Spherical Cap Harmonic Analysis

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The solution of Laplace's equation, in spherical coordinates, is developed for the boundary value problem appropriate to fitting the geomagnetic field over a spherical cap. The solution involves associated Legendre functions of integral order but nonintegral degree. The basis functions comprise two infinite sets, within each of which the functions are mutually orthogonal. The series for the expansion of the potential can by design be differentiated term by term to yield uniformly convergent series for the field components. The method is demonstrated by modeling the International Geomagnetic Reference Field 1980 at the earth's surface and upward continuing it to 300 and 600 km. The rate of convergence of the series is rapid, and standard errors of fit as low as the order of a nanotesla can be obtained with a reasonable number of coefficients. Upward continuation suffers from not considering data outside the cap, the deterioration being confined to the boundary at low continuation altitudes but spreading inward over the cap with increasing altitudes. At 600 km the standard error of upward continuation is about 5 times the standard error of fit. Both the fit and the upward continuation can be greatly improved at a given truncation level by subtraction of a known spherical harmonic potential determined from data from the whole earth.

Introduction

The problem of determining the geomagnetic field at a particular point in space, given a particular mathematical model, is reasonably straightforward. Spherical harmonic models, such as the International Geomagnetic Reference Fields (IGRF's) [IAGA Division 1 Working Group 1, 1981], enable the magnetic field to be calculated easily by computer, and at the same time they satisfy the necessary constraints that the curl and divergence of the field be zero. These constraints are equivalent to requiring that the field be the gradient of a potential, i.e., the gradient of a function that satisfies Laplace's differential equation.

The inverse problem of deriving a mathematical model that satisfies these same potential constraints, given a set of magnetic field observations, is in practice not so straightforward. When observations are available over either the whole sphere or (as will be shown in this paper) a hemisphere, the problem can be solved by the usual method of spherical harmonic analysis in terms of Legendre polynomials in colatitude and trigonometric functions in longitude [e.g., Chapman and Bartels, 1940, chapter XVII]. When observations are available, or analysis is required, over only a small portion of the earth's surface, however, these same Legendre polynomials and trigonometric functions are no longer the most appropriate basis functions for fitting a potential field model over that restricted area. In fact, the resulting least squares matrix of normal equations becomes, in this case, badly ill conditioned and cannot be solved with a sufficient degree of accuracy, often not at all.

The purpose of this paper is to solve analytically the boundary value problem appropriate to fitting a differentiable potential over a spherical cap. With the introduction of two sets of orthogonal basis functions the resulting expansion series can be differentiated term by term to give the geomagnetic field components. If the potential does not need to be differentiated with respect to colatitude, to give the north component, only one set of orthogonal basis functions is required. The method is termed spherical cap harmonic analysis. The usual method,

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applied to the whole sphere, is referred to as ordinary spherical harmonic analysis.

ALTERNATIVE METHODS

One method to circumvent directly the problem of ill conditioning in the ordinary spherical harmonic least squares matrix is to generate values by some other means (national charts or other spherical harmonic models) on the portion of the surface where there were previously no data [Nagy, 1981; Dawson et al., 1981]. Most of the coefficients in this method of representation, however, are required solely to fit already modeled data over an area in which there is absolutely no interest. Statistics on goodness of fit, etc., are difficult to ascertain because of the mixture of data and generated values, and requirements on computer time and memory become excessive with solutions of high degree.

Another method is to convert from spherical to rectangular coordinates, the harmonic solution involving trigonometric functions in two coordinates (x and y) and an exponential function in the third (z). This method, called the method of rectangular harmonic analysis, works reasonably well over small areas of the earth's surface [Alldredge, 1981]. The difficulty for large areas is that the natural decrease of the earth's field with radial distance r (for internal sources) is not preserved. Furthermore, the exponential function, for large degrees and a large range in z, can have a large range of values and hence destroy the numerical significance of the summations in the least squares matrix.

