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Notes and Correspondence
On the correlation functions associated with polynomials of the diffusion operator

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Correlation functions (CFs) associated with the inverse background-error correlations (iBECs) represented by polynomials of the diffusion operator D are obtained analytically for the binomial approximations of the Gaussian BEC and in the general case of a quadratic polynomial of D. The respective analytical expressions for one-, two- and three-dimensional cases have two tuning parameters, which provide enough freedom in adjusting the CFs' shape to experimental data. The polynomial coefficients of the corresponding iBEC operator are obtained in terms of these tuning parameters and may be useful in the design of the BEC models for variational data assimilation. Published in 2011 by John Wiley & Sons Ltd.

Key Words: variational data assimilation; correlation modelling

Received 1 February 2011; Revised 2 July 2011; Accepted 5 July 2011; Published online in Wiley Online Library 16 August 2011

Citation: Yaremchuk M, Smith S. 2011. On the correlation functions associated with polynomials of the diffusion operator. *Q. J. R. Meteorol. Soc.* **137**: 1927–1932. DOI:10.1002/qj.893

1. Introduction

Modelling of the inverse background-error correlations (iBECs) of random fields by differential operators has gained considerable attention in recent years, primarily due to computational efficiency of their implementation in the iterative minimization algorithms used in variational data assimilation (e.g. Xu, 2005; Pannekoucke and Massart, 2008; Mirouze and Weaver, 2010). Of particular interest are the iBEC models described by positive-definite polynomials of the diffusion operator

$$\mathsf{D} = \nabla \nu \nabla \, , \tag{1}$$

where ν is the symmetric positive-definite spatially varying diffusion tensor. This type of iBEC model is attractive for several reasons: (a) it allows straightforward control of inhomogeneity and anisotropy via the diffusion tensor; (b) it is computationally competitive in many applications; and (c) it is easier to develop with regard to keeping the positive-definiteness property of the BEC operator. In contrast, in the traditional approach of the 'direct' correlation modelling where spatial correlations are specified by prescribed analytical functions, care should be taken to maintain positive definiteness of the respective correlation operator, especially in anisotropic and/or inhomogeneous cases (e.g. Gaspari *et al.*, 2006; Gregori *et al.*, 2008).

Because of the above-mentioned properties, polynomials of D have been extensively used for approximating Gaussian-shaped BECs by either explicit (e.g. Derber and Rosati, 1989; Egbert *et al.*, 1994; Weaver and Courtier, 2001; Weaver *et al.*, 2003) or implicit (Ngodock *et al.*, 2000; DiLorenzo *et al.*, 2007) integration schemes. In the latter case, the BEC operator is obtained via iBEC representation by a binomial of D. Second-order polynomials of D were considered recently by Hristopulos (2003) and Hristopulos and Elogne (2007, 2009) for construction of the correlation models for geostatistical and other applications. Our research (Yaremchuk *et al.*, 2011) also indicates that low-order iBEC models can provide extra computational savings in three-dimensional variational (3D-Var) analysis while keeping the predictive skill of oceanographic assimilation systems. A comprehensive treatment of representing the iBECs by the polynomials of D was given by Xu

(2005), who obtained Taylor expansions approximating the propagator of the diffusion equation in one, two and three dimensions and obtained recursive relations for the polynomial coefficients associated with spatially homogeneous correlation functions.

It should be noted that, among the numerous classes of analytic correlation functions (CFs), only a few can be effectively implemented within the operator-based approach, because the corresponding iBEC is represented by a polynomial of $\mathbf{D}$. In many geophysical applications, however, details of the shape of a CF are poorly known because of insufficient statistics. As a consequence, in most cases, heuristic CFs can be adequately approximated using only one or two scalar parameters that define a family of analytic correlation functions. Therefore, analytic CFs, with inverses that can be described by low-order polynomials of $\mathbf{D}$, are of significant practical interest.

