6.10 APPLICATIONS OF SPATIALLY RECURSIVE DIGITAL FILTERS TO THE SYNTHESIS OF INHOMOGENEOUS AND ANISOTROPIC COVARIANCE OPERATORS IN A STATISTICAL OBJECTIVE ANALYSIS

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1. INTRODUCTION

The problem of inverting the very large system of equations implied by the variational principle defining a statistical objective analysis scheme is normally tackled by an iterative numerical method, such as the suitably preconditioned conjugate-gradient or quasi-Newton techniques. At each iteration, there is a requirement to convolve the background error covariance with a gridded field in order to recover another gridded field. Essentially, the background covariance becomes a filtering operator. This particular step, while it is only one of the several algebraic steps that constitute a single iteration cycle, is typically the one that dominates the computational cost in 3D-variational analysis. It is therefore very important to be able to execute it efficiently.

The synthesis of covariance operators by carefully constructed combinations of simpler, one-dimensional filters can be an efficient and versatile approach. To avoid the principal grid directions imposing a spurious anisotropic imprint on the morphology of the synthesized covariance function, each basic one-dimensional filter kernel must closely approximate a Gaussian. Recursive filters are able to mimic this profile efficiently and accurately, as we shall demonstrate. The covariance profile itself is not restricted to be of Gaussian type since, by superposition of a few Gaussian components of different scales, it is possible to produce a range of 'fat-tailed' covariance profiles that are arguably better suited to practical data assimilation. Also, a negative-Laplacian operator applied to a bell-shaped function yields negative side-lobes, which is another way by which it might be desirable to generalize a simple smoothing filter in order to simulate realistic error covariances.

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Recent developments of the recursive filtering technique allow us to consistently extend the synthesis of covariances to incorporate geographically adaptive modifications of covariance scale and amplitude, and general degrees of local stretching and compression in both two and three dimensions at arbitrary orientations. We describe some of these techniques in this paper.

2. HOMOGENEOUS RECURSIVE FILTERS

2.1 *Filters in one dimension*

Let $K/\delta x^2$ denote the finite difference operator:

$$K(\psi)_i/\delta x^2 = -(\psi_{i-1} - 2\psi_i + \psi_{i+1})/\delta x^2, \qquad (1)$$

approximating the differential operator, $-d^2/dx^2$, on a line-grid of uniform spacing δx. The spectral representation of the operator at wavenumber k (wavelength $2\pi/k$) is

$$\hat{K}(k) = \left(2\sin\left(\frac{k\delta x}{2}\right)\right)^2. \qquad (2)$$

Inverting this relationship, we obtain a formula for k^2 in terms of, $\hat{K}$:

$$k^2 = \frac{4}{\delta x^2}\left(\arcsin\left(\frac{\hat{K}^{1/2}}{2}\right)\right)^2. \qquad (3)$$

Clearly, the same formula relates operator $-d^2/dx^2$ to operator K; in fact, the algebraic manipulations we set forth here can be regarded as an application of the 'calculus of operators' (Dahlquist and Björck 1974, p. 311). Using the standard expansion:

$$\arcsin(z) = \sum_{i=0}^{\infty} \gamma_i z^{2i+1}, \quad |z| < 1 \qquad (4)$$

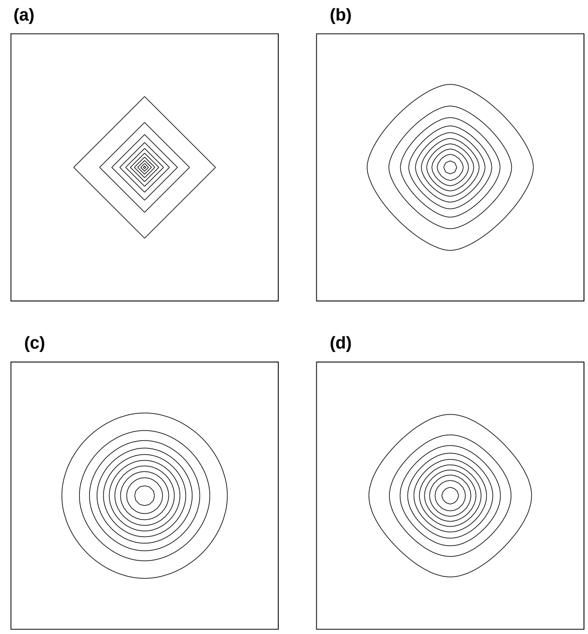

Figure 1. Sequential application of quasi-Gaussian recursive filters of order n in two dimensions. (a) $n = 1$; (b) $n = 2$; (c) $n = 4$; (d) four applications of filters with $n = 1$ with scale parameter adjusted to make the result comparable with the other single-pass filters. Contours are shown at multiples of odd integers.

