3A.5 EFFICIENT SITUATION-DEPENDENT COVARIANCE GENERATION USING RECURSIVE FILTERS AND THE METHODS OF RIEMANNIAN GEOMETRY

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1. INTRODUCTION

The recursive filter method for data assimilation began with its use as a provider of convenient and highly efficient quasi-diffusive smoothers in 'successive corrections' empiral analysis schemes (Purser and McQuigg 1982, Hayden and Purser 1986) but it was soon recognized that the method could be easily adapted to the generation of covariances in an optimal analysis (Purser 1983, Lorenc 1992). The filters themselves, in conjunction with the so-called two-dimensional 'Triad' or three-dimensional 'Hexad' methods (Purser 2005), may be regarded as an accelerated algorithm for simulating the finite-time outcome of a general (anisotropic and inhomogeneous) diffusive process resolved on the analysis grid. Derber and Rosati (1989) and Egbert et al. (1994) have also proposed simulated diffusion as a model for (ocean) covariance generation and the former scheme was generalized to fully anisotropic diffusivities by Weaver and Courtier (2001).

2. DIFFUSIVE PROCESSES AND METRICS

The result of diffusion in a Euclidean domain with homogeneous (but not necessarily isotropic) diffusivity tensor is, after any finite duration, a Gaussian distribution whose amplitude is exactly predictable. The centered second moment measure of the spread of the distribution is what we refer to as the 'aspect tensor'; it is, of course, directly proportional to the diffusivity tensor, but increases linearly with duration of the diffusive process. Since we are using diffusion as an idealized model process, and do not intend it to have any physical significance, we may choose the duration, t, conveniently to ensure that the aspect tensor becomes numerically identical to the diffusivity, in which case, our duration will be $t = 1/2$. Real covariances are generally not shaped like Gaussians, but a wider variety of covariance profiles are attainable by the superposition of a small number of the Gaussian 'building blocks' in what amounts to a kind of (inverse) discrete Laplace transform; of the distributions with spherical or ellipsoidal contours, the Gaussians are, by far, the easiest to generate, which is why they are chosen as the raw materials of more complex distributions.

The case where the intended aspect-tensor is *not* spatially homogeneous is challenging in two ways: first, we are now presented with the dilemma of choosing *which* choice of metric to use with the given coordinates that form the framework for the simulated diffusion process; second, we must find some way of estimating the amplitude of the result of this diffusion which is now *not* given accurately by the Gaussian amplitude formula. To take the example of vertical covariances in the atmosphere, even if the vertical scale (the aspect tensor) is a uniform physical distance, we shall obtain a different diffusion equation if we assume the 'capacity' of the space to hold the diffused substance is proportional to physical volume than if we assume it is proportional to the mass of air (whose own density with height changes). More generally, we see the ambiguity of in the general tensorial form of the diffusion equation:

$$\frac{\partial P}{\partial t} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \sqrt{g} D^{ij} \frac{\partial P}{\partial x^j},$$

in which changes in the metric assumptions that determine g (the square-root of the determinant of the covariant metric tensor, g_{ij}) do not directly affect the aspect tensor (which we will continue to identify with the diffusivity, D^{ij}), but the details of the diffusive process, and especially the resulting amplitude, are certainly altered by any change in g.

A perfect resolution to the metrical ambiguity is simply to decree that D^{ij} itself *defines* the metric tesnor (and by implication, the g). In this way, we standardize the diffusion equation to the special

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form:

$$\frac{\partial P}{\partial t} = \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^i}\sqrt{g}g^{ij}\frac{\partial P}{\partial x^j}.$$

What this equations says is that, the diffusion problem the recursive filters (or alternative methods) are tuned to solve is the problem of *uniform* and *isotropic* diffusion, but acting in a decidedly *non-Euclidean* and *non-homogeneous* space! But this choice has the additional benefit of helping us with the second challenge, that of determining the amplitude. There still is no analytic solution that we can look up, but this standardized form of the Riemannian-space diffusion, with unit and isotropic diffusivity, is one which lends itself to an asymptotic approximate solution expressible as an expansion in diagnostics of the intrinsic local geometrical properties of the space itself – essentially its 'curvature', and higher-order generalizations of this concept.