When field data are available on, and interest is confined to, the earth's surface, the field components are sometimes expressed in terms of polynomials in the two surface coordinates only, ignoring the third (radial or z) coordinate. Near-surface, such as aeromagnetic, data are generally reduced to the surface by means of the inverse cube relationship [Chapman, 1936, chapter I]; this results in an exact correction for the dipole term but only a partial correction for higher-order terms (the inverse cube reduction approximates the downward increase of the nth degree term by 3/(n + 2) of its actual value [Serson, 1966]). The only potential constraint that can be applied here, in the absence of vertical gradient information, is that the vertical component of the curl of the field be zero. This results in a constraint between the horizontal north (B_N)

and horizontal east (B_E) components:

$$\frac{\partial B_N}{\partial \lambda} + \frac{\partial (B_E \sin \theta)}{\partial \theta} = 0 \tag{1}$$

where θ and λ are the colatitude and east longitude. When the component B_N and the pseudo-component B_E sin θ are expressed as polynomials in θ and λ , the constraint is easily applied [Tsubokawa, 1952; Fougere and McClay, 1957; Reilly and Burrows, 1973; Dawson and Newitt, 1977]. Fitting other components (even simply B_N and B_E) or using coordinates other than θ and λ requires approximate methods [Zmuda and McClay, 1956; Haines, 1967; Le Mouel, 1970]. In any case, (1) is an incomplete criterion, ignoring the relationships between B_N and B_E and the vertical component B_V . Of course, these latter relationships, resulting from equating the divergence and the two horizontal components of the curl to zero, may be used to give estimates, at the surface, of the vertical gradients of the three field components [Tsubokawa, 1952; Haines, 1968].

Finally, the potential constraint can be ignored completely, and polynomials can be derived with completely uncoupled coefficients [Finlayson, 1973; Fabiano et al., 1979], or, in fact, the charts may simply be hand-drawn or computer-contoured, each component being analyzed numerically rather than mathematically and hence being processed independently of the others [Dawson and Dalgetty, 1966; Sucksdorff et al., 1971]. Again, this is usually done for surface and near-surface data only, ignoring the radial variation. In this case, the "mutual consistency" constraint (equation (1)) can be tested, either from the charts themselves [Chapman, 1942; Davids and Bernstein, 1945; Cullington, 1954] or analytically [Tsubokawa, 1952; Cullington, 1954; Haines, 1968]. In the analytical case, when the polynomial coefficients are derived by least squares, the statistical significance of the nonzero curl can also be tested [Haines, 1968].

A method that may be applicable to the fitting of magnetic observations on the earth's surface is the method of "harmonic splines" [Shure et al., 1982]. This method has been developed to give optimally smooth models at the surface of the core, although presumably the surface of the earth, or any other reference surface, could be used. The difficulty with the method is that the number of basis functions is equal to the number of observations, and so the method is practical only when the number of data are less than a few hundred. (An approximation technique, however, that gives models that are almost optimally smooth, has been described [Parker and Shure, 1982] in an attempt to overcome this difficulty.) Furthermore, it is not clear how well conditioned the inverse matrix would be over areas other than the whole sphere or a hemisphere, since the method does involve ordinary spherical harmonic basis functions of integral degree. In fact, it would seem that the spherical cap harmonic basis functions introduced here could be incorporated in the harmonic spline method to analyze small areas of the reference surface. Similar remarks apply to other inverse methods (reviewed, for example, by Whaler and Gubbins [1981] and Gubbins [1983]).

Spherical harmonic functions can be defined so that they are orthogonal over certain restricted areas of the sphere [Kelvin and Tait, 1896, chapter 1, Appendix B, sections f and g]. These functions generally involve associated Legendre functions of nonintegral degree that are orthogonal over a given range of colatitude [Kelvin and Tait, 1896, chapter 1, Appendix B, sections 1, m, and n; Smythe, 1950, sect. 5.26]. In cases of axial symmetry, of course, only the zonal functions of

nonintegral degree are required [Hobson, 1931, sections 23 and 259; Hall, 1949; Jackson, 1975, section 3.4].

