefficient are tied by the relation D + H = d + 1.

The generalized Cauchy family allows a wide range of 'roughness' and 'persistence' behaviors controlled by the parameters α and β , respectively. On the other hand, this family does not allow a wide range of smoothness behaviors, since a random field with correlation function $C_{\alpha,\beta,\theta}(r)$ is non-differentiable in mean square when $\alpha \in (0, 2)$ and infinitely differentiable when $\alpha = 2$, with no possible intermediate behaviors [19].

4.5.2 The Confluent Hypergeometric Family

Recently, [13] derived a new family of isotropic correlation functions in \mathbb{R}^d , for all $d \ge 1$, that display long-range dependence. The construction involves mixing the Matérn correlation functions (in a parametrization different than (4.5)) over the (new) squared range parameter, with the IG(α , $\beta^2/2$) distribution as the mixing distribution⁴. Specifically, their correlation function is given by

$$\begin{split} H_{\alpha,\beta,\nu}(r) &= \int_0^\infty M_{\phi/\sqrt{2\nu},\nu}(r) \frac{\beta^{2\alpha}}{2^{\alpha}\Gamma(\alpha)} \phi^{-2(\alpha+1)} e^{-\frac{\beta^2}{2\phi^2}} d\phi^2 \\ &= \frac{\beta^{2\alpha}\Gamma(\nu+\alpha)}{\Gamma(\nu)\Gamma(\alpha)} \int_0^\infty x^{\nu-1} (x+\beta^2)^{-(\nu+\alpha)} e^{-\frac{\nu r^2}{x}} dx \\ &= \frac{\Gamma(\nu+\alpha)}{\Gamma(\nu)} U\Big(\alpha, 1-\nu, \nu\Big(\frac{r}{\beta}\Big)^2\Big), \end{split}$$

where α , β , $\nu > 0$ and U(a, b, c) is the confluent hypergeometric function of the second kind ([1, 13.2]), so this family was named the Confluent Hypergeometric family; see [13] for details.

It was shown by [13] that the Confluent Hypergeometric and Matérn covariance functions with the same parameter ν have the same asymptotic behavior as $r \rightarrow 0$. Hence, like the Matérn family, a random field with correlation function $H_{\alpha,\beta,\nu}(r)$ is $[\nu]$ -times mean square differentiable [20], and the fractal dimension of realizations from this random field is [7, 16]

$$D = \begin{cases} d+1-\nu \text{ if } \nu \in (0,1) \\ d & \text{ if } \nu \ge 1 \end{cases} \quad (D \in [d,d+1)).$$

So this model allows any degree of smoothness and roughness which is controlled by the parameter v.

Additionally, it was shown by [13] that

$$H_{\alpha,\beta,\nu}(r) \sim ar^{-2\alpha}L(r^2), \quad \text{as } r \to \infty,$$

for some a > 0, where $L(x) := (x/(x + \beta^2/(2\nu)))^{\nu+\alpha}$ is a slowly varying function at infinity. Then, for any $d \in \mathbb{N}$, $H_{\alpha,\beta,\nu}(r)$ satisfies (4.4) when $\alpha \in (0, d/2]$. Hence, unlike the Matérn family, the Confluent Hypergeometric correlation functions display long-range dependence when $\alpha \in (0, d/2]$. In this case, they decay hyperbolically fast with increasing distance, with the rate of decay controlled by the parameter α , and the Hurst coefficient [16] is

$$H = d/2 + \alpha \in (d/2, d].$$

⁴ The symbol IG(α , $\beta^2/2$) denotes the inverse gamma distribution with shape parameter α and scale parameter $\beta^2/2$.

The random field has short-term dependence when $\alpha > d/2$. Like the generalized Cauchy family, *D* and *H* in the Confluent Hypergeometric family can vary independently of each other and they can take any value in their respective ranges of possible values. But in contrast to the former, the latter family allows a wide range of smoothness behaviors.

4.6 Discussion

Correlation functions displaying short-range dependence are the most often used in geostatistical applications. This practice is mainly due to the following:

- (I) Correlation families displaying long-range dependence are fewer and less known in geostatistics than short-range correlation families.
- (II) The detection of long-range dependence requires abundant data collected over large regions, which is often not available.
- (III) The main goal in many geostatistical applications is spatial interpolation based on densely collected data, in which case the behavior of the correlation function at short distances is much more important than the behavior at large distances.

Nevertheless, recent developments in theory and applications have shown that correlation functions displaying long-range dependence have a role to play in geo-statistics.

When the goal is spatial extrapolation or interpolation with sparsely located data, short-range correlation models may provide less satisfactory predictive inferences. In this case, the effect of the correlation function on the optimal linear predictor is negligible, as this predictor is essentially the estimated mean function. This is an unwanted outcome because it is rarely the case in applications that the modeler has strong confidence in the proposed mean function, even when this is constant. In an analysis of carbon dioxide measured in the United States by satellite, [13] found that, for spatial extrapolation, predictive inference based on the Confluent Hypergeometric family was better than that based on the Matérn family (when ν was fixed at the same value in both families). On the other hand, for spatial interpolation, predictive inference based on both families was about the same. These behaviors are explained by the fact that both families are equally flexible in modeling smoothness of the random field, while only the confluent hypergeometric family can model both short- and long-range dependence.

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