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NORMALIZATION OF THE DIFFUSIVE FILTERS THAT REPRESENT THE INHOMOGENEOUS COVARIANCE OPERATORS OF VARIATIONAL ASSIMILATION, USING ASYMPTOTIC EXPANSIONS AND TECHNIQUES OF NON-EUCLIDEAN GEOMETRY; PART II: RIEMANNIAN GEOMETRY AND THE GENERIC PARAMETRIX EXPANSION METHOD

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Abstract

This note is the second part of a study which develops the geometrical ideas that underly the 'parametrix expansion' asymptotic method for estimating the shape of the impulse response function of the diffusion equation in a smoothly curved non-Euclidean space. This part of the study develops the algebraic tools required to treat the general n-dimensional case in Riemannian geometry. Notations are developed both to facilitate the hand calculations for the low-order expansion terms, and to enable the bulk of the algebraic manipulations to be automated, should it become desirable to carry out the asymptotic expansion to a higher order. The general procedure is illustrated by exhibiting, in moderate detail, the algebraic operations required to obtain the first two coefficients for the amplitude adjustment quotient in the n-dimensional case, and for the important special cases of two and three dimensions where the curvature terms upon which the formulas depend take on simpler forms.

1. Introduction

Part I of this study (Purser 2008) considered the problem of estimating the amplitude of the 'heat kernel' (describing the result of diffusion applied for a given finite time to an initial impuse) in the special cases of highly symmetric intrinsically curved geometries. This topic is of considerable importance in modern data assimilation because the covariances we employ in three-dimensional variational assimilation ('3DVar') often use such heat-kernels, or quasi-Gaussians, as their basic building blocks; if the amplitude is mis-specified, the variance of the error in the background field is automatically wrong. NCEP uses recursive filters (e.q., Wu at al. 2002). For ocean data assimilation, explicit simulations of the diffusion process have been proposed (Derber and Rosati 1989; Weaver and Courtier 2001). When the recursive filter parameters, or the diffusivities, are permitted to vary smoothly in space, a method is needed to regulate the resulting rather unpredictable amplitudes. The examples of Part I served to introduce and exemplify the easiest applications of the 'parametrix expansion method', an asymptotic method of approximation for the ratio of the curved-space and Euclidean space kernel amplitude. At each stage of the parametrix expansion, the approximation to this ratio is constructed as some polynomial in the appropriate curvature tensor together with its first few covariant derivatives. In order to generalize the results we obtained to Riemannian geometries unconstrained by artificial conditions of symmetry we need, first, to develop some of the algebraic machinery of Riemannian geometry, and then to extend the parametrix method introduced in Part I to this more general situation.

Accordingly, in this Part II we introduce the notation and some of the relevant geometrical techniques in section 2 before developing the general parametrix expansion method for n dimensional Riemannian geometry in section 3. As in Part I, we adapt the simplest form of the parametrix expansion, which exhibits serious divergence even at first or second order when the diagnostics on which it depends become excessive, so that the adapted expansions, while still consistent with the formal asymptotic expansion, are inhibited from diverging strongly. The best of these practical 'robust' formulations in two dimensions were determined through the careful trials documented in Part I, and have been generalized here to the more complicated three-dimensional (3D) parametrix expansions. We describe these generalizations, and test them in idealized synthetic Riemannian geometries in section 4. We also speculate on how a practical 4D algorithm would look. We conclude with a review of the progress made and some promising avenues for future extensions and refinements of the methods proposed. Four appendices are provided to contain the more specialized technical material relating to the main text.

2. Tensors, Riemann metrics, curvature, and the shape of space

This section reviews tensor analysis and Riemannian geometry. While some of this material may be found in various standard texts of differential geometry, such as Kreyszig (1991), Synge and Schild (1949), Lovelock and Rund (1989), Burke (1985), or within texts devoted to the theory of General Relativity, such as Misner et al. (1970), Hawking and Ellis (1973), we give emphasis to the special parts of this subject that will become relevant in the applications to the parametrix expansion method described in section 3. Conventions of sign and notation vary from one author to another, so we establish our own notational conventions here. We develop and extend the concept of intrinsic curvature to include 'shape tensors' that generalize the celebrated 'Riemann' (or, sometimes, 'Riemann-Christoffel') fourth-rank curvature to the tensors of still higher rank that describe the local, but higher degree, variations of a space's intrinsic geometry. In this way we establish the geometrical tools that we shall employ to analyze the asymptotic behavior of uniform diffusive processes in smoothly curved spaces.

(a) *The metric and the rules of tensor transformation*

A coordinate system, $\boldsymbol{x} \equiv \{x^i\}$, for a point in n dimensions of a Riemannian space has a metric function associated with any pair of such points obtained implicitly by minimizing the integral of the infinitesimal distance element, ds, over all possible connecting paths, where:

$$ds^2 = g_{ij} dx^i dx^j. \tag{2.1}$$

Here we adopt the usual summation convention, tacitly assuming a summation from 1 to n for any repeated dummy indices that appear in the same term (where they must appear once in the upper 'contravariant' index position and once in the lower 'covariant' position, as both i and j do in (2.1) above). The 'metric' is the symmetric tensor field whose covariant (or 'type [0,2]') representation comprises the quantities g_{ij} at each point. The corresponding symmetric contravariant (or 'type-[2,0]') metric tensor, g^{ij}, is the inverse of g_{ij}. The mixed (or 'type-[1,1]') metric tensor field, g_i^k, is therefore at every point indistinguishable from the Kronecker 'δ' symbol or, in matrix form, the identity operator, with components:

$$g_i^k = \delta_i^k = \begin{cases} 1 & : \quad i = k, \\ 0 & : \quad i \neq k. \end{cases} \tag{2.2}$$

The local volume element is

$$d\tau = \sqrt{g}\, dx^1 \dots dx^n, \tag{2.3}$$

where g is the determinant of the covariant metric:

$$g = |g_{\bullet\bullet}|. \tag{2.4}$$

Vectors and tensors are directional quantities existing within the space and possessing geometrical relationships with the local orientations of the space that exist independently of any particular choice of the coordinates. For example, the gradient vector field $\boldsymbol{V}$ of a given scalar field, ϕ, is the same physical quantity associated with the same local direction at a particular point, regardless of the coordinates used as a convenience to define the numerical magnitudes of the components involved, and the resulting consistent behavior of such a vector field must be reflected in the manner in which one representation of the vectors is transformed into another. The use of covariant and contravariant vector and tensor representations simply facilitates their consistent transformations among alternative coordinates by employing the most convenient convention – one that ties the local basis vectors to the local derivatives of the associated coordinate frames. For example, the field of the vector corresponding to $\boldsymbol{V}$, the gradient of ϕ, is written for a coordinate system, $\{x^i\}$, in terms of its covariant components as simply the partials:

$$V_i = \frac{\partial \phi}{\partial x^i}. \tag{2.5}$$

Thus, the transformation of this representation to the equivalent covariant representation corresponding to another coordinate system, $\{\hat{x}^\alpha\}$, is nothing more than the usual 'chain-rule':

$$\hat{V}_\alpha = \hat{a}^i_{\ \alpha} V_i, \tag{2.6}$$

where the Jacobian matrix $\hat{a}$ denotes the partials of the x^i with respect to the $\hat{x}^\alpha$:

$$\hat{a}^i_{\ \alpha} = \frac{\partial x^i}{\partial \hat{x}^\alpha}. \tag{2.7}$$

Any other vector representation that consistently transforms as (2.6) is referred to as a 'covariant vector'. The inverse of the Jacobian matrix of the transformation is the Jacobian of the reverse coordinate transformation:

$$a^\alpha_{\ i} = \frac{\partial \hat{x}^\alpha}{\partial x^i}, \tag{2.8}$$

and it is this operator that transforms the coordinate differentials from the frame $\{x^i\}$ to the frame $\{x^\alpha\}$:

$$d\hat{x}^\alpha = a^\alpha_{\ i} dx^i. \tag{2.9}$$

Eq. (2.9) supplies the prototypical transformation idiom of the 'contravariant vectors'. In order that the infinitesimal line element length ds, and other scalars obtained by contractions of tensors with vectors, remain invariant with respect to changes in coordinates, we deduce that the covariant, mixed and contravariant tensors of second rank (such as the metric tensors) must transform according to the rules:

$$\hat{T}_{\alpha\beta} = \hat{a}^i_{\ \alpha} \hat{a}^j_{\ \beta} T_{ij}, \tag{2.10a}$$
$$\hat{T}^\alpha_{\ \beta} = a^\alpha_{\ i} \hat{a}^j_{\ \beta} T^i_{\ j}, \tag{2.10b}$$
$$\hat{T}^{\alpha\beta} = a^\alpha_{\ i} a^\beta_{\ j} T^{ij}. \tag{2.10c}$$

(*b*) *Christoffel symbols and covariant derivatives*

The shortest distance definition implicitly defines the shortest path, or 'geodesic', along which ds is integrated to give the finite distance between a pair of points. The equation for such a geodesic, given some initial direction and rate of change, dx^i/ds, is:

$$\frac{d^2x^i}{ds^2} = -\Gamma^i_{\ jk}\frac{dx^j}{ds}\frac{dx^k}{ds}, \tag{2.11}$$

where $\Gamma^i_{\ jk}$ denotes the Christoffel symbol of the second kind (type-[1,2]). This entity, and its lowered index counterpart, the Christoffel index of the first kind, $\Gamma_{i\,jk}$ (type-[0,3]), are defined in terms of the first partial derivatives of the metric:

$$\Gamma^i_{\ jk} = g^{il}\Gamma_{l\,jk}, \tag{2.12}$$

where,

$$\Gamma_{l\,jk} = \frac{1}{2}\left(\frac{\partial g_{lk}}{\partial x^j} + \frac{\partial g_{lj}}{\partial x^k} - \frac{\partial g_{jk}}{\partial x^l}\right). \tag{2.13}$$

In expressions where spatial partial derivatives are understood to be with respect to just a single fixed set of coordinates then the 'comma' notation conveniently abbreviates expressions and places all their subscripts in a single typographic line. Thus, the expression (2.13) appears in this notation,

$$\Gamma_{l\,ik} = \frac{1}{2}\left(g_{lk,j} + g_{lj,k} - g_{jk,l}\right). \tag{2.14}$$

With these definitions, one may verify that the solution of the geodesic equation of (2.11) leads to a uniform parameterization of it in the sense that:

$$\frac{d}{ds}\left(g_{ij}\frac{dx^i}{ds}\frac{dx^j}{ds}\right) = 0. \tag{2.15}$$

From definition (2.12), an important contraction of the Christoffel symbol is:

$$\Gamma^i_{\ ij} = \frac{1}{2g}g_{,j} = \frac{1}{2}(\ln g)_{,j}. \tag{2.16}$$

From the transformation rules of the metric, it is found that the above-defined entities, Γ, are *not* tensors, but attributes of the local curvature of the particular coordinates being used. They provide an especially natural definition of a 'connection', which enables the construction of sets of spatial derivatives of fields of vectors (and hence of tensors) that are themselves properly tensorial in their rules of transformation. (The partials of a vector or tensor field by themselves do *not* possess this property in general.)

We shall employ the notation, $V_{i|j}$, for the covariant derivative of a covariant vector V_i with respect to x^j. The covariant derivative of a contravariant vector, V^i, is then:

$$V^i_{|j} = V^i_{,j} + \Gamma^i_{\ jk}V^k, \tag{2.17}$$

and its contraction provides the standard divergence of vector $\boldsymbol{V}$ which, from (2.16), becomes:

$$V^i_{|i} = V^i_{,i} + \frac{1}{2g}g_{,i}V^i \equiv \frac{1}{\sqrt{g}}\left(\sqrt{g}V^i\right)_{,i}. \tag{2.18}$$

Covariant differentiation also applies to tensors, for example:

$$T^{ij}_{\ \ |k} = T^{ij}_{\ \ ,k} + \Gamma^{i}_{\ lk}T^{lj} + \Gamma^{j}_{\ lk}T^{il}, \tag{2.19a}$$

$$T^{i}_{\ j|k} = T^{i}_{\ j,k} + \Gamma^{i}_{\ lk}T^{l}_{\ j} - \Gamma^{l}_{\ jk}T^{i}_{\ l}, \tag{2.19b}$$

$$T_{ij|k} = T_{ij,k} - \Gamma^{l}_{\ ik}T_{lj} - \Gamma^{l}_{\ jk}T_{il}. \tag{2.19c}$$

The corresponding covariant derivatives of tensors of higher ranks follow the obvious generalization (see Lovelock and Rund 1989). The metric tensor is notable in that its covariant derivative vanishes. In a Riemann space, the representations of vectors and tensors are freely convertible between their various combinations of contravariant and covariant forms simply by applying the appropriate contractions with metric tensors:

$$V^i = g^{ij}V_j. \tag{2.20}$$

For repeated covariant differentiation of a generic quantity, ( ), we shall write

$$(\ )_{|ij} \equiv \Big[(\ )_{|i}\Big]_{|j}, \tag{2.21}$$

and note that, in general, covariant differentiation does **not** commute:

$$(\ )_{|ij} \neq (\ )_{|ji}, \tag{2.22}$$

an exception being the case where the quantity ( ) in (2.22) is a scalar (the resulting tensor is known as the 'Hessian').

(*c*) *Riemann curvature as a measure of noncommutation of covariant derivatives*

The noncommutation of the covariant derivative is a symptom of the intrinsic curvature of the space. In the case of a covariant vector, V_j, a direct calculation shows that,

$$(V_{j|k})_{|l} - (V_{j|l})_{|k} = R^{i}_{\ jkl}V_i, \tag{2.23}$$

where the new type [1,3] tensorial object,

$$R^{i}_{\ jkl} = \Gamma^{i}_{\ jl,k} - \Gamma^{i}_{\ jk,l} + \Gamma^{m}_{jl}\Gamma^{i}_{\ mk} - \Gamma^{m}_{jk}\Gamma^{i}_{\ ml}, \tag{2.24}$$

is the Riemann curvature tensor. Implicit in this definition is the result that, given an infinitesimal quadrilateral circuit generated by the ordered displacements, da^k and db^l, the change in vector, initially $\boldsymbol{V}$, upon being parallel-transported around the circuit, $\boldsymbol{x}, \boldsymbol{x}+\boldsymbol{da}, \boldsymbol{x}+\boldsymbol{da}+\boldsymbol{db}, \boldsymbol{x}+\boldsymbol{db}, \boldsymbol{x}$, is:

$$\Delta V^i = -R^{i}_{\ jkl}\, V^j\, da^k\, db^l. \tag{2.25}$$

This interpretation is discussed in Synge and Schild (1949). Further insight into the meaning of the curvature tensor, associated tensors and their generalizations, is gained by the introduction of the normal geodesic coordinates.

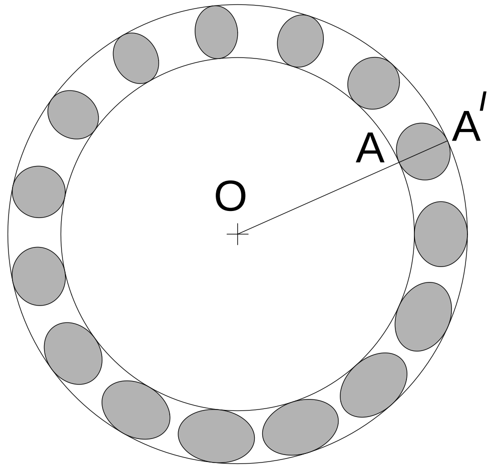

Figure 1. Schematic depiction of the train of 'Huygens wavelets' separating two successive 'wavefronts' of constant distance from the origin in normal geodesic coordinates. In the limit of infinitesimal separation of the two wavefronts, the wavelets exhibit elliptical shapes characteristic of the local representation of the metric tensor which, in order to maintain the points of tangency, A and A', in line with the center, O, must have this radial vector as an eigenvector and with unit eigenvalue.

(*d*) *Normal coordinates and 'shape' tensors of rank four*

In the neighborhood around a point of interest, $\boldsymbol{O}$, we construct a new coordinate system $\{\hat{x}^\alpha\}$ having $\boldsymbol{O}$ as its origin and locally possessing, as far as is possible, the familiar properties of a Cartesian coordinate set. The matrices formed by the metric tensors at $\boldsymbol{O}$ are the identity matrix and the geodesics through $\boldsymbol{O}$ are mapped to 'straight lines' in the sense that the coordinates $\hat{x}^\alpha$ preserve the same mutual ratio along the extent of any such geodesic. Also, the square of the distance from $\boldsymbol{O}$ is just the sum of squares of these coordinates. Points a fixed distance, s, from $\boldsymbol{O}$ therefore comprise the surface of a 'hypersphere' in the Cartesian interpretation of these normal coordinates.

The 'Huygens wavelet' construction of Fig. 1 schematically illustrates conditions on the infinitesimal spherical wavelets which must hold if they are to separate, with tangential contact, a pair of concentric spherical wave fronts. The straightness of the mapped radial geodesic OAA' in normal coordinates implies that the radial vector at each point is an eigenvector, with unit eigenvalue, of the local mapped metric, $\hat{g}_{ij}$. If this were not so, the points of tangency of the elliptically-mapped wavelets in the Cartesian map-space would lie on different radials for the outer wavefront than for the inner. If we introduce both doubly superscripted and doubly subscripted versions of the Kronecker symbol, with the stipulation that the index-raising/lowering actions of the metric tensors do *not* apply to them:

$$\left.\begin{array}{c}\delta^{ij}\\[2ex]\delta_{ij}\end{array}\right\} = \left\{\begin{array}{ccc}1 & : & i=j\\[2ex] 0 & : & i\neq j\end{array}\right. , \tag{2.26}$$

then we can state the eigenvector property with strict adherence to tensorial index notation:

$$\delta^{ij} g_{jk} x^k = g^{ij} \delta_{jk} x^k = x^i. \tag{2.27}$$

The normal coordinate vector is therefore an eigenvector of both the covariant and contravariant metric tensor everywhere, and with a unit eigenvalue.

We can expand the representation of g_{ij} as a Taylor series:

$$g_{ij}(\boldsymbol{x}) = \delta_{ij} + J_{ij\,k}x^k + J_{ij\,kl}x^k x^l + J_{ij\,klm}x^k x^l x^m \ldots, \tag{2.28}$$

where all the successive J are tensors and have coefficients assumed to be symmetric, both under transposition of the leading pair of indices, i and j, and also under permutation among any of the remaining indices. They will be referred to 'Jacobi shape tensors'. We emphasize that the definition of each tensor from (2.28) associates it only with the particular origin $\boldsymbol{O}$ chosen. While it is clearly possible to extend each J to a 'tensor field' by associating each new evaluation of it with its own locally-defined prescription corresponding to the new version of (2.28) that has as its origin this new evaluation point, we shall restrict our study to the case of a single fixed normal coordinate frame and will never assume tensors J to have any spatial extension; in particular, we shall not be obliged to differentiate these J.

Since the eigen-condition (2.27) holds for all neighboring $\boldsymbol{x}$, each row and each column of the contribution to $g_{\bullet\bullet}$ from any given J term must be reducible to a superposition of polynomials times vectors which are both linear in $\boldsymbol{x}$, and orthogonal to it. At each location $\boldsymbol{x}$, such vectors, $\boldsymbol{U}$, can always be expressed as a superposition of the form:

$$U_i = U_{pq}\left(\delta_i^p\delta_j^q - \delta_j^p\delta_i^q\right)x^j. \tag{2.29}$$

No loss of generality is incurred by assuming U_{pq} in (2.29) to be antisymmetric, $U_{pq} = -U_{qp}$, which implies that the rank of the implied linear space of $\boldsymbol{U}$ is $n(n-1)/2$ for a physical space of dimension n.

We find that no nonvanishing term, $J_{ij\,k}x^k$, can be formed with both row i and column j contributions to the metric being of the necessary form (2.29), so this term drops out. The general quadratic term may be expressed as a superposition of basic terms of the kind:

$$M_{ij}^{pq\,rs} = \left(\delta_i^p\delta_k^q - \delta_k^p\delta_i^q\right)\left(\delta_j^r\delta_l^s - \delta_l^r\delta_j^s\right)x^k x^l, \tag{2.30}$$

that is,

$$\begin{aligned} J_{ik\,jl}x^j x^l &= \frac{1}{4}Q_{pqrs}M_{ik}^{pq\,rs} \\ &= \frac{1}{4}(Q_{ij\,kl} - Q_{ji\,kl} - Q_{ij\,lk} + Q_{ji\,lk})x^j x^l, \end{aligned} \tag{2.31}$$

provided we respect the symmetry of the metric tensor by requiring:

$$Q_{ij\,kl} = Q_{kl\,ij}. \tag{2.32}$$

Again, we lose no generality by also requiring the antisymmetries:

$$Q_{ij\,kl} = -Q_{ji\,kl} = -Q_{ij\,lk}, \tag{2.33}$$

so that,

$$J_{ik\,jl}x^j x^l \equiv Q_{ij\,kl}x^j x^l. \tag{2.34}$$

Like J, Q is a tensor defined only locally and will never be differentiated. On the basis of these symmetries alone, we seem to have as many distinct components as there are independent elements in a symmetric matrix of order $n(n-1)/2$. However, the matrices of quadratic polynomials, $\boldsymbol{M}$, possess a further symmetry among each subset of such matrices sharing the same four upper indices (p, q, r, s) whenever these indices are all distinct (which can only happen in four or more dimensions). We see this by first symmetrizing these matrices:

$$\overline{M}_{ik}^{pq\,rs} = M_{ik}^{pq\,rs} + M_{ik}^{rs\,pq}, \tag{2.35}$$

and abbreviating the components of $\boldsymbol{x}$ associated with the representative index subset by $w \equiv x^p$, $x \equiv x^q$, $y \equiv x^r$ and $z \equiv x^s$. Matrices $\overline{\boldsymbol{M}}$ with these upper indices in any permutation have nonvanishing components only in rows i and columns k that also correspond to this same 4-dimensional subspace. Displaying only these active rows and columns and cyclically permuting the trailing three upper indices we find:

$$\overline{\boldsymbol{M}}^{pq\,rs} = \begin{bmatrix} 0, & 0, & xz, & -xy \\ 0, & 0, & -wz, & wy \\ xz, & -wz, & 0, & 0 \\ -xy, & wy, & 0, & 0 \end{bmatrix}, \tag{2.36a}$$

$$\overline{\boldsymbol{M}}^{pr\,sq} = \begin{bmatrix} 0, & -yz, & 0, & xy \\ -yz, & 0, & wz, & 0 \\ 0, & wz, & 0, & -wx \\ xy, & 0, & -wx, & 0 \end{bmatrix}, \tag{2.36b}$$

$$\overline{\boldsymbol{M}}^{ps\,qr} = \begin{bmatrix} 0, & yz, & -xz, & 0 \\ yz, & 0, & 0, & -wy \\ -xz, & 0, & 0, & wx \\ 0, & -wy, & wx, & 0 \end{bmatrix}, \tag{2.36c}$$

whose sum vanishes:

$$\overline{\boldsymbol{M}}^{pq\,rs} + \overline{\boldsymbol{M}}^{pr\,sq} + \overline{\boldsymbol{M}}^{ps\,qr} = \boldsymbol{O}. \tag{2.37}$$

This cancellation still occurs when the four upper indices are *not* distinct, but these cases are already dealt with by the other symmetry conditions. The number of independent instances of the new symmetry (sometimes referred to as Bianchi's algebraic identity) is equal to the number of ways of choosing four indices from the available n; the number of degrees of freedom of independent variations of the metric up to second degree in the expansion is therefore correspondingly reduced to:

$$F(n) = \binom{n(n-1)/2+1}{2} - \binom{n}{4} = n^2(n^2-1)/12. \tag{2.38}$$

So as not to incur ambiguity in the coefficients, $Q_{ij\,kl}$, in these cases where the indices are distinct, we can impose the rule that they obey the same cyclic symmetry:

$$Q_{ij\,kl} + Q_{ik\,lj} + Q_{il\,jk} = 0, \tag{2.39}$$

and then the representation, by $Q_{ij\,kl}$, of the quadratic variation of the metric $\boldsymbol{g}_{\bullet\bullet}$ is rendered unique.

