

Matérn Class Tensor-Valued Random Fields and Beyond

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Abstract We construct classes of homogeneous random fields on a three-dimensional Euclidean space that take values in linear spaces of tensors of a fixed rank and are isotropic with respect to a fixed orthogonal representation of the group of 3×3 orthogonal matrices. The constructed classes depend on finitely many isotropic spectral densities. We say that such a field belongs to either the Matérn or the dual Matérn class if all of the above densities are Matérn or dual Matérn. Several examples are considered.

Keywords Homogeneity · Isotropy · Group representation · Spectral density

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1 Introduction

Random functions of more than one variable, or *random fields*, were introduced in the 20th years of the past century as mathematical models of physical phenomena like turbulence, see, e.g., [9, 20, 39]. To explain how random fields appear in continuum physics, consider the following example.

Example 1 Let $E = E^3$ be a three-dimensional Euclidean point space, and let V be the translation space of E with an inner product (\cdot, \cdot) . Following [43], the elements A of E are called the *places* in E . The symbol $B - A$ is the vector in V that translates A into B .

Let $\mathcal{B} \subset E$ be a subset of E occupied by a material, e.g., a turbulent fluid or a deformable body. The temperature is a rank 0 tensor-valued function $T: \mathcal{B} \rightarrow \mathbb{R}^1$. The velocity of a fluid

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is a rank 1 tensor-valued function $\mathbf{v}: \mathcal{B} \rightarrow V$. The strain tensor is a rank 2 tensor-valued function $\varepsilon: \mathcal{B} \rightarrow \mathcal{S}^2(V)$, where $\mathcal{S}^2(V)$ is the linear space of symmetric rank 2 tensors over V . The piezoelectricity tensor is a rank 3 tensor-valued function $\mathbf{D}: \mathcal{B} \rightarrow \mathcal{S}^2(V) \otimes V$. The elastic modulus is a rank 4 tensor-valued function $\mathbf{C}: \mathcal{B} \rightarrow \mathcal{S}^2(\mathcal{S}^2(V))$. Denote the range of any of the above functions by \mathbf{V} . Physicists call \mathbf{V} for ranks 2 or 3 or 4 the *constitutive tensor space*. It is a subspace of the tensor power $V^{\otimes r}$, where r is a nonnegative integer. The form

$$(\mathbf{x}_1 \otimes \cdots \otimes \mathbf{x}_r, \mathbf{y}_1 \otimes \cdots \otimes \mathbf{y}_r) = (\mathbf{x}_1, \mathbf{y}_1) \cdots (\mathbf{x}_r, \mathbf{y}_r)$$

can be extended by linearity to the inner product on $V^{\otimes r}$ and then restricted to \mathbf{V} .

At microscopic length scales, *spatial randomness* of the material needs to be taken into account. Mathematically, there is a probability space $(\Omega, \mathfrak{F}, \mathbf{P})$ and a function $\mathbf{T}(A, \omega): \mathcal{B} \times \Omega \rightarrow \mathbf{V}$ such that for any fixed $A_0 \in \mathbf{V}$ and for any Borel set $B \subseteq \mathbf{V}$ the inverse image $\mathbf{T}^{-1}(A_0, B)$ is an event. The map $\mathbf{T}(\mathbf{x}, \omega)$ is a *random field*.

Translate the whole body \mathcal{B} by a vector $\mathbf{x} \in V$. The random fields $\mathbf{T}(A + \mathbf{x})$ and $\mathbf{T}(A)$ have the same finite-dimensional distributions. It is therefore convenient to assume that there is a random field defined *on all of* E such that its restriction to \mathcal{B} is equal to $\mathbf{T}(A)$. For brevity, denote the new field by the same symbol $\mathbf{T}(A)$ (but this time $A \in E$). The random field $\mathbf{T}(A)$ is *strictly homogeneous*, that is, the random fields $\mathbf{T}(A + \mathbf{x})$ and $\mathbf{T}(A)$ have the same finite-dimensional distributions. In other words, for each positive integer n , for each $\mathbf{x} \in V$, and for all distinct places $A_1, \dots, A_n \in E$ the random elements $\mathbf{T}(A_1) \oplus \cdots \oplus \mathbf{T}(A_n)$ and $\mathbf{T}(A_1 + \mathbf{x}) \oplus \cdots \oplus \mathbf{T}(A_n + \mathbf{x})$ of the direct sum on n copies of the space \mathbf{V} have the same probability distribution.

Let K be the material symmetry group of the material body \mathcal{B} acting in V . The group K is a subgroup of the orthogonal group $O(V)$. For simplicity, we assume that the material is fully symmetric, that is, $K = O(V)$. Fix a place $O \in \mathcal{B}$ and identify E with V by the map f that maps $A \in E$ to $A - O \in V$. Then K acts in E and rotates the body \mathcal{B} by

$$g \cdot A = f^{-1}gfA, \quad g \in O(V), \quad A \in \mathcal{B}.$$

Let U be the restriction of the orthogonal representation $g \mapsto g^{\otimes r}$ of the group $O(V)$ to the subspace \mathbf{V} of the space $V^{\otimes r}$. The group K acts in \mathbf{V} by $\mathbf{v} \mapsto U(g)\mathbf{v}$, $g \in K$. Under the action of K in E , the point A_0 becomes $g \cdot A_0$. Under the action of K in \mathbf{V} , the random tensor $\mathbf{T}(A_0)$ becomes $U(g)\mathbf{T}(A_0)$. The random fields $\mathbf{T}(g \cdot A)$ and $U(g)\mathbf{T}(A)$ must have the same finite-dimensional distributions, because $g \cdot A_0$ is the same material point in a different place. Note that this property does not depend on a particular choice of the place O , because the field is strictly homogeneous. We call such a field *strictly isotropic*.

Assume that the random field $\mathbf{T}(A)$ is *second-order*, that is

$$\mathbf{E}[\|\mathbf{T}(A)\|^2] < \infty, \quad A \in E.$$

Define the *one-point correlation tensor* of the field $\mathbf{T}(A)$ by

$$\langle \mathbf{T}(A) \rangle = \mathbf{E}[\mathbf{T}(A)]$$

and its *two-point correlation tensor* by

$$\langle \mathbf{T}(A), \mathbf{T}(B) \rangle = \mathbf{E}[(\mathbf{T}(A) - \langle \mathbf{T}(A) \rangle) \otimes (\mathbf{T}(B) - \langle \mathbf{T}(B) \rangle)].$$

Assume that the field $\mathbf{T}(A)$ is *mean-square continuous*, that is, its two-point correlation tensor $\langle \mathbf{T}(A), \mathbf{T}(B) \rangle: E \times E \rightarrow \mathbf{V} \otimes \mathbf{V}$ is a continuous function.

Note that [35] had shown that any finite-variance isotropic random field on a compact group is necessarily mean-square continuous under standard measurability assumptions, and hence

its covariance function is continuous. In the related settings, the characterisation of covariance function for a real homogeneous isotropic random field in d -dimensional Euclidean space was given in the classical paper by [40], where it was conjectured that the only form of discontinuity which could be allowed for such a function would occur at the origin. This conjecture was proved by [7] for $d \geq 2$. This result was widely used in Geostatistics (see, i.e., [13], among the others), who argued that the homogenous and isotropic random field could be expressed as a mean-square continuous component and what they called “nugget effect”, e.g. a purely discontinuous component. In fact this latter component should be necessarily non-measurable (see, i.e., [18, Example 1.2.5]). The relation between measurability and mean-square continuity in non-compact situation is still unclear even for scalar random fields. That is why we assume in this paper that our random fields are mean-square continuous, and hence their covariance functions are continuous.

If the field $T(A)$ is strictly homogeneous, then its one-point correlation tensor is a constant tensor in V , while its two-point correlation tensor is a function of the vector $B - A$, i.e., a function on V . Call such a field *wide-sense homogeneous*.

Similarly, if the field $T(A)$ is strictly isotropic, then we have

$$\begin{aligned} \langle T(g \cdot A) \rangle &= U(g)\langle T(A) \rangle, \\ \langle T(g \cdot A), T(g \cdot B) \rangle &= (U \otimes U)(g)\langle T(A), T(B) \rangle. \end{aligned} \tag{1}$$

Definition 1 A random field $T(A)$ is called *wide-sense isotropic* if its one-point and two-point correlation tensors satisfy (1).

For simplicity, identify the field $\{T(A) : A \in E\}$ defined on E with the field $\{T'(x) : x \in V\}$ defined by $T'(x) = T(O + x)$. Introduce the Cartesian coordinate system (x, y, z) in V . Use the introduced system to identify V with the coordinate space \mathbb{R}^3 and $O(V)$ with $O(3)$. Call \mathbb{R}^3 the *space domain*. The action of $O(3)$ on \mathbb{R}^3 is the matrix-vector multiplication.

Definition 1 was used by many authors including [36,42,46].

There is another definition of isotropy.

Definition 2 [46] A random field $T(A)$ is called a *multidimensional scalar wide-sense isotropic* if its one-point correlation tensor is a constant, while the two-point correlation tensor $\langle T(x), T(y) \rangle$ depends only on $\|y - x\|$.

It is easy to see that Definition 2 is a particular case of Definition 1 when the representation U is trivial, that is, maps all elements $g \in K$ to the identity operator.

In the case of $r = 0$, the complete description of the two-point correlation functions of scalar homogeneous and isotropic random fields is as follows. Recall that a measure μ defined on the Borel σ -field of a Hausdorff topological space X is called *Borel measure*.

Theorem 1 *Formula*

$$\langle T(x), T(y) \rangle = \int_0^\infty \frac{\sin(\lambda\|y - x\|)}{\lambda\|y - x\|} d\mu(\lambda) \tag{2}$$

establishes a one-to-one correspondence between the set of two-point correlation functions of homogeneous and isotropic random fields $T(x)$ on the space domain \mathbb{R}^3 and the set of all finite Borel measures μ on the interval $[0, \infty)$.

Theorem 1 is a translation of the result proved by [40] to the language of random fields. This translation is performed as follows. Assume that $B(x)$ is a two-point correlation function of a homogeneous and isotropic random field $T(x)$. Let n be a positive integer, let x_1, \dots, x_n

be n distinct points in \mathbb{R}^3 , and let c_1, \dots, c_n be n complex numbers. Consider the random variable $X = \sum_{j=1}^n c_j [T(\mathbf{x}_j) - \langle T(\mathbf{x}_j) \rangle]$. Its variance is non-negative:

$$E[X^2] = \sum_{j,k=1}^n c_j \overline{c_k} \langle T(\mathbf{x}_j), T(\mathbf{x}_k) \rangle \geq 0.$$

In other words, the two-point correlation function $\langle T(\mathbf{x}), T(\mathbf{y}) \rangle$ is a non-negative-definite function. Moreover, it is continuous, because the random field $T(\mathbf{x})$ is mean-square continuous, and depends only on the distance $\|\mathbf{y} - \mathbf{x}\|$ between the points \mathbf{x} and \mathbf{y} , because the field is homogeneous and isotropic. [40] proved that Eq. (2) describes all of such functions.

Conversely, assume that the function $\langle T(\mathbf{x}), T(\mathbf{y}) \rangle$ is described by Equation (2). The centred Gaussian random field with the two-point correlation function (2) is homogeneous and isotropic. In other words, there is a link between the theory of random fields and the theory of positive-definite functions.

In what follows, we consider the fields with absolutely continuous spectrum.

Definition 3 ([17]) A homogeneous and isotropic random field $T(\mathbf{x})$ has an *absolutely continuous spectrum* if the measure μ is absolutely continuous with respect to the measure $4\pi\lambda^2 d\lambda$, i.e., there exist a nonnegative measurable function $f(\lambda)$ such that

$$\int_0^\infty \lambda^2 f(\lambda) d\lambda < \infty$$

and $d\mu(\lambda) = 4\pi\lambda^2 f(\lambda) d\lambda$. The function $f(\lambda)$ is called the *isotropic spectral density* of the random field $T(\mathbf{x})$.