One type of area on the sphere over which spherical harmonic functions may be orthogonalized is that of a spherical cap. The region over a spherical cap of half angle θ_0 , between the radial distances r=a and r=b, is depicted in Figure 1. Satellite magnetic data from such a region (with $\theta_0=50^\circ$ and $b-a\approx 200$ km) are being analyzed [Coles et al., 1982] at the Earth Physics Branch, Ottawa, as one of Canada's contributions to the Magsat program [Langel, 1980]. The solution, in spherical coordinates, of Laplace's equation appropriate to the fitting of the geomagnetic field throughout such a region is developed in this paper.

First, the solution will be derived for an arbitrary differentiable potential, subject to boundary conditions that enable it to be expanded in a uniformly convergent series of basis functions. These basis functions will be shown to comprise two infinite sets, within each of which the functions are mutually orthogonal. The series can be differentiated term by term with respect to θ , λ , and r to give uniformly convergent series for the field components B_N , B_E , and B_V . The formulas for computing the associated Legendre functions of integral order and nonintegral degree are then derived. Finally, the method is demonstrated by fitting, over the spherical cap north of 40° N, the derivatives of a known potential field.

The nonlinear problem of determining potential field coefficients from values of declination, inclination, horizontal intensity, or total force is not discussed in this paper, nor is the conversion from geodetic to geocentric coordinates. Both of these subjects have been treated by Cain et al. [1965].

THE POTENTIAL

A solution, in spherical coordinates, of Laplace's equation for internal sources is given when m = 0 by

$$V_{n}^{m}(r, \theta, \lambda) = a \left(\frac{a}{r}\right)^{n+1} P_{n}^{m}(\cos \theta) \left\{g_{n}^{m} + h_{n}^{m}\lambda\right\}$$
 (2)

and when $m \neq 0$ by

$$V^{m}_{n}(r, \theta, \lambda) = a \left(\frac{a}{r}\right)^{n+1} P^{m}_{n}(\cos \theta)$$

$$\cdot \left\{ g^{m}_{n} \cos (m\lambda) + h^{m}_{n} \sin (m\lambda) \right\} \tag{3}$$

where r is the radial distance, θ is the colatitude, and λ is the longitude. The radius r=a defines a reference sphere, generally taken as the earth's surface, on which the potential is to be expanded. The functions P_n^m are known as associated Legendre functions of the first kind. This solution is found by separating the variables and solving the individual eigenvalue problems [e.g., Smythe, 1950, sections 5.12 and 5.14]. The parameters n and m are generally referred to as the degree and order, respectively, and represent the coupling between the three separated differential equations. The constants g_n^m and h_n^m , generally referred to as spherical harmonic coefficients, denote the amplitudes of the respective harmonics.

The eigenvalues, which here are m^2 and n(n+1), are determined, as in all eigenvalue problems, by the boundary conditions. Until these conditions are introduced, the solutions (2) and (3) are quite general, and n and m may be integral or nonintegral, real or complex, rational or irrational. The form of the solutions (2) and (3), however, anticipate some of the boundary results. For example, terms in $(r/a)^n$ for external sources are not included nor are the associated Legendre functions of the second kind for describing singular or nonanalytic functions.

The requirement here is that a differentiable potential function V is to be represented over a spherical cap in terms of functions of the form given in (2) and (3). That is, n and m must be determined so that the functions V^m_n constitute basis functions in θ and λ and can therefore be summed or integrated to give an expression for V. This is always possible when the boundary conditions on the separated differential equations in θ and λ are of the self-adjoint Sturm-Liouville type [e.g., Churchill, 1963, sections 32-34; Davis, 1963, section 2.4].