By the manner of its construction, $Q_{ij\,kl}$, possesses the attributes of a fourth-rank tensor when the normal coordinates $\boldsymbol{x}$ are transformed by orthogonal rotations (which leave all the defining properties of the normal coordinates invariant). This Q is the first of the series of what we can generically refer to as the 'Riemann shape tensors'. The reason for this choice of terminology is, as we show below, that the rank-four instance of Q turns out to be nothing more than a multiple of the Riemann curvature; likewise, a multiple of the rank-four instance of J, is known as the Jacobi curvature tensor (Misner et al. 1970), which justifies our naming the J family the 'Jacobi shape tensors'.

It is instructive to see what numerical values emerge for Q in the case of a space in 2D with constant Gaussian curvature, κ. For $\kappa > 0$ this represents an ordinary sphere of radius $1/\sqrt{\kappa}$. Let ϕ denote the colatitude and θ the longitude. Taking $\boldsymbol{O}$ to be the 'pole', we write the two normal coordinates $x \equiv \hat{x}^1$, $y \equiv \hat{x}^2$,

$$\begin{aligned} x &= \kappa^{-\frac{1}{2}}\phi\cos\theta, &\text{(2.40a)}\\ y &= \kappa^{-\frac{1}{2}}\phi\sin\theta. &\text{(2.40b)}\end{aligned}$$

Expressing the metric definition,

$$ds^2 = \kappa^{-1}d\phi^2 + \kappa^{-1}(\sin\phi)^2 d\theta^2, \tag{2.41}$$

and defining the radial distance,

$$r = (x^2 + y^2)^{\frac{1}{2}}, \tag{2.42}$$

so that

$$\begin{aligned} d\phi &= \frac{\kappa^{\frac{1}{2}}}{r}(x\,dx + y\,dy), &\text{(2.43a)}\\ d\theta &= \frac{1}{r^2}(-y\,dx + x\,dy), &\text{(2.43b)}\end{aligned}$$

we find that:

$$ds^2 = (dx^2 + dy^2) - \frac{1}{r^2}\left\{1 - \left[\frac{\sin(\kappa^{\frac{1}{2}}r)}{\kappa^{\frac{1}{2}}r}\right]^2\right\}\left(y^2dx^2 - 2xy\,dx\,dy + x^2dy^2\right). \tag{2.44}$$

We can use the expansion,

$$\begin{aligned} (\frac{\sin\phi}{\phi})^2 &= \frac{1}{2\phi^2}(1 - \cos\ 2\phi)\\ &= 1 - \frac{1}{3}\phi^2 + \frac{2}{45}\phi^4 + \mathcal{O}(\phi^6), &\text{(2.45)}\end{aligned}$$

to express the metric, $\boldsymbol{g}_{\bullet\bullet}$:

$$\boldsymbol{g}_{\bullet\bullet} = \boldsymbol{I} - \left(\frac{\kappa}{3} - \frac{2\kappa^2 r^2}{45}\right)\boldsymbol{M} + \text{higher order terms}, \tag{2.46}$$

where $\boldsymbol{M}$ is the essentially unique nontrivial example in 2D of a matrix of the construction (2.30), such as is given by indices, $(p, q, r, s) = (1, 2, 1, 2)$. Explicitly,

$$\boldsymbol{M} = \begin{bmatrix} y^2, & -xy \\ -xy, & x^2 \end{bmatrix}. \tag{2.47}$$

Hence, in this example, $Q_{12\,12} = -\kappa/3$, and a rescaling to make this curvature component match the Gaussian curvature is obtained by simply multiplying the components of Q by -3:

$$\hat{Q}_{ij\,kl} = -3Q_{ij\,kl}. \tag{2.48}$$

Note that the classical hyperbolic geometry is obtained by formally taking $\kappa < 0$, whereupon,

$$[\sin(\kappa^{\frac{1}{2}}r)]^2 = [i\ \sinh((-\kappa)^{\frac{1}{2}}r)]^2 = -[\sinh(|\kappa|^{\frac{1}{2}}r)]^2. \tag{2.49}$$

Returning to the general case, although the Christoffel symbols vanish in the normal coordinates at $\boldsymbol{O}$, their derivatives, expressible as second derivatives of the metric, do not. From the special condition at $\boldsymbol{O}$ which allows the simplification:

$$R_{ij\,kl} = \Gamma_{i\,jl,k} - \Gamma_{i\,jk,l} \tag{2.50}$$

and

$$\Gamma_{i\,jl,k} = J_{il\,jk} + J_{ij\,kl} - J_{jl\,ik}, \tag{2.51}$$

we obtain:

$$\begin{aligned} R_{ij\,kl} &= J_{il\,jk} - J_{jl\,ik} - J_{ik\,jl} + J_{jk\,il}, \\ &= \frac{1}{2}\left(Q_{ij\,lk} + Q_{ik\,lj} - Q_{ji\,lk} - Q_{jk\,li} - Q_{ij\,kl} - Q_{il\,kj} + Q_{ji\,kl} + Q_{jl\,ki}\right) \\ &= -3Q_{ij\,kl} \equiv \hat{Q}_{ij\,kl}. \end{aligned} \tag{2.52}$$

In other words, the same rescaling that allows the relevant components of Q to match the Gaussian curvature of two-dimensional sections brings this tensor into exact numerical correspondence with the Riemann tensor. This exercise confirms that the fourth-rank *Jacobi* shape tensor, J, retains all the information contained in its *Riemann* counterpart, $Q_{ij\,kl}$, and that the latter is indeed a fixed multiple of the Riemann curvature tensor.

In order to determine how many degrees of freedom can be exercised at a higher degree of the expansion of the metric in powers of the normal coordinate components, it helps to consider the pattern formed by the 'lexicographic' ordering of the components of $R_{i'j'\,k'l'}$ that are each strictly independent of any entries that have preceded them in the lexicon. Fig. 2 depicts the bottom corner of the generic pattern for an arbitrary number of spatial dimensions, n, in the form of a matrix indexed by 'rows' and 'columns' formed by the leading and trailing **pairs** of indices respectively. Owing to the (anti-)symmetries: $R_{i'j'\,k'l'} = -R_{j'i'\,k'l'}$ and $R_{i'j'\,k'l} = -R_{i'j'\,l'k'}$, these 'rows' and 'columns' can be restricted in the lexicon to just the $n(n+1)/2$ index pairs with $i' < j'$ (rows), and likewise, $k' < l'$ (columns). The lexicographic ordering of the serially-independent tensor elements is obtained by 'reading' rows from left to right and from the top row downward, where, for n dimensions, the top row lies just below the nth heavy horizontal line from the bottom. By virtue of the paired-index matrix symmetry, $R_{i'j'\,k'l'} = R_{k'l'\,i'j'}$, the entries of the lexicon are confined to the upper triangular portion (including the main diagonal) of this matrix. But the Bianchi algebraic symmetry, $R_{i'j'\,k'l'} + R_{i'k'\,l'j'} + R_{i'l'\,j'k'} = 0$ allows putative entries $R_{i'j'\,k'l'}$ in this portion of the matrix for which $j' > l'$ (and only these otherwise qualifying candidates) to be excused on the basis of their being equivalent to the sum of two terms occurring earlier in the lexicon, namely:

$$R_{i'j'\,k'l'} = -R_{i'k'\,l'j'} + R_{i'l'\,k'j'}.$$

This excluding condition carves out the regular pattern of isolated forbidden regions we see shaded in Fig. 2.

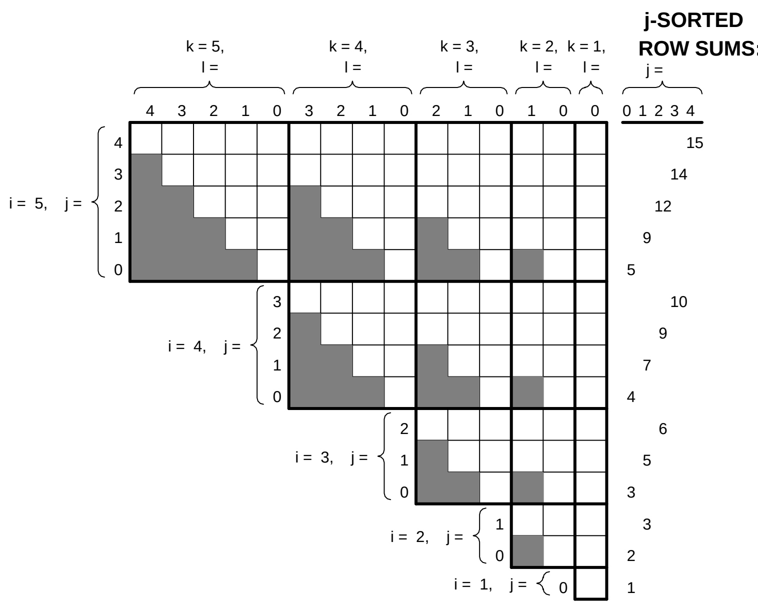

Figure 2. Lexicographic matrix arrangement showing the pattern of serially independent entries of the index sequences of the generic Riemann curvature tensor. In n dimensions, the indices of the tensor, $R_{i'j'\,k'l'}$, are here expressed in the form of the complementary indices: $\{i, j, k, l\} = \{n - i', n - j', n - k', n - l'\}$. The white spaces are assigned only to those elements of the tensor which, in a lexicographic ordering, are independent of entries that appear earlier in the lexicon. The row-sums of white squares listed to the right of the matrix, and later reproduced as the quantities '$T(i, j)$' of Table 1, are used to infer the number of independent components of the higher-rank generalizations of shape tensors that quantify the higher degree departures from flatness of the Riemannian space, as discussed in the text.

TABLE 1. TABLE OF ROW SUMS, $T(i,j)$.

i	$j=0$	1	2	3	4	5
1	1					
2	2	3				
3	3	5	6			
4	4	7	9	10		
5	5	9	12	14	15	
6	6	11	15	18	20	21

TABLE 2. TABLE OF CUMULATIVE ROW SUMS, $U(i,j)$.

i	$j=0$	1	2	3	4	5
1	1					
2	3	3				
3	6	8	6			
4	10	15	15	10		
5	15	24	27	24	15	
6	21	35	42	42	35	21

(e) *Degrees of freedom and symmetries for shape tensors of rank* > 4

Also shown in Fig. 2 are the row-counts of the lexicographic entries, sorted by j, which we shall be using presently. Denoting this tally, $T(i,j)$, it is easily verified that:

$$T(i,j) = \frac{(2i-j)(j+1)}{2}. \tag{2.53}$$

We next consider the third-degree polynomial terms for the metric tensor. Again, in order that this contribution to the metric has $\boldsymbol{x}$ as a null vector everywhere, it must be expressible:

$$J_{ik\,jlm} x^j x^l x^m = \frac{1}{4} Q_{pq\,rs\,t} (\delta_i^p \delta_j^q - \delta_j^p \delta_i^q)\,(\delta_k^r \delta_l^s - \delta_l^r \delta_k^s)\,x^j x^l x^t \tag{2.54}$$

and the symmetries involving the first four indices of this fifth-rank tensor Q can be required, without loss of generality, to be exactly those inherited from its fourth-rank counterpart (or equivalently, those of the Riemann tensor). However, we cannot assume that the number of independent degrees of freedom at this order is just $n \times F(n)$, because the factor,

$$(\delta_k^r \delta_l^s - \delta_l^r \delta_k^s)\,x^l x^t = (\delta_k^r x^s - \delta_k^s x^r)\,x^t \tag{2.55}$$

has a linear dependency under cyclic permutation of the indices, r, s and t. As was the case with the Bianchi algebraic identity, this new symmetry can be imposed on the coefficients $Q_{pq\,rs\,t}$ in order to keep them unambiguous:

$$Q_{pq\,rs\,t} + Q_{pq\,st\,r} + Q_{pq\,tr\,s} = 0. \tag{2.56}$$

The implication of this symmetry for the derivatives of the Riemann tensor is what is known as the 'Bianchi derivative identity':

$$R_{ij\,kl|m} + R_{ij\,lm|k} + R_{ij\,mk|l} = 0. \tag{2.57}$$

This identity reduces the number of independent elements of the tensors Q of fifth rank and higher from what a naive extrapolation might have led us to expect.

We can extend the lexicographic convention for the ordering of tensors Q of rank higher than four in the natural way, but it is convenient temporarily to adopt an alternative convention, just to facilitate the counting of independent components (obviously the choice of lexicographic ordering convention cannot change the number of independent degrees of freedom in the tensors represented). Suppose we construct the alternative extended lexicon for the serially-independent components of the tensor, Q of rank $4+M$ according to the rule that the trailing M indices (beyond the fourth) are ordered *first* (as if they were placed at the front) while the first four indices, i, j, k, l, are ordered as if, as a group, they were placed in the trailing position. There are exactly $\binom{j+M-1}{M}$ lexicographically-ordered strings of the M trailing indices that do not exceed second index, $j \leq n$. (Note that if the last one of these M indices were to exceed j, and hence i, then the Bianchi cyclic symmetry associated with these three indices would imply that this tensor component could be replaced by a linear combination of the two others which both have lexicographic precedence, and so the original component could not itself then qualify for the $(4+M)$-digit lexicon of serially-independent Q components.) We have seen from Fig. 2 that the number of entries in the Riemann tensor lexicon whose first index is i and whose second index is $j > i$ is $T(n-i, n-j)$. The number of entries in the Riemann tensor lexicon whose second index equals j is therefore $U(n-1, n-j)$, where:

$$\begin{aligned} U(i,j) &= \sum_{i'=j+1}^{i} T(i',j), \\ &= (j+1)(i-j)(i+1)/2, \quad 0 \leq j < i. \end{aligned} \tag{2.58}$$

Some of these $U(i,j)$ are listed in Table 2. We are therefore able to deduce the size, $F(n,M)$, of the $(4+M)$-digit lexicon, that is, the number of independent degrees of freedom in the 'shape tensor' of rank $4+M$ for a space of dimension n. We use the lemma (readily proved by induction):

$$\sum_j \binom{j}{a}\binom{c-j}{b} = \binom{c+1}{a+b+1}, \quad a,b \geq 0, \quad c \geq a+b, \tag{2.59}$$

to simplify the summation for $F(n,M)$:

$$\begin{aligned} F(n,M) &= \sum_{j=2}^{n} \binom{j+M-1}{M} U(n-1, n-j) \\ &= \sum_j \binom{j+M-1}{M} \frac{n(j-1)(n+1-j)}{2} \\ &= \frac{n(M+1)}{2} \sum_j \binom{j}{M+1}\binom{n+M-j}{1} \end{aligned}$$

$$= \frac{n(M+1)}{2}\binom{n+M+1}{M+3}. \tag{2.60}$$

In the special case, $M = 0$, we confirm that the formula correctly reproduces the numbers $F(n)$ of (2.38), as required. A list of some of the values of $F(n, M)$ is given in Table 3.

TABLE 3. The number $F(n, M)$ of independent degrees of freedom of the shape tensor of rank $4 + M$ of generic Riemannian space of dimension n.

n	$M = 0$	1	2	3	4
2	1	2	3	4	5
3	6	15	27	42	60
4	20	60	126	224	360
5	50	175	420	840	1500

TABLE 4. Q-tensor component dependencies lexicographic reduction rules.

Index inequality	Substitution rule for $\tilde{Q}_{12\,\ldots} \equiv Q_{i_1 i_2\,\ldots}$
$i_1 = i_2$	0
$i_3 = i_4$	0
$i_1 > i_2$	$-\tilde{Q}_{21\,34\,\ldots}$
$i_3 > i_4$	$-\tilde{Q}_{12\,43\,\ldots}$
$i_1 > i_3$	$+\tilde{Q}_{32\,14\,\ldots} - \tilde{Q}_{31\,24\,\ldots}$
$i_2 > i_4$	$+\tilde{Q}_{14\,32\,\ldots} - \tilde{Q}_{13\,42\,\ldots}$
`IF M > 0:`	
$i_3 > i_5$	$+\tilde{Q}_{12\,54\,3\ldots} - \tilde{Q}_{12\,53\,4\ldots}$
$i_p > i_{p+1}, \quad p > 4$	$+\tilde{Q}_{\ldots,p+1,p,\ldots}$ (`index transposition`)

Returning to the usual lexicographic ordering convention for the components of Q tensors, a component can be said to be 'reducible' with respect to the lexicographic convention if it can generally be expressed as a linear combination of other components that enjoy lexicographic precedence. A reducible component can be recognized if it satisfies one of the inequalities listed in Table 4. Also given there is the substitution rule that gives the magnitude of the reducible component in terms of other components that occur earlier than it in the lexicon. The substituted components can themselves be reducible in this sense, so the rules given by this table must be iterated until no further substitutions occur in order to express each component in irreducible terms.

(*f*) *Notational development and some relationships connecting Q and J tensors*

The corresponding Jacobi shape tensors, J, of rank $\alpha = M + 4$ can also be ordered lexicographically and, although we shall not use such a lexicon, it is useful to clarify the symmetries of J that the lexicographic reduction rules for these quantities would need to respect. First, when dealing with a generic number of tensor-style indices, $i_1, \ldots i_\alpha$, we shall find it convenient to use the shorthand notation:

$$J_{i_1 i_2 \ldots i_\alpha} \equiv \tilde{J}_{12 \ldots \alpha}, \tag{2.61}$$

and likewise for other indexed tensor-like symbols. For the generic index i_β, we shall refer to the number or function, β, as its 'index label'. Associating the indices with numerical labels certainly makes it easier to automate the lexicographic comparisons, but it also simplifies some of the combinatoric expressions we use as shortcuts to hand calculations. Note that when we encounter the Kronecker symbol written '$\tilde{\delta}^{12}$' it is *not* invariably zero (as it obviously would be without the *tilde*); instead, we should consistently interpret this symbol to mean:

$$\tilde{\delta}^{12} = \begin{cases} 1 & : \quad i_1 = i_2, \\ 0 & : \quad i_1 \neq i_2. \end{cases} \tag{2.62}$$

When, as later, we have occasion to employ multiple instances of these superscripted Kronecker symbols in a term, it becomes convenient to adopt abbreviations of the kind exemplified by:

$$\tilde{\delta}^{aa'\,bb'\,cc'} \equiv \tilde{\delta}^{aa'}\tilde{\delta}^{bb'}\tilde{\delta}^{cc'}.$$

A more substantial economy results from the exploitation of combinatoric principles based on the symmetries of the tensorial quantities we deal with. When given an index list together with a pattern of partitioning of this set into ordered subsets of given sizes, it is convenient to adopt a shorthand 'combinatorial index' notation for the sum of the instances of an indexed quantity when all possible combinations of the given set of indices distributed amongst the partitions are exercised (but index order *inside* each subset is not distinguished). The subsets of a given size, β, will be denoted by this β inside parentheses in the index position. Thus, for example, $\tilde{A}_{1(2)(1)}$ is understood to expand to the sum of three $(= 2 + 1)$ terms. To be written this way, A *must* already be a quantity known to exhibit symmetry with respect to transposition of its middle pair of indices. At times, it is necessary to make explicit the 'parent set'. Here, the parent set, which we can denote '(3)', comprises the three hidden index labels involved in the combination. Suppose, for example, the hidden indices involved are, i_4, i_7 and i_8. Then, when the necessity to make this parent set known arises, we shall define it with the notation,

$$(3) \equiv \{4, 7, 8\}.$$

The explicit expansion of what, in combinatoric notation, is condensed into a *single* term, is then:

$$\begin{aligned} \tilde{A}_{1(2)(1)} &\equiv \tilde{A}_{1478} + \tilde{A}_{1487} + \tilde{A}_{1784}, \\ &\equiv A_{i_1\,i_4\,i_7\,i_8} + A_{i_1\,i_4\,i_8\,i_7} + A_{i_1\,i_7\,i_8\,i_4}. \end{aligned}$$

Note that index label, '1', being *not* included in parentheses, remains fixed through all the different combinations. The combinatorial index notation can equally be applied to terms with conventional (alphabetic) tensor subscripts and superscripts, instead of index labels we used in this example.