Example 2 (The Matérn two-point correlation function) Consider a two-point correlation function of a scalar random field $T(\mathbf{x})$ of the form

$$\langle T(\mathbf{x}), T(\mathbf{y}) \rangle = M_{\nu,a}(\mathbf{x}, \mathbf{y}) = \frac{2^{1-\nu}\sigma^2}{\Gamma(\nu)} (a \|\mathbf{x} - \mathbf{y}\|)^\nu K_\nu(a \|\mathbf{x} - \mathbf{y}\|), \tag{3}$$

where $\sigma^2 > 0, a > 0, \nu > 0$ and $K_\nu(z)$ is the Bessel function of the third kind of order ν . Here, the parameter ν measures the differentiability of the random field; the parameter σ is its variance and the parameter a measures how quickly the correlation function of the random field decays with distance. The corresponding isotropic spectral density is

$$f(\lambda) = f_{\nu,a,\sigma^2}(\lambda) = \frac{\sigma^2 \Gamma(\nu + \frac{3}{2}) a^{2\nu}}{2\pi^{3/2} (a^2 + \lambda^2)^{\nu + \frac{3}{2}}}, \quad \lambda \geq 0.$$

Note that Example 2 demonstrates another link, this time between the theory of random fields and the theory of special functions.

In this paper, we consider the following problem. How to define the Matérn two-point correlation tensor for the case of $r > 0$? A particular answer to this question can be formulated as follows.

Example 3 (Parsimonious Matérn model, [12]) We assume that the vector random field

$$T(\mathbf{x}) = (T_1(\mathbf{x}), \dots, T_m(\mathbf{x}))^\top, \quad \mathbf{x} \in \mathbb{R}^3,$$

has the two-point correlation tensor $B(\mathbf{x}, \mathbf{y}) = (B_{ij}(\mathbf{x}, \mathbf{y}))_{1 \leq i, j \leq m}$. It is not straightforward to specify the cross-covariance functions $B_{ij}(\mathbf{x}), 1 \leq i, j \leq m, i \neq j$, as non-trivial,

valid parametric models because of the requirement of their non-negative definiteness. In the multivariate Matérn model, each marginal covariance function

$$B_{ii}(\mathbf{x}, \mathbf{y}) = \sigma_i^2 M_{v_i, a_i}(\mathbf{x}, \mathbf{y}), \quad i = 1, \dots, m,$$

is of the type (3) with the isotropic spectral density $f_{ii}(\lambda) = f_{v_i, a_i, \sigma_i^2}(\lambda)$.

Each cross-covariance function

$$B_{ij}(\mathbf{x}, \mathbf{y}) = B_{ji}(\mathbf{x}, \mathbf{y}) = b_{ij} \sigma_i \sigma_j M_{v_{ij}, a_{ij}}(\mathbf{x}, \mathbf{y}), \quad 1 \leq i, j \leq m, \quad i \neq j$$

is also a Matérn function with co-location correlation coefficient b_{ij} , smoothness parameter v_{ij} and scale parameter a_{ij} . The spectral densities are

$$f_{ij}(\mathbf{x}) = f_{v_{ij}, a_{ij}, b_{ij} \sigma_i \sigma_j}(\mathbf{x}), \quad 1 \leq i, j \leq m, \quad i \neq j.$$

The question then is to determine the values of v_{ij} , a_{ij} and b_{ij} so that the non-negative definiteness condition is satisfied. Let $m \geq 2$. Suppose that

$$v_{ij} = \frac{1}{2}(v_i + v_j), \quad 1 \leq i, j \leq m, \quad i \neq j,$$

and that there is a common scale parameter in the sense that there exists an $a > 0$ such that

$$a_i = \dots = a_m = a, \quad \text{and } a_{ij} = a \text{ for } 1 \leq i, j \leq m, \quad i \neq j.$$

Then the multivariate Matérn model provides a valid second-order structure in \mathbb{R}^3 if

$$b_{ij} = \beta_{ij} \left[\frac{\Gamma(v_i + \frac{3}{2})}{\Gamma(v_i)} \frac{\Gamma(v_j + \frac{3}{2})}{\Gamma(v_j)} \right]^{1/2} \frac{\Gamma(\frac{1}{2}(v_i + v_j))}{\Gamma(\frac{1}{2}(v_i + v_j) + \frac{3}{2})}$$

for $1 \leq i, j \leq m, i \neq j$, where the matrix $(\beta_{ij})_{i,j=1,\dots,m}$ has diagonal elements $\beta_{ii} = 1$ for $i = 1, \dots, m$, and off-diagonal elements $\beta_{ij}, 1 \leq i, j \leq m, i \neq j$ so that it is symmetric and non-negative definite.

Example 4 (Flexible Matérn model) Consider the vector random field $\mathbf{T}(\mathbf{x}) \in \mathbb{R}^m, \mathbf{x} \in \mathbb{R}^3$ with the two-point covariance tensor

$$\langle T_i(\mathbf{x}), T_j(\mathbf{y}) \rangle = B_{ij}(\mathbf{x}, \mathbf{y}) = \bar{B}_{ij}(\mathbf{y} - \mathbf{x}) = \sigma_{ij} M_{v_{ij}, a_{ij}}(\mathbf{x}, \mathbf{y}), \quad 1 \leq i, j \leq m,$$

where again

$$M_{v,a}(\mathbf{x}, \mathbf{y}) = \frac{2^{1-v} \sigma^2}{\Gamma(v)} (a \|\mathbf{y} - \mathbf{x}\|)^v K_v(a \|\mathbf{y} - \mathbf{x}\|).$$

Denote by \mathcal{N} the set of all nonnegative-definite matrices. Assume that the matrix $\Sigma = (\sigma_{ij})_{1 \leq i, j \leq m} = (\sigma_{ij}) \in \mathcal{N}$, and denote $\sigma_i^2 = \sigma_{ii}, i = 1, \dots, m$.

Then the spectral density $F = (f_{ij})_{1 \leq i, j \leq m}$ has the entries

$$\begin{aligned} f_{ij}(\boldsymbol{\lambda}) &= \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{-i(\boldsymbol{\lambda}, \mathbf{h})} \bar{B}_{ij}(\mathbf{h}) \, d\mathbf{h} \\ &= \sigma_{ij} a_{ij}^{2v_{ij}} \frac{1}{(a_{ij} + \|\boldsymbol{\lambda}\|^2)^{v_{ij} + \frac{3}{2}}} \frac{\Gamma(v_{ij} + \frac{3}{2})}{\Gamma(v_{ij})}, \quad 1 \leq i, j \leq m, \quad \boldsymbol{\lambda} \in \mathbb{R}^3. \end{aligned}$$

We need to find some conditions on parameters $a_{ij} > 0, v_{ij} > 0$, under which $F \in \mathcal{N}$. The general conditions can be found in [2, 8].

Recall that a symmetric, real $m \times m$ matrix $\Theta = (\theta_{ij})_{1 \leq i, j \leq m}$, is said to be *conditionally negative definite* [3], if the inequality

$$\sum_{i=1}^m \sum_{j=1}^m c_i c_j \theta_{ij} \leq 0$$

holds for any real numbers c_1, \dots, c_m , subject to

$$\sum_{i=1}^m c_i = 0.$$

In general, a necessary condition for the above inequality is

$$\theta_{ii} + \theta_{jj} \leq 2\theta_{ij}, \quad i, j = 1, \dots, m,$$

which implies that all entries of a conditionally negative definite matrix are nonnegative whenever its diagonal entries are non-negative. If all its diagonal entries vanish, a conditionally negative definite matrix is also named a Euclidean distance matrix. It is known that $\Theta = (\theta_{ij})_{1 \leq i, j \leq m}$ is conditionally negative definite if and only if an $m \times m$ matrix S with entries $\exp\{-\theta_{ij}u\}$ is positive definite, for every fixed $u \geq 0$ (cf. [3, Theorem 4.1.3]), or $S = e^{-u\Theta}$, where e^Λ is an Hadamard exponential of a matrix Λ .

Some simple examples of conditionally negative definite matrices are

- (i) $\theta_{ij} = \theta_i + \theta_j$;
- (ii) $\theta_{ij} = \text{const}$;
- (iii) $\theta_{ij} = |\theta_i - \theta_j|$;
- (iv) $\theta_{ij} = |\theta_i - \theta_j|^2$
- (v) $\theta_{ij} = \max\{\theta_i, \theta_j\}$;
- (vi) $\theta_{ij} = -\theta_i\theta_j$.

Recall that the Hadamard product of two matrices A and B is the matrix $A \circ B = (A_{ij} \cdot B_{ij})_{1 \leq i, j \leq m}$. By Schur theorem if $A \in \mathcal{N}$, $B \in \mathcal{N}$, then so is $A \circ B$.

Then

$$F = \Sigma \circ A \circ B \circ C,$$

where one need to find conditions under which

$$A = \left(\frac{1}{(1 + \|\lambda\|^2 / a_{ij}^2)^{v_{ij} + \frac{3}{2}}} \right)_{1 \leq i, j \leq m} \geq 0, \quad B = \left(\frac{1}{a_{ij}^3} \right)_{1 \leq i, j \leq m} \geq 0,$$

$$C = \left(\frac{\Gamma(v_{ij} + \frac{3}{2})}{\Gamma(v_{ij})} \right)_{1 \leq i, j \leq m} \geq 0.$$

We consider first the case 1, in which we assume that

$$a_i = \dots = a_m = a, \quad 1 \leq i, j \leq m.$$

Then

$$A = e^{-\frac{3}{2}} \left(\exp \left\{ -v_{ij} \log \left(1 + \frac{\|\lambda\|^2}{a^2} \right) \right\} \right)_{1 \leq i, j \leq m} \geq 0,$$

if and only if the matrix

$$Y = (-v_{ij})_{1 \leq i, j \leq m}$$

is conditionally negative definite (see above examples (i)–(vi)), then for such $(-v_{ij})_{1 \leq i, j \leq m}$, we have to check that the matrix $C = (\Gamma(v_{ij} + \frac{3}{2})/\Gamma(v_{ij}))_{1 \leq i, j \leq m} \geq 0$. This class is not empty, since it includes the case of the so-called parsimonious model: $v_{ij} = \frac{v_i + v_j}{2}$ (see Example 3).

Recall that a Hermitian matrix $A = (a_{ij})_{i, j=1, \dots, p}$ is *conditional non-negative* if $\mathbf{x}^\top A \mathbf{x}^* \geq 0$, for all $\mathbf{x} \in \mathbb{C}^p$ such that $\sum_{i=1}^p x_i = 0$, and \mathbf{x}^* is the complex conjugate of \mathbf{x} .

Thus, for the case 1, the following multivariate Matérn models are valid under the following conditions (see, [2,8]):

(A1) Assume that

- (i) $a_i = \dots = a_m = a, 1 \leq i, j \leq m$;
- (ii) $-v_{ij}, 1 \leq i, j \leq m$; form conditionally non-negative matrices;
- (iii) $\sigma_{ij} \frac{\Gamma(v_{ij} + \frac{3}{2})}{\Gamma(v_{ij})}, 1 \leq i, j \leq m$; form non-negative definite matrices.

Consider the case 2:

$$v_{ij} = v > 0, \quad 1 \leq i, j \leq m.$$

Then the following multivariate Matérn models are valid under the following conditions [2]:

(A2) either

- (a) $-a_{ij}^2, 1 \leq i, j \leq m$, form a conditionally non-negative matrix and $\sigma_{ij} a_{ij}^{2v}, 1 \leq i, j \leq m$, form non-negative definite matrices; or
- (b) $-a_{ij}^{-2}, 1 \leq i, j \leq m$, form a conditionally non-negative matrix and $\sigma_{ij}/a_{ij}^3, 1 \leq i, j \leq m$, form non-negative definite matrices.