When all longitudes λ are represented in the data, the (Sturm-Liouville) boundary conditions on λ are those of continuity:

$$V_{n}^{m}(r, \theta, \lambda) = V_{n}^{m}(r, \theta, \lambda + 2\pi)$$
$$\frac{\partial V_{n}^{m}(r, \theta, \lambda)}{\partial \lambda} = \frac{\partial V_{n}^{m}(r, \theta, \lambda + 2\pi)}{\partial \lambda}$$

These conditions restrict the value of m to be real and integral and require that $h^0_n = 0$. They therefore exclude the exponential, or hyperbolic trigonometric, functions associated with imaginary values of m; this in fact is why the trigonometric form was chosen in (3) for the solution in λ . The case of integral m applies both to ordinary spherical harmonics over the entire sphere and to spherical harmonics over the spherical cap.

The boundary condition on θ is, at $\theta = 0$, one of regularity:

$$\frac{\partial V^{m}_{n}(r, 0, \lambda)}{\partial \theta} = 0 \qquad m = 0 \tag{4}$$

$$V^{m}_{n}(r, 0, \lambda) = 0 \qquad m \neq 0 \tag{5}$$

This condition permits an arbitrary potential that is independent of longitude at $\theta = 0$. It is satisfied by the Legendre functions of the first kind and excludes those of the second kind. Again, this condition is the same for both spherical harmonics over the entire sphere and those over a spherical cap.

The boundary condition on θ at $\theta = \theta_0$ is similar when $\theta_0 = \pi$, the case of ordinary spherical harmonics:

$$\frac{\partial V_{n}^{m}(r, \pi, \lambda)}{\partial \theta} = 0 \qquad m = 0$$
 (6)

$$V^{m}_{n}(r, \pi, \lambda) = 0 \qquad m \neq 0 \tag{7}$$

This condition dictates that n must be real and integral, whereupon the (infinite series) Legendre functions $P^m_n(\cos \theta)$ reduce to the familiar (finite series) Legendre polynomials.

A second linearly independent solution (involving a Legendre function of the second kind) has a singularity at $\theta = 0$ and at $\theta = \pi$, and so by (4)–(7) cannot be included in the solution (equations (2) and (3)) for the whole sphere.

For the spherical cap, with $\theta_0 \neq \pi$, the potential V at θ_0 and its derivative with respect to θ must be arbitrary:

$$V(r, \theta_0, \lambda) = f(r, \lambda) \tag{8}$$

$$\frac{\partial V(r, \, \theta_0, \, \lambda)}{\partial \theta} = g(r, \, \lambda) \tag{9}$$

where of course the functions f and g are subject to the same conditions on r and λ as V and $\partial V/\partial \theta$, respectively. It will be shown shortly that these boundary conditions on θ are satisfied by choosing all values of n such that

$$\frac{\partial V_{n}^{m}(r,\,\theta_{0},\,\lambda)}{\partial\theta} = 0 \tag{10}$$

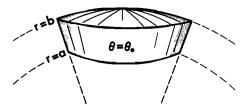


Fig. 1. Spherical cap of half angle θ_0 . Colatitude (θ) and radial (r) extent denotes region over which magnetic data are to be analyzed. Total region is bounded by the surfaces r=a, r=b, and $\theta=\theta_0$.

and all values of n such that

$$V^{m}_{n}(r, \theta_{0}, \lambda) = 0 \tag{11}$$

for all m. These conditions in turn are satisfied by Legendre functions $P_n^m(\cos\theta)$ of real but not necessarily integral degree, both those that have zero slope at $\theta = \theta_0$ and those that are zero at $\theta = \theta_0$. Since V_n^m and $\partial V_n^m/\partial\theta$ cannot simultaneously be zero [e.g., MacRobert, 1967, chapter V, section 5], it will be shown that the functions satisfying (10) enable (8) to hold, and those satisfying (11) enable (9) to hold. Since the different real values of n for which these equations hold depend separately on m, they will be denoted by $n_k(m)$, the k being an integer subscript chosen in some way to order the various roots n at a given m. Here the index k has been chosen to start at m, analogous to the case of integral n. Defined in this way, the $n_k(m)$ for which (k-m) = even are the roots of (10) and those for which (k-m) = odd are the roots of (11), when these equations are considered as equations in n.