An isolated single pair of parentheses in the index list of a term, i.e., the parent set, clearly translates to only a single instance of that term, however large the number in parentheses (size of the parent set); at the opposite extreme, if a term's index list contains α distinct occurrences of '(1)' (but no other parenthetic indices) then this combinatorial term actually signifies $\alpha!$ separate explicit-index terms. More generally, for a parent set, (α), the number of explicit-index terms into which a sequence of combinatorial-index terms expands, when the latter consists of the partitioning sequence, β_i, with $\alpha = \sum_{i=1}^{P} \beta_i$, is the multinomial: $\alpha!/(\beta_1! \ldots \beta_P!)$. Consistency with these rules requires that the occurrence of a '(0)' means that *no* explicit index exists at this position, but the term itself remains; however, a '(-1)' combinatorial index will invariably be interpretted as implying that the term itself is annihiliated. When the context makes the interpretation of a quantity's indices unambiguous as index labels, rather than actual indices, we may sometimes omit the 'tilde' in the interests of typographic clarity.

The symmetry of any J tensor of rank $\alpha + 2$ under transposition of its first pair of indices could be signified in this notation by:

$$2!\tilde{J}_{(2)\;3\ldots\alpha+2} = \tilde{J}_{(1)(1)\;3\ldots\alpha+2},$$

Alternatively, its symmetry with respect to permutation of its remaining α indices could be signified by:

$$\alpha!\tilde{J}_{12\;(\alpha)} = \tilde{J}_{12\;(1)_1\ldots(1)_\alpha}.$$

Denote

$$x^{i_3 i_4 \ldots i_{\alpha+2}} \equiv \tilde{x}^{34\ldots\alpha+2},$$

and, since the terms in the Taylor expansion of $\tilde{g}_{12}$ at degree α sum to:

$$\tilde{J}_{12\;34\ldots\alpha+2}\tilde{x}^{34\ldots\alpha+2} = \tilde{Q}_{13\;24\;\ldots\alpha+2}\tilde{x}^{34\ldots\alpha+2}, \tag{2.63}$$

the result of differentiating α times to recover these coefficients is the relationship, written now with conventional tensor indices, i and j:

$$\begin{aligned} \alpha! J_{ij\;(\alpha)} &= Q_{i(1)_1\;j(1)_2\;\ldots(1)_\alpha} \\ &= (\alpha-2)! Q_{i(1)\;j(1)\;(\alpha-2)}, \quad \alpha \geq 2, \end{aligned} \tag{2.64}$$

(since Q is symmetric with respect to permutation of its trailing $\alpha - 2$ indices). From this result we are able to obtain:

Lemma 1:

$$J_{(1)i\;(\alpha)} = J_{i(1)\;(\alpha)} = 0. \quad \alpha \geq 2. \tag{2.65}$$

□

Proof:

We exploit the antisymmetry of Q with respect to transposition of its leading pair of indices:

$$\begin{aligned} J_{(1)i\;(\alpha)} &\propto Q_{(1)(1)\;i(1)\;(\alpha-2)} \\ &= 0, \quad \alpha \geq 2. \end{aligned} \tag{2.66}$$

□

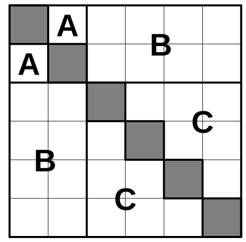

Figure 3. Among the index permutations of a shape tensor, J, any component may be identified by the specification of just the leading pair of index labels and therefore mapped to off-diagonal components of a symmetric matrix. Equation (2.65) may be interpretted as saying that the nondiagonal row- and column-sums of the matrix vanish. Let one of these J components be selected, say $\tilde{J}_{12\,\ldots}$, which maps to the matrix elements marked 'A' in the figure. Denote by 'B' the index-permuted elements of $\tilde{J}$ possessing either the index label, '1' or '2', which maps to the two portions of the matrix as marked. The remaining index-permuted elements, containing neither index label '1' nor '2' map to the region of the matrix marked 'C'. The 'B' elements clearly sum to twice the negative-sum of the A element and to twice the negative sum of the 'C' elements.

An interpretation of this symmetry and its consequences is given in Fig. 3.

Let the numerical indices of $\tilde{J}$ be ordered to reflect the lexicographic ranking of the pool of indices used to indicate the components of J, but let the actual indices of a particular component of J be denoted respectively, $j_1, \ldots, j_\alpha$. For the particular component to belong to the J-lexicon it is clearly necessary that $j_1 \leq j_2$, since every J tensor is symmetrical with respect to these first two indices. Likewise, from symmetry with respect to the remaining $\alpha - 2$ indices, we have a series of inequalities, $j_3 \leq j_4, \ldots \leq j_{\alpha-1} \leq j_\alpha$. But (2.65) implies that the indices of a lexicographically irreducible component also satisfies the inequality, $j_2 < j_\alpha$, since it is otherwise expressible as a linear superposition of components with the same j_1 but smaller j_2. Finally, by a consideration of what (2.65) implies for the components whose leading and trailing pair of indices are the four indices that rank last lexicographically amongst the indices present, it is straightforward to prove that an irreducible component must also satisfy $j_1 < j_{\alpha-1}$. We will not attempt to provide a table, analogous to Table 4, for the J-lexicon reduction rules as these are rather more complicated and will not be applied in this study. However, from the criteria of lexicographic irreducibility we have obtained we can immediately assert the following lemma:

Lemma 2:

The number of components of the J tensor of rank α that are irreducible according to the above criteria is equal to the number of independent components of the corresponding Q shape tensor. The lexicographic rules we have discovered for J are therefore sufficient.

□

The proof of this lemma is given in Appendix A.

In addition to the generic formula (2.64) enabling J to be expressed in terms of Q, we clearly need an inverse of this formula to facilitate evaluation of the Q tensor of rank α from the derivatives, at the origin, of the covariant metric. The requisite formula is given by:

Theorem 1:

$$\tilde{Q}_{12\,34\,\dots\alpha} = \frac{\alpha-3}{\alpha-1}(\tilde{J}_{13\,24\dots\alpha} - \tilde{J}_{23\,14\dots\alpha} - \tilde{J}_{14\,23\dots\alpha} + \tilde{J}_{24\,13\dots\alpha}). \tag{2.67}$$

□

A proof of this important identity is given in Appendix A. It is partly from this result that we can deduce that the successive covariant derivatives of the Riemann tensor take the form:

$$\tilde{R}_{12\,34|5\dots\alpha} = -(\alpha-4)!\binom{\alpha-1}{2}\tilde{Q}_{12\,34\,5\dots\alpha} + \mathcal{N}, \tag{2.68}$$

where $\mathcal{N}$ denotes the additional nonlinear terms in R and its covariant derivatives up to degree $\alpha-6$ when $\alpha \geq 6$. This observation that the Taylor expansion coefficients of the metric tensor in normal coordinates are each a polynomial in the Riemann tensor and its covariant derivatives was apparently first made by the celebrated geometer and pioneering group-theorist, E. Cartan (e.g., see Berger et al. 1971).

As we shall often use the tensors obtained when shape tensors, Q, are contracted with respect to their first and third indices, it is convenient to establish a notation for them. We shall also use the further contractions obtained when, in addition, the second and fourth indices of Q are contracted. Therefore, we define:

$$\overline{Q}_{24\,5\dots\alpha} = \tilde{\delta}^{aa'}\tilde{Q}_{a2\,a'4\,5\dots\alpha}, \tag{2.69a}$$

$$\overline{\overline{Q}}_{5\dots\alpha} = \tilde{\delta}^{aa'\,bb'}\tilde{Q}_{ab\,a'b'\,5\dots\alpha} = \tilde{\delta}^{bb'}\overline{Q}_{bb'\,5\dots\alpha}, \tag{2.69b}$$

where it is understood that the quantity $\overline{\overline{Q}}$ reduces to a scalar in the case where $\alpha = 4$. Note that $\overline{Q}$ is symmetric with respect to its leading pair of indices. (Note also that $\overline{Q}$ and $\overline{\overline{Q}}$ exhibit the first examples where typographic clarity prompts us to relax the 'tilde' convention.) We directly obtain from (2.64):

$$\begin{aligned} \alpha!\delta^{aa'}\tilde{J}_{aa'\,(\alpha)} &= (\alpha-2)!\overline{Q}_{(1)(1)\,(\alpha-2)} \\ &= 2(\alpha-2)!\overline{Q}_{(2)\,(\alpha-2)}, \quad \alpha \geq 2. \end{aligned} \tag{2.70}$$

Less obvious is the following identity, whose range of α-validity extends down to $\alpha = 2$ since we interpret a combinatoric subscript index, '(-1)' in a factor to imply the annihilation of the term to which it belongs:

Lemma 3:

$$\alpha!\delta^{aa'}\tilde{J}_{a1\,a'(\alpha-1)} = (\alpha-2)!\left[2\overline{Q}_{(2)\,1(\alpha-3)} - (\alpha-1)\overline{Q}_{1(1)\,(\alpha-2)}\right], \quad \alpha \geq 2 \tag{2.71}$$

□

The proof, once again, is provided in Appendix A and, from this result, as a direct corollary, we also obtain:

$$\alpha!\delta^{aa'}\tilde{J}_{a(1)\,a'(\alpha-1)} = -2(\alpha-2)!\overline{Q}_{(2)\,(\alpha-2)}, \quad \alpha \geq 2, \tag{2.72}$$

which we shall put to use in Appendix B to derive quantities employed by the parametrix expansion of section 3.

(*g*) *The Ricci tensor*

Analogous to the contracted form, $\overline{Q}$, of the Q tensor, an important contraction of the full Riemann tensor leads to the symmetric 'Ricci tensor':

$$R_{ij} = R^k_{i\,kj} \equiv R_i^{\;k}{}_{jk}, \tag{2.73}$$

whose $n(n+1)/2$ nontrivially distinct components are sufficient to define all the curvature in $n \leq 3$ dimensions. Different sign conventions are employed by different authors, but we shall follow that of Lovelock and Rund (1989) which associates a positive Ricci scalar (contraction of the Ricci tensor) with a positive Gaussian curvature in the two-dimensional case. [Synge and Schild (1949) and Kreyszig (1991) adopt the opposite sign convention for the Ricci quantities.]

The Ricci tensor may be related directly to the derivatives of the metric tensor and Christoffel symbol:

$$R_{ij} = \frac{1}{2}\left((\ln g)_{,k}\Gamma^k_{ij} - (\ln g)_{,ij}\right) + \Gamma^k_{ij,k} - \Gamma^k_{il}\Gamma^l_{jk}. \tag{2.74}$$

The further contraction leads to the 'Ricci scalar':

$$R = R^i_i \equiv g^{ij}R_{ij}. \tag{2.75}$$

The Ricci tensor inherits the Bianchi derivative identity in the form:

$$R^i_{j|i} = \frac{1}{2}R_{|j}. \tag{2.76}$$

In $n = 2$ dimensions,

$$R = 2\kappa \tag{2.77}$$

where κ is the Gaussian curvature. In 2D, κ or R suffice to recover all the Riemann and Ricci curvature components:

$$R_{ij\,kl} = (g_{ik}g_{jl} - g_{il}g_{jk})R/2, \tag{2.78a}$$
$$R_{ij} = g_{ij}R/2 \tag{2.78b}$$

In $n = 3$ dimensions, the Ricci tensor suffices to recover the Riemann tensor according to:

$$R_{ij\,kl} = g_{ik}R_{jl} + g_{jl}R_{ik} - g_{il}R_{jk} - g_{jk}R_{il} - (g_{ik}g_{jl} - g_{il}g_{jk})R/2. \tag{2.79}$$

In the special cases of n-dimensional hyperbolic and elliptic geometries with constant and isotropic curvature, one can quantify this curvature as the Gaussian curvature κ on any two-dimensional geodesic 'section'. In these special cases,

$$R_{ij\,kl} = (g_{ik}g_{jl} - g_{il}g_{jk})\kappa, \tag{2.80}$$

so that the Ricci tensor and scalar become:

$$R_{ij} = (n-1)\kappa g_{ij}, \tag{2.81}$$

and

$$R = n(n-1)\kappa. \tag{2.82}$$

3. The heat kernel in a Riemannian manifold

The solution to the diffusion equation from an initial unit impulse, is known by mathematicians as the 'heat kernel'. The mathematical behavior of the heat kernel in Riemannian geometry has stimulated a enormous amount of research amongst geometers and topologists owing to the insights it provides, both locally and globally, about the geometrical characteristics of the manifold on which the diffusion occurs (McKean 1970; Grigor'yan and Noguchi 1998; Rosenberg 1997). Recent applications have also been found in statistical information theory (Laffetry and Lebanon 2005) and, in a sense, our own interest in the behavior of heat kernels in a curved space also relates to the manipulation and characterization of information, though the Riemannian manifold in our context is a smooth deformation of the actual physical space in which we are attempting to assimilate meteorological data. Nevertheless, the same asymptotic methods recur in all these applications and of central importance is the so-called 'parametrix expansion' which we have already discussed in special geometries in Part I. Here we extend the study of this asymptotic approximation method to more general Riemannian geometries of three or more dimensions.

An approximate solution, P_0, in the normal coordinates is given by pretending these to be Cartesian coordinates of a Euclidean geometry, so that the familar Gaussian formula is obtained:

$$P_0(t;\boldsymbol{x}) = \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{r^2}{4t}\right), \tag{3.1}$$

where

$$r^2 = \delta_{ij} x^i x^j, \tag{3.2}$$

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 spatial coordinates:

$$\frac{\partial P_0}{\partial t} = \left(\frac{r^2}{4t^2} - \frac{n}{2t}\right) P_0, \tag{3.3a}$$

$$\frac{\partial P_0}{\partial x^i} = -\frac{\delta_{ij} x^j}{2t} P_0, \tag{3.3b}$$

$$\frac{\partial^2 P_0}{\partial x^i \partial x^j} = \left(\frac{\delta_{ik}\delta_{jl} x^k x^l}{4t^2} - \frac{\delta_{ij}}{2t}\right) P_0. \tag{3.3c}$$

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

$$\delta^{ij} \frac{\partial^2 P_0}{\partial x^i \partial x^j} = \left(\frac{\delta_{ij} x^i x^j}{4t^2} - \frac{n}{2t}\right) P_0, \tag{3.4}$$

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

$$\frac{\partial P_0}{\partial t} = \delta^{ij} \frac{\partial^2 P_0}{\partial x^i \partial x^j}. \tag{3.5}$$

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

$$P(t; \boldsymbol{x}) = P_0(t; \boldsymbol{x}) T(t; \boldsymbol{x}), \tag{3.6}$$

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

$$\begin{aligned} \frac{\partial P}{\partial t} &= \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \sqrt{g} g^{ij} \frac{\partial P}{\partial x^j} \\ &= W^i \frac{\partial P}{\partial x^i} + g^{ij} \frac{\partial^2 P}{\partial x^i \partial x^j}, \end{aligned} \tag{3.7}$$

where,

$$W^i = g^{ij} \left(\frac{1}{2} \frac{\partial g_{kl}}{\partial x^j} - \frac{\partial g_{jk}}{\partial x^l} \right) g^{kl} = -\Gamma^i{}_{kl} g^{kl}. \tag{3.8}$$

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:

$$T(t; \boldsymbol{x}) = 1 + \sum_{s, \boldsymbol{p} \geq 0} \hat{T}_{s;\boldsymbol{p}} t^s \boldsymbol{x}^{\boldsymbol{p}}, \tag{3.9}$$

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

$$\hat{T}_{0;\boldsymbol{0}} = 0, \tag{3.10}$$

but the nontrivial coefficients in this expansion must be inferred by first expanding the derivatives in the diffusion equation (3.7) as applied to the product $P_0 T$.

We proceed by multiplying the expanded terms of (3.7) by t/P_0, having made the substitutions (3.3a)–(3.3c):

$$\begin{aligned} 0 &= \frac{t}{P_0} \left(\frac{\partial P}{\partial t} - W^i \frac{\partial P}{\partial x^i} - g^{ij} \frac{\partial^2 P}{\partial x^i \partial x^j} \right) \\ &= \left[\frac{r^2}{4t} - \frac{n}{2} - g^{ij} \delta_{ik} \delta_{jl} \frac{x^k x^l}{4t} + \frac{\delta^{ij} \delta_{ij}}{2} \right] (1 + T) \\ &\quad + t \left[\frac{\partial T}{\partial t} + g^{ij} x^k \delta_{jk} \frac{\partial T}{\partial x^i} - \delta^{ij} \frac{\partial^2 T}{\partial x^i \partial x^j} \right] \\ &\quad + \frac{1}{2} \left[(g^{ij} - \delta^{ij}) \delta_{ij} + W^i \delta_{ik} x^k \right] (1 + T) \\ &\quad - t \left[W^i \frac{\partial T}{\partial x^i} + (g^{ij} - \delta^{ij}) \frac{\partial^2 T}{\partial x^i \partial x^j} \right]. \end{aligned} \tag{3.11}$$

We exploit the eigen condition (2.27) to show that the expression within the first square brackets on the right vanishes, and to simplify terms in the second and third square brackets. Also, we organize the remaining expression into: the part, $\mathcal{T}$, linear in T and not involving the metric terms; the part, $\mathcal{G}$, linear in the metric terms but not involving T; the remaining 'bilinear' terms, $\mathcal{Q}$, (linear separately in T and the metric terms). It is convenient to abbreviate successive partial derivatives with respect to time, t, by '$\mathcal{T}_1$', '$\mathcal{T}_2$', etc., but spatial partial derivatives with respect to x^p by '$\mathcal{T}_{,p}$', etc, as we did in section 2 and the appendices. Thus, for example, according to this notation,

$$\frac{\partial^4 \mathcal{T}}{\partial t^2 \partial x^p \partial x^q} \equiv \mathcal{T}_{2,pq},$$

and, in generic expressions, $\mathcal{T} \equiv \mathcal{T}_0$. Also, we define $x_i = g_{ij}x^j = \delta_{ij}x^j$ so that $x_{i,p} = \delta_{ip}$. As in Part I, we obtain

$$\mathcal{T} + \mathcal{G} + \mathcal{Q} = 0 \tag{3.12}$$

but now with

$$\begin{aligned}
\mathcal{T} &= tT_1 + x^i T_{,i} - t\delta^{ij}T_{,ij}, && (3.13a)\\
\mathcal{G} &= \frac{1}{2}\left[-n + \delta_{ij}g^{ij} + x_i W^i\right], && (3.13b)\\
\mathcal{Q} &= \mathcal{G}T - t\left[W^i T_{,i} + (g^{ij} - \delta^{ij})T_{,ij}\right]. && (3.13c)
\end{aligned}$$

We group the derivatives by their successive 'slab-degrees', h, meaning the sum of the spatial degrees plus twice the temporal degree (see Part I). We proceed by writing each of the general derivative of a given slab-degree, followed by the evaluation at the space-time origin, henceforth denoted by $\boldsymbol{O}$, of these derivatives. Thus, at $h = 0$ we have the trivial:

$$\mathcal{T}|_0 = \mathcal{G}|_0 = \mathcal{Q}|_0 = 0. \tag{3.14}$$

At $h = 1$:

$$\begin{aligned}
\mathcal{T}_{,p} &= tT_{1,p} + T_{,p} + x^i T_{,ip} - t\delta^{ij}T_{,ijp}, && (3.15a)\\
\mathcal{G}_{,p} &= \frac{1}{2}\left[\delta_{ij}g^{ij}_{,p} + \delta_{ip}W^i + x_i W^i_{,p}\right], && (3.15b)\\
\mathcal{Q}_{,p} &= \mathcal{G}_{,p}T + \mathcal{G}T_{,p}\\
&\quad -t\left[W^i_{,p}T_{,i} + W^i T_{,ip} + g^{ij}_{,p}T_{,ij} + (g^{ij} - \delta^{ij})T_{,ijp}\right]. && (3.15c)
\end{aligned}$$

These terms also evaluate to zero at $\boldsymbol{O}$:

$$\mathcal{T}_{,p}|_0 = \mathcal{G}_{,p}|_0 = \mathcal{Q}_{,p}|_0 = 0. \tag{3.16}$$

At $h = 2$:

$$\begin{aligned}
\mathcal{T}_{,pq} &= tT_{1,pq} + 2T_{,pq} + x^i T_{,ipq} - t\delta^{ij}T_{,ijpq},\\
\mathcal{G}_{,pq} &= \frac{1}{2}\left[\delta_{ij}g^{ij}_{,pq} + \delta_{ip}W^i_{,q} + \delta_{iq}W^i_{,p} + x_i W^i_{,pq}\right],\\
\mathcal{Q}_{,pq} &= \mathcal{G}_{,pq}T + \mathcal{G}_{,p}T_{,q} + \mathcal{G}_{,q}T_{,p} + \mathcal{G}T_{,pq}\\
&\quad -t\left[W^i_{,pq}T_{,i} + W^i_{,p}T_{,iq} + W^i_{,q}T_{,ip} + W^i T_{,ipq}\right.\\
&\quad \left.+g^{ij}_{,pq}T_{,ij} + g^{ij}_{,p}T_{,ijq} + g^{ij}_{,q}T_{,ijp} + (g^{ij} - \delta^{ij})T_{,ijpq}\right],
\end{aligned}$$

we begin to see the generic patterns that occur in the combinations of the terms. The combinatorial index notation alleviates a considerable algebraic burden as we progress to higher orders of derivatives and allows these equations to be rewritten equivalently:

$$\begin{aligned}
\mathcal{T}_{,(2)} &= tT_{1,(2)} + 2T_{,(2)} + x^i T_{,i(2)} - t\delta^{ij} T_{,ij(2)}, && (3.17a)\\
\mathcal{G}_{,(2)} &= \frac{1}{2}\left[\delta_{ij} g^{ij}_{\ ,(2)} + \delta_{i(1)} W^i_{\ ,(1)} + x_i W^i_{\ ,(2)}\right], && (3.17b)\\
\mathcal{Q}_{,(2)} &= \mathcal{G}_{,(2)} T + \mathcal{G}_{,(1)} T_{,(1)} + \mathcal{G} T_{,(2)} \\
&\quad -t\left[W^i_{\ ,(2)} T_{,i} + W^i_{\ ,(1)} T_{,i(1)} + W^i T_{,i(2)}\right. \\
&\quad \left.+g^{ij}_{\ ,(2)} T_{,ij} + g^{ij}_{\ ,(1)} T_{,ij(1)} + (g^{ij} - \delta^{ij}) T_{,ij(2)}\right]. && (3.17c)
\end{aligned}$$

Also at $h = 2$ we have:

$$\begin{aligned}
\mathcal{T}_1 &= tT_2 + T_1 + x^i T_{1,i} - t\delta^{ij} T_{1,ij} - \delta^{ij} T_{,ij}, && (3.18a)\\
\mathcal{G}_1 &= 0, && (3.18b)\\
\mathcal{Q}_1 &= \mathcal{G} T_1 - t\left[W^i T_{1,i} + (g^{ij} - \delta^{ij}) T_{1,ij}\right] \\
&\quad - \left[W^i T_{,i} + (g^{ij} - \delta^{ij}) T_{,ij}\right]. && (3.18c)
\end{aligned}$$

At $\boldsymbol{O}$, only a few terms survive:

$$\begin{aligned}
\mathcal{T}_{,(2)}|_0 &= 2T_{,(2)} && (3.19a)\\
\mathcal{G}_{,(2)}|_0 &= \frac{1}{2}\left[\delta_{ij} g^{ij}_{\ ,(2)} + \delta_{i(1)} W^i_{\ ,(1)}\right], && (3.19b)\\
\mathcal{Q}_{,(2)}|_0 &= 0 && (3.19c)
\end{aligned}$$

$$\begin{aligned}
\mathcal{T}_1|_0 &= T_1 - \delta^{ij} T_{,ij}, && (3.20a)\\
\mathcal{G}_1|_0 &= 0, && (3.20b)\\
\mathcal{Q}_1|_0 &= 0. && (3.20c)
\end{aligned}$$

Exploiting these results and the condition requiring the vanishing of $(\mathcal{T} + \mathcal{G} + \mathcal{Q})_{,(2)}$ and $(\mathcal{T}_1 + \mathcal{G}_1 + \mathcal{Q}_1)$ at $\boldsymbol{O}$, we are able to deduce:

Theorem 2:

$$T_1 = \frac{1}{6} R. \qquad (3.21)$$

□

A proof of this theorem is given in Appendix C. This generalizes to n dimensions the first-order result we found in Part I for the surfaces ($n = 2$) of constant curvature.