These classes of Matérn models are not empty since in the case of parsimonious model they are consistent with [12, Theorem 1]. For the parsimonious model from this paper ($v_{ij} = \frac{v_i + v_j}{2}, 1 \leq i, j \leq m$), the following multivariate Matérn models are valid under conditions

(A3) either

- (a) $v_{ij} = \frac{v_i + v_j}{2}, a_{ij}^2 = \frac{a_i^2 + a_j^2}{2}, 1 \leq i, j \leq m$, and $\sigma_{ij} a_{ij}^{2v_{ij}}/\Gamma(v_{ij}), 1 \leq i, j \leq m$, form non-negative definite matrices;
or
- (b) $v_{ij} = \frac{v_i + v_j}{2}, a_{ij}^{-2} = \frac{a_i^{-2} + a_j^{-2}}{2}, 1 \leq i, j \leq m$, and $\sigma_{ij}/a_{ij}^3/\Gamma(v_{ij}), 1 \leq i, j \leq m$, form non-negative definite matrices;

The most general conditions and new examples can be found in [2,8]. The paper by [11] reviews the main approaches to building multivariate correlation and covariance structures, including the multivariate Matérn models.

Example 5 (Dual Matérn models) Adapting the so-called duality theorem (see, i.e., [10]), one can show that under the conditions A1, A2 or A3

$$\frac{1}{(1 + \|\mathbf{h}\|^2)^{v_{ij} + \frac{3}{2}}} = \int_{\mathbb{R}^3} e^{i(\boldsymbol{\lambda}, \mathbf{h})} s_{ij}(\boldsymbol{\lambda}) d\boldsymbol{\lambda}, \quad 1 \leq i, j \leq m,$$

where

$$s_{ij}(\boldsymbol{\lambda}) = \frac{1}{(2\pi)^3 2^{v_{ij}-1} \Gamma(v_{ij} + \frac{3}{2})} (\|\boldsymbol{\lambda}\|)^{v_{ij}} K_{v_{ij}}(\|\boldsymbol{\lambda}\|), \quad \boldsymbol{\lambda} \in \mathbb{R}^3, \quad 1 \leq i, j \leq m,$$

is the valid spectral density of the vector random field with correlation structure $((1 + \|\mathbf{h}\|^2)^{-(\nu_{ij} + \frac{3}{2})})_{1 \leq i, j \leq m} = (D_{ij}(\mathbf{h}))_{1 \leq i, j \leq m}$. We will call it the *dual Matérn model*.

Note that for the Matérn models

$$\int_{\mathbb{R}^3} \bar{B}_{ij}(\mathbf{x}) d\mathbf{x} < \infty.$$

This condition is known as short range dependence, while for the dual Matérn model, the long range dependence is possible:

$$\int_{\mathbb{R}^3} D_{ij}(\mathbf{h}) d\mathbf{h} = \infty, \quad \text{if } 0 < \nu_{ij} < \frac{3}{2}.$$

When $m = 3$, the random field of Example 3 is scalar isotropic but not isotropic. How to construct examples of homogeneous and *isotropic* vector and tensor random fields with Matérn two-point correlation tensors?

To solve this problem, we develop a sketch of a general theory of homogeneous and isotropic tensor-valued random fields in Sect. 2. This theory was developed by [30,33]. In particular, we explain another two links: one leads from the theory of random fields to classical invariant theory, other one was established recently and leads from the theory of random fields to the theory of convex compacta.

In Sect. 3, we give examples of Matérn homogeneous and isotropic tensor-valued random fields. Finally, in Appendices we shortly describe the mathematical terminology which is not always familiar to specialists in probability: tensors, group representations, and classical invariant theory. For different aspects of theory of random fields see also [24,25].

2 A Sketch of a General Theory

Let r be a nonnegative integer, let V be an invariant subspace of the representation $g \mapsto g^{\otimes r}$ of the group $O(3)$, and let U be the restriction of the above representation to V . Consider a homogeneous V -valued random field $T(\mathbf{x}), \mathbf{x} \in \mathbb{R}^3$. Assume it is isotropic, that is, satisfies (1). It is very easy to see that its one-point correlation tensor $\langle T(\mathbf{x}) \rangle$ is an arbitrary element of the isotypic subspace of the space V that corresponds to the trivial representation. In particular, in the case of $r = 0$ the representation U is trivial, and $\langle T(\mathbf{x}) \rangle$ is an arbitrary real number. In the case of $r = 1$ we have $U(g) = g$. This representation does not contain a trivial component, therefore $\langle T(\mathbf{x}) \rangle = \mathbf{0}$. In the case of $r = 2$ and $U(g) = S^2(g)$ the isotypic subspace that corresponds to the trivial representation is described in Example 12, we have $\langle T(\mathbf{x}) \rangle = CI$, where C is an arbitrary real number, and I is the identity operator in \mathbb{R}^3 , and so on.

Can we quickly describe the two-point correlation tensor in the same way? The answer is positive. Indeed, the second equation in (1) means that $\langle T(\mathbf{x}), T(\mathbf{y}) \rangle$ is a measurable covariant of the pair (g, U) . The integrity basis for polynomial invariants of the defining representation contains one element $I_1 = \|\mathbf{x}\|^2$. By the Wineman–Pipkin theorem (Appendix A, Theorem 6), we obtain

$$\langle T(\mathbf{x}), T(\mathbf{y}) \rangle = \sum_{l=1}^L \varphi_l(\|\mathbf{y} - \mathbf{x}\|^2) T_l(\mathbf{y} - \mathbf{x}),$$

where $T_l(\mathbf{y} - \mathbf{x})$ are the basic covariant tensors of the representation U .

For example, when $r = 1$, the basis covariant tensors of the defining representations are δ_{ij} and $x_i x_j$ by the result of [44] mentioned in Appendix C. We obtain the result by [39]:

$$\langle \mathbb{T}(\mathbf{x}), \mathbb{T}(\mathbf{y}) \rangle = \varphi_1(\|\mathbf{y} - \mathbf{x}\|^2) \delta_{ij} + \varphi_2(\|\mathbf{y} - \mathbf{x}\|^2) \frac{(y_i - x_i)(y_j - x_j)}{\|\mathbf{y} - \mathbf{x}\|^2}.$$

When $r = 2$ and $U(g) = \mathbf{S}^2(g)$, the three rank 4 isotropic tensors are $\delta_{ij} \delta_{kl}$, $\delta_{ik} \delta_{jl}$, and $\delta_{il} \delta_{jk}$. Consider the group Σ of order 8 of the permutations of symbols i, j, k , and l , generated by the transpositions (ij) , (kl) , and the product $(ik)(jl)$. The group Σ acts on the set of rank 4 isotropic tensors and has two orbits. The sums of elements on each orbit are basis isotropic tensors:

$$L^1_{ijkl} = \delta_{ij} \delta_{kl}, \quad L^2_{ijkl} = \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}.$$

Consider the case of degree 2 and of order 4. For the pair of representations $(g^{\otimes 4}, (\mathbb{R}^3)^{\otimes 4})$ and (g, \mathbb{R}^3) we have 6 covariant tensors:

$$\delta_{il} x_j x_k, \delta_{jk} x_i x_l, \delta_{jl} x_i x_k, \delta_{ik} x_j x_l, \delta_{kl} x_i x_j, \delta_{ij} x_k x_l.$$

The action of the group Σ has 2 orbits, and the symmetric covariant tensors are

$$\|\mathbf{x}\|^2 L^3_{ijkl}(\mathbf{x}) = \delta_{il} x_j x_k + \delta_{jk} x_i x_l + \delta_{jl} x_i x_k + \delta_{ik} x_j x_l,$$

$$\|\mathbf{x}\|^2 L^4_{ijkl}(\mathbf{x}) = \delta_{kl} x_i x_j + \delta_{ij} x_k x_l.$$

In the case of degree 4 and of order 4 we have only one covariant:

$$\|\mathbf{x}\|^4 L^5_{ijkl}(\mathbf{x}) = x_i x_j x_k x_l.$$

The result by [28]

$$\langle \mathbb{T}(\mathbf{x}), \mathbb{T}(\mathbf{y}) \rangle = \sum_{m=1}^5 \varphi_m(\|\mathbf{y} - \mathbf{x}\|^2) L^m_{ijkl}(\mathbf{y} - \mathbf{x})$$

easily follows.

The case of $r = 3$ will be considered in details elsewhere.

When $r = 4$ and $U(g) = \mathbf{S}^2(S^2(g))$, the situation is more delicate. A linear relations between isotropic tensors, called *syzygies*, appear. There are 8 symmetric isotropic tensors connected by 1 syzygy, 13 basic covariant tensors of degree 2 and of order 8 connected by 3 syzygies, 10 basic covariant tensors of degree 4 and of order 8 connected by 2 syzygies, 3 basic covariant tensors of degree 6 and of order 8, and 1 basic covariant tensor of degree 8 and of order 8, see [31, 32] for details. It follows that there are

$$(8 - 1) + (13 - 3) + (10 - 2) + 3 + 1 = 29$$

linearly independent basic covariant tensors. The result by [29] includes only 15 of them and is therefore incomplete.

How to find the functions φ_m ? In the case of $r = 0$, the answer is given by Theorem 1:

$$\varphi_1(\|\mathbf{y} - \mathbf{x}\|^2) = \int_0^\infty \frac{\sin(\lambda \|\mathbf{y} - \mathbf{x}\|)}{\lambda \|\mathbf{y} - \mathbf{x}\|} d\mu(\lambda).$$

In the case of $r = 1$, the answer has been found by [46]:

$$\varphi_1(\|\mathbf{y} - \mathbf{x}\|^2) = \frac{1}{\rho^2} \left(\int_0^\infty j_2(\lambda \rho) d\Phi_2(\lambda) - \int_0^\infty j_1(\lambda \rho) d\Phi_1(\lambda) \right),$$

$$\varphi_2(\|\mathbf{y} - \mathbf{x}\|^2) = \int_0^\infty \frac{j_1(\lambda\rho)}{\lambda\rho} d\Phi_1(\lambda) + \int_0^\infty \left(j_0(\lambda\rho) - \frac{j_1(\lambda\rho)}{\lambda\rho} \right) d\Phi_2(\lambda), \tag{4}$$

where $\rho = \|\mathbf{y} - \mathbf{x}\|$, j_n are the spherical Bessel functions, and Φ_1 and Φ_2 are two finite measures on $[0, \infty)$ with $\Phi_1(\{0\}) = \Phi_2(\{0\})$.

In the general case, we proceed in steps. The main idea is simple. We describe all homogeneous random fields and throw away those that are not isotropic. The homogeneous random fields are described by the following result.

Theorem 2 *Formula*

$$\langle \mathbf{T}(\mathbf{x}), \mathbf{T}(\mathbf{y}) \rangle = \int_{\mathbb{R}^3} e^{i(\mathbf{p}, \mathbf{y} - \mathbf{x})} d\mu(\mathbf{p}) \tag{5}$$

establishes a one-to-one correspondence between the set of the two-point correlation tensors of homogeneous random fields $\mathbf{T}(\mathbf{x})$ on the space domain \mathbb{R}^3 with values in a complex finite-dimensional space $\mathbf{V}_{\mathbb{C}}$ and the set of all measures μ on the Borel σ -field $\mathfrak{B}(\mathbb{R}^3)$ of the wavenumber domain \mathbb{R}^3 with values in the cone of nonnegative-definite Hermitian operators in $\mathbf{V}_{\mathbb{C}}$.

This theorem was proved by [22,23] for one-dimensional stochastic processes. Kolmogorov’s results have been further developed by [4–6,27] among others.

We would like to write as many formulae as possible in a coordinate-free form, like (5). To do that, let J be a *real structure* in the space $\mathbf{V}_{\mathbb{C}}$, that is, a map $j: \mathbf{V}_{\mathbb{C}} \rightarrow \mathbf{V}_{\mathbb{C}}$ with

- $J(\mathbf{x} + \mathbf{y}) = J(\mathbf{x}) + J(\mathbf{y}), \mathbf{x}, \mathbf{y} \in \mathbf{V}_{\mathbb{C}}$.
- $J(\alpha\mathbf{x}) = \bar{\alpha}J(\mathbf{x}), \mathbf{x} \in \mathbf{V}_{\mathbb{C}}, \alpha \in \mathbb{C}$.
- $J(J(\mathbf{x})) = \mathbf{x}, \mathbf{x} \in \mathbf{V}_{\mathbb{C}}$.