A second linearly independent solution involves $P_n^m(-\cos\theta)$ which has a singularity at $\theta=0$, and so again cannot be included in the solution (2) and (3) (for m=0 see Smythe [1950, section 5.22] and Duff and Naylor [1966, section 9.6]). In fact, the singularity in $P_n^m(\cos\pi)$, for $n \neq \text{integer}$, prohibits, at $\theta_0=\pi$, the solution of (11) for m=0 and of (10) for $m\neq 0$; the boundary conditions then revert simply to (6) and (7).

The boundary condition on r, for internal sources, is

$$\lim_{r\to\infty} V^m_n(r,\,\theta,\,\lambda)=0$$

This condition requires the real part of n to be not less than -1.

For m = 0, then, $n \ge -1$. The harmonic of order m = 0 and degree n = -1 is simply the constant term in the expansion of the potential. This term cannot be determined when only derivatives of the potential are available. In this case, it is omitted, and $n \ge 0$.

Since the solutions for m < 0 are the same as those for m > 0, they are redundant and are also omitted. In this case, n > m.

By superposition, the general solution in spherical coordinates of Laplace's equation over the spherical cap is

$$V = \sum_{m=0}^{\infty} \sum_{k=m}^{\infty} a \left(\frac{a}{r}\right)^{n_k(m)+1} P^m_{n_k(m)}(\cos \theta) \cdot \left\{ g^m_k \cos (m\lambda) + h^m_k \sin (m\lambda) \right\}$$
(12)

where the g^m_n , h^m_n have been reindexed to g^m_k , h^m_k and it is understood that h^o_k is zero a priori.

Since the eigenvalue problem in λ and the two eigenvalue problems in θ (one with boundary conditions (4), (5), and (10), the other with (4), (5), and (11)) are each of the self-adjoint Sturm-Liouville type, the eigenfunction solutions form in each case, by the Sturm-Liouville theorem, an orthogonal set of

basis functions for a very general class of functions [e.g., Churchill, 1963, sections 32-34; Davis, 1963, section 2.4]. The $V_{n_k(m)}^m(r, \theta, \lambda)$ can thus be divided into two infinite sets of basis functions, one with (k-m) = even and the other with (k-m) = odd, such that the functions in each set are mutually orthogonal over the spherical cap. Of course, the θ orthogonalization, as in the case of ordinary spherical harmonics, is taken with respect to the functional argument $\cos \theta$, giving the weight function $\sin \theta$ when taken with respect to θ :

$$\int_{0}^{\theta_0} P^m_{n_j(m)}(\cos \theta) P^m_{n_k(m)}(\cos \theta) \sin \theta \ d\theta = 0$$

for $j \neq k$ (and where j - m and k - m are either both odd or both even). This is a necessary consequence of the separated differential equation in θ .

Functions in one set are not θ orthogonal to those in the other, and in fact it can be shown that

$$\int_0^{\theta_0} P^m_{n_j(m)}(\cos \theta) P^m_{n_k(m)}(\cos \theta) \sin \theta \ d\theta$$

$$= \frac{\sin \theta_0 P^m_{n_j(m)}(\cos \theta_0) \{ [dP^m_{n_k(m)}(\cos \theta_0)]/d\theta \}}{[n_k(m) - n_j(m)][n_k(m) + n_j(m) + 1]}$$

for j - m = even and k - m = odd.