where

$$\gamma_i = \frac{1}{(2i+1)} . \frac{(2i-1)!!}{(2i)!!}, \tag{5}$$

we may obtain a power expansion for $k^2\delta x^2$, and thence, the expansions for the term, $(k^2\delta x^2)^i$:

$$(k^2\delta x^2)^i = \sum_{j\geq i} b_{i,j}(\hat{K})^j. \tag{6}$$

A tabulation of the coefficients $b_{i,j}$ is given in Purser et al. (2001).

Consider the differential operator:

$$\mathcal{D}_{(n)} = 1 - \frac{a^2}{2}\frac{d^2}{dx^2} \cdots + \frac{1}{n!}\left(-\frac{a^2}{2}\frac{d^2}{dx^2}\right)^n, \tag{7}$$

whose spectral representation is

$$\hat{\mathcal{D}}_{(n)} = 1 + \sigma^2\left(\frac{k^2\delta x^2}{2}\right) \cdots + \frac{\sigma^{2n}}{n!}\left(\frac{k^2\delta x^2}{2}\right)^n, \tag{8}$$

where $\sigma = a/\delta x$. Since,

$$\lim_{n\to\infty} \hat{\mathcal{D}}_{(n)} = \exp\left(\frac{a^2k^2}{2}\right), \tag{9}$$

the substitution of each power series (6) up to degree n for the powers of k^2 into (8) gives us a way of approximating this exponential function in terms of $\hat{K}$:

$$\hat{\mathcal{D}}^*_{(n)} = 1 + \frac{\sigma}{2}\sum_{j=1}^{n} b_{1,j}\hat{K}^j \ldots \frac{1}{n!}\left(\frac{\sigma^2}{2}\right)^n b_{n,n}\hat{K}^n. \tag{10}$$

Correspondingly, there is a finite difference operator, $\mathcal{D}^*_{(n)}$, composed of the nth-degree expansion of K implied by this approximation which, following a rearrangement of terms, we may write:

$$\mathcal{D}^*_{(n)} = 1 + b_{1,1}\frac{\sigma^2}{2}K + \ldots + \left[\sum_{j=1}^{n}\frac{b_{j,n}}{j!}\left(\frac{\sigma^2}{2}\right)^j\right]K^n. \tag{11}$$

Owing to the positivity of all the coefficients $b_{i,j}$, this operator is guaranteed a well-defined inverse.

The reciprocal of the function $\exp(a^2k^2/2)$ in (9) is a Gaussian function in k and is the Fourier transform of a convolution operator (on the line x) whose kernel is also of Gaussian form. Provided we can find a practical way to invert the operator equation,

$$\mathcal{D}^*_{(n)}\boldsymbol{s} = \boldsymbol{p}, \tag{12}$$

for a given input distribution, $\boldsymbol{p}$, the resulting output, $\boldsymbol{s}$, will be an approximation to the convolution of $\boldsymbol{p}$ by the Gaussian function whose spectral transform is the reciprocal of the right-hand-side of (11). The approximation, $(\mathcal{D}^*_{(n)})^{-1}$, to this convolution is what we refer to as a 'quasi-Gaussian filter'. The common centered second-moment of operator $\mathcal{D}_{(n)}$ and its approximation, $\mathcal{D}^*_{(n)}$, is exactly $-a^2$, so a is a convenient measure of the intrinsic distance scale of the smoothing filter implied by the inversion of (12). A useful fact is that the square of the intrinsic scale of the composition of sequential smoothing filters is the sum of squares of the scales of the individual components. Also, as a consequence of the statisticians' 'central limit theorem' applied to convolutions in general, the effective convolution-kernel of such a composition of several identical filter-factors resembles a Gaussian more closely than does the representative factor. Thus, provided it becomes feasible to invert (12), we possess the means to convolve a gridded input distribution with a smooth quasi-Gaussian kernel, at least in one dimension.