Any tensor $\mathbf{x} \in \mathbf{V}_{\mathbb{C}}$ can be written as $\mathbf{x} = \mathbf{x}^+ + \mathbf{x}^-$, where

$$\mathbf{x}^+ = \frac{1}{2}(\mathbf{x} + J\mathbf{x}), \quad \mathbf{x}^- = \frac{1}{2}(\mathbf{x} - J\mathbf{x}).$$

Denote

$$\mathbf{V}^+ = \{ \mathbf{x} \in \mathbf{V}_{\mathbb{C}} : J\mathbf{x} = \mathbf{x} \}, \quad \mathbf{V}^- = \{ \mathbf{x} \in \mathbf{V}_{\mathbb{C}} : J\mathbf{x} = -\mathbf{x} \}.$$

Both sets \mathbf{V}^+ and \mathbf{V}^- are real vector spaces. If the values of the random field $\mathbf{T}(\mathbf{x})$ lie in \mathbf{V}^+ , then the measure μ satisfies the condition

$$\mu(-A) = \mu^{\top}(A) \tag{6}$$

for all Borel subsets $A \subseteq \mathbb{R}^3$, where $-A = \{ -\mathbf{p} : \mathbf{p} \in A \}$.

Next, the following Lemma can be proved. Let $\mathbf{p} = (\lambda, \varphi_{\mathbf{p}}, \theta_{\mathbf{p}})$ be the spherical coordinates in the wavenumber domain.

Lemma 1 *A homogeneous random field described by (5) and (6) is isotropic if and only if its two-point correlation tensor has the form*

$$\langle \mathbf{T}(\mathbf{x}), \mathbf{T}(\mathbf{y}) \rangle = \frac{1}{4\pi} \int_0^\infty \int_{S^2} e^{i(\mathbf{p}, \mathbf{y} - \mathbf{x})} f(\lambda, \varphi_{\mathbf{p}}, \theta_{\mathbf{p}}) \sin \theta_{\mathbf{p}} d\varphi_{\mathbf{p}} d\theta_{\mathbf{p}} d\nu(\lambda), \tag{7}$$

where ν is a finite measure on the interval $[0, \infty)$, and where f is a measurable function taking values in the set of all symmetric nonnegative-definite operators on \mathbf{V}^+ with unit trace and satisfying the condition

$$f(g\mathbf{p}) = \mathbf{S}^2(U)(g) f(\mathbf{p}), \quad \mathbf{p} \in \mathbb{R}^3, \quad g \in \mathbf{O}(3). \tag{8}$$

When $\lambda = 0$, condition (8) gives $f(\mathbf{0}) = \mathbf{S}^2(U)(g)f(\mathbf{0})$ for all $g \in O(3)$. In other words, the tensor $f(\mathbf{0})$ lies in the isotypic subspace of the space $\mathbf{S}^2(V^+)$ that corresponds to the trivial representation of the group $O(3)$, call it H_1 . The intersection of H_1 with the set of all symmetric nonnegative-definite operators on V^+ with unit trace is a convex compact set, call it C_1 .

When $\lambda > 0$, condition (8) gives $f(\lambda, 0, 0) = \mathbf{S}^2(U)(g)f(\lambda, 0, 0)$ for all $g \in O(2)$, because $O(2)$ is the subgroup of $O(3)$ that fixes the point $(\lambda, 0, 0)$. In other words, consider the restriction of the representation $\mathbf{S}^2(U)$ to the subgroup $O(2)$. The tensor $f(\lambda, 0, 0)$ lies in the isotypic subspace of the space $\mathbf{S}^2(V^+)$ that corresponds to the trivial representation of the group $O(2)$, call it H_0 . We have $H_1 \subset H_0$, because $O(2)$ is a subgroup of $O(3)$. The intersection of H_0 with the set of all symmetric nonnegative-definite operators on V^+ with unit trace is a convex compact set, call it C_0 .

Fix an orthonormal basis $T^{0,1,0}, \dots, T^{0,n_0,0}$ of the space H_1 . Assume that the space $H_0 \ominus H_1$ has the non-zero intersection with the spaces of n_1 copies of the irreducible representation U^{2g} , n_2 copies of the irreducible representation U^{4g} , ..., n_r copies of the irreducible representation U^{2rg} of the group $O(3)$, and let $T^{2\ell,n,m}$, $-2\ell \leq m \leq 2\ell$, be the tensors of the Gordenko basis of the n th copy of the representation $U^{2\ell g}$. We have

$$f(\lambda, 0, 0) = \sum_{\ell=0}^r \sum_{n=1}^{n_\ell} f_{\ell n}(\lambda) T^{2\ell,n,0} \tag{9}$$

with $f_{\ell n}(\lambda) = 0$ for $\ell > 0$ and $1 \leq n \leq n_\ell$. By (8) we obtain

$$f(\lambda, \varphi_{\mathbf{p}}, \theta_{\mathbf{p}}) = \sum_{\ell=0}^r \sum_{n=1}^{n_\ell} f_{\ell n}(\lambda) \sum_{m=-2\ell}^{2\ell} U_{m0}^{2\ell g}(\varphi_{\mathbf{p}}, \theta_{\mathbf{p}}) T^{2\ell,n,m}.$$

Equation (7) takes the form

$$\begin{aligned} \langle T(\mathbf{x}), T(\mathbf{y}) \rangle &= \frac{1}{2\sqrt{\pi}} \sum_{\ell=0}^r \sum_{n=1}^{n_\ell} \sum_{m=-2\ell}^{2\ell} \int_0^\infty \int_{S^2} e^{i(\mathbf{p}, \mathbf{y}-\mathbf{x})} f_{\ell n}(\lambda) \frac{1}{\sqrt{4\ell+1}} \\ &\times S_{2\ell}^m(\varphi_{\mathbf{p}}, \theta_{\mathbf{p}}) T^{2\ell,n,m} \sin \theta_{\mathbf{p}} d\varphi_{\mathbf{p}} d\theta_{\mathbf{p}} d\nu(\lambda), \end{aligned} \tag{10}$$

where we used the relation

$$U_{m0}^{2\ell g}(\varphi_{\mathbf{p}}, \theta_{\mathbf{p}}) = \sqrt{\frac{4\pi}{4\ell+1}} S_{2\ell}^m(\varphi_{\mathbf{p}}, \theta_{\mathbf{p}}).$$

Substitute the *Rayleigh expansion*

$$e^{i(\mathbf{p}, \mathbf{r})} = 4\pi \sum_{\ell=0}^\infty \sum_{m=-\ell}^\ell i^\ell j_\ell(\|\mathbf{p}\| \cdot \|\mathbf{r}\|) S_\ell^m(\theta_{\mathbf{p}}, \varphi_{\mathbf{p}}) S_\ell^m(\theta_{\mathbf{r}}, \varphi_{\mathbf{r}})$$

into (10). We obtain

$$\begin{aligned} \langle T(\mathbf{x}), T(\mathbf{y}) \rangle &= 2\sqrt{\pi} \sum_{\ell=0}^r \sum_{n=1}^{n_\ell} \sum_{m=-2\ell}^{2\ell} \int_0^\infty (-1)^\ell j_{2\ell}(\lambda \|\mathbf{r}\|) f_{\ell n}(\lambda) \frac{1}{\sqrt{4\ell+1}} \\ &\times S_\ell^m(\varphi_{\mathbf{r}}, \theta_{\mathbf{r}}) T^{2\ell,n,m} d\nu(\lambda), \end{aligned}$$

where $\mathbf{r} = \mathbf{y} - \mathbf{x}$. Returning back to the matrix entries $U_{m0}^{2\ell g}(\varphi_{\mathbf{r}}, \theta_{\mathbf{r}})$, we have

$$\langle \mathbb{T}(\mathbf{x}), \mathbb{T}(\mathbf{y}) \rangle = \int_0^\infty \sum_{\ell=0}^r (-1)^\ell j_{2\ell}(\lambda \|\mathbf{r}\|) \sum_{n=1}^{n_\ell} f_{\ell n}(\lambda) M^{2\ell, n}(\varphi_{\mathbf{r}}, \theta_{\mathbf{r}}) \, d\nu(\lambda), \tag{11}$$

where

$$M^{2\ell, n}(\varphi_{\mathbf{r}}, \theta_{\mathbf{r}}) = \sum_{m=-2\ell}^{2\ell} U_{m0}^{2\ell g}(\varphi_{\mathbf{r}}, \theta_{\mathbf{r}}) \mathbb{T}^{2\ell, n, m}.$$

It is easy to check that the function $M^{2\ell, n}(\varphi_{\mathbf{r}}, \theta_{\mathbf{r}})$ is a covariant of degree 2ℓ and of order $2r$. Therefore, the M -function is a linear combination of basic symmetric covariant tensors, or L -functions:

$$M^{2\ell, n}(\varphi_{\mathbf{r}}, \theta_{\mathbf{r}}) = \sum_{k=0}^{\ell} \sum_{q=1}^{q_{kr}} c_{nkq} \frac{L^{2k, q}(\mathbf{y} - \mathbf{x})}{\|\mathbf{y} - \mathbf{x}\|^{2k}},$$

where q_{kr} is the number of linearly independent symmetric covariant tensors of degree $2k$ and of order $2r$. The right hand side is indeed a polynomial in sines and cosines of the angles $\varphi_{\mathbf{r}}$ and $\theta_{\mathbf{r}}$. Equation (11) takes the form

$$\begin{aligned} \langle \mathbb{T}(\mathbf{x}), \mathbb{T}(\mathbf{y}) \rangle &= \int_0^\infty \sum_{\ell=0}^r (-1)^\ell j_{2\ell}(\lambda \|\mathbf{r}\|) \sum_{n=1}^{n_\ell} f_{\ell n}(\lambda) \\ &\quad \times \sum_{k=0}^{\ell} \sum_{q=1}^{q_{kr}} c_{nkq} \frac{L^{2k, q}(\mathbf{y} - \mathbf{x})}{\|\mathbf{y} - \mathbf{x}\|^{2k}} \, d\nu(\lambda). \end{aligned}$$

Recall that $f_{\ell n}(\lambda)$ are measurable functions such that the tensor (9) lies in \mathcal{C}_1 for $\lambda = 0$ and in \mathcal{C}_0 for $\lambda > 0$. The final form of the two-point correlation tensor of the random field $\mathbb{T}(\mathbf{x})$ is determined by geometry of convex compacta \mathcal{C}_0 and \mathcal{C}_1 . For example, in the case of $r = 1$ the set \mathcal{C}_0 is an interval (see [33]), while \mathcal{C}_1 is a one-point set inside this interval. The set \mathcal{C}_0 has two extreme points, and the corresponding random field is a sum of two uncorrelated components given by Eq. (12) below. The one-point set \mathcal{C}_1 lies in the middle of the interval, the condition $\Phi_1(\{0\}) = \Phi_2(\{0\})$ follows. In the case of $r = 2$, the set of extreme points of the set \mathcal{C}_0 has three connected components: two one-point sets and an ellipse, see [33], and the corresponding random field is a sum of three uncorrelated components.

In general, the two-point correlation tensor of the field has the simplest form when the set \mathcal{C}_0 is a simplex. We use this idea in Examples 6 and 8 below.

3 Examples of Matérn Homogeneous and Isotropic Random Fields

Example 6 Consider a centred homogeneous scalar isotropic random field $T(\mathbf{x})$ on the space \mathbb{R}^3 with values in the two-dimensional space \mathbb{R}^2 . It is easy to see that both \mathcal{C}_0 and \mathcal{C}_1 are equal to the set of all symmetric nonnegative-definite 2×2 matrices with unit trace. Every such matrix has the form

$$\begin{pmatrix} x & y \\ y & 1 - x \end{pmatrix}$$

with $x \in [0, 1]$ and $y^2 \leq x(1 - x)$. Geometrically, C_0 and C_1 are the balls

$$\left(x - \frac{1}{2}\right)^2 + y^2 = \frac{1}{4}.$$

Inscribe an equilateral triangle with vertices

$$C^1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad C^{2,3} = \frac{1}{4} \begin{pmatrix} 1 & \pm\sqrt{3} \\ \pm\sqrt{3} & 3 \end{pmatrix}$$

into the above ball. The function $f(\mathbf{p})$ takes the form

$$f(\mathbf{p}) = \sum_{m=1}^3 a_m(\|\mathbf{p}\|)C^m,$$

where $a_m(\|\mathbf{p}\|)$ are the barycentric coordinates of the point $f(\mathbf{p})$ inside the triangle. The two-point correlation tensor of the field takes the form

$$\langle T(\mathbf{x}), T(\mathbf{y}) \rangle = \sum_{m=1}^3 \int_0^\infty \frac{\sin(\lambda\|\mathbf{y} - \mathbf{x}\|)}{\lambda\|\mathbf{y} - \mathbf{x}\|} C^m d\Phi_m(\lambda),$$

where $d\Phi_m(\lambda) = a_m(\lambda)d\nu(\lambda)$ are three finite measures on $[0, \infty)$, and ν is the measure of Eq. (7). Define $d\Phi_m(\lambda)$ as Matérn spectral densities of Example 2 (resp. dual Matérn spectral densities of Example 5). We obtain a scalar homogeneous and isotropic Matérn (resp. dual Matérn) random field.