Based on the results of the recent studies, this note presents analytical expressions for the CFs corresponding to two types of the iBEC models: the first type is the mth-order binomial of $\mathbf{D}$, which approximates the Gaussian-shaped CF; and the second type is a quadratic function of $\mathbf{D}$ that is capable of reproducing negative lobes in the CFs. The obtained CFs generalize earlier results of Hristopulos and Elogne (2007; hereinafter HE07) and Mirouze and Weaver (2010), and may facilitate practical design of the cost functions in variational data assimilation problems, as they give explicit relationships between the shape of the CFs and the structure of the corresponding iBEC operators in the analytic form.

2. CFs generated by the polynomials of the homogeneous diffusion operator

Consider an anisotropic homogeneous diffusion operator (1) in $\mathbb{R}^n, n = 1, \ldots, 3$ with $\boldsymbol{x} \in \mathbb{R}^n$ representing points in the physical space and $\boldsymbol{k}$ representing points in the wavenumber space. By the appropriate coordinate transformation (e.g. Xu, 2005; HE07) the problem can be reduced to considering isotropic BEC operators of the form $F(-\Delta)$, where F is a positive function and Δ is the Laplacian operator. In the general case of an inhomogeneous operator, such transformation cannot be found, but local transformations of this type can be useful in constructing the BEC operator.

In this note, the following two classes of the iBEC operators are considered: the first is represented by the binomial

$$\mathbf{B}^{-1} = (\mathbf{I} - \alpha_0 \Delta)^m, \tag{2}$$

and the other by the second-order polynomial in Δ:

$$\mathbf{B}^{-1} = \mathbf{I} - \alpha_1 \Delta + \alpha_2 \Delta^2. \tag{3}$$

Here $\mathbf{I}$ is the identity operator and α_i are the real numbers, constrained by the positive definiteness requirement of $\mathbf{B}^{-1}$. In the binomial case (2), this constraint is $\alpha_0 \geq 0$. For the quadratic polynomial (3), the positive-definiteness requirement can be taken into account explicitly by diagonalizing $\mathbf{B}^{-1}$ via the Fourier transform. In the Fourier representation, $\mathbf{B}^{-1}$ acts as multiplication by the polynomial in $k^2 \equiv |\boldsymbol{k}|^2$, and the positive-definiteness property translates into the requirement for the spectral polynomial

$$B^{-1}(k) = 1 + \alpha_1 k^2 + \alpha_2 k^4 \tag{4}$$

to be positive for all $k^2 \equiv |\boldsymbol{k}|^2$ (e.g. Reed and Simon, 1975). This constraint is equivalent to the statement that the polynomial in the right-hand side of (4) must not have real positive roots. Since we are considering biquadratic polynomials with real coefficients, these roots are symmetric with respect to both real and imaginary axes. Thus, without loss of generality (except for the special case of imaginary roots, which is treated later), $B^{-1}(k)$ can also be represented in the form

$$B^{-1}(k) = \gamma\{a^2 + (k-b)^2\}\{a^2 + (k+b)^2\}, \tag{5}$$

where a and b are real numbers defining the inverse decorrelation scales of the covariance operator, and $\gamma = (a^2 + b^2)^{-2}$. The correspondence between α_1, α_2 and a, b can easily be established:

$$\alpha_1 = 2(a^2 - b^2)(a^2 + b^2)^{-2}; \quad \alpha_2 = (a^2 + b^2)^{-2} \tag{6}$$

Compared to the spectral representation (4) considered in HE07, the representation (5) has the advantage that its free parameters are not constrained by the positive-definiteness requirement. The reciprocal of $B^{-1}(k)$ provides the spectral representation of the BEC operator:

$$B(k) = \left[\gamma\{a^2 + (k-b)^2\}\{a^2 + (k+b)^2\}\right]^{-1}. \tag{7}$$

In a special case when both roots are on the imaginary axis, the diagonal of $\mathbf{B}^{-1}$ can be represented by

$$B^{-1}(k) = \tilde{\gamma}(a^2 + k^2)(b^2 + k^2), \tag{8}$$

where $\tilde{\gamma} = (ab)^{-2}$ and the weighting factors before the Laplacians are given by

$$\tilde{\alpha}_1 = (a^2 + b^2)(ab)^{-2}, \qquad \tilde{\alpha}_2 = (ab)^{-2}. \tag{9}$$

The corresponding spectrum can be reduced to the difference of the respective first-order (one-parameter) spectra

$$\begin{aligned} B(k) &= \frac{1}{\tilde{\gamma}(a^2 + k^2)(b^2 + k^2)} \\ &= \frac{\tilde{\gamma}^{-1}}{b^2 - a^2}\left(\frac{1}{a^2 + k^2} - \frac{1}{b^2 + k^2}\right) \end{aligned}$$

considered in the next section.