We shall use τ as the subscript denoting the number of derivatives of a term with respect to t and use α and β to denote the number of generic spatial derivatives in the context of the combinatorial index notation. Then, in general, the parametrix expansion is built up by ensuring that, for each combination of temporal (τ) and spatial (α) differencing,

$$\mathcal{T}_{\tau,(\alpha)} + \mathcal{G}_{\tau,(\alpha)} + \mathcal{Q}_{\tau,(\alpha)} = 0, \tag{3.22}$$

at $\boldsymbol{O}$. The set of equations for $\tau = 0$ but arbitrary spatial degree, α, are:

$$\begin{aligned}
\mathcal{T}_{,(\alpha)} &= tT_{1,(\alpha)} + \alpha T_{,(\alpha)} + x^i T_{,i(\alpha)} - t\delta^{ij} T_{,ij(\alpha)}, &(3.23\text{a})\\
\mathcal{G}_{,(\alpha)} &= \frac{1}{2}\left(\delta_{ij} g^{ij}_{,(\alpha)} + \delta_{i(1)} W^i_{,(\alpha-1)} + x_i W^i_{,(\alpha)}\right), &(3.23\text{b})\\
\mathcal{Q}_{,(\alpha)} &= \sum_{\beta=0}^{\alpha} \mathcal{G}_{,(\alpha-\beta)} T_{,(\beta)}\\
&\quad -t\left[\sum_{\beta=0}^{\alpha}\left(W^i_{,(\alpha-\beta)} T_{,i(\beta)} + g^{ij}_{,(\alpha-\beta)} T_{,ij(\beta)}\right) - \delta^{ij} T_{,ij(\alpha)}\right]. &(3.23\text{c})
\end{aligned}$$

The generic equations when $\tau > 0$ are:

$$\begin{aligned}
\mathcal{T}_{\tau,(\alpha)} &= tT_{\tau+1,(\alpha)} + (\alpha+\tau) T_{\tau,(\alpha)} + x^i T_{\tau,i(\alpha)} - t\delta^{ij} T_{\tau,ij(\alpha)} - \tau\delta^{ij} T_{\tau-1,ij(\alpha)}, &(3.24\text{a})\\
\mathcal{G}_{\tau,(\alpha)} &= 0, &(3.24\text{b})\\
\mathcal{Q}_{\tau,(\alpha)} &= \sum_{\beta=0}^{\alpha} \mathcal{G}_{,(\alpha-\beta)} T_{\tau,(\beta)}\\
&\quad -t\left[\sum_{\beta=0}^{\alpha}\left(W^i_{,(\alpha-\beta)} T_{\tau,i(\beta)} + g^{ij}_{,(\alpha-\beta)} T_{\tau,ij(\beta)}\right) - \delta^{ij} T_{\tau,ij(\alpha)}\right]\\
&\quad -\tau\left[\sum_{\beta=0}^{\alpha}\left(W^i_{,(\alpha-\beta)} T_{\tau-1,i(\beta)} + g^{ij}_{,(\alpha-\beta)} T_{\tau-1,ij(\beta)}\right) - \delta^{ij} T_{\tau-1,ij(\alpha)}\right]. &(3.24\text{c})
\end{aligned}$$

At $\boldsymbol{O}$, where $t = 0$, $x^i = 0$, $W^i = 0$, $g^{ij} = \delta^{ij}$, $g^{ij}_{,(1)} = 0$, $T = 0$, $T_{,(1)} = 0$, the surviving terms are just:

$$\begin{aligned}
\mathcal{T}_{,(\alpha)}|_0 &= \alpha T_{,(\alpha)}, &(3.25\text{a})\\
\mathcal{G}_{,(\alpha)}|_0 &= \frac{1}{2}\left(\delta_{ij} g^{ij}_{,(\alpha)} + \delta_{i(1)} W^i_{,(\alpha-1)}\right), &(3.25\text{b})\\
\mathcal{Q}_{,(\alpha)}|_0 &= \sum_{\beta=2}^{\alpha-2} \mathcal{G}_{,(\alpha-\beta)} T_{,(\beta)}, &(3.25\text{c})
\end{aligned}$$

and, for $\tau > 0$:

$$\begin{aligned}
\mathcal{T}_{\tau,(\alpha)}|_0 &= (\alpha+\tau) T_{\tau,(\alpha)} - \tau\delta^{ij} T_{\tau-1,ij(\alpha)}, &(3.26\text{a})\\
\mathcal{G}_{\tau,(\alpha)}|_0 &= 0, &(3.26\text{b})\\
\mathcal{Q}_{\tau,(\alpha)}|_0 &= \sum_{\beta=0}^{\alpha-2} \mathcal{G}_{,(\alpha-\beta)} T_{\tau,(\beta)}
\end{aligned}$$

$$-\tau \left[\sum_{\beta=0}^{\alpha-1} W^{i}_{,(\alpha-\beta)} T_{\tau-1,i(\beta)} + \sum_{\beta=0}^{\alpha-2} g^{ij}_{,(\alpha-\beta)} T_{\tau-1,ij(\beta)} \right]. \tag{3.26c}$$

The order of evaluations at a generic slab index, h, are as follows. First, we use (3.25b) to construct a formula for $\mathcal{G}_{,(h)}$ at $\boldsymbol{O}$ expressed in terms of various Q shape tensors up to rank $h+2$. Then, since $\mathcal{Q}_{,(h)}$ is expressible [from (3.25c)] in terms of quantities known from evaluations at earlier values of the slab index, we can determine:

$$T_{,(h)} = -\frac{1}{h} \left(\mathcal{G}_{,(h)} + \mathcal{Q}_{,(h)} \right) \Big|_0 \tag{3.27}$$

from the requirement that the right-hand sides in the first set, (3.25a)–(3.25c), of equations at this h sum to zero. From the corresponding requirement pertaining to the subsequent sets, (3.26a)–(3.26c), we then evaluate each $\mathcal{Q}_{\tau,(h-2\tau)}$ for $\tau \leq h/2$, followed by,

$$T_{\tau,(h-2\tau)} = \frac{1}{h-\tau} \left(\tau \delta^{ij} T_{\tau-1,ij(h-2\tau)} - \mathcal{Q}_{\tau,(h-2\tau)} \right), \quad \tau \leq h/2. \tag{3.28}$$

For even h, the last quantity evaluated, $T_{h/2}$, is a new coefficient in the amplitude expansion. As we have seen, it is always possible to express each Q-type shape tensor in terms of the Riemann tensor and its covariant derivatives; therefore the amplitude expansion coefficient can be likewise expressed.

At $h = 2\tau + \alpha = 3$, the relevant equations evaluated at $\boldsymbol{O}$ give the two sets:

$$\begin{aligned} \mathcal{T}_{,(3)}|_0 &= 3T_{,(3)}, && (3.29a)\\ \mathcal{G}_{,(3)}|_0 &= \frac{1}{2}\left[\delta_{ij} g^{ij}_{,(3)} + \delta_{i(1)} W^{i}_{,(2)}\right], && (3.29b)\\ \mathcal{Q}_{,(3)}|_0 &= 0, && (3.29c) \end{aligned}$$

and,

$$\begin{aligned} \mathcal{T}_{1,(1)}|_0 &= 2T_{1,(1)} - \delta^{ij} T_{,ij(1)}, && (3.30a)\\ \mathcal{G}_{1,(1)}|_0 &= 0, && (3.30b)\\ \mathcal{Q}_{1,(1)}|_0 &= 0, && (3.30c) \end{aligned}$$

from which it is possible to obtain explicit formulas for $\mathcal{G}_{,(3)}$, $T_{,(3)}$ and $T_{1,(1)}$. These terms would be required (in the expressions for $\mathcal{Q}_{\tau,(\alpha)}$ at $h > 4$, but are not immediately pertinent to evaluating the next coefficient, T_2, of relevance to the filter normalization problem; for this, we must press on to consider the next slab, $h = 4$, where we find that, at $\boldsymbol{O}$:

$$\begin{aligned} \mathcal{T}_{,(4)}|_0 &= 4T_{,(4)}, && (3.31a)\\ \mathcal{G}_{,(4)}|_0 &= \frac{1}{2}\left[\delta_{ij} g^{ij}_{,(4)} + \delta_{i(1)} W^{i}_{,(3)}\right], && (3.31b)\\ \mathcal{Q}_{,(4)}|_0 &= \mathcal{G}_{,(2)} T_{,(2)}; && (3.31c) \end{aligned}$$

$$\mathcal{T}_{1,(2)}|_0 = 3T_{1,(2)} - \delta^{ij}T_{,ij(2)}, \quad (3.32a)$$
$$\mathcal{G}_{1,(2)}|_0 = 0, \quad (3.32b)$$
$$\mathcal{Q}_{1,(2)}|_0 = \mathcal{G}_{,(2)}T_1 - \left[W^i_{,(1)}T_{,i(1)} + g^{ij}_{,(2)}T_{,ij}\right]; \quad (3.32c)$$

$$\mathcal{T}_2|_0 = 2T_2 - 2\delta^{ij}T_{1,ij}, \quad (3.33a)$$
$$\mathcal{G}_2|_0 = 0, \quad (3.33b)$$
$$\mathcal{Q}_2|_0 = 0. \quad (3.33c)$$

From the vanishing of these $h=4$ derivatives of $(\mathcal{T}+\mathcal{G}+\mathcal{Q})$ evaluated at $\boldsymbol{O}$, together with relevant intermediate terms that were calculated in the course of proving theorem 2, we can show the following.

Theorem 3:

$$T_2 = \frac{1}{180}\left(12\nabla^2 R + 5R^2 - 2R_{ij}R^{ij} + 2R_{ijkl}R^{ijkl}\right). \quad (3.34)$$

□

As shown in Berger et al. (1971) this formula, being expressed in Riemann and Ricci tensors, is valid in any number $n \geq 2$ of dimensions. Our proof, exploiting the combinatorial shorthand developed in section 2 and Appendix B in order to make the calculations (just!) manageable, is set out in Appendix C in sufficient detail to show how the corresponding calculations could be extended, by automatic symbol manipulation, to even higher degrees of the parametrix expansion if required. This formula specializes, when $n \leq 3$, to one involving only the Ricci tensor and scalar:

$$T_2 = \frac{1}{60}\left(2R_{ij}R^{ij} + R^2 + 4\nabla^2 R\right). \quad (3.35)$$

In $n=2$ dimensions, where:

$$\begin{aligned} T_2 &= \frac{1}{30}(R^2 + 2\nabla^2 R) \\ &= \frac{2}{15}(\kappa^2 + \nabla^2\kappa), \end{aligned} \quad (3.36)$$

the second order parametrix expansion for the amplitude at the standard time, $t = 1/2$, becomes:

$$\begin{aligned} T(\frac{1}{2}, 0) &\approx 1 + \frac{T_1}{2} + \frac{T_2}{8} \\ &= 1 + \frac{\kappa}{6} + \frac{1}{60}(\kappa^2 + \nabla^2\kappa), \end{aligned} \quad (3.37)$$

in perfect agreement with the form we deduced in Part I using the less general geometrical methods.

We can also make the substitutions (2.80), (2.81) and (2.82) for the isotropic curvature case to obtain, for the special case of 3D uniform curvature:

$$T_2 = \kappa^2, \quad (3.38)$$

which is also consistent with the second-order term in the expansion obtained for this case in Part I.

4. Robust implementations and experimental validation

(*a*) *Robust implementations*

In Part I we showed how some of the problems with the tendency for the asymptotic approximations to diverge for large excursions of the diagnostics on which they depend can be controlled, without compromising the formal validity of the approximation, by substituting for each diagnostic a 'saturation function' of it. The tested forms of the saturation function of a diagnostic, x, say, behaves like x itself to first and second order for small values of x, but smoothly diverge from x so that their absolute magnitude never exceeds some finite limit proportional to a specified 'saturation parameter', s. The simple and effective form suggested for the saturation function was:

$$\mathrm{SAT}_1(s,x) = \frac{x}{[1+(x/s)^2]^{1/2}}, \tag{4.1}$$

which asymptotes to the constant limits, $\pm s$, as $x \to \pm\infty$. Each contributing diagnostic in the asymptotic estimate is associated with its own characteristic saturation parameter in general. We also showed in Part I that a further safeguard against the possibility of the computed amplification factor becoming negative, or involving a division by zero, or becoming excessively large and positive, was to employ a form for the divisor of the amplitude correction that involved a function that behaved like the exponential function for small arguments, retained the positivity of the exponential function for all arguments, but neither grew nor decayed as rapidly as the true exponential. This 'pseudo-exponential function' was defined:

$$\widetilde{\exp}(x) = x + \sqrt{1+x^2}. \tag{4.2}$$

From the large number of amplitude-approximating formulations tested in Part I, the best first-order scheme, which we denoted, E_1, and the two second-order schemes that tied for 'best', which we denoted, E_2 and H_2, can be adapted, with the incorporation of the saturation function SAT_1 and the pseudo-exponential function, $\widetilde{\exp}$, to the corresponding 3D approximations. Since in this Part II we shall always use the preferred saturation function, SAT_1, for every term that contributes to the argument of the pseudo-exponential function, it is convenient to denote the value of the saturation function of x by the 'effective x', $\widetilde{x}$:

$$\widetilde{x} = \mathrm{SAT}_1(s,x) \tag{4.3}$$

and we shall always make clear which saturation parameter, s, is being invoked. Thus, for schemes, E_1 and E_2, we shall take the effective Ricci scalar, $\widetilde{R}$ to be the evaluation of the saturation function of R with parameter, s_R. For the term involving the contraction of the Ricci tensor with itself, we take the saturation parameter of $\widetilde{R_{ij}R^{ij}}$ to be just $(s_R)^2$. The effective Laplacian of the Ricci scalar, $\widetilde{\nabla^2 R}$, is likewise obtained from SAT_1 applied to the true Laplacian and with a saturation parameter we denote by s_L. With these notations assumed, the modifications to the amplitude, b_0, obtained from the direct application of the usual Gaussian amplitude formula after the Riemannian-space diffusion has been completed are now given for schemes E_1 and E_2 respectively by:

$$e_1 = b_0/\widetilde{\exp}\left[\widetilde{R}/12\right], \tag{4.4a}$$

$$e_2 = b_0/\widetilde{\exp}\left[\widetilde{R}/12 - \widetilde{R}^2/720 + \widetilde{R_{ij}R^{ij}}/240 + \widetilde{\nabla^2 R}/120\right], \tag{4.4b}$$

It would be possible for each of the four saturation function terms of E_2 individually to possess distinct tuned parameters, of course, but preliminary experiments in which this was done showed very little relative advantage compared to this formulation where only two independent parameters are used.

The experimental configuration of Part I that we denoted H_2 was a variant on E_2 that applied the saturation function separately to the two eigenvalues of the Hessian of the scalar curvature before summing them to form the effective Laplacian of the last term. We shall do the same here except that, in this 3D case, there are now more opportunities to take advantage of the separation by eigen-decomposition of the various tensorial components so that the saturation function can be applied to each piece individually. Even the first-order term which, in 3D, consists only of (pseudo-exponential of) the term linear in the Ricci scalar, offers an opportunity to dissect this simple term into three eigenvalues of the Ricci tensor, with the saturation function applied to each one. But this suggests that, in 3D, we should add a first-order 'H'-type scheme — H_1, which replaces the single term of scheme E_1. The second-order scheme, H_2, also contains this first-order term's eigen-decomposition of the Ricci tensor but, in the terms quadratic in the Ricci tensor, it is desirable to avoid the appearance of the term that, in the formula (4.4b) for e_2, is of the opposite (negative) sign from the other positive terms. By separating the quadratic contribution of the Ricci scalar from the quadratic contribution of the *trace-free* part of the Ricci tensor, not only is any negative-signed term avoided, but the term involving the square of the Ricci scalar actually vanishes entirely (as we could have anticipated from our study of the 3D constant-curvature case in Part I, where the entire asymptotic expansion was shown to be given exactly by the Taylor series of the exponential function of just half the sectional curvature, or equivalently, of our first-order term, $R/12$).

We denote the eigenvalues of the Ricci tensor by $\rho_{(\alpha)}$, where $\sum_{\alpha=1}^{3} \rho_{(\alpha)} = R$, and the eigenvalues of the corresponding trace-free part of the Ricci tensor by $\sigma_{(\alpha)} = \rho_{(\alpha)} - R/3$. The eigenvalues satisfy:

$$g^{ij} R_{jk} (V^{(R)})^k_{(\alpha)} = (V^{(R)})^i_{(\alpha)} \rho_{(\alpha)}, \quad \alpha = 1, 2, 3, \tag{4.5}$$

for eigenvectors, $(V^{(R)})^i$, of the Ricci tensor R_{ij}. Similarly, and essentially as we did in Part I, we can also define the eigenvalues of the Hessian of the scalar curvature. The scalar curvature we use in the 3D case is just the Ricci scalar. We recall the tensorial definition of the Hessian operator from Part I:

$$\mathcal{H}_{ij}(R) = \left(\frac{\partial^2 R}{\partial x^i \partial x^j} - \Gamma^k_{ij} \frac{\partial R}{\partial x^k} \right). \tag{4.6}$$

The eigenvalues, $\eta_{(\alpha)}$ of this $\mathcal{H}_{ij}$ are defined to satisfy:

$$g^{ij} \mathcal{H}_{jk} (V^{(H)})^k_{(\alpha)} = (V^{(H)})^i_{(\alpha)} \eta_{(\alpha)}, \quad \alpha = 1, 2, 3. \tag{4.7}$$

As in Part I, we can employ a Cholesky decomposition (Golub and Van Loan 1989) of the metric to transform both non-standard eigen-problems, (4.5) and (4.7), into the simpler and more familiar standard eigen-problems involving a single symmetric matrix.

For the 'H_2' schemes, we use the same saturation parameter, which we again denote s_R, for both the $\rho_{(\alpha)}$ and the $\sigma_{(\alpha)}$, from which, via the function SAT_1, we obtain their effective quantities, $\widetilde{\rho}_{(\alpha)}$ and $\widetilde{\sigma}_{(\alpha)}$. Similarly, we introduce another saturation parameter, s_H, and, applying SAT_1 with this parameter to each of the $\eta_{(\alpha)}$, obtain their effective counterparts, $\widetilde{\eta}_{(\alpha)}$. We are now in a position to define the schemes H_1 and H_2:

$$h_1 = b_0/\widetilde{\exp}\left[\sum_{\alpha=1}^{3}\widetilde{\rho}_{(\alpha)}/12\right], \tag{4.8a}$$

$$h_2 = b_0/\widetilde{\exp}\left[\sum_{\alpha=1}^{3}\left(\widetilde{\rho_{(\alpha)}}/12+\widetilde{\sigma}^2_{(\alpha)}/240+\widetilde{\eta}_{(\alpha)}/120\right)\right]. \tag{4.8b}$$

(b) *Experimental validation*

The schemes we have described were compared for various idealized smooth random synthetic geometries. The geometries were periodic in the three coordinates of the finite differencing grid used to resolve them, the grid dimensions being $24 \times 24 \times 24$. The metric tensors were constructed as the exponentials of random symmetric matrices which were themselves generated by spatially smoothing symmetric 'white-noise' matrices. The spatial smoothing used in this synthesis was given an approximately Gaussian spectral profile and characteristic spatial scale (or smoothness parameter), S. The amplitude of this variation was here arbitrarily parameterized to be proportional to a convenient 'variance parameter', 'V'. The control experiment, denoted as in Part I by A_0 took the contravariant metric to be the diffusivity and the grid geometry to be Cartesian, but all the other experiments assumed 3D Riemannian geometry and a filter representing isotropic diffusion with unit diffusivity within this geometry, diffusion proceeding for a half-unit of time, as explained in earlier sections. Experiment 'A_0' denotes the result of normalizing the amplitude by the 3D Gaussian amplitude formula valid in Euclidean geometry for a homogeneous diffusion with the diffusivity that happens to occur at each of the chosen sample test points. These sample points, of which there were 32 in all experiments, formed a face-centered cubic sub-lattice of the computational grid – a configuration chosen to keep the sample points as far away from their nearest neighbors as possible so that the diffusion of impulsive (delta-function) initial distributions of 'diffused substance' would not strongly interfere with one another when diffused simultaneously. The Riemannian geometry diffusion experiments were similarly conducted with the trivial default normalization representing the 'zero-order' parametrix expansion denoted (again, as in Part I) by B_0. The non-trivial parametrix expansions of first and second order, denoted by the schemes E_1, E_2, H_1 and H_2 have already been described. The results from two series of geometric realizations are gathered into table 5 in two sets of four vertical columns. These two sets of columns differ only in the random number 'seed' used to produce the series of random numbers, so the geometries created in the corresponding columns are stochastically equivalent realizations.