Example 7 Using (4) and the well-known formulae

$$j_0(t) = \frac{\sin t}{t}, \quad j_1(t) = \frac{\sin t}{t^2} - \frac{\cos t}{t}, \quad j_2(t) = \left(\frac{3}{t^2} - 1\right) \frac{\sin t}{t} - \frac{3 \cos t}{t^2},$$

we write the two-point correlation tensor of rank 1 homogeneous and isotropic random field in the form

$$\langle \mathbf{v}(\mathbf{x}), \mathbf{v}(\mathbf{y}) \rangle = B_{ij}^{(1)}(\mathbf{r}) + B_{ij}^{(2)}(\mathbf{r}),$$

where $\mathbf{r} = \mathbf{y} - \mathbf{x}$, and

$$\begin{aligned} B_{ij}^{(1)}(\mathbf{x}, \mathbf{y}) &= \int_0^\infty \left[\left(-\frac{3 \sin(\lambda\|\mathbf{r}\|)}{(\lambda\|\mathbf{r}\|)^3} + \frac{\sin(\lambda\|\mathbf{r}\|)}{\lambda\|\mathbf{r}\|} + \frac{3 \cos(\lambda\|\mathbf{r}\|)}{(\lambda\|\mathbf{r}\|)^2} \right) \frac{r_i r_j}{\|\mathbf{r}\|^2} \right. \\ &\quad \left. + \left(\frac{\sin(\lambda\|\mathbf{r}\|)}{(\lambda\|\mathbf{r}\|)^3} - \frac{\cos(\lambda\|\mathbf{r}\|)}{(\lambda\|\mathbf{r}\|)^2} \right) \delta_{ij} \right] d\Phi_1(\lambda), \\ B_{ij}^{(2)}(\mathbf{x}, \mathbf{y}) &= \int_0^\infty \left[\left(\frac{3 \sin(\lambda\|\mathbf{r}\|)}{(\lambda\|\mathbf{r}\|)^3} - \frac{\sin(\lambda\|\mathbf{r}\|)}{\lambda\|\mathbf{r}\|} - \frac{3 \cos(\lambda\|\mathbf{r}\|)}{(\lambda\|\mathbf{r}\|)^2} \right) \frac{r_i r_j}{\|\mathbf{r}\|^2} \right. \\ &\quad \left. + \left(\frac{\sin(\lambda\|\mathbf{r}\|)}{\lambda\|\mathbf{r}\|} - \frac{\sin(\lambda\|\mathbf{r}\|)}{(\lambda\|\mathbf{r}\|)^3} + \frac{\cos(\lambda\|\mathbf{r}\|)}{(\lambda\|\mathbf{r}\|)^2} \right) \delta_{ij} \right] d\Phi_2(\lambda). \end{aligned} \tag{12}$$

Now assume that the measures Φ_1 and Φ_2 are described by Matérn densities:

$$d\Phi_i(\lambda) = 2\pi\lambda^2 \frac{\sigma_i^2 \Gamma(v_i + \frac{3}{2}) a_i^{2v_i}}{2\pi^{3/2} (a_i^2 + \lambda^2)^{v_i + \frac{3}{2}}}, \quad i = 1, 2.$$

It is possible to substitute these densities to (12) and calculate the integrals using [37, Eq. 2.5.9.1]. We obtain rather long expressions that include the generalised hypergeometric function ${}_1F_2$.

The situation is different for the dual model:

$$d\Phi_i(\lambda) = \frac{1}{(2\pi)^2 2^{v_i-1} \Gamma(v_i + 3/2)} \lambda^{v_i+2} K_{v_i}(\lambda).$$

Using [38, Eqs. 2.16.14.3, 2.16.14.4], we obtain

$$\begin{aligned} B_{ij}^{(k)}(\mathbf{x}, \mathbf{y}) = & C_k \left(-\frac{3\pi \Gamma(2\nu_k)}{4\|\mathbf{r}\|^3(1 + \|\mathbf{r}\|^2)^{\nu_k/2}} \left[P_{\nu_k-1}^{-\nu_k} \left(\frac{\|\mathbf{r}\|}{\sqrt{1 + \|\mathbf{r}\|^2}} \right) \right. \right. \\ & \left. \left. - P_{\nu_k-1}^{-\nu_k} \left(-\frac{\|\mathbf{r}\|}{\sqrt{1 + \|\mathbf{r}\|^2}} \right) \right] + \frac{2^{\nu_k} \sqrt{\pi} \Gamma(\nu_k + 3/2)}{(1 + \|\mathbf{r}\|^2)^{\nu_k+3/2}} \right. \\ & \left. + \frac{3 \cdot 2^{\nu_k-1} \sqrt{\pi} \Gamma(\nu_k + 1/2)}{(1 + \|\mathbf{r}\|^2)^{\nu_k+1/2}} \right) \frac{r_i r_j}{\|\mathbf{r}\|^2} \\ & + C_1 \left(\frac{\pi \Gamma(2\nu_k)}{4\|\mathbf{r}\|^3(1 + \|\mathbf{r}\|^2)^{\nu_1/2}} \left[P_{\nu_k-1}^{-\nu_k} \left(\frac{\|\mathbf{r}\|}{\sqrt{1 + \|\mathbf{r}\|^2}} \right) \right. \right. \\ & \left. \left. - P_{\nu_k-1}^{-\nu_k} \left(-\frac{\|\mathbf{r}\|}{\sqrt{1 + \|\mathbf{r}\|^2}} \right) \right] - \frac{2^{\nu_k} \sqrt{\pi} \Gamma(\nu_k + 1/2)}{(1 + \|\mathbf{r}\|^2)^{\nu_k+3/2}} \right) \delta_{ij}, \end{aligned}$$

where

$$C_k = \frac{1}{(2\pi)^2 2^{\nu_k-1} \Gamma(\nu_k + 3/2)}, \quad k = 1, 2.$$

Example 8 Consider the case when $r = 2$ and $U(g) = \mathbf{S}^2(g)$. In order to write down symmetric rank 4 tensors in a compressed matrix form, consider an orthogonal operator τ acting from $\mathbf{S}^2(\mathbf{S}^2(\mathbb{R}^3))$ to $\mathbf{S}^2(\mathbb{R}^6)$ as follows:

$$\tau f_{ijkl} = \begin{pmatrix} f_{-1-1-1-1} & f_{-1-100} & f_{-1-111} & \sqrt{2}f_{-1-1-10} & \sqrt{2}f_{-1-101} & \sqrt{2}f_{-1-11-1} \\ f_{00-1-1} & f_{0000} & f_{0011} & \sqrt{2}f_{00-10} & \sqrt{2}f_{0001} & \sqrt{2}f_{001-1} \\ f_{11-1-1} & f_{1100} & f_{1111} & \sqrt{2}f_{11-10} & \sqrt{2}f_{1101} & \sqrt{2}f_{111-1} \\ \sqrt{2}f_{-10-1-1} & \sqrt{2}f_{-1000} & \sqrt{2}f_{-1011} & 2f_{-10-10} & 2f_{-1001} & 2f_{-101-1} \\ \sqrt{2}f_{01-1-1} & \sqrt{2}f_{0100} & \sqrt{2}f_{0111} & 2f_{01-10} & 2f_{0101} & 2f_{011-1} \\ \sqrt{2}f_{1-1-1-1} & \sqrt{2}f_{1-100} & \sqrt{2}f_{1-111} & 2f_{1-1-10} & 2f_{1-101} & 2f_{1-11-1} \end{pmatrix},$$

see [16, Eq. (44)]. It is possible to prove the following. The matrix $\tau f_{ijkl}(\mathbf{0})$ lies in the interval C_1 with extreme points C^1 and C^2 , where the nonzero elements of the symmetric matrix C^1 lying on and over the main diagonal are as follows:

$$C_{11}^1 = C_{12}^1 = C_{13}^1 = C_{22}^1 = C_{23}^1 = C_{33}^1 = \frac{1}{3},$$

while those of the matrix C^2 are

$$\begin{aligned} C_{11}^2 = C_{22}^2 = C_{33}^2 &= \frac{2}{15}, & C_{44}^2 = C_{55}^2 = C_{66}^2 &= \frac{1}{5}, \\ C_{12}^2 = C_{13}^2 = C_{23}^2 &= -\frac{1}{15}. \end{aligned}$$

The matrix $\tau f_{ijkl}(\lambda, 0, 0)$ with $\lambda > 0$ lies in the convex compact set C_0 . The set of extreme points of C_0 contains three connected components. The first component is the one-point set $\{D^1\}$ with

$$D_{44}^1 = D_{66}^1 = \frac{1}{2}.$$

The second component is the one-point set $\{D^2\}$ with

$$D_{11}^2 = D_{33}^2 = \frac{1}{4}, \quad D_{55}^2 = \frac{1}{2}, \quad D_{13}^2 = -\frac{1}{4}.$$

The third component is the ellipse $\{D^\theta : 0 \leq \theta < 2\pi\}$ with

$$D_{11}^\theta = D_{33}^\theta = D_{13}^\theta = \frac{1}{2} \sin^2(\theta/2), \quad D_{22}^\theta = \cos^2(\theta/2),$$

$$D_{12}^\theta = D_{23}^\theta = \frac{1}{2\sqrt{2}} \sin(\theta).$$

Choose three points D^3, D^4, D^5 lying on the above ellipse. If we allow the matrix $\tau_{f_{ijkl}}(\lambda, 0, 0)$ with $\lambda > 0$ to take values in the simplex with vertices $D^i, 1 \leq i \leq 5$, then the two-point correlation tensor of the random field $\varepsilon(\mathbf{x})$ is the sum of five integrals. The more the four-dimensional Lebesgue measure of the simplex in comparison with that of C_0 , the wider class of random fields is described.

Note that the simplex should contain the set C_1 . The matrix C^1 lies on the ellipse and corresponds to the value of $\theta = 2 \arcsin(\sqrt{2/3})$. It follows that one of the above points, say D^3 , must be equal to C^1 . If we choose D^4 to correspond to the value of $\theta = 2(\pi - \arcsin(\sqrt{2/3}))$, that is,

$$D_{11}^4 = D_{33}^4 = D_{13}^4 = \frac{1}{6}, \quad D_{22}^4 = \frac{2}{3}, \quad D_{12}^4 = D_{23}^4 = -\frac{1}{3},$$

then

$$C^2 = \frac{2}{5}(D^1 + D^2) + \frac{1}{5}D^4,$$

and C^2 lies in the simplex. Finally, choose D^5 to correspond to the value of $\theta = \pi$, that is

$$D_{11}^5 = D_{33}^5 = D_{13}^5 = \frac{1}{2}.$$

The constructed simplex is not the one with maximal possible Lebesgue measure, but the coefficients in formulas are simple.