3. THE PARAMETRIX EXPANSION METHOD

The asymptotic expansion method that gives successive approximations to the amplitude adjustment factor that must be applied, as a correction, to the Gaussian amplitude formula, is called the 'Parametrix Expansion' method. It is a technique whose generality extends beyond just the diffusion equation, having been proposed more than a century ago by the Italian geometer, E. E. Levi (1907) and refined by Hilbert (1912). More recently, and in the *same* context as our diffusion, or 'heat kernel' problem, it is finding numerous applications in abstract geometry and topology (e.g., Gilkey 1984, Rosenberg 1997). Only a cursory discussion of the technique will be given here; for technical details, the interested reader is referred to the Gilkey and Rosenberg books or to Purser (2008) where the algebraic development is more fully expounded.

Normal coordinates about a point in a Riemannian geometry are, in a sense, the closest possible local coordinates to being Cartesian (again, for more rigorous definitions, see the above-quoted references). An approximate solution, P_0, in the normal coordinates of an n-dimensional manifold is given by pretending these to be Cartesian coordinates of a Euclidean geometry, so that the familar Gaussian formula is obtained:

$$P_0(t;\mathbf{x}) = \frac{1}{(4\pi t)^{n/2}}\exp\left(-\frac{r^2}{4t}\right),$$

where

$$r^2 = \delta_{ij}x^i x^j,$$

is the square of the radial distance. It is easy to verify the following partial derivatives of this solution, where the independent variables now include time t in addition to the n spatial coordinates:

$$\frac{\partial P_0}{\partial t} = \left(\frac{r^2}{4t^2} - \frac{n}{2t}\right)P_0,$$

$$\frac{\partial P_0}{\partial x^i} = -\frac{\delta_{ij}x^j}{2t}P_0,$$

$$\frac{\partial^2 P_0}{\partial x^i \partial x^j} = \left(\frac{\delta_{ik}\delta_{jl}x^k x^l}{4t^2} - \frac{\delta_{ij}}{2t}\right)P_0.$$

From the trace of the last of these equations we obtain:

$$\delta^{ij}\frac{\partial^2 P_0}{\partial x^i \partial x^j} = \left(\frac{\delta_{ij}x^i x^j}{4t^2} - \frac{n}{2t}\right)P_0,$$

and thereby verify that P_0 does indeed obey the Euclidean form of the diffusion equation:

$$\frac{\partial P_0}{\partial t} = \delta^{ij}\frac{\partial^2 P_0}{\partial x^i \partial x^j}.$$

The time-dependent solution we are more interested in, expressed as $P(t;\mathbf{x})$, the product of the known $P_0(t,\mathbf{x})$ and a smooth modulating function $T(t,\mathbf{x})$:

$$P(t;\mathbf{x}) = P_0(t;\mathbf{x})T(t;\mathbf{x}),$$

is the one initialized by a unit impulse at the normal coordinate origin and that obeys the diffusion equation discussed in Part I of Purser(2008):

$$\frac{\partial P}{\partial t} = \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^i}\sqrt{g}g^{ij}\frac{\partial P}{\partial x^j}$$

$$= W^i\frac{\partial P}{\partial x^i} + g^{ij}\frac{\partial^2 P}{\partial x^i \partial x^j},$$

where,

$$W^i = g^{ij}\left(\frac{1}{2}\frac{\partial g_{kl}}{\partial x^j} - \frac{\partial g_{jk}}{\partial x^l}\right)g^{kl} = -\Gamma^i{}_{kl}g^{kl}.$$