Because of homogeneity, the matrix elements of $\mathbf{B}$ depend only on the distance $r = |\boldsymbol{x}|$ from the diagonal. They can be computed by applying the inverse Fourier transform to $\mathbf{B}(k)$:

$$B^n(r) = (2\pi)^{-n} \int_{\mathbb{R}^n} B(k) \exp(-\mathrm{i}\boldsymbol{k}\boldsymbol{x})\, \mathrm{d}\boldsymbol{k}. \tag{10}$$

By integrating over the directions in $\mathbb{R}^n$ (see the Appendix), (10) can be reduced to

$$B^n(r) = (2\pi)^{-n/2} \int_0^\infty B(k) k^{n-1} (kr)^{-s} J_s(kr)\, \mathrm{d}k, \tag{11}$$

where J denotes the Bessel function of the first kind and $s = n/2 - 1$. The respective matrix elements of the correlation operator (correlation functions) are obtained by normalization:

$$C^n(r) = B^n(r)/B^n(0). \quad (12)$$

In practical applications, the diffusion operator is not homogeneous, and the analytic representations (4)–(11) cannot be obtained. However, the action of the BEC operator on a state vector can be computed numerically at a relatively low cost. The major problem with such modelling is the efficient estimation of the diagonal elements

$$\mathbf{B}^n(\boldsymbol{x},\boldsymbol{x}) \equiv \int_{\mathbb{R}^n} \mathbf{B}^n(\boldsymbol{x},\boldsymbol{y})\,\delta(\boldsymbol{x}-\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}, \quad (13)$$

which are necessary to rescale $\mathbf{B}$ to have its diagonal elements equal to unity. In practice, the rescaling factors $N^n(\boldsymbol{x})$ are defined as reciprocals of $\mathbf{B}^n(\boldsymbol{x},\boldsymbol{x})$.

Taking the integral in (13) numerically is expensive, because the convolutions with the δ-functions have to be performed at all numerical grid points $\boldsymbol{x}$. However, reasonable approximations for $N^n(\boldsymbol{x})$ can be obtained by using the homogeneous analytical versions of (13) (e.g. Purser *et al.*, 2003; Mirouze and Weaver, 2010). Therefore, analytical formulae describing homogeneous BEC operators are of significant practical interest. Another benefit of the analytical models, is their ability to provide guidance in the design of the correlation functions. In the case considered, the type of spectral polynomial defines the CF's shape as a function of α_i. Conversely, it provides the values of α_i after the CF parameters are (optimally) fitted to the available data. In this note, two types of such polynomials are considered: the first type describes power approximations of the Gaussian-shaped CF, and the second is a general second-order polynomial given by (5) and (8).

3. Power approximations of the Gaussian-shaped CF

An important family of one-parameter correlation spectra provides approximations to the Gaussian-shaped correlation function:

$$B^n_m(k) = \left(1+\frac{a^2k^2}{2m}\right)^{-m} \approx \exp\left(-\frac{a^2k^2}{2}\right). \quad (14)$$

Although the binomial approximation (14) converges fast enough (e.g. Abramowitz and Stegun, 1972), only small values of m are of practical interest. In this section we derive the binomial-generated CFs and the correction coefficient needed for efficient approximation of the Gaussian CF when m is small.