Theorem 3 *Let $\varepsilon(\mathbf{x})$ be a random field that describes the stress tensor of a deformable body. The following conditions are equivalent.*

1. *The matrix $\tau_{f_{ijkl}}(\lambda, 0, 0)$ with $\lambda > 0$ takes values in the simplex described above.*
2. *The correlation tensor of the field has the spectral expansion*

$$\langle \varepsilon(\mathbf{x}), \varepsilon(\mathbf{y}) \rangle = \sum_{n=1}^5 \int_0^\infty \sum_{q=1}^5 \tilde{N}_{nq}(\lambda, \|\mathbf{r}\|) L_{ijkl}^q(\mathbf{r}) d\Phi_n(\lambda),$$

where the non-zero functions $\tilde{N}_{nq}(\lambda, r)$ are given in Table 1, and where $\Phi_n(\lambda)$ are five finite measures on $[0, \infty)$ with

$$\Phi_1(\{0\}) = \Phi_2(\{0\}) = 2\Phi_4(\{0\}), \quad \Phi_5(\{0\}) = 0.$$

Assume that all measures Φ_n are absolutely continuous and their densities are either the Matérn or the dual Matérn densities. The two-point correlation tensors of the corresponding random fields can be calculated in exactly the same way as in Example 7.

Table 1 The functions $\tilde{N}_{nq}(\lambda, r)$

n	q	$N_{nq}(\lambda, r)$
1	1	$-\frac{1}{15}j_0(\lambda r) - \frac{2}{21}j_2(\lambda r) - \frac{1}{35}j_4(\lambda r)$
1	2	$\frac{1}{10}j_0(\lambda r) + \frac{1}{14}j_2(\lambda r) - \frac{1}{35}j_4(\lambda r)$
1	3	$-\frac{3}{28}j_2(\lambda r) + \frac{1}{7}j_4(\lambda r)$
1	4	$\frac{1}{7}j_2(\lambda r) + \frac{1}{7}j_4(\lambda r)$
1	5	$-j_4(\lambda r)$
2	1	$-\frac{1}{15}j_0(\lambda r) + \frac{4}{21}j_2(\lambda r) + \frac{1}{140}j_4(\lambda r)$
2	2	$\frac{1}{10}j_0(\lambda r) - \frac{1}{7}j_2(\lambda r) + \frac{1}{140}j_4(\lambda r)$
2	3	$\frac{3}{14}j_2(\lambda r) - \frac{1}{28}j_4(\lambda r)$
2	4	$-\frac{2}{7}j_2(\lambda r) - \frac{1}{28}j_4(\lambda r)$
2	5	$\frac{1}{4}j_4(\lambda r)$
3	1	$\frac{1}{3}j_0(\lambda r)$
4	1	$-\frac{1}{135}j_0(\lambda r) - \frac{4}{21}j_2(\lambda r) + \frac{3}{70}j_4(\lambda r)$
4	2	$\frac{1}{90}j_0(\lambda r) + \frac{1}{7}j_2(\lambda r) + \frac{3}{70}j_4(\lambda r)$
4	3	$-\frac{3}{14}j_2(\lambda r) - \frac{3}{14}j_4(\lambda r)$
4	4	$\frac{2}{7}j_2(\lambda r) - \frac{3}{14}j_4(\lambda r)$
4	5	$\frac{3}{2}j_4(\lambda r)$
5	1	$\frac{1}{5}j_0(\lambda r) - \frac{2}{7}j_2(\lambda r) + \frac{1}{70}j_4(\lambda r)$
5	2	$\frac{1}{30}j_0(\lambda r) + \frac{2}{21}j_2(\lambda r) + \frac{1}{70}j_4(\lambda r)$
5	3	$\frac{1}{14}j_2(\lambda r) - \frac{1}{14}j_4(\lambda r)$
5	4	$\frac{5}{21}j_2(\lambda r) - \frac{1}{14}j_4(\lambda r)$
5	5	$\frac{1}{2}j_4(\lambda r)$

Introduce the following notation:

$$\begin{aligned} \mathbb{T}_{ijkl}^{0,1} &= \frac{1}{3}\delta_{ij}\delta_{kl}, \\ \mathbb{T}_{ijkl}^{0,2} &= \frac{1}{\sqrt{5}}\sum_{n=-2}^2 g_{2[1,1]}^{n[i,j]}g_{2[1,1]}^{n[k,l]}, \\ \mathbb{T}_{ijkl}^{2,1,m} &= \frac{1}{\sqrt{6}}(\delta_{ij}g_{2[1,1]}^{m[k,l]} + \delta_{kl}g_{2[1,1]}^{m[i,j]}), \quad -2 \leq m \leq 2, \\ \mathbb{T}_{ijkl}^{2,2,m} &= \sum_{n,q=-2}^2 g_{2[2,2]}^{m[n,q]}g_{2[1,1]}^{n[i,j]}g_{2[1,1]}^{q[k,l]}, \quad -2 \leq m \leq 2, \\ \mathbb{T}_{ijkl}^{4,1,m} &= \sum_{n,q=-4}^4 g_{4[2,2]}^{m[n,q]}g_{2[1,1]}^{n[i,j]}g_{2[1,1]}^{q[k,l]}, \quad -4 \leq m \leq 4, \end{aligned}$$

where $g_{N_1[N_1, N_2]}^{n_1[n_1, n_2]}$ are the so called *Godunov–Gordienko coefficients* described in [14]. Introduce the following notation:

$$G_{\ell' m' p}^{\ell'' m} = \sqrt{(2\ell' + 1)(2\ell'' + 1)}g_{p[\ell', \ell'']}^{m[m', m'']}g_{m[\ell', \ell'']}^{0[0,0]}.$$

Consider the five nonnegative-definite matrices A^n , $1 \leq n \leq 5$, with the following matrix entries:

$$\begin{aligned}
 a_{\ell' m' ij}^{\ell'' m'' kl, 1} &= \left(\frac{1}{\sqrt{5}} T_{ijkl}^{0,2} G_{\ell' m' 0}^{\ell'' m'' 0} - \frac{1}{5\sqrt{14}} \sum_{m=-2}^2 T_{ijkl}^{2,2,m} G_{\ell' m' 2}^{\ell'' m'' m} - \frac{2\sqrt{2}}{9\sqrt{35}} \sum_{m=-4}^4 T_{ijkl}^{4,1,m} G_{\ell' m' 4}^{\ell'' m'' m} \right), \\
 a_{\ell' m' ij}^{\ell'' m'' kl, 2} &= \left(\frac{1}{\sqrt{5}} T_{ijkl}^{0,2} G_{\ell' m' 0}^{\ell'' m'' 0} + \frac{\sqrt{2}}{5\sqrt{7}} \sum_{m=-2}^2 T_{ijkl}^{2,2,m} G_{\ell' m' 2}^{\ell'' m'' m} + \frac{1}{9\sqrt{70}} \sum_{m=-4}^4 T_{ijkl}^{4,1,m} G_{\ell' m' 4}^{\ell'' m'' m} \right), \\
 a_{\ell' m' ij}^{\ell'' m'' kl, 3} &= T_{ijkl}^{0,1} G_{\ell' m' 0}^{\ell'' m'' 0}, \\
 a_{\ell' m' ij}^{\ell'' m'' kl, 4} &= \left(\frac{1}{9\sqrt{5}} T_{ijkl}^{0,2} G_{\ell' m' 0}^{\ell'' m'' 0} - \frac{\sqrt{2}}{5\sqrt{7}} \sum_{m=-2}^2 T_{ijkl}^{2,2,m} G_{\ell' m' 2}^{\ell'' m'' m} + \frac{\sqrt{2}}{3\sqrt{35}} \sum_{m=-4}^4 T_{ijkl}^{4,1,m} G_{\ell' m' 4}^{\ell'' m'' m} \right), \\
 a_{\ell' m' ij}^{\ell'' m'' kl, 5} &= \left(\left(\frac{2}{3} T_{ijkl}^{0,1} + \frac{1}{3\sqrt{5}} T_{ijkl}^{0,2} \right) G_{\ell' m' 0}^{\ell'' m'' 0} + \left(\frac{2}{9} \sum_{m=-2}^2 T_{ijkl}^{2,1,m} - \frac{\sqrt{2}}{9\sqrt{7}} \sum_{m=-2}^2 T_{ijkl}^{2,2,m} \right) G_{\ell' m' 2}^{\ell'' m'' m} \right. \\
 &\quad \left. + \frac{\sqrt{2}}{9\sqrt{35}} \sum_{m=-4}^4 T_{ijkl}^{4,1,m} G_{\ell' m' 4}^{\ell'' m'' m} \right),
 \end{aligned}$$

and let L^n be infinite lower triangular matrices from Cholesky factorisation of the matrices A^n .

Theorem 4 *The following conditions are equivalent.*

1. The matrix $\tau f_{ij\ell m}(\lambda, 0, 0)$ with $\lambda > 0$ takes values in the simplex described above.
2. The field $\varepsilon(\mathbf{x})$ has the form

$$\varepsilon_{ij}(\rho, \theta, \varphi) = C\delta_{ij} + 2\sqrt{\pi} \sum_{n=1}^5 \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \int_0^{\infty} j_{\ell}(\lambda\rho) dZ_{\ell mij}^n(\lambda) S_{\ell}^m(\theta, \varphi),$$

where

$$Z_{\ell mij}^n(A) = \sum_{(\ell', m', k, l) \leq (\ell, m, i, j)} Z_{\ell' m' kl}^n(A),$$

and where $Z_{\ell' m' kl}^n$ is the sequence of uncorrelated scattered random measures on $[0, \infty)$ with control measures Φ_n .

The idea of proof is as follows. Write down the Rayleigh expansion for $e^{i(\mathbf{p}, \mathbf{x})}$ and for $e^{-i(\mathbf{p}, \mathbf{y})}$ separately, substitute both expansions into (10) and use the following result, known as the *Gaunt integral*:

$$\begin{aligned}
 \int_{S^2} S_{\ell_1}^{m_1}(\theta, \varphi) S_{\ell_2}^{m_2}(\theta, \varphi) S_{\ell_3}^{m_3}(\theta, \varphi) \sin \theta \, d\varphi \, d\theta &= \sqrt{\frac{(2\ell_1 + 1)(2\ell_2 + 1)}{4\pi(2\ell_3 + 1)}} \\
 &\quad \times g_{\ell_3[\ell_1, \ell_2]}^{m_3[m_1, m_2]} g_{\ell_3[\ell_1, \ell_2]}^{0[0, 0]}.
 \end{aligned}$$

This theorem can be proved exactly in the same way, as its complex counterpart, see, for example, [34]. Then apply Karhunen’s theorem, see [19].

In order to simulate such fields numerically, one can use simulation algorithms based on spectral expansions. One of such algorithms is described in [21] and realised using MATLAB®, see also references herein. Other software, like R, may be used as well. In comparison

with [21], only one new problem appears, that is, calculation of the Godunov–Gordienko coefficients $g_{N[N_1, N_2]}^{n[n_1, n_2]}$. An algorithm for calculation of the above coefficients is given in [41]. It was realised by the second named author using MATLAB and used for calculation of the syzygies and spectral expansions.

The significance of the Matérn class of tensor-valued random fields follows from the fact that scalar random fields with such a correlation structures are solutions of the fractional analogs of the stochastic Helmholtz equations and hence they are widely used in applications of isotropic random fields on Euclidean space as well spherical random fields obtained as the restriction of isotropic random fields onto the sphere, see [26, Example 2]. For an application of spherical tensor random fields to estimation of parameters of Cosmic Microwave Background one can also propose an analogous of the Matérn class tensor-valued correlation structure, a paper by the authors is currently in preparation.

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Appendix A: Tensors

There are several equivalent definitions of tensors. Surprisingly, the most abstract of them is useful in the theory of random fields.

Let r be a nonnegative integer, and let V_1, \dots, V_r be linear spaces over the same field \mathbb{K} . When $r = 0$, define the tensor product of the empty family of spaces as \mathbb{K}^1 , the one-dimensional linear space over \mathbb{K} .

Theorem 5 (The universal mapping property) *There exist a unique linear space $V_1 \otimes \dots \otimes V_r$, and a unique linear operator $\tau : V_1 \times V_2 \times \dots \times V_r \rightarrow V_1 \otimes \dots \otimes V_r$ that satisfy the universal mapping property: for any linear space W and for any multilinear map $\beta : V_1 \times V_2 \times \dots \times V_r \rightarrow W$, there exists a unique linear operator $B : V_1 \otimes \dots \otimes V_r \rightarrow W$ such that $\beta = B \circ \tau$:*

$$\begin{array}{ccc}
 V_1 \times V_2 \times \dots \times V_r & \xrightarrow{\tau} & V_1 \otimes \dots \otimes V_r \\
 & \searrow \beta & \downarrow B \\
 & & W
 \end{array}$$

In other words: *the construction of the tensor product of linear spaces reduces the study of multilinear mappings to the study of linear ones.*

Remark 1 In mathematical jargon, the above diagram is *commutative*: all directed paths with the same start and endpoints lead to the same result by composition. That is: $\beta = B \circ \tau$.