The upper section of the table contains the best rms errors in the normalized amplitudes averaged over the 32 sample points out of all the combinations of the relevant saturation param-

TABLE 5. Table of rms errors of the normalized amplitudes of diffusion equation filters in smooth random geometries whose statistical characteristics are governed by a scale parameter, S and a variance parameter, V. The method A_0 refers to the Gauss-formula normalization of the filter assuming variable tensor diffusivity in Euclidean geometry, B_0 the uncorrected amplitude when the filter is rewritten as an isotropic filter in the Riemannian geometry whose metric equals the diffusivity assumed for A_0 experiments. The first-order correction methods E_1 and H_1 use the Riemannian geometry method with the first-order parametrix expansion stabilized by saturation functions as explained in the text. The methods E_2 and H_2 are two variants of the correspondingly stabilized 2nd-order parametrix methods. The numbers given are the rms errors of the adjusted amplitudes averaged over the 32 sample points of the domain. In the unstarred experiments the best (i.e., smallest) rms statistic are quoted for a range of combinations of the relevant saturation parameters, s_R for the Ricci scalar (used by E_1 and E_2) or the eigenvalues of the Ricci tensor (used by H_1 and H_2, s_L (used by E_2) and s_H (used by H_2), as the text explains. For the starred experiments, the saturation parameters are fixed to values which appear to give reasonably good results overall for the experiments to which they apply. These very roughly optimized values are as follow: $s_R = 2$ for E_1 and E_2; $s_R = 1$ for H_1 and H_2; $s_L = 6$ for E_2; $s_H = 5$ for H_2. Finally, some statistics of each realization of the Riemannian geometry are given. These are: the dimensionless measure of the total valume of the triply periodic domain; the minimum and maximum values of the Ricci scalar; the minimum and maximum of the Laplacian of the Ricci scalar. The columns are arranged roughly in ascending order of numerical difficulty with the largest characteristic scales of curvature variation at the left, subdivided by the two grades of amplitude of this stochastic curvature.

$[S, V]$:	[96, 1]	[96, 2]	[48, 1]	[48, 2]	[96, 1]	[96, 2]	[48, 1]	[48, 2]
A_0	0.1062	0.1634	0.2347	0.3445	0.0807	0.1207	0.3455	0.5515
B_0	0.0655	0.0921	0.1005	0.1360	0.0565	0.0823	0.1504	0.2064
E_1	0.0200	0.0364	0.0752	0.1128	0.0255	0.0437	0.0907	0.1370
E_2	0.0089	0.0222	0.0640	0.1067	0.0094	0.0242	0.0828	0.1335
H_1	0.0178	0.0324	0.0703	0.1017	0.0217	0.0377	0.0734	0.1151
H_2	0.0080	0.0168	0.0603	0.0874	0.0076	0.0171	0.0668	0.1000
E_1^*	0.0210	0.0427	0.0929	0.1225	0.0298	0.0450	0.0916	0.1376
E_2^*	0.0265	0.0480	0.0670	0.1072	0.0145	0.0349	0.0864	0.1379
H_1^*	0.0178	0.0347	0.0922	0.1132	0.0303	0.0423	0.0790	0.1151
H_2^*	0.0280	0.0484	0.0603	0.0876	0.0221	0.0354	0.0786	0.1203
volume:	260	289	245	268	187	180	216	227
$R_{\min}$:	-6.0	-11.4	-41.1	-81.5	-5.0	-9.5	-64.5	-139.4
$R_{\max}$:	2.5	3.5	11.1	19.3	2.8	4.1	14.4	26.7
$\nabla^2 R_{\min}$:	-25.3	-56.0	-808.7	-3118.1	-34.7	-109.4	-1256.7	-5123.9
$\nabla^2 R_{\max}$:	65.0	182.3	1651.4	5523.2	65.7	195.2	4027.4	14148.8

eters of each respective scheme (note that, owing to the larger dimensionality of the problem, we are not able to reproduce the large sample numbers we could achieve in the corresponding 2D experiments of Part I). The second section of the table lists the rms errors obtained instead for the four parametrix expansion schemes when their saturation parameters were held fixed to values judged to be close to an overall optimum. For these fixed-parameter schemes we have labeled E_1^* and E_2^*, their parameters were $s_R = 2$ and $s_L = 6$. For the schemes we have labeled H_1^* and H_2^*, the parameters were kept fixed at $s_R = 1$ and $s_H = 5$.

Some idea of the variability of the geometry is imparted by inspection of the third section of the table. There one will find the total volume of the periodic domain (in intrinsic dimensionless units supplied by the metric itself), the minimum and maximum values attained by the Ricci scalar in each realization, and the extremes attained by the Laplacian of this quantity, again, all in intrinsic or dimensionless units. Large values of the Laplacian found to the right of each set of four columns are indicative of a 'choppiness' of the curvature, whose amplitude is indicated by the relative magnitudes of the Ricci scalar. In all of the realizations the curvature is of a considerable magnitude (even with the smaller variance parameter cases, $V=1$) and the relatively abrupt changes of curvature implied by the smaller scale parameter cases, $S=48$, are particularly challenging for any filter normalization technique. For the Euclidean method, scheme A_0, rms errors are usually larger than ten percent and sometimes exceed fifty percent. Just by formulating the diffusion problem in the Riemannian geometry without further correction (experiments B_0) already reduces these errors substantially. For the smoother geometries ($S=96$) the parametrix method taken to second-order, whether by the E_2 or the H_2 scheme, produce further spectacular improvements in the amplitude estimates. As expected, for the more variable and shorter scale ($S=48$) random realizations, the advantages of the higher order schemes are not as great, but they still seem significant and are generally better than their first-order counterparts, E_1 or H_1. This confirms that the use of the pseudo-exponential function formulations with the 'effective' arguments that are moderated through their saturation functions does indeed make even the second-order parametrix methods numerically robust.

To a greater extent than was evident in the equivocal results we obtained in two dimensions, these 3D results suggest that the H schemes are significantly better than the corresponding E schemes at both first and second orders. Of course, the results presented use relatively simple and crudely tuned parametrizations and it is not hard to see how refinements could be made in several ways. Nevertheless, the rms statistics presented here, if borne out in practice, show that the robust implementations of the parametrix method can provide a satisfactory solution to the problem of 'calibrating' the synthetic covariances of a spatially adaptive data assimilation in three dimensions, and indicate that methods analogous to the H schemes might well be equally beneficial in the case of four dimensions.

(*c*) *Speculations on the form of practical normalization in four dimensions*

Based on the indications in 3D that it is beneficial, for robustness, to break down each term in the parametrix expansion formula into separate eigenvalue contributions prior to the application of the saturation function, we speculate that this approach continued into the 4D context will also lead to promising algorithms for normalizing the adaptive quasi-diffusive filters. In 4D we cannot avoid having to deal with contributions from the fourth-rank curvature tensor. However, just as we are able to break down the Ricci tensor into a trace-free part, plus the isotropic part associated with the Ricci scalar, the Riemann tensor itself can likewise be broken down into parts associated with the Ricci scalar and the trace-free Ricci tensor respectively, plus the residual totally trace-free 'Weyl tensor'. Each part may then be associated with a superposition of its eigen-components.

If we write S_{ij} for the trace-free portion of the Ricci tensor:

$$S_{ij} = R_{ij} - \frac{1}{n} R\, g_{ij}, \tag{4.9}$$

whose eigenvalues we have already denoted by '$\sigma_{(\alpha)}$', then the part of the Riemann tensor attributable to S_{ij} is:

$$S_{ij\,kl} = \frac{1}{n-2}\left(S_{ik}g_{jl} + S_{jl}g_{ik} - S_{il}g_{jk} - S_{jk}g_{il}\right), \quad n \geq 3, \tag{4.10}$$

while the part attributable to the Ricci scalar is:

$$U_{ij\,kl} = \frac{R}{n(n-1)}\left(g_{ik}g_{jl} - g_{il}g_{jk}\right), \quad n \geq 2. \tag{4.11}$$

The residual part, which is orthogonal to both S and U, is the Weyl tensor:

$$W_{ij\,kl} = R_{ij\,kl} - S_{ij\,kl} - U_{ij\,kl}, \tag{4.12}$$

which has a presence only in dimensions $n \geq 4$.

We find that:

$$R_{ij}R^{ij} = S_{ij}S^{ij} + \frac{1}{n}R^2, \tag{4.13}$$

and that

$$R_{ij\,kl}R^{ij\,kl} = W_{ij\,kl}W^{ij\,kl} + \frac{4}{n-2}S_{ij}S^{ij} + \frac{2}{n(n-1)}R^2. \tag{4.14}$$

Up to second-order the parametrix expansion is therefore equivalent to:

$$\begin{aligned} T(\frac{1}{2},0) &\approx 1 + \frac{T_1}{2} + \frac{T_2}{8} \\ &\approx \exp\left[\frac{R}{12} + \frac{1}{720}\left(-\frac{(n-3)}{n(n-1)}R^2 + \frac{(6-2)}{(n-2)}S_{ij}S^{ij} + W_{ij\,kl}W^{ij\,kl}\right) + \frac{\nabla^2 R}{120}\right], \end{aligned} \tag{4.15}$$

which is universally valid for *all* $n \geq 2$, provided we omit the term quadratic in S_{ij} when $n = 2$ (and remember that $W_{ij\,kl}$ vanishes at $n \leq 3$). In the particular case of four dimensions, where:

$$T(\frac{1}{2},0) \approx \exp\left(R/12 - R^2/8640 + S_{ij}S^{ij}/720 + W_{ij\,kl}W^{ij\,kl}/720 + \nabla^2 R/120\right), \tag{4.16}$$

we propose that an appropriate corresponding form of the robust scheme, H_2, is:

$$h_2 = b_0/\widetilde{\exp}\left[\sum_{\alpha=1}^{4}\left(\widetilde{\rho_{(\alpha)}}/12 + \widetilde{\sigma}^2_{(\alpha)}/720 + \widetilde{\eta}_{(\alpha)}/120\right) - \left(\sum_{\alpha=1}^{4}\widetilde{\rho}_{(\alpha)}\right)^2/8640 + \sum_{\alpha=1}^{6}\widetilde{\omega}^2_{(\alpha)}/720\right]. \tag{4.17}$$

The six quantities, $\widetilde{\omega}_{(\alpha)}$, are derived by applying the saturation function, with a new parameter, s_W, to each of the six eigenvalues, $\omega_{(\alpha)}$, of the Weyl tensor. In this case, the Weyl tensor is regarded as a symmetric operator, but in the six-dimensional space of 'bivectors' (Penrose and Rindler 1988), with the eigen-problem defined:

$$g^{ip}g^{jq}W_{pq\,kl}V^{kl}_{(\alpha)} = V^{ij}_{(\alpha)}\omega_{(\alpha)}. \tag{4.18}$$

In this context, the $V^{ij}_{(\alpha)}$ are six contravariant tensor representations of the Weyl tensor's anti-symmetric 'eigen-bivectors', which are discussed in greater detail in Appendix D.

The geometry of the eigen-structure of the Weyl tensor has several surprising features which we analyse and discuss in Appendix D. One peculiarity of the Weyl tensor in four dimensions is that it can be split into a 'self-dual' piece and a complementary 'anti-self-dual' piece. While a single saturation parameter, $s_W \approx 1$, for this Weyl tensor contribution would presumably suffice to maintain the robustness of this more general form of the implementation of the amplitude adjustment, it might transpire that, upon refinement and tuning, the best results would require different saturation parameter values to be chosen for the self-dual and anti-self-dual portions. But the investigation of this subtle question lies far beyond the scope of this note.

5. Conclusion

Following on from the more specialized applications of the parametrix expansion treated in Part I, this Part II provides a survey of the relevant portions of the general n-dimensional Riemannian geometry before describing the systematic approach by which the parametrix expansion may be carried out in its full generality. Even at the second order of expansion, which we have presented here in detail, the algebraic manipulations of the tensorial quantities needed in the course of taking the necessary intermediate steps become extremely cumbersome. However, we are rewarded by the one-line result, (3.34), of remarkable simplicity and which, as is discussed in Berger et al (1971), Gilkey (1984) and Rosenberg (1997), is valid to any number of spatial dimensions. In principle, the formal techniques we have described here could be extended to higher orders of the expansion, but it would not be practical to carry out the requisite manipulations without the aid of automated symbolic manipulation software configured for this problem. Luckily, there is no pressing practical need for such high-order expansions of the parametrix method in our context of normalizing the quasi-diffusive filters for use in data assimilation because, as we saw in the results of numerical experiments in Part I, the chief advantages of the method are gained from the very lowest orders of the asymptotic series. Even posing the diffusion problem as one of isotropic diffusion in the implied Riemannian geometry without *any* degree of asymptotic expansion (just using the Gaussian amplitude formula) yields a very significant gain in the accuracy of the filter amplitude normalization. Moreover, even at second order, the series sum often tends not to improve significantly, or even to show signs of divergence, when the excursions of the aspect tensor field occur too suddenly. However, as in Part I, we have extended the study of the first- and second-order parametrix methods beyond their purely formal mathematical aspects and have developed empirical modifications, still fully consistent with the asymptotic expansions, but which effectively immunize the expansions, to a considerable degree, against the ill-effects of the large, or abrupt excursions of the curvature diagnostics which would otherwise cause the application of these approximations to fail.

Preliminary experiments fully justify the approach we have taken and suggest directions for extending the method to four dimensions should this become desirable. Future experience with the practical implementation of the these methods will, no doubt, reveal unsuspected further problems to solve and provide a better feel for the relative advantages of first-order versus second-order (or higher) approximations in the practical context where reliability and robustness are generally of greater importance than improvements in rms measures of amplitude accuracy.

While the diagnostics upon which the formal asymptotic expansions are based are strictly local (ultimately, combinations of various *in situ* values of the higher derivatives of the metric tensor), there is no reason in principle that a more general set of *non-local* diagnostics could be not exploited instead. For example, it costs very little to apply the (un-normalized) anisotropic smoother; this provides a means of locally averaging the values of the curvature diagnostics which, in this study and in other formal studies of the parametrix expansion, have been strictly confined to their immediate in situ evaluations. A modification of the expansion series to accommodate the more general smoothed or averaged diagnostics would obviously be needed, but, by effectively 'feeling' and blending the local variablity of the original curvature dignostics, the more general method might automatically lead to a more representative and robust normalization requiring less of the kinds of interventions, with empirical 'saturation functions' that we have devoted effort to developing and describing here. Again, this extension of the present method must be deferred for future consideration.

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Appendix A

Proofs of theorems relating J and Q shape tensors

Proof of lemma 2:

Let the actual indices of a particular component of the Q tensor be denoted respectively, $q_1, \dots, q_\alpha$. We recall the complete criteria of lexicographic irreducibility of the component Q and list them in the following arrangement:

$$q_1 \leq q_3 \leq q_5 \leq q_6 \dots \leq q_\alpha, \tag{A.1a}$$
$$q_2 \leq q_4, \tag{A.1b}$$
$$q_1 < q_2, \tag{A.1c}$$
$$q_3 < q_4. \tag{A.1d}$$

Now we list the criteria of irreducibility of the component of the corresponding J:

$$j_\alpha \geq j_{\alpha-1} \geq j_{\alpha-2} \geq j_{\alpha-3} \dots \geq j_3, \tag{A.2a}$$
$$j_2 \geq j_1, \tag{A.2b}$$
$$j_\alpha > j_2, \tag{A.2c}$$
$$j_{\alpha-1} > j_1. \tag{A.2d}$$

There is evidently a perfect 'isomorphism' between these two networks of inequalities except that the sense of all the inequalities of the one set is reversed with respect to all the corresponding inequalities of the other set. (Although, for low rank Q and J, some of the train of inequalities in the respective first lines becomes redundant in each set, it is always *corresponding* inequalities that drop out, leaving the isomorphism intact.) The same pattern of qualifying criteria implies the same number of lexicographically independent components for the two tensors; therefore the lexicographic rules for J are complete.

□

Proof of Theorem 1:

The result has been shown to be true in the case $\alpha = 4$ when we obtained (2.52). For the case of shape tensors of rank $\alpha \geq 5$ let us define

$$\tilde{S}_{13245\ldots\alpha} = (\tilde{J}_{12\,345\ldots\alpha} - \tilde{J}_{32\,145\ldots\alpha} - \tilde{J}_{14\,325\ldots\alpha} + \tilde{J}_{34\,125\ldots\alpha}). \tag{A.3}$$

By direct substitution of (A.3) we can easily verify that $\tilde{S}$ satisfies all the symmetries we require of a Q-type shape tensor of this rank, viz:

$$\begin{aligned}
\tilde{S}_{1324\ldots\alpha} + \tilde{S}_{3124\ldots\alpha} &= 0, && \text{(A.4a)}\\
\tilde{S}_{1324\ldots\alpha} + \tilde{S}_{1242\ldots\alpha} &= 0, && \text{(A.4b)}\\
\tilde{S}_{1324\ldots\alpha} + \tilde{S}_{3214\ldots\alpha} + \tilde{S}_{2134\ldots\alpha} &= 0, && \text{(A.4c)}\\
\tilde{S}_{1324\ldots\alpha} + \tilde{S}_{1243\ldots\alpha} + \tilde{S}_{1432\ldots\alpha} &= 0, && \text{(A.4d)}\\
\tilde{S}_{13245\ldots\alpha} + \tilde{S}_{13452\ldots\alpha} + \tilde{S}_{13524\ldots\alpha} &= 0, && \text{(A.4e)}
\end{aligned}$$

and

$$(\alpha-4)!\tilde{S}_{1324(\alpha-4)} = \tilde{S}_{1324(1)_1\ldots(1)_{\alpha-4}}. \tag{A.5}$$

consider

$$\begin{aligned}
Z &= \tilde{S}_{1(1)2(1)(\alpha-4)}\\
&= \tilde{J}_{12(1)(1)(\alpha-4)} - \tilde{J}_{(1)21(1)(\alpha-4)} - \tilde{J}_{1(1)(1)2(\alpha-4)} + \tilde{J}_{(1)(1)12(\alpha-4)}.
\end{aligned} \tag{A.6}$$

The first of the four terms on right-hand side of (A.6) expands to $(\alpha-2)(\alpha-3)$ instances of $\tilde{J}_{12(\alpha-2)}$. Numbering the indices in these terms up to α, then in the expansion of the second term, the first explicit index is always some $\beta \in \{3, 4, \ldots, \alpha\}$ and, by symmetry, any one of such values must occur in a proportion, $1/(\alpha-2)$ of these terms, or, $(\alpha-3)$ times. Therefore from the property (2.65), the sum of the terms into which the second term of (A.6) expands is $(\alpha-3)\tilde{J}_{12(\alpha-2)}$. By a similar argument, the third term also expands with a sum of an equal amount. In the fourth term, both the first two indices of its expansion are neither 1 nor 2 and each such index pairs occurs just twice. By applying the result (2.65) to all possible leading index pairs, to pairs containing a single '1' or a single '2' and to the pair '12' itself, we find that the sum of the terms into which the fourth term of (A.6) expands give $2\tilde{J}_{12(\alpha-2)}$. The schematic diagram of Fig. 3 and its accompanying caption clarify this issue. In summary, we find that

$$
\begin{aligned}
Z &= [(\alpha-2)(\alpha-3)+2(\alpha-3)+2]\,\tilde{J}_{12\,(\alpha-2)}, \\
&= (\alpha-1)(\alpha-2)\tilde{J}_{12\,(\alpha-2)}.
\end{aligned}
\tag{A.7}
$$

But, from (2.64),

$$
\begin{aligned}
\tilde{Q}_{1(1)2(1)(\alpha-4)} &= (\alpha-2)(\alpha-3)\tilde{J}_{12\,(\alpha-2)}, \\
&= \frac{\alpha-3}{\alpha-1}Z,
\end{aligned}
\tag{A.8}
$$

and since the symmetries of $\tilde{S}$ have been shown to conform to those of $\tilde{Q}$, whose independent degrees of freedom are, moreover, equal in number to those of $\tilde{J}$, we confirm that the theorem is true; that is:

$$
\tilde{Q}_{12\,34\,\ldots\alpha} = \frac{\alpha-3}{\alpha-1}(\tilde{J}_{13\,24\ldots\alpha} - \tilde{J}_{23\,14\ldots\alpha} - \tilde{J}_{14\,23\ldots\alpha} + \tilde{J}_{24\,13\ldots\alpha}). \qquad \square.
$$

Proof of lemma 3:
From (2.64), we can express the contracted $\tilde{J}$:

$$
\alpha!\delta^{aa'}\tilde{J}_{a1\,a'(\alpha-1)} = (\alpha-2)!\delta^{aa'}\left[\tilde{Q}_{aa'1(1)(\alpha-2)} + \tilde{Q}_{a(1)1a'(\alpha-2)} + \tilde{Q}_{a(1)1(1)a'(\alpha-3)}\right]. \tag{A.9}
$$

By index-transposition symmetry, the first term on the right vanishes. By the Bianchi symmetry, the index 'a'' in the third term can be brought forward in two substituted terms, and a further application of index-transposition symmetry then gives us:

$$
\begin{aligned}
\alpha!\delta^{aa'}\tilde{J}_{a1\,a'(\alpha-1)} &= (\alpha-2)!\delta^{aa'}\left[-\tilde{Q}_{a(1)a'1(\alpha-2)} + \tilde{Q}_{a(1)a'(1)1(\alpha-3)} - \tilde{Q}_{a(1)a'1(1)(\alpha-3)}\right], \\
&= (\alpha-2)!\left[\overline{Q}_{(1)(1)\,1(\alpha-3)} - (\alpha-1)\overline{Q}_{1(1)\,(\alpha-2)}\right],
\end{aligned}
\tag{A.10}
$$

whose first right-hand term may be simplified by virtue of the transposition symmetry with respect to the leading pair of indices to give the form as given by (2.71). $\square$

Appendix B

Special notation and combinatorial short-cuts for quantities derived from the metric

The quantities g^{ij}, $\Gamma^{i}{}_{jk}$, and W^i and their (spatial) partial derivativess in the normal coordinates share a special algebraic property that allows them to be constructed as 'chains' or 'trees' of factors alternating between contravariant metric, $g^{\bullet\bullet}$, ('superscript factors') and partial derivatives of covariant metric, $g_{\bullet\bullet}$ ('subscript factors'). They are 'trees' in the sense that, reading from left to right, each differentiated subscript factor is linked by a contracted dummy index (of 'a-type') to a superscript factor that immediately precedes it, while each superscript factor except the first is linked by another contracted dummy index (of 'b-type') to one of the subscript factors that precede it (though not always necessarily the one immediately before this contravariant metric; the special case where the linkage *is* simply consecutive gives what we call a 'chain'). Moreover, in each such term, the factors and indices can be arranged such that the b-type links never cross: the order of the appearance of dummy subscripts belonging to b-type links is the same as the order of the superscript factors they point to. Every term begins with a superscript factor but may end with factors of either type. Owing to this special construction, such a term can be coded in a way in which the internal contracted indices of both a-type and b-type are implicit.