Substituting (14) into (11), integrating over k and normalizing the result by $\mathbf{B}^n(0)$ yields the correlation functions of the Matern family (Stein, 1999) enumerated by $s = m - n/2$ and scaled by $a_* = a/\sqrt{2m}$:

$$C^n_m(\rho) = \frac{\rho^s K_s(\rho)}{2^{s-1}\Gamma(s)}, \quad (15)$$

where $\rho = r/a_*$, Γ is the gamma function and K stands for the modified Bessel function of the second kind (e.g. Abramowitz and Stegun, 1972). The respective normalization factors are

$$N^n_m = \frac{\Gamma(m)}{\Gamma(s)}(2\sqrt{\pi}a_*)^n. \quad (16)$$

In the limiting case $m \to \infty$, the correlation functions (15) take the Gaussian form:

$$C^n_\infty = \exp(-r^2/2a^2); \qquad n = 1, \ldots \quad (17)$$

Consecutive approximations of the Gaussian CF by (15) are shown in Figure 1. It is remarkable that, when $m = 1$, the correlation functions (15) have singularities at $\rho = 0$ in both two and three dimensions (also Table I). This means that *in the continuous case* the first-order approximations become invalid when $n > 1$. Numerically, however, the correlation functions do exist for $n > 1$, but their decorrelation scale is limited by the grid size δ (the corresponding CF is shown by the dotted line in Figure 1(a)). This occurs because the numerical analogue of the δ-function is never singular, but has a finite amplitude inversely proportional to the volume of a grid cell, therefore resulting in a finite value of the convolution (13) even if it is infinite in the continuous case. After normalization by that finite value, the CF is 1 at $r = 0$, but its effective decorrelation scale remains proportional to the local grid size δ if $a \gg \delta$.

It is also noteworthy that the mth-order correlation functions in 3D coincide with the $(m-1)$th-order CFs in 1D. In particular, the 1D second-order autoregression, or SOAR function, widely used in operational analyses, corresponds to the third-order approximation of the Gaussian function in 3D.

Figure 1(a) shows that low-order power approximations (14) underestimate the decorrelation scale a of the target Gaussian function. This unpleasant property can be corrected by optimizing the value of a in (14) to obtain the best fit with the Gaussian CF. Because the Gaussian and its approximating functions are both positive and have similar shapes, a reasonable optimization criterion is to set their integral decorrelation scales equal to each other:

$$\begin{aligned}\int_0^\infty C^n_m(\rho)\,\mathrm{d}r &\equiv \frac{a_{\mathrm{opt}}}{\sqrt{2m}}\int_0^\infty C^n_m(y)\,\mathrm{d}y \\ &= \int_0^\infty \exp\left(-\frac{r^2}{2a^2}\right)\mathrm{d}r = a\sqrt{\frac{\pi}{2}}.\end{aligned} \quad (18)$$

Expression (18) shows that $a_{\mathrm{opt}} = \xi^n_m a$, with the rescaling coefficient

$$\xi^n_m = \sqrt{\pi m}\left[\int_0^\infty C^n_m(y)\,\mathrm{d}y\right]^{-1} = \frac{\Gamma(s)}{\Gamma(s+1/2)}\sqrt{m}. \quad (19)$$

The values of ξ^n_m for $m < 4$ and their respective approximation errors are assembled in Table I.

The coefficients ξ^n_m along with relationship (14) provide an expression for estimating α_0 in the binomial iBEC model (2) which approximates the Gaussian-shaped correlation function with a given radius a:

$$\alpha_0 = (\xi^n_m a)^2/2m \quad (20)$$

4. Two-parameter correlation functions

In the general case of the two-parameter approximation (5) there are two complex roots located symmetrically with