The tensor product $\mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_r$ of the vectors $\mathbf{v}_i \in V_i, 1 \leq i \leq r$, is defined by

$$\mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_r = \tau(\mathbf{v}_1, \dots, \mathbf{v}_r).$$

Let $V_1, \dots, V_r, W_1, \dots, W_r$ be finite-dimensional linear spaces, and let $A_i \in L(V_i, W_i)$ for $1 \leq i \leq r$. The tensor product of linear operators, $A_1 \otimes \dots \otimes A_r$, is a unique element of the space $L(V_1 \otimes \dots \otimes V_r, W_1 \otimes \dots \otimes W_r)$ such that

$$(A_1 \otimes \dots \otimes A_r)(\mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_r) := A_1(\mathbf{v}_1) \otimes \dots \otimes A_r(\mathbf{v}_r), \quad \mathbf{v}_i \in V_i.$$

If all the spaces $V_i, 1 \leq i \leq r$, are copies of the same space V , then we write $V^{\otimes r}$ for the r -fold tensor product of V with itself, and $\mathbf{v}^{\otimes r}$ for the tensor product of r copies of a vector $\mathbf{v} \in V$. Similarly, for $A \in L(V, V)$ we write $A^{\otimes r}$ for the r -fold tensor product of A with itself. Note that $A^{\otimes 0}$ is the identity operator in the space \mathbb{K}^1 .

Appendix B: Group Representations

Let G be a topological group. A *finite-dimensional representation* of G is a pair (ρ, V) , where V is a finite-dimensional linear space, and $\rho: G \rightarrow GL(V)$ is a continuous group homomorphism. Here $GL(V)$ is the *general linear group of order n* , or the group of all invertible $n \times n$ matrices. In what follows, we omit the word “finite-dimensional” unless infinite-dimensional representations are under consideration.

In a coordinate form, a representation of G is a continuous group homomorphism $\rho: G \rightarrow GL(n, \mathbb{K})$ and the space \mathbb{K}^n .

Let $W \subseteq V$ be a linear subspace of the space V . W is called an *invariant subspace* of the representation (ρ, V) if $\rho(g)\mathbf{w} \in W$ for all $g \in G$ and $\mathbf{w} \in W$. The restriction of ρ to W is then a representation (σ, W) of G . Formula

$$\tau(g)(\mathbf{v} + W) := \rho(g)\mathbf{v} + W$$

defines a representation $(\tau, V/W)$ of G in the quotient space V/W .

In a coordinate form, take a basis for W and complete it to a basis for V . The matrix of $\rho(g)$ relative to the above basis is

$$\rho(g) = \begin{pmatrix} \sigma(g) & * \\ 0 & \tau(g) \end{pmatrix}. \tag{13}$$

Let (ρ, V) and (τ, W) be representations of G . An operator $A \in L(V, W)$ is called an *intertwining operator* if

$$\tau(g)A = A\rho(g), \quad g \in G. \tag{14}$$

The intertwining operators form a linear space $L_G(V, W)$ over \mathbb{K} .

The representations (ρ, V) and (τ, W) are called *equivalent* if the space $L_G(V, W)$ contains an invertible operator. Let A be such an operator. Multiply (14) by A^{-1} from the right. We obtain

$$\tau(g) = A\rho(g)A^{-1}, \quad g \in G.$$

In a coordinate form, $\tau(g)$ and $\rho(g)$ are matrices of the same presentation, written in two different bases, and A is the transition matrix between the bases.

A representation (ρ, V) with $V \neq \{\mathbf{0}\}$ is called *reducible* if there exists an invariant subspace $W \notin \{\{\mathbf{0}\}, V\}$. In a coordinate form, all blocks of the matrix (13) are nonempty. Otherwise, the representation is called *irreducible*.

Example 9 Let $G = O(3)$. The mapping $g \mapsto g^{\otimes r}$ is a representation of the group G in the space $(\mathbb{R}^3)^{\otimes r}$. When $r = 0$, this representation is called *trivial*, when $r = 1$, it is called *defining*. When $r \geq 2$, this representation is reducible.

From now on we suppose that the topological group G is compact. There exists an inner product (\cdot, \cdot) on V such that

$$(\rho(g)\mathbf{v}, \rho(g)\mathbf{w}) = (\mathbf{v}, \mathbf{w}), \quad \mathbf{v}, \mathbf{w} \in V.$$

In a coordinate form, we can choose an orthonormal basis in V . If V is a complex linear space, then the representation (ρ, V) takes values in $U(n)$, the group of $n \times n$ unitary matrices, and we speak of a *unitary representation*. If V is a real linear space, then the representation (ρ, V) takes values in $O(n)$, and we speak of an *orthogonal representation*.

Let (π, V) and (ρ, W) be representations of G . The *direct sum of representations* is the representation $(\pi \oplus \rho, V \oplus W)$ acting by

$$(\pi \oplus \rho)(g)(\mathbf{v} \oplus \mathbf{w}) := \pi(g)\mathbf{v} \oplus \rho(g)\mathbf{w}, \quad g \in G, \quad \mathbf{v} \in V, \quad \mathbf{w} \in W.$$

In a coordinate form, we have

$$\pi \oplus \rho(g) = \begin{pmatrix} \pi(g) & 0 \\ 0 & \rho(g) \end{pmatrix}. \tag{15}$$

Consider the action $\pi \otimes \rho$ of the group G on the set of tensor products $\mathbf{v} \otimes \mathbf{w}$ defined by

$$(\pi \otimes \rho)(g)(\mathbf{v} \otimes \mathbf{w}) := \pi(g)\mathbf{v} \otimes \rho(g)\mathbf{w}, \quad g \in G, \quad \mathbf{v} \in V, \quad \mathbf{w} \in W.$$

This action may be extended by linearity to the *tensor product of representations* $(\pi \otimes \rho, V \otimes W)$. In a coordinate form, $(\pi \otimes \rho)(g)$ is a rank 4 tensor with components

$$T_{ijkl}(g) = \pi_{ij}(g)\rho_{kl}(g), \quad g \in G.$$

A representation (σ, V) of a group G is called *completely reducible* if for every invariant subspace $W \subset V$ there exists an invariant subspace $U \subset V$ such that $V = W \oplus U$. In a coordinate form, any basis $\{\mathbf{w}_1, \dots, \mathbf{w}_p\}$ for W can be completed to a basis $\{\mathbf{w}_1, \dots, \mathbf{w}_p, \mathbf{u}_1, \dots, \mathbf{u}_q\}$ for V such that the span of the vectors $\mathbf{u}_1, \dots, \mathbf{u}_q$ is invariant. The matrix $\sigma(g)$ in the above basis has the form (15). Any representation of a compact group is completely reducible.

Let (ρ, V) be an irreducible representation of a group G . Denote by $[\rho]$ the equivalence class of all representations of G equivalent to (ρ, V) and by \hat{G} the set of all equivalence classes of irreducible representations of G . For any finite-dimensional representation (σ, V) of G , there exists finitely many equivalence classes $[\rho_1], \dots, [\rho_k] \in \hat{G}$ and uniquely determined positive integers m_1, \dots, m_k such that (σ, V) is equivalent to the direct sum of m_1 copies of the representation $(\rho_1, V_1), \dots, m_k$ copies of the representation (ρ_k, V_k) . The direct sum $m_i V_i$ of m_i copies of the linear space V_i is called the *isotypic subspace* of the space V that corresponds to the representation (ρ_i, V_i) . The numbers m_i are called the *multiplicities* of the irreducible representation (ρ_i, V_i) in (σ, V) . The decompositions $V = \sum m_i V_i$ and $\sigma = \sum m_i \rho_i$ are called the *isotypic decompositions*.

Assume that a compact group G is *easy reducible*. This means that for any three irreducible representation (ρ, V) , (σ, W) , and (τ, U) of G the multiplicity m_τ of τ in $\rho \otimes \sigma$ is equal to either 0 or 1. For example, the group $O(3)$ is easy reducible. Assume $m_\tau = 1$. Let $\{\mathbf{e}_i^\rho : 1 \leq i \leq \dim \rho\}$ be an orthonormal basis in V , and similarly for σ and τ . There are two natural bases in the space $V \otimes W$. The *coupled basis* is

$$\{\mathbf{e}_i^\rho \otimes \mathbf{e}_j^\sigma : 1 \leq i \leq \dim \rho, 1 \leq j \leq \dim \sigma\}.$$

The *uncoupled basis* is

$$\{\mathbf{e}_k^\tau : m_\tau = 1, 1 \leq k \leq \dim \tau\}.$$

In a coordinate form, the elements of the space $V \otimes W$ are matrices with $\dim \rho$ rows and $\dim \sigma$ columns. The coupled basis consists of matrices having 1 in the i th row and j th column, and all other entries equal to 0. Denote by $c_{\tau[\rho,\sigma]}^{k[i,j]}$ the coefficients of expansion of the vectors of uncoupled basis in the coupled basis:

$$\mathbf{e}_k^\tau = \sum_{i=1}^{\dim \rho} \sum_{j=1}^{\dim \sigma} c_{\tau[\rho,\sigma]}^{k[i,j]} \mathbf{e}_i^\rho \otimes \mathbf{e}_j^\sigma. \tag{16}$$

The numbers $c_{\tau[\rho,\sigma]}^{k[i,j]}$ are called the *Clebsch–Gordan coefficients* of the group G . In the coupled basis, the vectors of the uncoupled basis are matrices $c_{\tau[\rho,\sigma]}^k$ with matrix entries $c_{\tau[\rho,\sigma]}^{k[i,j]}$, the *Clebsch–Gordan matrices*.

Example 10 (Irreducible unitary representations of $SU(2)$) Let ℓ be a non-negative integer or half-integer (the half of an odd integer) number. Let (ρ_0, \mathbb{C}^1) be the trivial representation, and let $(\rho_{1/2}, \mathbb{C}^2)$ be the defining representation of $SU(2)$. The representation $(\rho_\ell, \mathbb{C}^{2\ell+1})$ with $\ell = 1, 3/2, 2, \dots$, is the symmetric tensor power $\rho_\ell = \mathbf{S}^{2\ell}(\rho_{1/2})$. No other irreducible unitary representations exist.

We may realise the representations ρ_ℓ in the space $\mathcal{P}^{2\ell}(\mathbb{C}^2)$ of homogeneous polynomials of degree 2ℓ in two formal complex variables ξ and η over the two-dimensional complex linear space \mathbb{C}^2 . The group $SU(2)$ consists of the matrices

$$g = \begin{pmatrix} \alpha & \beta \\ -\bar{\beta} & \bar{\alpha} \end{pmatrix}, \quad \alpha, \beta \in \mathbb{C}, \quad |\alpha|^2 + |\beta|^2 = 1. \tag{17}$$

The representation ρ_ℓ acts as follows:

$$(\rho_\ell(g)h)(\xi, \eta) = h(\bar{\alpha}\xi - \beta\eta, \bar{\beta}\xi + \alpha\eta), \quad h \in \mathcal{P}^{2\ell}(V).$$

Note that $\rho_\ell(-E) = E$ if and only if ℓ is integer.