An illustrative example is the contravariant metric $g^{\bullet\bullet}$ itself, together with its partial derivatives.

$$\begin{aligned} g^{i_1 i_2}{}_{,i_3} &= -g^{i_1 a_1} g_{a_1 b_2, i_3} g^{b_2 i_2}, && \text{(B.1)} \\ g^{i_1 i_2}{}_{,i_3 i_4} &= +g^{i_1 a_1} g_{a_1 b_2, i_4} g^{b_2 a_2} g_{a_2 b_3, i_3} g^{b_3 i_2} \\ &\quad -g^{i_1 a_1} g_{a_1 b_2, i_3 i_4} g^{b_2 i_2} \\ &\quad +g^{i_1 a_1} g_{a_1 b_2, i_3} g^{b_2 a_2} g_{a_2 b_3, i_4} g^{b_3 i_2}, && \text{(B.2)} \end{aligned}$$

whose resultant terms are all 'chains' in the sense defined above.

We could encode these expressions more concisely using a shorthand notation in which the two superscripts associated with each $g^{\bullet\bullet}$, if of the contracted 'a' or 'b' kind, are implicit, but unwritten. We could also omit the subscript 'a' indices without loss of information, provided we somehow distinguish the case (as above) where this 'a' occurs to the left of the comma from more general cases we shall need to deal with where the 'a' index may alternatively follow the comma. Also, since the 'b'-type subscripts all occur in proper numerical order, which also corresponds to the order of occurrence of the later $g^{\bullet\bullet}$ to which they connect by index-contraction, we would lose no information by placing an anonymous 'bullet' subscript in their place. Finally, since each $g^{\bullet\bullet}$ and differentiated $g_{\bullet\bullet}$ alternate, with the $g^{\bullet\bullet}$ invariably coming first, we need only mark the start of each such pair, and the terminating $g^{\bullet\bullet}$, if present, with a special punctuation, leaving in between only the trimmed-down subscript lists. We therefore adopt an encoding where the contravariant metric by itself, or at the end of a term is written as a special '|' or '/' punctuation and, as we have done in some expressions already, each un-paired index, such as i_2, is replaced by its own index label, in this case '2', as in the 'tilde' notation. For the trivial example,

$$g^{i_1 i_2} \equiv \tilde{g}^{12} \equiv |^{12}. \tag{B.3}$$

In the partial derivative expression of (B.1) we can simply write

$$g^{i_1 i_2}{}_{,i_3} \equiv \tilde{g}^{12}_{,3} \equiv -\,|_{\bullet\,3}|^{12} \tag{B.4}$$

and, keeping the interior of each expression free of the unpaired superscripts, encode (B.2) as:

$$g^{i_1 i_2}{}_{,i_3 i_4} \equiv \tilde{g}^{12}_{,34} \equiv \Big[|_{\bullet\,4}|_{\bullet\,3}| - |_{\bullet\,34}| + |_{\bullet\,3}|_{\bullet\,4}|\Big]^{12}. \tag{B.5}$$

The rules for successive partial differentiation are evidently very simple since, in a term, every superscript factor and every subscript factor is differentiated in its place in the chain to contribute a new term, also a chain, in the result expression. This is just an application of the rule of Leibniz. The derivative of each superscript factor is defined:

$$|_{,p} = -|_{\bullet\,p}|, \tag{B.6}$$

while the derivative of the index string representing the subscript factor just entails appending the new differentiation index to the list of subscripts. In the case of the three terms making up ${\Gamma^{i_1}}_{i_2 i_3} \equiv {\tilde{\Gamma}^1}_{23}$, two of these terms already conform to what our '$|$' notation can deal with, but in the third term,

$$-\frac{1}{2} g^{i_1 a_1} g_{i_2 i_3, a_1},$$

the index, a_1, now couples the superscript factor to the *differentiated* position of the subscript factor. However, we can conveniently signify this distinction by replacing the '$|$' by a '$/$' marking the start of the 'bifactor'. Thus, the complete encoding of the Christoffel symbol becomes:

$$\tilde{\Gamma}^1_{23} \equiv \left[\frac{1}{2} \Big(|_{2\,3} + |_{3\,2} - /_{23} \Big) \right]^1 . \tag{B.7}$$

The third term could equally be written with a '$/_{32}$' since the leading pair of indices to the right of any '$/$' are transposable (corresponding to the symmetry of the covariant metric tensor); but this is clearly not true of the '$|$'-type bifactors. However, for more complex bifactors of α written indices (which can include bullets), we are permitted to permute the trailing $\alpha - 1$ indices of a $|$-type bifactor, and the trailing $\alpha - 2$ indices of a $/$-type bifactor (i.e., the ones that correspond to the spatial derivative indices).

For the quantity W^i defined in (3.8) it is convenient to consider its parts separately, that is,

$$W^i = \frac{1}{2} X^i - Y^i \tag{B.8}$$

where, although X and Y may be written in different ways in the shorthand notation, we shall adopt a style in which the second contracted index of the last superscript factor is always written as the reserved symbol, '$\circ$', with its existence as a matching superscript on the final '$|$' of each term taken as implicit. In other respects, this '$\circ$' index is treated as just another numerical index label, allowing us to express X and Y:

$$\tilde{X}^1 = /_{\bullet\circ}|^1, \tag{B.9a}$$
$$\tilde{Y}^1 = |_{\bullet\,\circ}|^1. \tag{B.9b}$$

It will be observed that Y^i is the contraction of the negative derivative of the contravariant metric that we can symbolize:

$$\tilde{Y}^1 = -|^1_{,\circ}. \tag{B.10}$$

We have seen how the application of Leibniz rule for the construction of partial derivatives of a multifactor term leads to a proliferation of terms in the result. Nevertheless, in view of the fact that higher derivatives of the W^i and g^{ij} terms figure so prominently in the parametrix expansion procedure of section 3, it is worth devoting some effort to establishing a systematic formulaic description of the generic higher derivatives of the two parts, X^i and Y^i, of W^i, together with the derivatives of the metric, g^{ij}. In order to proceed it is necessary to introduce a notation for some additional combinatoric functions associated with the theory of partitions. First, we consider the ways in which a set of α items (which will end up being our indices of partial differentiation) may be arranged in ordered nonempty subsets. For the qth such

TABLE 6. ORDERED PARTITIONS OF α UP TO $\alpha = 4$.

α	q	$\sigma_{1,q,\alpha}$	$\sigma_{2,q,\alpha}$	$\sigma_{3,q,\alpha}$	$\sigma_{4,q,\alpha}$	$\nu_{q,\alpha}$	$\mu_{q,\alpha}$
1	$E_0 = 1$	1				1	1
2	1	2				1	1
	$E_1 = 2$	1	1			2	2
3	1	3				1	1
	2	2	1			2	3
	3	1	2			2	3
	$E_2 = 4$	1	1	1		3	6
4	1	4				1	1
	2	3	1			2	4
	3	2	2			2	6
	4	2	1	1		2	12
	5	1	3			2	4
	6	1	2	1		3	12
	7	1	1	2		3	12
	$E_3 = 8$	1	1	1	1	4	24

arrangement we let $\sigma_{p,q,\alpha}$ measure the size of the pth subset, and let $\nu_{q,\alpha}$, record the number of subsets. Clearly, for the case of $\alpha = 1$ item, only the single trivial arrangement is possible:

$$\nu_{1,1} = 1, \tag{B.11}$$

and

$$\sigma_{1,1,1} = 1. \tag{B.12}$$

But, if $E_{\alpha-1}$ denotes the number of the ordered partitions of α, i.e., the maximum index q at this α, then we may recursively define, for any $\alpha > 1$:

$$\nu_{q,\alpha} = \begin{cases} \nu_{q,\alpha-1} & : \quad q \le E_{\alpha-2} \\ \nu_{q-E_{\alpha-2},\alpha-1} + 1 & : \quad q > E_{\alpha-2}. \end{cases}, \quad q = 1, \ldots E_{\alpha-1}, \tag{B.13}$$

$$\sigma_{p,q,\alpha} = \begin{cases} \sigma_{p,q,\alpha-1} + 1 & : \quad p = 1, \quad q \le E_{\alpha-2} \\ 1 & : \quad p = 1, \quad q > E_{\alpha-2} \\ \sigma_{p,q,\alpha-1} & : \quad p > 1, \quad q \le E_{\alpha-2} \\ \sigma_{p-1,q-E_{\alpha-2},\alpha-1} & : \quad p > 1, \quad q > E_{\alpha-2} \end{cases}, \quad q = 1, \ldots E_{\alpha-1}. \tag{B.14}$$

The number $E_{\alpha-1}$ of such arrangements for a given α is also subject to a recurrence:

$$E_\alpha = E_{\alpha-1} + E_{\alpha-1} = 2E_{\alpha-1}, \tag{B.15}$$

and, since $E_0 = 1$, it is simply the indicated power of two: $E_\alpha = 2^\alpha$. This suggests that a binary indexing of the partitions at each α may be natural. Putting the α items to be partitioned in a row offers $\alpha - 1$ intermediate positions where a separating partition is either present or absent. If the presence or absence at each location is signified by a '1' or a '0', then one does indeed obtain a binary indexing. (The resulting binary index is one less than our index q).

TABLE 7. Ordered 'Fibonacci' partitions of α up to $\alpha = 6$ conditional upon each subset being of a size greater than one.

α	q	$\hat{\sigma}_{1,q,\alpha}$	$\hat{\sigma}_{2,q,\alpha}$	$\hat{\sigma}_{3,q,\alpha}$	$\hat{\nu}_{q,\alpha}$	$\hat{\mu}_{q,\alpha}$
2	$F_1 = 1$	2			1	1
3	$F_2 = 1$	3			1	1
4	1	4			1	1
	$F_3 = 2$	2	2		2	6
5	1	5			1	1
	2	3	2		2	10
	$F_4 = 3$	2	3		2	10
6	1	6			1	1
	2	4	2		2	15
	3	3	3		2	20
	4	2	4		2	15
	$F_5 = 5$	2	2	2	3	90

Table 6 displays the examples of these functions for $\alpha \leq 4$ together with the multinomial quantity,

$$\mu_{q,\alpha} = \alpha!/\prod_{p=1}^{\nu_{q,\alpha}} (\sigma_{p,q,\alpha})!, \tag{B.16}$$

which quantifies the number of distinct ways the α items may be distributed among subsets of these given sizes.

We can use these combinatorial functions to formulate expressions for the successive derivatives of the quantities g^{ij}, X^i and Y^i that appear in the parametrix expansion of section 3. First, we introduce a notation for a superscript factor meta-symbol, $\dagger$, which becomes either a $/$ or a $|$ depending on whether or not its subscripts include the reserved subscript symbol, '$\circ$'. Let set, $\mathcal{L}$, stand for a part of the subscript list and let $\mathcal{L}^- = \mathcal{L} \setminus \{\circ\}$ denote the part of it that excludes the reserved subscript, $\circ$. Then the action of meta-symbol, $\dagger$, which always occurs in association with a leading subscript, $\bullet$, is defined:

$$\dagger_{\bullet\mathcal{L}} \equiv \begin{cases} /_{\bullet\circ\mathcal{L}^-} & : \quad \circ \in \mathcal{L}, \\ |_{\bullet\mathcal{L}} & : \quad \circ \notin \mathcal{L}. \end{cases} \tag{B.17}$$

With this augmentation to our shorthand and combinatorial index notations we can immediately formulate the degree-α partial derivative of $\tilde{X}^1 \equiv X^{i_1}$:

$$\tilde{X}^1_{,(\alpha)} = -\left[\sum_{q=1}^{E_\alpha}\left(\prod_{p=1}^{\nu_{q,\alpha+1}} -\dagger_{\bullet(\sigma_{p,q,\alpha+1})}\right)\Big|\right]^1, \quad \text{where } (\sigma_{1,1,\alpha+1}) \equiv \{\circ\} \cup (\alpha). \tag{B.18}$$

The factors of the product are consistently ordered from left to right with increasing p. In other words, the partitioning occurring here involves a given set of α generic indices, plus the special index, $\circ$ understood to be contracted with the final $|$ of the concatenation implied by the product operator in (B.18). The corresponding equation for the repeated derivative of Y^i is similarly structured, but simpler now that the mode-switching '†' meta-symbol is not involved:

$$\tilde{Y}^1_{,(\alpha)} = -\left[\sum_{q=1}^{E_\alpha}\left(\prod_{p=1}^{\nu_{q,\alpha+1}} -|_{\bullet(\sigma_{p,q,\alpha+1})}\right)|\right]^1, \quad \text{where } (\sigma_{1,1,\alpha+1}) \equiv \{\circ\} \cup (\alpha). \tag{B.19}$$

Finally, a similar construction formulates the derivatives of the contravariant metric itself:

$$\tilde{g}^{12}_{,(\alpha)} \equiv \left[\sum_{q=1}^{E_{\alpha-1}}\left(\prod_{p=1}^{\nu_{q,\alpha}} -|_{\bullet(\sigma_{p,q,\alpha})}\right)|\right]^{12}, \quad \text{where } (\sigma_{1,1,\alpha}) \equiv (\alpha). \tag{B.20}$$

However, if we intend only to evaluate these quantities at $\boldsymbol{O}$, then the contributions associated with partitions containing a subset of size one disappear, since these factors translate into a singly-differentiated metric. Therefore, it is convenient to formalize the special case in which only partitions into subsets of size two or more are retained. The number of subsets of the qth partition in this case will be denoted $\hat{\nu}_{q,\alpha}$ and the size of the pth subset of this partition by $\hat{\sigma}_{p,q,\alpha}$. Then, the recurrences are initialized by the values:

$$\hat{\nu}_{1,2} = 1, \tag{B.21}$$

and

$$\hat{\sigma}_{1,1,2} = 2, \tag{B.22}$$

and continue for $\hat{\nu}$:

$$\hat{\nu}_{q,\alpha} = \begin{cases} \hat{\nu}_{q,\alpha-1} & : \; q \le F_{\alpha-2} \\ \hat{\nu}_{q-F_{\alpha-2},\alpha-2} + 1 & : \; q > F_{\alpha-2} \end{cases}, \quad q = 1, \ldots F_{\alpha-1} \tag{B.23}$$

and for $\hat{\sigma}$:

$$\hat{\sigma}_{p,q,\alpha} = \begin{cases} \hat{\sigma}_{p,q,\alpha-1} + 1 & : \; p = 1, \quad q \le F_{\alpha-2} \\ 2 & : \; p = 1, \quad q > F_{\alpha-2} \\ \hat{\sigma}_{p,q,\alpha-1} & : \; p > 1, \quad q \le F_{\alpha-2} \\ \hat{\sigma}_{p-1,q-F_{\alpha-2},\alpha-2} & : \; p > 1, \quad q > F_{\alpha-2}. \end{cases}, \quad q = 1, \ldots F_{\alpha-1} \tag{B.24}$$

The superficial similarities between these two sets of recurrence equations and the corresponding (B.13), (B.14) are obvious, but the subtle differences have important effects. $F_{\alpha-1}$ is now the number of arrangements of the ordered subsets for each α and the recurrence relation it satisfies is:

$$F_\alpha = F_{\alpha-1} + F_{\alpha-2}, \tag{B.25}$$

which, with F_0=0 and $F_1 = 1$, generates the Fibonacci sequence.

The equations for X^i, Y^i and g^{ij} evaluated at $\boldsymbol{O}$ can now be simplified, taking modified forms of (B.18), (B.19), (B.20), but with F, $\hat{\nu}$ and $\hat{\sigma}$ replacing E, ν and σ. As α increases, the economy of terms achieved by this substitution become more and more dramatic.

To show how the formalism may be applied in practice, consider the evaluation, at $\boldsymbol{O}$ of the quantity, $\tilde{\delta}_{1a}\tilde{X}^a{}_{,(3)}$. Since $F_3 = 2$, we obtain a summation over two partition-classes of terms which can then be made more specific through the appropriate interpretation of the switching operator, †:

$$\begin{aligned}
\tilde{\delta}_{1a}\tilde{X}^a{}_{,(3)}|_0 &= \tilde{\delta}_{1a}\left[\sum_{q=1}^{2}\left(\prod_{p=1}^{\hat{\nu}_{q,4}} -\dagger_{\bullet(\hat{\beta}_{p,q,4})}\right)|\right]^a, \quad (\hat{\beta}_{1,1,4}) \equiv \{\circ\}\cup(3), \\
&= \tilde{\delta}_{1a}\left[/_{\bullet\circ\,(3)}| - \left(/_{\bullet\circ\,(1)}|_{\bullet\,(2)}| + |_{\bullet\,(2)}/_{\bullet\circ\,(1)}|\right)\right]^a \\
&= 24\tilde{\delta}^{aa'}\tilde{J}_{aa'\,1(3)} - 4\tilde{\delta}^{aa'\,bb'}\left(\tilde{J}_{ab\,1(1)}\tilde{J}_{a'b'\,(2)} + \tilde{J}_{1a(2)}\tilde{J}_{bb'a'(1)}\right), \\
&= 8\overline{Q}_{1(1)\,(2)} - 2\tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a1\,b(1)}\tilde{Q}_{a'(1)\,b'(1)} - 2\tilde{\delta}^{aa'}\overline{Q}_{(1)a}\tilde{Q}_{1(1)\,a'(1)}. \qquad \text{(B.26)}
\end{aligned}$$

While this expression, through the corresponding W expression it contributes to, comes into play at orders of the parametric expansion higher than second, the second order parametrix coefficient itself (T_2) requires only the combination in which the index label we have marked '1' is replaced by the '(1)' of a larger combination. Lemma 1 can then be invoked to simplify the intermediate computations, or we can act on (B.26) directly to obtain:

$$\tilde{\delta}_{(1)a}\tilde{X}^a{}_{,(3)}|_0 = 16\overline{Q}_{(2)(2)} - 2\tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a(1)\,b(1)}\tilde{Q}_{a'(1)\,b'(1)}. \qquad \text{(B.27)}$$

Similar manipluations can be performed to obtain the corresponding Y expression, and hence the W expression, all of them expressed as combinations of the Q tensors. Likewise, we can derive the needed derivatives of the contravariant metric. Without providing the full step-by-step details (which should, by now, hold no mystery), we simply state the results relevant to the second-order parametrix expansion:

$$\begin{aligned}
\tilde{\delta}_{1a\,2b}\tilde{g}^{ab}_{,(2)}|_0 &= -\tilde{Q}_{1(1)\,2(1)}, && \text{(B.28a)} \\
\tilde{\delta}_{aa'}\tilde{g}^{aa'}_{,(2)}|_0 &= -2\overline{Q}_{(2)}, && \text{(B.28b)} \\
\tilde{\delta}_{aa'}\tilde{g}^{aa'}_{,(4)}|_0 &= -4\overline{Q}_{(2)\,(2)} + \tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a(1)\,b(1)}\tilde{Q}_{a'(1)\,b'(1)}, && \text{(B.28c)}
\end{aligned}$$

and

$$\begin{aligned}
\tilde{\delta}_{1a}\tilde{W}^a_{,(1)}|_0 &= 2\overline{Q}_{1(1)}, && \text{(B.29a)} \\
\tilde{\delta}_{(1)a}\tilde{W}^a_{,(1)}|_0 &= 4\overline{Q}_{(2)}, && \text{(B.29b)} \\
\tilde{\delta}_{(1)a}\tilde{W}^a_{,(3)}|_0 &= 12\overline{Q}_{(2)\,(2)} - 2\tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a(1)\,b(1)}\tilde{Q}_{a'(1)b'(1)}. && \text{(B.29c)}
\end{aligned}$$

From the definition of the Riemann tensor arranged as:

$$\tilde{R}^1{}_{2\,34} = \tilde{\Gamma}^1_{24,3} - \tilde{\Gamma}^1_{23,4} + \tilde{\Gamma}^1_{3a}\tilde{\Gamma}^a_{24} - \tilde{\Gamma}^1_{4a}\tilde{\Gamma}^a_{23}, \qquad \text{(B.30)}$$

it is not difficult to see that the product terms on the right-hand side are expressible in the new notation. The full expansion is:

$$
\begin{aligned}
\tilde{R}^{1}_{\;2\,34} \;=\;& \Big[\frac{1}{2}\Big(-\,|_{3\,24} + |_{4\,23} + /_{23\,4} - /_{24\,3}\Big) \\
+\;& \frac{1}{4}\Big(+\,|_{3\,\bullet}|_{2\,4} + |_{3\,\bullet}|_{4\,2} - |_{3\,\bullet}/_{24} - |_{4\,\bullet}|_{2\,3} - |_{4\,\bullet}|_{3\,2} + |_{4\,\bullet}/_{23} \\
& -|_{\bullet 3}|_{2\,4} - |_{\bullet\,3}|_{4\,2} + |_{\bullet\,3}/_{24} + |_{\bullet\,4}|_{2\,3} + |_{\bullet\,4}|_{3\,2} - |_{\bullet\,4}/_{23} \\
& -/_{3\bullet}|_{2\,4} - /_{3\bullet}|_{4\,2} + /_{3\bullet}/_{24} + /_{4\bullet}|_{2\,3} + /_{4\bullet}|_{3\,2} - /_{4\bullet}/_{23}\Big)\Big]^{1} .
\end{aligned}
\tag{B.31}
$$

Of these terms, only the first four survive evaluation at $\boldsymbol{O}$, where they yield the expressions in J or in Q tensors equivalent to those given by (2.52).