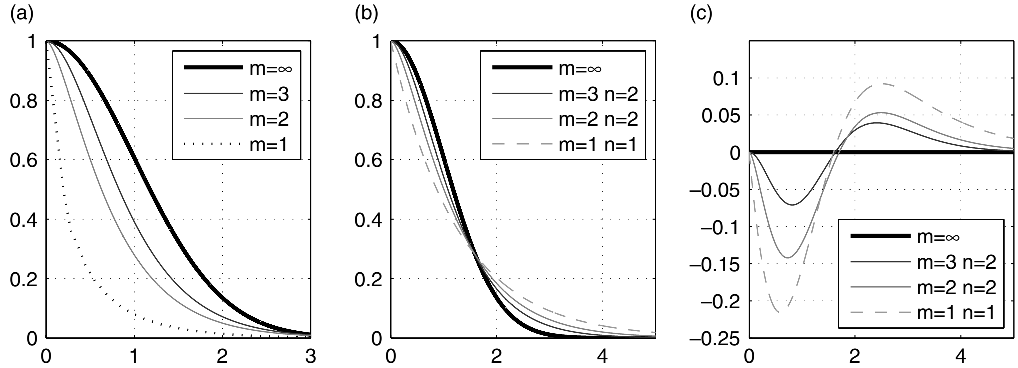

Figure 1. (a) Power approximations (14) of the Gaussian CF in two dimensions ($n = 2$). The CF for $m = 1$ is shown by the dotted line for the numerical realization with the grid step $\delta = a/4$. (b) Same approximations, but with optimally adjusted correlation radii for various combinations of m and n. (c) Differences between the Gaussian CF and its approximation shown in (b). The horizontal axes are scaled by a.

Table I. Correlation functions associated with the power approximations (14) of the Gaussian CF in n dimensions. The CFs for $n = 1, 3$ are rewritten in terms of elementary functions for convenience. The correlation radius adjustment coefficients ξ_m^n are shown below the formulae together with (in bold) the corresponding relative errors in approximation of the Gaussian CF.

	$n = 1$	$n = 2$	$n = 3$
$m = 1$	$\exp(-\rho)$ $\sqrt{\pi}$ **0.33**	$K_0(\rho)$ --	$\exp(-\rho)/\rho$ --
$m = 2$	$(1+\rho)\exp(-\rho)$ $\sqrt{\pi/2}$ **0.13**	$\rho K_1(\rho)$ $\sqrt{8/\pi}$ **0.19**	$\exp(-\rho)$ $\sqrt{2\pi}$ **0.33**
$m = 3$	$(1+\rho+\rho^2/3)\exp(-\rho)$ $\sqrt{27\pi/8}$ **0.08**	$\rho^2 K_2(\rho)/2$ $\sqrt{16/3\pi}$ **0.10**	$(1+\rho)\exp(-\rho)$ $\sqrt{3\pi/4}$ **0.13**
$m = \infty$	$\exp(-r^2/2a^2)$	$\exp(-r^2/2a^2)$	$\exp(-r^2/2a^2)$

respect to imaginary axis. Plugging (7) into (11), integrating over k, and renormalizing yields the following CFs:

$$C^n(a,b,r) = \frac{1}{\mathrm{i}\beta_n}\left\{z^s K_s(\bar{z}) - \bar{z}^s K_s(z)\right\}, \tag{21}$$

where $z = (a + \mathrm{i}b)r$, the overline denotes the complex conjugation, $s = 1 - n/2$, and the coefficients β_n are

$$\beta_{1,3} = b\sqrt{\frac{2\pi}{a^2+b^2}}, \qquad \beta_2 = 2\arctan\left(\frac{b}{a}\right). \tag{22}$$

Note that, despite a seemingly complex-valued expression in the right-hand side of (21), its imaginary part is identically zero. Similar to the binomial case, 1D and 3D two-parameter CFs can also be expressed in terms of elementary functions:

$$C^1(a,b,r) = \frac{\sqrt{a^2+b^2}}{b} \times \exp(-ar)\cos\left\{br - \arctan\left(\frac{a}{b}\right)\right\}, \tag{23}$$

$$C^3(a,b,r) = \exp(-ar)\frac{\sin(br)}{br} \tag{24}$$

Figure 2 shows the dependence of the correlation functions (21) on the magnitude of b for various n. As can be seen from (23) and (24), CFs in 1D and 3D have equidistant zeros separated by π/b except for the first zero which is $\pi/2b$ away from the origin for $n = 3$, and depends on both a and b for $n = 1$. Although analytical expressions are quite different for $n = 2$ and $n = 3$, the behaviour of the CFs is rather similar. In the 1D case, the first zero is somewhat farther away from the origin and the CF is less damped.