Here, Γ denotes the Christoffel symbol of the second kind (e.g. Synge and Schild 1949, Kreysig 1991). The idea is that, for small t, the solutions P and P_0 are very alike and the modulating function, T, is close to unity. As t increases, the T remains smooth so that it can be approximated by a power series expansion in both time and space. We write the vector of nonnegative integer exponents of the spatial coordinates in such an expansion as $\boldsymbol{p}$, so that the generic form of the power expansion of T becomes:

$$T(t;\mathbf{x}) = 1 + \sum_{s,\boldsymbol{p}\geq 0}\hat{T}_{s;\boldsymbol{p}}t^s\mathbf{x}^{\boldsymbol{p}},$$

with the obvious meaning attached to the vector exponents on the right. Naturally,

$$\hat{T}_{0;\mathbf{0}} = 0,$$

but the other components must be established, step by step, through iterative back substitutions that enable the coefficients in both the time and the space parts of the expansion of $T(t; \mathbf{x})$ to remain consistent with both sides of the diffusion equataion. If we denote the temporal set of coefficients,

$$T_s \equiv \hat{T}_{s;\mathbf{0}},$$

we find, after a considerable mass of algebraic substitutions (see Purser 2008), that:

$$T_1 = \frac{1}{6}R,$$

$$T_2 = \frac{1}{180}\left(12\nabla^2 R + 5R^2 - 2R_{ij}R^{ij} + 2R_{ijkl}R^{ijkl}\right).$$

where R, R^{ij}, and R^{ijkl} are the Ricci scalar, Ricci tensor, and Riemann-Christoffel curvature tensor, respectively.

In two dimensions, where the Riemann curvature is expressible in terms of the Ricci curvature, we obtain,

$$T_2 = \frac{1}{60}\left(2R_{ij}R^{ij} + R^2 + 4\nabla^2 R\right),$$

which further reduces in two-dimensions to

$$T_2 = \frac{1}{30}(R^2 + 2\nabla^2 R)$$
$$= \frac{2}{15}(\kappa^2 + \nabla^2 \kappa),$$

where $\kappa = R/2$ is the Gaussian curvature.

The desired parametrix expansion for the amplitude factor comes from the evaluation of T at $t = \frac{1}{2}$. For example, in two dimensions, the second-order expansion becomes:

$$T(\frac{1}{2}, 0) \approx 1 + \frac{T_1}{2} + \frac{T_2}{8}$$
$$= 1 + \frac{\kappa}{6} + \frac{1}{60}(\kappa^2 + \nabla^2 \kappa).$$

4. PRACTICAL IMPLEMENTATION

The parametrix method, being of the asymptotic kind, does not generally yield a converging solution. In practical applications it is therefore necessary to implement the procedure with safeguards to protect against the wildly divergent expansions that result from locally large values of the implied curvature (coming from second derivatives of the aspect tensor) or of the spatial derivatives of curvature. The robust implementation employs 'saturation functions' of the curvature diagnostics in place of the quantities themselves where, by 'saturation function' we mean a function similar to the hyperbolic tangent, rising monotonically to a finite plateau. By such methods it is possible to immunize the amplitude estimation procedure, to a large degree, and ensure that it works reliably to produce covariances of approximately the intended amplitude for all reasonable spatial variations of the adaptive aspect tensors.

5. DISCUSSION

The amplitude estimation procedure outlined here is being implemented at NCEP in a reformulation of the recursive filter covariance generator that uses the given aspect tensor to define the effective metric, and hence the necessary curvature diagnostics, of the Riemannian geometry. If successful, it is intended that the method will eventually become a part of the various operational analyses. But another potential application of adaptive filters with well-controlled amplitudes is to the problem of characterizing analysis error (or at least the ratio between analysis error and background error), which is generally much less spatially homogeneous than is the background error, and therefore intrinsically harder to characterize adequately. Should the representation of analysis error/back ground error ratio prove to be feasible by these filters, then it should, in principle, be possible also to apply them to the related problem of better preconditioning the minimization algorithm for the analysis. These aspects of the adaptive filters will be examined in the future.

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