Brevity is evidently not the main strength of this notation; rather it is the simplicity of the rules of syntax and combination, which make this notation relatively straighforward to mechanize. The terms (B.31) are listed systematically, with the four single-bifactor terms placed first, followed by all the two-bifactor terms. Within each group, the terms are listed lexicographically, with '|' having precedence over '/', and named digits having precedence over bullets. Establishing a convention of lexicographic precedence (though not necessarily this one) simplifies sorting, which in turn facililates the gathering of algebraically similar terms.

Being a true tensor, $\tilde{R}^{1}_{234}$ generates other tensors by repeated covariant differentiation. Moreover, the pattern, in which only the leading index is a superscript, is preserved. By induction, we are then justified in expecting the entire sequence of covariant derivatives to be expressible in our notation if we can show that the first covariant derivative is. The first covariant derivative of the Riemann tensor can be written in the form:

$$
\tilde{R}^{1}_{\;2\,34|5} = \tilde{R}^{1}_{\;2\,34,5} + \tilde{\Gamma}^{1}_{\;5a}\tilde{R}^{a}_{\;2\,34} - \tilde{R}^{1}_{\;a\,34}\tilde{\Gamma}^{a}_{\;25} - \tilde{R}^{1}_{\;2\,a4}\tilde{\Gamma}^{a}_{\;35} - \tilde{R}^{1}_{\;2\,3a}\tilde{\Gamma}^{a}_{\;45}, \tag{B.32}
$$

from which it is clear that all terms in the result will indeed be expressible in our machinable notation, but now as nontrivial 'trees' rather than just the 'chains' we have encountered so far in each expanded term.

Appendix C

Practical application of the combinatoric notation and identities to obtain the parametrix expansion terms.

The application of the combinatorial formulas of Appendix B allowed us to derive the successive derivatives of g^{ij} and of W^i needed to carry out the parametrix expansion method of section 3. We now use these quantities to establish the proofs of theorems 2 and 3.

Proof of Theorem 2:

The statement of the theorem is given in Eq. (3.21). Using (B.28b) and (B.29b) in (3.19b), we find:

$$
\mathcal{G}_{,(2)}|_0 = \overline{Q}_{(2)}, \tag{C.1}
$$

and thus,

$$T_{,(2)} = -\frac{1}{2}\overline{Q}_{(2)}. \tag{C.2}$$

Equation (3.20a) then implies that:

$$T_1 = -\frac{1}{2}\overline{\overline{Q}}. \tag{C.3}$$

Recall that $Q_{ij\,kl} = -(1/3)R_{ij\,kl}$, so, in terms of the Ricci scalar, R, we have indeed proved that

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

as required.

□

Before deriving the next coefficient in the parametrix expansion of the amplitude, we state the exact relationship that connects the rank-six shape tensor, Q, to the second covariant derivative of the Riemann tensor:

Lemma 4:

$$\tilde{R}_{12\,34|56}\Big|_0 = -20\tilde{Q}_{12\,34\,56} + \frac{1}{9}\sum_{\alpha=1}^{28} c_\alpha \tilde{\delta}^{aa'}\,\tilde{R}_{p_\alpha q_\alpha\, r_\alpha a}\tilde{R}_{s_\alpha t_\alpha\, u_\alpha a'}\Big|_0, \tag{C.4}$$

(where α is a counting index, *not* a vector component, and where the c_α are the set of numerical coefficients of each quadratic combination, *not* a spatial vector.) The coefficients and index permutations are given in table 8.

□

TABLE 8. Coefficients and index permutations of the quadratic combinations of the Riemann tensor in the second covariant derivative of the Riemann tensor.

α	c	prq	stu	α	c	pqr	stu	α	c	pqr	stu	α	c	pqr	stu	α	c	pqr	stu
1	3	123	456	5	-3	134	256	11	3	143	256	17	2	153	246	23	2	163	245
2	-6	123	465	6	6	134	265	12	-6	143	265	18	-4	153	264	24	-4	163	254
3	-3	124	356	7	-1	135	246	13	1	145	236	19	-2	154	236	25	-2	164	235
4	6	124	365	8	2	135	264	14	-2	145	263	20	4	154	263	26	4	164	253
				9	-1	136	245	15	1	146	235	21	3	156	234	27	-6	165	234
				10	2	136	254	16	-2	146	253	22	-3	156	243	28	6	165	243

Outline of the proof of lemma 4: The result in lemma 4 is obtained by mechanically carrying out the manipulations described in Appendix B that correspond to the covariant derivatives of the Riemann tensor when this tensor itself is encoded in the form given by (B.31). After performing the two symbolic covariant differentiations on this expression, the collected terms are 'evaluated' at $\boldsymbol{O}$. By this is meant the following sequence of algebraic operation. First, the removal of all the vanishing terms containing a factor corresponding to only a singly differentiated metric. Then a conversion in each remaining term of each bifactor into its implied J tensor. Next, each J tensor factor is expanded, using (2.64), to its equivalent Q-tensor representation. Each Q tensor is checked for lexicographic reducibility according to the rules set out in table 4 and rewritten, if necessary, in its unique equivalent irreducible form (conformable terms being gathered frequently throughout the process in order to keep their number manageable). Finally, rank-4 Q tensors in the expression are replaced by the Riemann tensor using (2.52). The corollary (2.68) to theorem 1 ensures that the only other Q term then remaining is the single instance of the rank-six tensor with indices in the same order as those of the twice-differentiated Riemann tensor. The coefficients of the numerous terms quadratic in the Riemann tensor are those that have been gathered in Table 8.

□

We obtain:

Lemma 5:

$$\nabla^2 R\Big|_0 \equiv \delta^{ij} R_{|ij}\Big|_0 = -20\delta^{ij}\overline{\overline{Q}}_{ij} + \frac{4R^{ij}R_{ij} + 6R_{ij\,kl}R^{ij\,kl}}{9}\Big|_0. \tag{C.5}$$

□

Proof: The result (C.5) is obtained by carrying out three pairs of index contractions: $(i_1 \equiv i_3)$; $(i_2 \equiv i_4)$; and $(i_5 \equiv i_6)$; in (C.4) and gathering the resulting conformable terms. The trace of the twice differentiated Ricci scalar is identified with the Laplacian of this scalar.

□

Proof of Theorem 3:

The statement of the theorem is given in Eq. (3.34). Using (B.28c) and (B.29c) in (3.31b), we find:

$$\mathcal{G}_{,(4)}|_0 = 4\overline{Q}_{(2)(2)} - \frac{1}{2}\tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a(1)b(1)}\tilde{Q}_{a'(1)\,b'(1)}, \tag{C.6}$$

and from (C.1), (C.2) and (3.31c) we get:

$$\mathcal{Q}_{,(4)}|_0 = -\frac{1}{2}\overline{Q}_{(2)}\overline{Q}_{(2)}. \tag{C.7}$$

Therefore, bringing in (3.31a), and setting $(\mathcal{T} + \mathcal{G} + \mathcal{Q})_{,(4)} = 0$ at $\boldsymbol{O}$, we get:

$$T_{,(4)} = -\overline{Q}_{(2)\,(2)} + \frac{1}{8}\overline{Q}_{(2)}\overline{Q}_{(2)} + \frac{1}{8}\tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a(1)\,b(1)}\tilde{Q}_{a'(1)\,b'(1)}. \tag{C.8}$$

We have already calculated all the factors on the right-hand side of (3.32c), which enables us to find:

$$\mathcal{Q}_{1,(2)}|_0 = -\frac{1}{2}\overline{Q}_{(2)}\overline{\overline{Q}} + \tilde{\delta}^{aa'}\overline{Q}_{a(1)}\overline{Q}_{a'(1)} - \frac{1}{2}\tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a(1)\,b(1)}\overline{Q}_{a'b'}. \tag{C.9}$$

From (C.8), we can obtain:

$$\begin{aligned}\tilde{\delta}^{aa'} T_{,aa'(2)}|_0 &= -\overline{\overline{Q}}_{(2)} - 2\tilde{\delta}^{aa'}\overline{Q}_{a(1)\,a'(1)} - \tilde{\delta}^{aa'}\overline{Q}_{(2)\,aa'}, \\ &+\frac{1}{2}\tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a(1)b(1)}\overline{Q}_{a'b'} + \frac{3}{4}\tilde{\delta}^{aa'\,bb'\,cc'}\tilde{Q}_{a(1)\,bc}\tilde{Q}_{a'(1)\,b'c'} \\ &+\frac{1}{4}\overline{Q}_{(2)}\overline{\overline{Q}} + \frac{1}{4}\tilde{\delta}^{aa'}\overline{Q}_{(1)a}\overline{Q}_{(1)a'}.\end{aligned} \tag{C.10}$$

Then the vanishing of $(\mathcal{T}_{1,(2)} + \mathcal{Q}_{1,(2)})$ at $\boldsymbol{O}$ implies that:

$$\begin{aligned}T_{1,(2)} &= -\frac{1}{3}\overline{\overline{Q}}_{(2)} - \frac{2}{3}\tilde{\delta}^{aa'}\overline{Q}_{a(1)\,a'(1)} - \frac{1}{3}\tilde{\delta}^{aa'}\overline{Q}_{(2)\,aa'} \\ &+\frac{1}{3}\tilde{\delta}^{aa'\,bb'}\tilde{Q}_{a(1)\,b(1)}\overline{Q}_{a'b'} + \frac{1}{4}\tilde{\delta}^{aa'\,bb'\,cc'}\tilde{Q}_{a(1)\,bc}\tilde{Q}_{a'(1)b'c'} \\ &+\frac{1}{4}\overline{Q}_{(2)}\overline{\overline{Q}} - \frac{1}{4}\tilde{\delta}^{aa'}\overline{Q}_{(1)a}\overline{Q}_{(1)a'}.\end{aligned} \tag{C.11}$$

Invoking (3.33a) and (2.52) we therefore obtain:

$$\begin{aligned}T_2 &= -\frac{4}{3}\tilde{\delta}^{aa'}\overline{\overline{Q}}_{aa'} + \frac{1}{4}\overline{\overline{Q}\overline{Q}} + \frac{1}{6}\tilde{\delta}^{aa'\,bb'}\overline{Q}_{ab}\overline{Q}_{a'b'} + \frac{1}{2}\tilde{\delta}^{aa'\,bb'\,cc'\,dd'}\tilde{Q}_{abcd}\tilde{Q}_{a'b'c'd'} \\ &= -\frac{4}{3}\tilde{\delta}^{aa'}\overline{\overline{Q}}_{aa'} + \frac{1}{36}R^2 + \frac{1}{54}R_{ij}R^{ij} + \frac{1}{18}R_{ijkl}R^{ijkl}.\end{aligned} \tag{C.12}$$

By combining this result with the expression (C.5) from lemma 5, we find that:

$$T_2 = \frac{1}{15}\delta^{ij}R_{|ij} + \frac{1}{36}R^2 - \frac{1}{90}R_{ij}R^{ij} + \frac{1}{90}R_{ijkl}R^{ijkl}, \tag{C.13}$$

which is equivalent to the result (3.34) asserted.

□

Appendix D

Geometry of the eigen-structure of the generic 4D Weyl tensor

D1. Separating the Weyl tensor from the Riemann tensor

In four dimensions the parametrix expansion continues to contain the Ricci tensor and scalar terms, but the quadratic term, $R_{ij\,kl}R^{ij\,kl}$ now includes additional contributions not expressible through Ricci components alone. Nevertheless, there is a sense in which the Ricci tensor still captures much of the information of the full Riemann, and we therefore wish to ensure that, to the fullest extent possible, this quadratic contribution is dealt with in the way that allows the saturation functions we have already defined for the Ricci tensor's eigenvalues to have their maximum effect. As discussed in section 4(c), we are therefore motivated to decompose the Riemann into the smallest part expressible in terms of the Ricci tensor, and the part left over, the Weyl tensor, $W_{ij\,kl}$:

$$R_{ij\,kl} = W_{ij\,kl} + T_{ij\,kl}, \tag{D.1}$$

where,

$$T_{ij\,kl} = S_{ij\,kl} + U_{ij\,kl}, \tag{D.2}$$

with $S_{ij\,kl}$ and $U_{ij\,kl}$ defined by (4.10) and (4.11) for $n = 4$ dimensions. The contraction of T is the Ricci tensor:

$$T^i{}_{j\,il} = R_{jl} = R^i{}_{j\,il}, \tag{D.3}$$

and where W and T are orthogonal in the sense:

$$W_{ij\,kl}T^{ij\,kl} = 0. \tag{D.4}$$

Having done this, we can examine the structure of W to see how best to extract characteristic scalars from it, to which we can apply the saturation function, with appropriate parameters.

The obvious characteristic quantities to use are the eigenvalues of W when W is interpreted as a symmetric operator in its first pairs of indices and its second pairs of indices. Since the Riemann tensor and its subdivisions W and T are antisymmetric in first pair and second pair of indices, the order of the 'matrix' to which the Weyl reduces is effectively only six in 4D (although, owing to the duplication of the antisymmetric components, we must take care to restore magnitudes of all trace-like quantities by including a factor of two).

D2. Eigen-structure of the Weyl tensor

The number of degrees of freedom we have in specifying the Riemann tensor in n dimensions is:

$$N_R(n) = n^2(n^2 - 1)/12, \tag{D.5}$$

while the Ricci tensor, $R^i{}_{j\,il}$, which can be any rank-2 symmetric tensor, has the number of degrees of freedom given by:

$$N_T(n) = n(n-1)/2, \tag{D.6}$$

leaving the number,

$$N_W(n) = N_R(n) - N_T(n) \tag{D.7}$$

left over for the degrees of freedom of the Weyl tensor. In 4D these numbers are:

$$N_R(n) = 20, \tag{D.8a}$$
$$N_T(n) = 10, \tag{D.8b}$$
$$N_W(n) = 10. \tag{D.8c}$$

Consequently, we seek a way of constructing tensors with the Weyl symmetries and possessing ten continuous parameters.

Consider the bivector, V_{ij}, in a local orthonormal coordinate frame, having the matrix representation (row i, column j):

$$V_{ij} = \begin{bmatrix} 0, & A, & B, & C \\ -A, & 0, & C, & -B \\ -B, & -C, & 0, & A \\ -C, & B, & -A, & 0 \end{bmatrix}. \tag{D.9}$$

Construct a contender for a portion of the Weyl tensor from the outer product of V with itself:

$$W^{(\zeta)}_{ij\,kl} = V_{ij}V_{kl}, \tag{D.10}$$

and consider the symmetries which the Weyl tensor needs to satisfy. First, consider the trace:

$$(W^{(\zeta)})^{i}{}_{j\,il} = V^{i}{}_{j}V_{il}. \tag{D.11}$$

Take the case where j and l are equal, say, $j = l = 1$, and we find that this trace becomes $A^2 + B^2 + C^2$, but when j and l differ, we find that the trace vanishes. In general:

$$V^{i}{}_{j}V_{il} = g_{jl}S^2, \tag{D.12}$$

where

$$S^2 = (A^2 + B^2 + C^2). \tag{D.13}$$

(Metric, g_{ij}, is equivalent to the Kronecker delta here since we are assuming normal coordinates.)

Next, consider the test of the Bianchi algebraic identity where we take the sum over cyclic permutation of the last three indices, j, k, l. Take the case where i and j are equal, say $i = j = 1$. Then

$$V_{11}V_{23} + V_{12}V_{31} + V_{13}V_{12} = 0 - AB + BA = 0. \tag{D.14}$$

For the case where all the indices are different, say, $i = 1$, $j = 2$, $k = 3$, $l = 4$, we get:

$$V_{12}V_{34} + V_{13}V_{42} + V_{14}V_{23} = A^2 + B^2 + C^2 = S^2, \tag{D.15}$$

and for other instances it is straightforward to verify that we obtain $\pm S^2$ according to whether the indices, i, j, k, l are an even $(= +S^2)$ or an odd $(= -S^2)$ permutation of $(1, 2, 3, 4)$. Introducing the Levi-Civita symbol, ϵ_{ijkl}, whose value is ± 1 according to whether the permutation is even or odd, we may express this result:

$$W^{(\zeta)}_{ij\,kl} + W^{(\zeta)}_{ik\,lj} + W^{(\zeta)}_{il\,jk} = \epsilon_{ij\,kl}S^2. \tag{D.16}$$

The other trace and permutation symmetries are equivalent to the ones we have checked and all give a violation for a tensor of the form $W^{(\zeta)}$ proportional to S^2. We can constrain the parameters A, B and C to make their sum of squares, S^2 equal to unity, and form a linear superposition by multiplying each such normalized $W^{(\zeta)}$ by a coefficient, $w^{+}_{(\zeta)}$. If we do this, the violation of the symmetries is directly proportional to the sum, $\sum_{\zeta} w^{+}_{(\zeta)}$, of the coefficients by which the normalized $W^{(\zeta)}$ are combined. Therefore, by ensuring that this sum vanishes, we guarantee a total tensor that satisfies all of the Weyl symmetries:

$$W^{+}_{ij\,kl} = \sum_{\zeta} V^{(\zeta)}_{ij}V^{(\zeta)}_{kl}w^{+}_{(\zeta)}, \quad \sum_{\zeta} w^{+}_{(\zeta)} = 0. \tag{D.17}$$

Each set, $(A, B, C)_{(\zeta)}$ forms a unit vector and an orthogonal triplet of such vectors produces a corresponding orthogonal triplet of the $W^{(\zeta)}$. It is therefore sufficient to sum ζ over only three instances to capture the full range of variability that this pattern of construction permits. Three degrees of freedom permit this orthogonal triple to be rotated, and the constraint that the three coefficients, $w^+_{(\zeta)}$, sum to zero implies that these coefficients collectively supply an additional two degrees of freedom in defining this class of Weyl tensors. In effect, the bivectors, $V^{(\zeta)}_{ij}$, act as the mutually-orthogonal eigenvectors of this part of the Weyl tensor, while the multiplying scalar coefficients act as the corresponding eigenvalues.

Even accounting for the fact that each $V^{(\zeta)}_{ij}$ contains the duplication of coefficients (with a sign change) upon taking the transpose, our construction in terms of $(A, B, C)^{(\zeta)}$ involves an additional duplication (i.e., each A, B, and C, appears four times in the matrix representation of the bivector) which we can exploit to form a new, and linearly independent class of eigen-bivectors. The new class can be written in the form:

$$U_{ij} = \begin{bmatrix} 0, & A, & B, & C \\ -A, & 0, & -C, & B \\ -B, & C, & 0, & -A \\ -C, & -B, & A, & 0 \end{bmatrix}. \tag{D.18}$$

By performing the same symmetry tests as before, we can verify that the new set of bivectors act as the eigen-bivectors of a distinct family of Weyl tensors requiring another five continuous independent degrees of freedom. We thus account for the ten degrees of freedom of the full Weyl tensor.