In the special case (8), the CFs can be expressed via the differences of the first-order CFs (15) discussed in section 3:

$$\widetilde{C}^1(a,b,r) = \frac{a\exp(-br) - b\exp(-ar)}{a-b}, \tag{25}$$

$$\widetilde{C}^2(a,b,r) = \frac{K_0(ar) - K_0(br)}{\log(b/a)}, \tag{26}$$

$$\widetilde{C}^3(a,b,r) = \frac{\exp(-ar) - \exp(-br)}{(b-a)r}. \tag{27}$$

In the expressions (25), (27) the representations of the Bessel functions in terms of elementary functions were used. Also note that $\widetilde{C}^{2,3}(r)$ are non-singular at $r = 0$ because the singularities are cancelled out by taking the difference in the numerator. In this special case, the second parameter gives little extra freedom in adjusting the shape of the CFs, because the resulting curves remain positive functions of r. The extra degree of freedom can be used to partly control, for example, the CF derivative at $r = 0$.

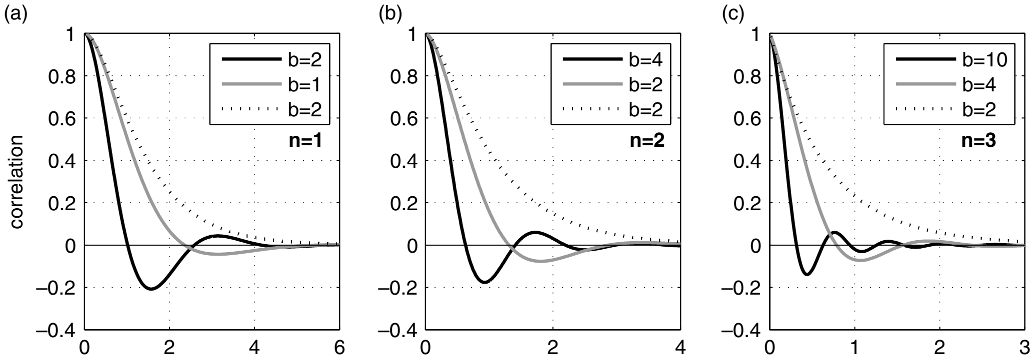

Figure 2. Two-parameter CFs corresponding to the quadratic inverse BEC (5) with $a = 1$. The horizontal axis is scaled by a. Dotted lines show CFs corresponding to the case (8) with two imaginary roots of the spectral polynomial.

The normalization constants for the functions (21) and (25)–(27) are respectively

$$N^1 = \frac{4a}{a^2 + b^2}, \quad N^2 = \frac{8\pi ab}{\beta_2 (a^2 + b^2)^2}, \quad N^3 = \frac{8\pi a}{(a^2 + b^2)^2} \tag{28}$$

and

$$\widetilde{N}^1 = \frac{2(a+b)}{ab}, \quad \widetilde{N}^2 = \frac{2\pi(a^2 - b^2)}{a^2 b^2 \log(a/b)}, \quad \widetilde{N}^3 = \frac{4\pi(a+b)}{a^2 b^2}. \tag{29}$$

Equations (21) and (25)–(27) provide explicit expressions for the CFs of the two-parameter BEC model. Combining them with the relationships (6)–(9) allows the parameters of inverse BEC operator (3) to be computed after the values of a and b are adjusted to experimental data using (21) or (25)–(27).

5. Summary and discussion

BEC modelling with diffusion operators is an efficient and flexible tool for evaluating matrix-vector products of large dimension which emerge in minimization algorithms of variational data assimilation. This note has discussed analytic relationships between the parameters controlling the shape of correlation functions and the polynomial coefficients characterizing the structure of the respective inverse BEC operator. The results may be helpful in designing the BEC operators in variational data assimilation algorithms.