As a matrix, $\mathcal{D}^*_{(n)}$ is banded and, for an infinite domain, symmetric. Conventionally, the linear inversion of a system such as (12) might be effected by employing an LU factorization (Dahlquist and Björck 1974) of $\mathcal{D}^*_{(n)}$,

$$\mathcal{D}^*_{(n)} \equiv \mathcal{A}\mathcal{B}, \tag{13}$$

with lower-triangular band matrix, $\mathcal{A}$ and upper-triangular band matrix $\mathcal{B}$, allowing the solution to proceed as two steps of recursive substitution. On an infinite grid, the same principle pertains, but with the guaranteed simplification of: (i) a translational symmetry ensuring that every row of $\mathcal{A}$ is identical (allowing for the trivial translation) and every row of $\mathcal{B}$ is identical; (ii) ordinary matrix symmetry by which we can ensure that $\mathcal{B}$ is simply the transpose of $\mathcal{A}$. In this case, the LU decomposition of $\mathcal{D}^*_{(n)}$ is also of the symmetric, or Cholesky type (Dahlquist and Björck 1974).

In the two stages of solution,

$$\mathcal{A}\boldsymbol{q} = \boldsymbol{p}, \tag{14a}$$

$$\mathcal{B}\boldsymbol{s} = \boldsymbol{q}, \tag{14b}$$

the explicit recursions of the back-substitutions are the following basic recursive filters:

$$q_i = \beta p_i + \sum_{j=1}^{n} \alpha_j q_{i-j}, \tag{15a}$$

$$s_i = \beta q_i + \sum_{j=1}^{n} \alpha_j s_{i+j}, \tag{15b}$$

which are conveniently referred to as the 'advancing' and 'backing' steps respectively since, in the first, index i must be treated in increasing order while, in the second, it must be treated in decreasing order.

2.2 *Filters in two dimensions*

Let x and y be horizontal Cartesian coordinates, k and l the associated wavenumber components. Then in two dimensions, we can exploit the factoring property of isotropic Gaussians:

$$\exp\left(-\frac{a^2\rho^2}{2}\right) = \exp\left(-\frac{a^2k^2}{2}\right)\exp\left(-\frac{a^2l^2}{2}\right), \tag{16}$$

where $\rho = (k^2 + l^2)^{1/2}$ is the total wavenumber. In terms of basic one-dimensional Gaussian smoothing filters, $\mathcal{D}^{(x)}_{(\infty)}$ and $\mathcal{D}^{(y)}_{(\infty)}$, operating in the x and y directions, a two-dimensional *isotropic* filter, G_a, also of Gaussian form, results from the successive application of the one-dimensional factors, $\mathcal{D}^{(x)}_{(\infty)}$ and $\mathcal{D}^{(y)}_{(\infty)}$. For example, an input field, χ, is smoothed to produce the output field, ψ, by the convolution:

$$\psi(\boldsymbol{x}_1) = \int\int G_a(\boldsymbol{x}_1, \boldsymbol{x}_2)\chi(\boldsymbol{x}_2)dx_2\, dy_2 \equiv G_a \star \chi, \tag{17}$$

where

$$G_a = \mathcal{D}^{(y)}_{(\infty)} \star \mathcal{D}^{(x)}_{(\infty)}. \tag{18}$$

The crucial significance of the Gaussian form for the one dimensional filters is that this form is the *only* shape which, upon combination by convolution in the x and y directions, produces an *isotropic* product filter.

Fig. 1 depicts the results obtained by smoothing a delta function placed at the center of a square grid. Fig. 1a shows the result of a single application of the first-order filter, $\mathcal{D}_{(1)}$, in the x and y directions. This result is clearly neither smooth nor even approximately isotropic. Figs. 1b and 1c show the results obtained by using the filters of orders two and four. We see that the appearance of isotropy is not adequately attained until the order exceeds two, but the fourth-order filter shown in Fig. 1c seems to provide an excellent approximation to the isotropic Gaussian. For applications in data assimilation, it is usually worth the cost of applying a filter of at least fourth-order if the filter is to be applied only once in each of the orthogonal grid directions. For a roughly equivalent cost, one may also apply the simple first-order filter four times in succession (but with a scale only a half as large in each instance); the result is shown in Fig. 1d, but is clearly inferior to the use of the single fourth-order filter.