In order to gain insight into the geometrical significance of the normalized eigen-bivectors we have constructed, we consider a canonical representation of a mutually orthogonal set of them defined as follows:

$$V^{(1)},\ V^{(2)},\ V^{(3)} = \begin{bmatrix} 0, & 1, & 0, & 0 \\ -1, & 0, & 0, & 0 \\ 0, & 0, & 0, & 1 \\ 0, & ,0, & -1, & 0 \end{bmatrix}, \begin{bmatrix} 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & -1 \\ -1, & 0, & 0, & 0 \\ 0, & 1, & 0, & 0 \end{bmatrix}, \begin{bmatrix} 0, & 0, & 0, & 1 \\ 0, & 0, & 1, & 0 \\ 0, & -1, & 0, & 0 \\ -1, & 0, & 0, & 0 \end{bmatrix} \tag{D.19}$$

$$U^{(1)},\ U^{(2)},\ U^{(3)} = \begin{bmatrix} 0, & 1, & 0, & 0 \\ -1, & 0, & 0, & 0 \\ 0, & 0, & 0, & -1 \\ 0, & ,0, & 1, & 0 \end{bmatrix}, \begin{bmatrix} 0, & 0, & 1, & 0 \\ 0, & 0, & 0, & 1 \\ -1, & 0, & 0, & 0 \\ 0, & -1, & 0, & 0 \end{bmatrix}, \begin{bmatrix} 0, & 0, & 0, & 1 \\ 0, & 0, & -1, & 0 \\ 0, & 1, & 0, & 0 \\ -1, & 0, & 0, & 0 \end{bmatrix} \tag{D.20}$$

A further analysis of each one of these bivectors through its own eigen-decomposition runs into the problems associated with its double degeneracy (two pairs of the conjugate imaginary eigenvalues, $\sqrt{-1}$). Fortunately, the canonical representation is simple enough to allow us to see that one natural decomposition uses the basis four-vectors themselves. We therefore define:

$$Q_1 \equiv (\boldsymbol{a}_1, \boldsymbol{b}_1, \boldsymbol{c}_1, \boldsymbol{d}_1) = \left(\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \right), \tag{D.21}$$

and note that the canonical eigen-bivectors are obtained:

$$\begin{aligned} \left[V^{(1)}, V^{(2)}, V^{(3)}\right] &= [(\boldsymbol{a}_1 \wedge \boldsymbol{b}_1 + \boldsymbol{c}_1 \wedge \boldsymbol{d}_1), \quad (\boldsymbol{a}_1 \wedge \boldsymbol{c}_1 + \boldsymbol{d}_1 \wedge \boldsymbol{b}_1), \quad (\boldsymbol{a}_1 \wedge \boldsymbol{d}_1 + \boldsymbol{b}_1 \wedge \boldsymbol{c}_1)], \\ \left[U^{(1)}, U^{(2)}, U^{(3)}\right] &= [(\boldsymbol{a}_1 \wedge \boldsymbol{b}_1 - \boldsymbol{c}_1 \wedge \boldsymbol{d}_1), \quad (\boldsymbol{a}_1 \wedge \boldsymbol{c}_1 - \boldsymbol{d}_1 \wedge \boldsymbol{b}_1), \quad (\boldsymbol{a}_1 \wedge \boldsymbol{d}_1 - \boldsymbol{b}_1 \wedge \boldsymbol{c}_1)], \end{aligned} \tag{D.22}$$

where the wedge product is defined for two column vectors, p and q:

$$\boldsymbol{p} \wedge \boldsymbol{q} = \boldsymbol{p}\boldsymbol{q}^{\mathsf{T}} - \boldsymbol{q}\boldsymbol{p}^{\mathsf{T}}. \tag{D.23}$$

While these equations make it transparent that the sums and differences of the corresponding V^{ζ} and U^{ζ} lead to 'simple' bivectors, each expressible as the wedge product of a single pair of vectors, it is perhaps less obvious that this property occurs with the pairing of *any* V^{ζ} with *any* U^{η}. Each of the six possible permutations leads to a different system of mutually orthogonal unit-vector pairs, $\{\pm\boldsymbol{a}, \pm\boldsymbol{b}, \pm\boldsymbol{c}, \pm\boldsymbol{d}\}$ from which right-handed orthogonal quartets can be selected to serve as the alternative principal components. For example, we can define two of the alternative right-handed orthogonal quartets:

$$2Q_2 \equiv 2(\boldsymbol{a}_2, \boldsymbol{b}_2, \boldsymbol{c}_2, \boldsymbol{d}_2) = \left(\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \end{bmatrix} \right), \tag{D.24}$$

$$2Q_3 \equiv 2(\boldsymbol{a}_3, \boldsymbol{b}_3, \boldsymbol{c}_3, \boldsymbol{d}_3) = \left(\begin{bmatrix} -1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ -1 \\ 1 \end{bmatrix} \right). \tag{D.25}$$

Then we find

$$\begin{aligned} \left[-V^{(3)}, -V^{(2)}, -V^{(1)}\right] &= [(\boldsymbol{a}_2 \wedge \boldsymbol{b}_2 + \boldsymbol{c}_2 \wedge \boldsymbol{d}_2), (\boldsymbol{a}_2 \wedge \boldsymbol{c}_2 + \boldsymbol{d}_2 \wedge \boldsymbol{b}_2), (\boldsymbol{a}_2 \wedge \boldsymbol{d}_2 + \boldsymbol{b}_2 \wedge \boldsymbol{c}_2)], \\ \left[-U^{(2)}, -U^{(1)}, -U^{(3)}\right] &= [(\boldsymbol{a}_2 \wedge \boldsymbol{b}_2 - \boldsymbol{c}_2 \wedge \boldsymbol{d}_2), (\boldsymbol{a}_2 \wedge \boldsymbol{c}_2 - \boldsymbol{d}_2 \wedge \boldsymbol{b}_2), (\boldsymbol{a}_2 \wedge \boldsymbol{d}_2 - \boldsymbol{b}_2 \wedge \boldsymbol{c}_2)], \end{aligned} \tag{D.26}$$

or, using the third basis set, Q_3:

$$\begin{aligned}\left[-V^{(2)}, -V^{(1)}, -V^{(3)}\right] &= [(\boldsymbol{a}_3 \wedge \boldsymbol{b}_3 + \boldsymbol{c}_3 \wedge \boldsymbol{d}_3), (\boldsymbol{a}_3 \wedge \boldsymbol{c}_3 + \boldsymbol{d}_3 \wedge \boldsymbol{b}_3), (\boldsymbol{a}_3 \wedge \boldsymbol{d}_3 + \boldsymbol{b}_3 \wedge \boldsymbol{c}_3)]\,, \\ \left[-U^{(3)}, -U^{(2)}, -U^{(1)}\right] &= [(\boldsymbol{a}_3 \wedge \boldsymbol{b}_3 - \boldsymbol{c}_3 \wedge \boldsymbol{d}_3), (\boldsymbol{a}_3 \wedge \boldsymbol{c}_3 - \boldsymbol{d}_3 \wedge \boldsymbol{b}_3), (\boldsymbol{a}_3 \wedge \boldsymbol{d}_3 - \boldsymbol{b}_3 \wedge \boldsymbol{c}_3)]\,.\end{aligned} \tag{D.27}$$

Note that the negatives of the Vs and Us remain valid eigen-bivectors. However, the new V-type triplets and the new U-type triplets separately retain the chiral senses of the two original triplets, and this remains true for every valid alternative choice of righthanded $\{a, b, c, d\}$. If we reverse the chiral sense of the set, Q_1, the U become the new V and vice versa (with possible index permutations and sign-flips). The new relationships between the V triplets and the U triplets are the two possible cyclic rotations of the original set of correspondences; there are three other possible permutations of 'odd' parity, and these correspond to the compositions we obtain when we consider the additional alternative quartets defined:

$$\sqrt{2}Q_4 \equiv \sqrt{2}(\boldsymbol{a}_4, \boldsymbol{b}_4, \boldsymbol{c}_4, \boldsymbol{d}_4) = \left(\begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ -1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix} \right), \tag{D.28}$$

$$\sqrt{2}Q_5 \equiv \sqrt{2}(\boldsymbol{a}_5, \boldsymbol{b}_5, \boldsymbol{c}_5, \boldsymbol{d}_5) = \left(\begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ -1 \end{bmatrix} \right), \tag{D.29}$$

$$\sqrt{2}Q_6 \equiv \sqrt{2}(\boldsymbol{a}_6, \boldsymbol{b}_6, \boldsymbol{c}_6, \boldsymbol{d}_6) = \left(\begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \\ -1 \end{bmatrix} \right). \tag{D.30}$$

Then, applying the standard pattern of composition:

$$\begin{aligned}\left[-V^{(1)}, V^{(3)}, V^{(2)}\right] &= [(\boldsymbol{a}_4 \wedge \boldsymbol{b}_4 + \boldsymbol{c}_4 \wedge \boldsymbol{d}_4), (\boldsymbol{a}_4 \wedge \boldsymbol{c}_4 + \boldsymbol{d}_4 \wedge \boldsymbol{b}_4), (\boldsymbol{a}_4 \wedge \boldsymbol{d}_4 + \boldsymbol{b}_4 \wedge \boldsymbol{c}_4)]\,, \\ \left[-U^{(1)}, U^{(2)}, -U^{(3)}\right] &= [(\boldsymbol{a}_4 \wedge \boldsymbol{b}_4 - \boldsymbol{c}_4 \wedge \boldsymbol{d}_4), (\boldsymbol{a}_4 \wedge \boldsymbol{c}_4 - \boldsymbol{d}_4 \wedge \boldsymbol{b}_4), (\boldsymbol{a}_4 \wedge \boldsymbol{d}_4 - \boldsymbol{b}_4 \wedge \boldsymbol{c}_4)]\,,\end{aligned} \tag{D.31}$$

$$\begin{aligned}\left[V^{(1)}, -V^{(2)}, -V^{(3)}\right] &= [(\boldsymbol{a}_5 \wedge \boldsymbol{b}_5 + \boldsymbol{c}_5 \wedge \boldsymbol{d}_5), (\boldsymbol{a}_5 \wedge \boldsymbol{c}_5 + \boldsymbol{d}_5 \wedge \boldsymbol{b}_5), (\boldsymbol{a}_5 \wedge \boldsymbol{d}_5 + \boldsymbol{b}_5 \wedge \boldsymbol{c}_5)]\,, \\ \left[U^{(3)}, -U^{(2)}, U^{(1)}\right] &= [(\boldsymbol{a}_5 \wedge \boldsymbol{b}_5 - \boldsymbol{c}_5 \wedge \boldsymbol{d}_5), (\boldsymbol{a}_5 \wedge \boldsymbol{c}_5 - \boldsymbol{d}_5 \wedge \boldsymbol{b}_5), (\boldsymbol{a}_5 \wedge \boldsymbol{d}_5 - \boldsymbol{b}_5 \wedge \boldsymbol{c}_5)]\,,\end{aligned} \tag{D.32}$$

$$
\begin{aligned}
\left[V^{(2)}, V^{(1)}, -V^{(3)}\right] &= [(\boldsymbol{a}_6 \wedge \boldsymbol{b}_6 + \boldsymbol{c}_6 \wedge \boldsymbol{d}_6), (\boldsymbol{a}_6 \wedge \boldsymbol{c}_6 + \boldsymbol{d}_6 \wedge \boldsymbol{b}_6), (\boldsymbol{a}_6 \wedge \boldsymbol{d}_6 + \boldsymbol{b}_6 \wedge \boldsymbol{c}_6)]\,, \\
\left[U^{(1)}, -U^{(2)}, -U^{(3)}\right] &= [(\boldsymbol{a}_6 \wedge \boldsymbol{b}_6 - \boldsymbol{c}_6 \wedge \boldsymbol{d}_6), (\boldsymbol{a}_6 \wedge \boldsymbol{c}_6 - \boldsymbol{d}_6 \wedge \boldsymbol{b}_6), (\boldsymbol{a}_6 \wedge \boldsymbol{d}_6 - \boldsymbol{b}_6 \wedge \boldsymbol{c}_6)]\,.
\end{aligned}
\tag{D.33}
$$

D3. Geometrical significance

The eight vertices formed by all of the plus and minus combinations of the members of a given set, Q_p, have a convex hull in the form of an 'orthoplex' (or 'cross polytope'), which is the n-dimensional analogue of the 3D octahedron. The three intersecting orthoplexes associated with Q_1, Q_2 and Q_3 have, as their convex hull, the regular polytope called the '24-cell' (Coxeter 1963). This is composed of 24 regular octahedra meeting eight at a time at every one of the 24 vertices. Neighboring vertices are 60 degrees apart about the center. This remarkable polytope is also self-dual, which means that the 24 unit vectors piercing the centers of the 24 octahedra form the vertices of a second 24-cell. The 24-cell dual to the one we identify with Q_1, Q_2 and Q_3 is itself identified in an exactly analgous manner, with the three sets, Q_4, Q_5 and Q_6. Thus, in the same way that a symmetric matrix has an eigenstructure whose vectors are always associated with a particular orthoplex of eigenvector directions, we see that the 4D Weyl tensor has a characteristic eigen-structure that we can always identify with a dual pair of 24-cells.

D4. Infinitesimal rotations

An infinitesimal rigid rotation of the sets Q_ζ induces a corresponding rotation of the eigen-bivectors, $V^{(\zeta)}$ and U^ζ. For example, let $(\alpha, \beta, \gamma, \alpha', \beta', \gamma')$ be the infinitesimal rotation parameters such that the first-order perturbation of a vector $\boldsymbol{q}$ gives a new vector $\boldsymbol{q}'$ defined:

$$
\begin{bmatrix} q'_1 \\ q'_2 \\ q'_3 \\ q'_4 \end{bmatrix} = \begin{bmatrix} 1, & \alpha, & \beta, & \gamma \\ -\alpha, & 1, & \gamma', & -\beta' \\ -\beta, & -\gamma', & 1, & \alpha' \\ -\gamma, & \beta', & -\alpha', & 1 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{bmatrix}. \tag{D.34}
$$

If we apply this rotation to, say, the set Q_1, we can apply the standard composition scheme to find the perturbations of the V and U bivectors. We find that these bivectors rotate according to the scheme:

$$V'^{(1)} = V^{(1)} - (\gamma + \gamma')V^{(2)} + (\beta + \beta')V^{(3)}, \tag{D.35a}$$

$$V'^{(2)} = V^{(2)} - (\alpha + \alpha')V^{(3)} + (\gamma + \gamma')V^{(1)}, \tag{D.35b}$$

$$V'^{(3)} = V^{(3)} - (\beta + \beta')V^{(1)} + (\alpha + \alpha')V^{(2)}, \tag{D.35c}$$

and

$$U'^{(1)} = U^{(1)} + (\gamma - \gamma')U^{(2)} - (\beta - \beta')U^{(3)}, \tag{D.36a}$$

$$
\begin{aligned}
U'^{(2)} &= U^{(2)} + (\alpha - \alpha')U^{(3)} - (\gamma - \gamma')U^{(1)}, && \text{(D.36b)}\\
U'^{(3)} &= U^{(3)} + (\beta - \beta')U^{(1)} - (\alpha - \alpha')U^{(2)}. && \text{(D.36c)}
\end{aligned}
$$

We see that the primed rotation parameters rotate the V and the U in the same sense, while the unprimed rotation parameters rotate the V and U in the opposite sense. This allows us to steer a 'path' through the six-dimensional manifold of proper rotations in 4D (the members of the orthogonal group, O_4^+) to obtain any combination of the two independent representations of the proper rotations (O_3^+) needed to characterize any valid orthogonal right-handed representation of the eigen-bivectors of the generic Weyl tensor.

D5. Chiral decomposition

From the pattern formed by the eigen-bivectors of the two parities, we can form projection operators that preserve the V-type and nullify the U-type or vice versa. First, define:

$$
J_{ij\,kl} = g_{ik}g_{jl} - g_{il}g_{jk}, \tag{D.37}
$$

and notice that, for any ζ,

$$
\begin{aligned}
\frac{1}{2}J_{ij}{}^{i'j'}V^{(\zeta)}_{i'j'} &= V^{(\zeta)}_{ij}, && \text{(D.38a)}\\
\frac{1}{2}J_{ij}{}^{i'j'}U^{(\zeta)}_{i'j'} &= U^{(\zeta)}_{ij}. && \text{(D.38b)}
\end{aligned}
$$

In contrast, one half of the Levi-Civita tensor acts upon the forms V and U:

$$
\begin{aligned}
\frac{1}{2}\epsilon_{ij}{}^{i'j'}V^{(\zeta)}_{i'j'} &= V^{(\zeta)}_{ij}, && \text{(D.39a)}\\
\frac{1}{2}\epsilon_{ij}{}^{i'j'}U^{(\zeta)}_{i'j'} &= -U^{(\zeta)}_{ij}. && \text{(D.39b)}
\end{aligned}
$$

Therefore, if we define:

$$
\begin{aligned}
(P^+)_{ij\,kl} &= (J_{ij\,kl} + \epsilon_{ijkl})/4, && \text{(D.40a)}\\
(P^-)_{ij\,kl} &= (J_{ij\,kl} - \epsilon_{ijkl})/4, && \text{(D.40b)}
\end{aligned}
$$

then it follows that:

$$
\begin{aligned}
(P^+)_{ij}{}^{i'j'}V^{(\zeta)}_{i'j'} &= V^{(\zeta)}_{ij}, && \text{(D.41a)}\\
(P^+)_{ij}{}^{i'j'}U^{(\zeta)}_{i'j'} &= 0, && \text{(D.41b)}\\
(P^-)_{ij}{}^{i'j'}V^{(\zeta)}_{i'j'} &= 0, && \text{(D.41c)}\\
(P^-)_{ij}{}^{i'j'}U^{(\zeta)}_{i'j'} &= U^{(\zeta)}_{ij}, && \text{(D.41d)}
\end{aligned}
$$

so that $P^{(+)}$ projects out the V parts, and $P^{(-)}$ projects out only the U parts of any bivectors. It also follows that, since,

$$W^{+}_{ij\,kl} = \sum_{\zeta=1}^{3} V^{(\zeta)}_{ij} V^{(\zeta)}_{kl} w^{+}_{(\zeta)}, \tag{D.42a}$$

$$W^{-}_{ij\,kl} = \sum_{\zeta=1}^{3} U^{(\zeta)}_{ij} U^{(\zeta)}_{kl} w^{-}_{(\zeta)}, \tag{D.42b}$$

define the structures of the positive and negative parity parts of the total Weyl tensor,

$$W_{ij\,kl} = W^{+}_{ij\,kl} + W^{-}_{ij\,kl}, \tag{D.43}$$

we can separate these contributions by applying the projection operators to the first pair and the second pair of the indices of W simultaneously:

$$W^{+}_{ij\,kl} = (P^{+})_{ij}^{\;\;i'j'} W_{i'j'\,k'l'} (P^{+})^{k'l'}_{\;\;\;\;kl}, \tag{D.44a}$$

$$W^{-}_{ij\,kl} = (P^{-})_{ij}^{\;\;i'j'} W_{i'j'\,k'l'} (P^{-})^{k'l'}_{\;\;\;\;kl}. \tag{D.44b}$$

The parts, W^{+} and W^{-}, are said to be 'self-dual' and 'anti-self-dual' respectively (duality is with respect to double-sided contraction with the Levi-Civita tensor). In General Relativity (GR), where the curved space has the Minkowski signature, the Weyl tensor describes the possible curvatures of space in the absence (locally) of matter or energy; the general classification of Weyl tensors (Petrov 1954, 1969, Penrose and Rindler 1988) is then complicated by the presence of a 'light-cone', but the existence of two independent states of polarization of gravitational waves of GR (Misner et al. 1970) would appear to relate to this implicit dichotomy of the Weyl tensor in four dimensions.

The chiral decomposition will work even when, owing to chance degeneracies in the eigenvalues of W, the eigenstructure consists of a pair of eigenvectors that mix a $V^{(\zeta)}$ with a $U^{(\eta)}$. This decomposition could conceivably be of practical value if it is found that the self-dual and anti-self-dual parts of W need to be treated with different saturation-function parameters in the amplitude correction procedure.

References

Berger, M, P. Gauduchon, and E. Mazet 1971 *Le Spectre d'une variété riemannienne,* Lecture Notes in Mathematics, vol. 194, Springer-Verlag, Berlin.

Burke, W. L. 1985 *Applied Differential Geometry.* Cambridge University Press. 414 pp.

Coxeter, H. S. M. 1963 *Regular Polytopes*, Dover, New York. 321 pp.

Derber, J. C., and A. Rosati 1989 A global ocean data assimilation system. *J. Phys. Ocean.,* **19,** 1333–1347.

Gilkey, P. B. 1984 *Invariance Theory, the Heat Equation, and the Atiyah-Singer Index Theorem.* Publish or Perish, Wilmington, DE, 345 pp.

Golub, G. H., and C. F. Van Loan 1989 *Matrix Computations.* Johns Hopkins, 642 pp.

Grigor'yan, A., and M. Noguchi	1998	The heat kernel on hyperbolic space. *Bull. London Math. Soc.,* **30,** 643–650.
Hawking, S. W., and G. F. R. Ellis	1973	*The Large Scale Structure of Space-Time.* Cambridge University Press. 391 pp.
Huygens, C.,	1962	*Treatise on Light,* Translated by S. P. Thompson from *Traité de la Lumière*, published in 1690. Dover, New York.
Kreyszig, E.	1991	*Differential Geometry* Dover, New York. 352 pp.
Lafferty, J., and G. Lebanon	2005	Diffusion kernels on statistical manifolds. *J. of Machine Learning Research,* **6,** 129–163.
Lovelock, D., and H. Rund	1989	*Tensors, Differential Forms, and Variational Principles*, Dover, New York. 366 pp.
McKean, H. P.	1970	An upper bound to the spectrum of Δ on a manifold of negative curvature. *J. Differential Geometry,* **4,** 359–366.
Misner, C. W., K. S. Thorne, and J. A. Wheeler	1970	*Gravitation.* W. H. Freeman & Co., New York. 1279 pp.
Penrose, R., and W. Rindler	1988	*Spinors and Space-Time: Volume 2, Spinor and Twistor Methods in Space-Time Geometry.* Cambridge University Press.
Petrov, A. Z.	1954	Classification of spaces defined gravitational fields. *Uch. Zapiski Kazan Gos. Univ.,* **144,** 55.
Petrov, A. Z.	1969	*Einstein Spaces.* Pergamon.
Purser, R. J.	2008	Normalization of the diffusive filters that represent the inhomogeneous covariance operators of variational assimilation, using asymptotic expansions and techniques of non-Euclidean geometry; Part I: Analytic solutions for symmetric cases and the validation of practical algorithms. NOAA/NCEP Office Note 456
Rosenberg, S.	1997	*The Laplacian on a Riemannian Manifold; London Mathematical Society Student Texts 31.* Cambridge, 174 pp.
Synge, J. L., and A. Schild	1949	*Tensor Calculus.* Dover, New York, 324 pp.
Weaver, A., and P. Courtier	2001	Correlation modelling on the sphere using a generalized diffusion equation. *Quart. J. Roy. Meteor. Soc.,* **127,** 1815–1846.
Wu, W.-S., R. J. Purser, and D. F. Parrish	2002	Three-dimensional variational analysis with spatially inhomogeneous covariances. *Mon. Wea. Rev.,* **130,** 2905–2916.