The *Wigner orthonormal basis* in the space $\mathcal{P}^{2\ell}(V)$ is as follows:

$$\mathbf{e}_m(\xi, \eta) := (-1)^{\ell+m} \sqrt{\frac{(2\ell+1)!}{(\ell+m)!(\ell-m)!}} \xi^{\ell+m} \eta^{\ell-m}, \quad m = -\ell, -\ell+1, \dots, \ell. \tag{18}$$

The matrix entries of the operators $\rho_\ell(g)$ in the above basis are called *Wigner D functions* and are denoted by $D_{mn}^\ell(g)$. The tensor product $\rho_{\ell_1} \otimes \rho_{\ell_2}$ is expanding as follows

$$\rho_{\ell_1}(g) \otimes \rho_{\ell_2}(g) = \sum_{\ell=|\ell_1-\ell_2|}^{\ell_1+\ell_2} \oplus \rho_\ell(g).$$

Example 11 (Irreducible unitary representations of $SO(3)$ and $O(3)$) Realise the linear space \mathbb{R}^3 with coordinates x_{-1}, x_0 , and x_1 as the set of traceless Hermitian matrices over \mathbb{C}^2 with entries

$$\begin{pmatrix} x_0 & x_1 + ix_{-1} \\ x_1 - ix_{-1} & -x_0 \end{pmatrix}.$$

The matrix (17) acts on the so realised \mathbb{R}^3 as follows:

$$\pi(g) \begin{pmatrix} x_0 & x_1 + ix_{-1} \\ x_1 - ix_{-1} & -x_0 \end{pmatrix} := g^* \begin{pmatrix} x_0 & x_1 + ix_{-1} \\ x_1 - ix_{-1} & -x_0 \end{pmatrix} g.$$

The mapping π is a homomorphism of $SU(2)$ onto $SO(3)$. The kernel of π is $\pm E$. Assume that (ρ, V) is an irreducible unitary representation of $SO(3)$. Then $(\rho \circ \pi, V)$ is an irreducible

unitary representation of $SU(2)$ with kernel $\pm E$. Then we have $\rho \circ \pi = \rho_\ell$ for some integer ℓ . In other words, every irreducible unitary representation (ρ_ℓ, V) of $SU(2)$ with integer ℓ gives rise to an irreducible unitary representation of $SO(3)$, and no other irreducible unitary representations exist. We denote the above representation of $SO(3)$ again by (ρ_ℓ, V) .

Let $SO(2)$ be the subgroup of $SO(3)$ that leaves the vector $(0, 0, 1)^\top$ fixed. The restriction of ρ_ℓ to $SO(2)$ is equivalent to the direct sum of irreducible unitary representations $(e^{im\varphi}, \mathbb{C}^1)$, $-\ell \leq m \leq \ell$ of $SO(2)$. Moreover, the space of the representation $(e^{im\varphi}, \mathbb{C}^1)$ is spanned by the vector $\mathbf{e}_m(\xi, \eta)$ of the Wigner basis (18). This is where their enumeration comes from.

The group $O(3)$ is the Cartesian product of its normal subgroups $SO(3)$ and $\{I, -I\}$. The elements of $SO(3)$ are rotations, while the elements of the second component are reflections. Therefore, any irreducible unitary representation of $O(3)$ is the outer tensor product of some (ρ_ℓ, V) by an irreducible unitary representation of $\{E, -E\}$. The latter group has two irreducible unitary representation: trivial (ρ_+, \mathbb{C}^1) and determinant (ρ_-, \mathbb{C}^1) . Denote $\rho_{\ell,+} := \rho_\ell \hat{\otimes} \rho_+$ and $\rho_{\ell,-} := \rho_\ell \hat{\otimes} \rho_-$. These are all irreducible unitary representations of $O(3)$.

Introduce the coordinates on $SO(3)$, the *Euler angles*. Any rotation g may be performed by three successive rotations:

- rotation $g_0(\psi)$ about the x_0 -axis through an angle ψ , $0 \leq \psi < 2\pi$;
- rotation $g_{-1}(\theta)$ about the x_{-1} -axis through an angle θ , $0 \leq \theta \leq \pi$,
- rotation $g_0(\varphi)$ about the x_0 -axis through an angle φ , $0 \leq \varphi < 2\pi$.

The angles ψ , θ , and φ are the *Euler angles*. The Wigner D functions are $D_{mn}^\ell(\varphi, \theta, \psi)$. The Wigner D functions D_{m0}^ℓ do not depend on ψ and may be written as $D_{m0}^\ell(\varphi, \theta)$. The *spherical harmonics* Y_ℓ^m are defined by

$$Y_\ell^m(\theta, \varphi) := \sqrt{\frac{2\ell + 1}{4\pi}} D_{m0}^\ell(\varphi, \theta). \tag{19}$$

Let (r, θ, φ) be the spherical coordinates in \mathbb{R}^3 :

$$\begin{aligned} x_{-1} &= r \sin \theta \sin \varphi, \\ x_0 &= r \cos \theta, \\ x_1 &= r \sin \theta \cos \varphi. \end{aligned} \tag{20}$$

The measure $d\Omega := \sin \theta d\varphi d\theta$ is the Lebesgue measure on the *unit sphere* $S^2 := \{\mathbf{x} \in \mathbb{R}^3 : \|\mathbf{x}\| = 1\}$. The spherical harmonics are orthonormal:

$$\int_{S^2} Y_{\ell_1}^{m_1}(\theta, \varphi) \overline{Y_{\ell_2}^{m_2}(\theta, \varphi)} d\Omega = \delta_{\ell_1 \ell_2} \delta_{m_1 m_2}.$$

Example 12 (Expansions of tensor representations of the group $O(3)$) Let $r \geq 2$ be a non-negative integer, and let Σ_r be the permutation group of the numbers $1, 2, \dots, r$. The action

$$\sigma \cdot (\mathbf{v}_1 \otimes \dots \otimes \mathbf{v}_r) := \mathbf{v}_{\sigma^{-1}(1)} \otimes \dots \otimes \mathbf{v}_{\sigma^{-1}(r)}, \quad \sigma \in \Sigma_r,$$

may be extended by linearity to an orthogonal representation of the group Σ_r in the space $(\mathbb{R}^3)^{\otimes r}$, call it $(\rho_r, (\mathbb{R}^3)^{\otimes r})$. Consider the orthogonal representation $(\tau, (\mathbb{R}^3)^{\otimes r})$ of the group $O(3) \times \Sigma_r$ acting by

$$\tau(g, \sigma)(\mathbf{T}) := \rho^{\otimes r}(g) \rho_r(\sigma)(\mathbf{T}), \quad \mathbf{T} \in (\mathbb{R}^3)^{\otimes r}.$$

The representation $(\tau, (\mathbb{R}^3)^{\otimes 2})$ of the group $O(3) \times \Sigma_2$ is the direct sum of three irreducible components

$$\tau = [\rho_{0,+}(g)\tau_+(\sigma)] \oplus [\rho_{1,+}(g)\varepsilon(\sigma)] \oplus [\rho_{2,+}(g)\tau_+(\sigma)],$$

where τ_+ is the trivial representation of the group Σ_2 , while ε is its non-trivial representation. The one-dimensional space of the first component is the span of the identity matrix and consists of scalars. The three-dimensional space of the second component is the space $\Lambda^2(\mathbb{R}^3)$ of 3×3 skew-symmetric matrices. Its elements are three-dimensional pseudo-vectors. Finally, the five-dimensional space of the third component consists of 3×3 traceless symmetric matrices (deviators). The second component is $(\Lambda^2(g), \Lambda^2(\mathbb{R}^3))$, and the direct sum of the first and third components is $(\mathcal{S}^2(g), \mathcal{S}^2(\mathbb{R}^3))$.

In general, the representation $(\tau, (\mathbb{R}^3)^{\otimes r})$ is reducible and may be represented as the direct sum of irreducible representations as follows:

$$\tau(g, \sigma) = \sum_{\ell=0}^r \sum_{q=1}^{N_r^\ell} \oplus U^{\ell x}(g)\rho_q(\sigma),$$

where q is called the *seniority index* of the component $U^{\ell x}(g)\rho_q(\sigma)$, see [1], and where $x = g$ for even r and $x = u$ for odd r . The number N_r^ℓ of copies of the representation $U^{\ell x}$ is given by

$$N_r^\ell = \sum_{k=0}^{\lfloor (r-\ell)/3 \rfloor} \binom{r}{k} \binom{2r-3k-\ell-2}{r-2}.$$

Appendix C: Classical Invariant Theory

Let V and W be two finite-dimensional linear spaces over the same field \mathbb{K} . Let (ρ, V) and (σ, W) be two representations of a group G . A mapping $h : W \rightarrow V$ is called a *covariant* or *form-invariant* or a *covariant tensor* of the pair of representations (ρ, V) and (σ, W) , if

$$h(\sigma(g)\mathbf{w}) = \rho(g)h(\mathbf{w}), \quad g \in G.$$

In other words, the diagram

$$\begin{array}{ccc} W & \xrightarrow{h} & V \\ \downarrow \sigma & & \downarrow \rho \\ W & \xrightarrow{h} & V \end{array}$$

is commutative, as explained in Remark 1.

If $V = \mathbb{K}^1$ and ρ is the trivial representation of G , then the corresponding covariant scalars are called *absolute invariants* (or just invariants) of the representation (σ, W) , hence the name *Invariant Theory*. Note that the set $\mathbb{K}[W]^G$ of invariants is an *algebra* over the field \mathbb{K} , that is, a linear space over \mathbb{K} with bilinear multiplication operation and a multiplication identity 1. The product of a covariant $h : W \rightarrow V$ and an invariant $f \in \mathbb{K}[W]^G$ is again a covariant. In other words, the covariant tensors of the pair of representations (ρ, V) and (σ, W) form a *module* over the algebra of invariants of the representation (σ, W) .

A mapping $h : W \rightarrow V$ is called *homogeneous polynomial mapping of degree d* if for any $\mathbf{v} \in V$ the mapping $\mathbf{w} \mapsto (h(\mathbf{w}), \mathbf{v})$ is a homogeneous polynomial of degree d in $\dim W$

variables. The mapping h is called a *polynomial covariant of degree d* if it is homogeneous polynomial mapping of degree d and a covariant.

Let (σ, W) be the defining representation of G , and (ρ, V) be the r th tensor power of the defining representation. The corresponding covariant tensors are said to have an *order r* . The covariant tensors of degree 0 and of order r of the group $O(n)$ are known as *isotropic tensors*.

The algebra of invariants and the module of covariant tensors were an object of intensive research. The first general result was obtained by [15]. The author proved that for any finite-dimensional complex representation of the group $G = \text{SL}(2, \mathbb{C})$ the algebra of invariants and the module of covariant tensors are finitely generated. In other words, there exists an *integrity basis*: a finite set of invariant homogeneous polynomials I_1, \dots, I_N such that every polynomial invariant can be written as a polynomial in I_1, \dots, I_N . An integrity basis is called *minimal* if none of its elements can be expressed as a polynomial in the others. A minimal integrity basis is not necessarily unique, but all minimal integrity bases have the same amount of elements of each degree.

The algebra of invariants is not necessarily free. Some polynomial relations between generators, called *syzygies* may exist.

The importance of polynomial invariants can be explained by the following result. Let G be a closed subgroup of the group $O(3)$, the group of symmetries of a material. Let $(\rho, V), (\rho_1, V_1), \dots, (\rho_N, V_N)$ be finitely many orthogonal representations of G in real finite-dimensional spaces. Let $T: V_1 \oplus \dots \oplus V_N \rightarrow V$ be an *arbitrary* (say, measurable) covariant of the pair ρ and $\rho_1 \oplus \dots \oplus \rho_N$. Let $\{I_k: 1 \leq k \leq K\}$ be an integrity basis for *polynomial invariants* of the representation ρ , and let $\{T_l: 1 \leq l \leq L\}$ be an integrity basis for *polynomial covariant tensors* of the pair ρ and $\rho_1 \oplus \dots \oplus \rho_N$. Following [45], we call T_l *basic covariant tensors*.

Theorem 6 [45] *A function $T: V_1 \oplus \dots \oplus V_N \rightarrow V$ is a measurable covariant of the pair ρ and $\rho_1 \oplus \dots \oplus \rho_N$ if and only if it has the form*

$$T(T_1, \dots, T_N) = \sum_{l=1}^L \varphi_l(I_1, \dots, I_K) T_l(T_1, \dots, T_N),$$

where φ_l are real-valued measurable functions of the elements of an integrity basis.

In 1939 in the first edition of [44] Weyl proved that any polynomial covariant of degree d and of order r of the group $O(n)$ is a linear combination of products of Kronecker’s deltas δ_{ij} and second degree homogeneous polynomials $x_i x_j$.

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