Although only homogeneous operators in boundaryless domains were considered, the relationships (15)–(16), (20)–(29) may provide reasonable guidance to constructing more realistic BEC operators, especially in cases when the typical scale of variability of the diffusion tensor is much larger than the local decorrelation scale ρ_c and/or most of the observations are separated from the boundaries by distances, exceeding ρ_c. In a similar way, weak inhomogeneity can be introduced by variable scaling factors $a(\boldsymbol{x})$, $b(\boldsymbol{x})$, and the local CF shapes can be assessed using (21)–(27).

Although generalizations of (21) for higher-order polynomials are possible, this study has been limited to quadratic polynomials for two reasons. First, the BEC operators encountered in geophysical fluid dynamics applications are rarely homogeneous and observational statistics are usually insufficient to capture the spatial dependence of the BEC structure. Therefore experimental estimates of the BECs are either limited to low-rank ensemble estimates or have to rely on the very rough assumption of homogeneity. Needless to say, in the latter case the structure of a sample CF should be elaborated with sufficiently low detalization which can be well accounted for by a two-parameter CF family. The second reason is that the use of higher-order polynomials considerably degrades the conditioning of the linear systems that are being solved in the assimilation process (Yaremchuk *et al.*, 2011) and, therefore, requires sophisticated preconditioners.

It should be noted that similar problems have been recently studied by many authors (e.g. Xu, 2005; Hristopulos and Elogne, 2007, 2009; Mirouze and Weaver, 2010). In particular, analytic formulae analogous to (23), (24), (25) and (27) were derived in a somewhat different setting by HE07 who considered iBECs of similar structure. Xu (2005) analyzed Taylor expansions of the Gaussian BEC operator and obtained recursive relations for the polynomial coefficients associated with an arbitrary CF. Mirouze and Weaver (2010) also demonstrated a possibility to generate oscillating CFs using higher-order polynomials in 1D.

The objective of this note was to present the accumulated information in concise form and to provide explicit relationships between the polynomial coefficients of the iBEC operators and the corresponding CF parameters that can be derived from experimental data. In addition to this, coefficients ξ_m^n for the power approximations of the Gaussian BEC operator, and the analytic expression (21) for the two-parameter model in arbitrary dimension, have been obtained. The latter includes, in particular, the 2D case formulae (26), (28), (29) absent in HE07, who considered only 1D and 3D cases.

We believe this note may facilitate further development of the BEC models in variational data assimilation. Moreover, since the described methodology can be used for the approximation of arbitrary self-adjoint operators with positive spectrum, results may also find applications beyond the BEC modelling in geophysical inverse problems.

Appendix

Let θ be the angle between $\boldsymbol{x}$ and $\boldsymbol{k}$ in $\mathbb{R}^n$ and $n > 2$. Then the integral (10) can be rewritten in spherical coordinates as

$$B^n(r) = (2\pi)^{-n} \int_0^\infty B(k) \int_{\Omega_{n-1}} \exp(-\mathrm{i}kr\cos\theta) k^{n-1} \, \mathrm{d}k \, \mathrm{d}\Omega_{n-1}, \tag{A.1}$$

where $d\Omega_{n-1}$ is the element of the surface area of the unit sphere. Since $\cos\theta$ changes symmetrically within the limits of integration, the imaginary part of the exponent vanishes. Furthermore, using the identity $d\Omega_{n-1} = d\Omega_{n-2} \cdot \sin^{n-2}\theta\, d\theta$, the integral (A.1) can be rewritten as

$$B^n(r) = (2\pi)^{-n}\int_0^\infty B(k)k^{n-1}\,dk \int_{\Omega_{n-2}} d\Omega_{n-2} \times \int_0^\pi \cos(kr\cos\theta)\sin^{n-2}\theta\, d\theta\,. \tag{A.2}$$

Integration over θ (3.715.21 of Gradshteyn and Ryzhik, 1980) and substitution of the formula for the surface of $(n-2)$-dimensional unit sphere into (A.2) yields (11).

The general relationship (11) also holds for $n = 1, 2$ although these cases require a special (less complicated) treatment.

Acknowledgements

This study was supported by the Office of Naval Research (program element 0602435N). Helpful comments of Prof. C. Bettie and Prof. D. Nechaev are acknowledged.

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