3. INHOMOGENEOUS FILTERS

We can generalize the conditions of homogeneity of the smoothing scales to incorporate the effects of a scale that can vary smoothly across the grid, again, without invalidating the property of self-adjointness. However, this additional generalization requires that, in all appearances of the operator, $(-(a^2/2)d^2/dx^2)$, in the counterpart to the polynomial (11) of this operator, a form of the second derivative factor is substituted which is self-adjoint even when a is a function of x. Of the qualifying possibilities, the one that is most convenient in practice and which leads to a substance-conserving filter, is the one most closely identified with the operation of a diffusive process:

$$-\frac{d}{dx}\frac{a^2(x)}{2}\frac{d}{dx}. \tag{19}$$

4. ANISOTROPIC FILTERS

In addition to spatial inhomogeneity, we would like to be able to stretch the local shape of the covariance function into the form of an ellipse (in two dimensions) or ellipsoid (in three dimensions). Except in the unnatural special cases where the principal axes for the stretching exactly coincide with the coordinate grid directions, we cannot achieve the desired shapes without including non-standard grid lines amongst the set of directions

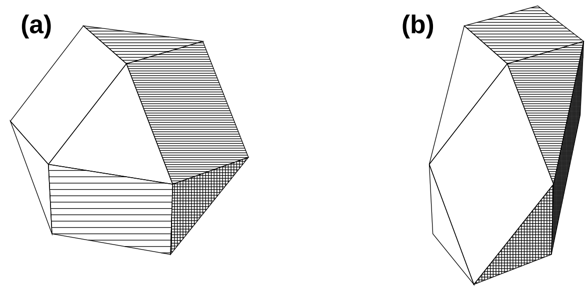

Figure 2. Geometric depiction of an iterative step in the Hexad algorithm, by which one skewed cuboctahedron in the grid has one antipodal pair of its 12 vertices (defining one of the active generalized grid lines) is replaced by another pair, forming another skewed cuboctahedron. The before (a) and after (b) pictures show that the topological configurations remain equivalent although disjoint regions of the space of aspect tensors are made accessible by positive smoothing confined to the two respective hexads of generalized grid lines. Generically, a given aspect tensor can be resolved into positive line-smoothing operations associated with only one hexad of this form.

along which recursive smoothing operators apply. For example, in three dimensions, the description of the requisite stretching generally involves six independent components of a symmetric 'aspect tensor' defining the spatial second moments. The essentially additive property of second moments under composition by spatially unbiased filters (which is an exact result in the case of spatially homogeneous smoothers) allows the six independent aspect tensor components to be resolved into a 'hexad' of generalized grid lines and their associated one-dimensional second moments of dispersion. A special convention for choosing this hexad, which we will briefly describe, ensures that this resolution of the aspect tensor is essentially unique.

On a grid represented by any 3-vector of integers, the directions of a feasible hexad are collectively the set generated by the integer displacements, $\boldsymbol{g}^{ip}$, for $p = 1, \dots 6$, where the triple product,

$$[\boldsymbol{g}^{(i1)}, \boldsymbol{g}^{(i3)}, \boldsymbol{g}^{(i5)}] = 1 \tag{20}$$

and

$$\boldsymbol{g}^{(i2)} = \boldsymbol{g}^{(i5)} - \boldsymbol{g}^{(i3)}, \tag{21a}$$

$$\boldsymbol{g}^{(i4)} = \boldsymbol{g}^{(i1)} - \boldsymbol{g}^{(i5)}, \tag{21b}$$

$$\boldsymbol{g}^{(i6)} = \boldsymbol{g}^{(i3)} - \boldsymbol{g}^{(i1)}, \tag{21cv}$$

In the context of such a hexad it requires only linear analysis to resolve the aspect tensor components into the additive components associated with each of the six generators of a given hexad. However, for the hexad to have validity as a smoother, all six of these projected components must also be non-negative. It can be shown that, for every positive-definite aspect tensor there is essentially always, and only, one way to associate positive projected components with the directions of a feasible hexad.

Geometrically, the 12 points comprising any feasible hexad of generators, together with their antipodes, have a convex-hull in the form of a linearly transformed *cuboctahedron*, two examples of which are shown in Fig. 2. In seeking the valid hexad for a given aspect tensor, when an invalid trial hexad (Fig 2a, say) projects a *negative* component of this tensor onto one of its six diameters, we step closer (e.g., Fig.2b) to the sought-after valid hexad by replacing only the generator associated with the offending line with a generator of the only possible alternative line which the defining hexad rules permit. The stepwise replacement of one trial hexad configuration by another therefore has a nice geometrical interpretation which is illustrated in Fig. 2 by the mutation from panel (a) to (b). A short chain of such iterations will usually suffice to find a given aspect tensor's unique hexad for which the desired anisotropy is obtained by smoothing along this hexad's six directions with the dispersion scales prescribed by the tensor's positive projection into these directions. There is an analogous 'triad algorithm' for the two-dimensional case.

5. ACKNOWLEDGMENTS

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