Mean square values could be computed, if required, from the formulas

$$\int_0^{\theta_0} [P^m_{n_k(m)}(\cos \theta)]^2 \sin \theta \, d\theta$$

$$= -\frac{\sin \theta_0}{2n_k(m) + 1} P^m_{n_k(m)}(\cos \theta_0) \frac{\partial}{\partial n} \frac{dP^m_{n_k(m)}(\cos \theta_0)}{d\theta}$$

when k - m is even, and

$$\int_{0}^{\theta_{0}} [P^{m}_{n_{k}(m)}(\cos \theta)]^{2} \sin \theta \ d\theta$$

$$= \frac{\sin \theta_{0}}{2n_{k}(m) + 1} \frac{dP^{m}_{n_{k}(m)}(\cos \theta_{0})}{d\theta} \frac{\partial}{\partial n} P^{m}_{n_{k}(m)}(\cos \theta_{0})$$

when k-m is odd. (The latter is given by Smythe [1950, section 5.26].) For purposes of fitting data and determining coefficients by least squares, mean cross and mean square values are not required and so have not been computed here. They would be required in a study of power spectra or when expressing the coefficients as integral transforms over the spherical cap.

To represent a potential function that does not have to be differentiated with respect to θ would require only equations (8) and (10), not (9) and (11). Only one set of orthogonal functions (denoted here by k-m= even) would then be required. The potential series itself would still be uniformly convergent, although its rate of convergence would reflect the error at the boundary in the first derivative with respect to θ .

It can now be simply shown that (8) and (9) follow from (10) and (11). First, substituting (11), satisfied for k - m = odd, into (12) at $\theta = \theta_0$ gives

$$V(r, \theta_0, \lambda) = \sum_{m=0}^{\infty} \sum_{\substack{k=m \\ k-m=\text{even}}}^{\infty} a \left(\frac{a}{r}\right)^{n_k(m)+1} P^m_{n_k(m)}(\cos \theta_0)$$

$$\cdot \left\{ g^m_k \cos (m\lambda) + h^m_k \sin (m\lambda) \right\}$$

$$= \sum_{k=0}^{\infty} a_k \cos (m\lambda) + b_k \sin (m\lambda)$$

where for example

$$a_m = \sum_{\substack{k=m\\k=m \text{ even}}}^{\infty} a \left(\frac{a}{r}\right)^{n_k(m)+1} P^m_{n_k(m)}(\cos \theta_0) g^m_k$$

Thus $V(r, \theta_0, \lambda)$ can be equated to a function $f(r, \lambda)$, with the same boundary constraints on r and λ as V, provided that the a_m , b_m are Fourier coefficients of the orthogonal eigenfunction expansion in λ of the function $f(r, \lambda)$.

Similarly, substituting (10), satisfied for k - m = even, into the derivative of (12) at $\theta = \theta_0$ gives

$$\frac{\partial V(r, \theta_0, \lambda)}{\partial \theta} = \sum_{m=0}^{\infty} c_m \cos(m\lambda) + d_m \sin(m\lambda)$$

where, for example,

$$c_m = \sum_{\substack{k=m+1\\k-m = \text{odd}}}^{\infty} a \left(\frac{a}{r}\right)^{n_k(m)+1} \frac{dP^m_{n_k(m)}(\cos\theta_0)}{d\theta} g^m_k$$

and where again the c_m , d_m are the Fourier coefficients in the expansion with respect to λ of the function $g(r, \lambda)$.

The θ , λ , r boundary conditions given above thus permit the representation by (12), on a spherical cap, of an arbitrary differentiable potential function, excluding the constant term. The upper limits for m and k, in an approximation or practical problem, can be taken as M and K, respectively, where $M \le K$, and, of course, the order of summation can be reversed, k incrementing from zero to K and K from zero to minimum (K, K). When the field is isotropic, the maximum order K is taken equal to the maximum index K. This will be the case followed here.

Including the constant term would permit the expansion of a very general function and its derivative on the surface r = a. This is the analogue to the expansion theorem for the whole sphere [Courant and Hilbert, 1953, chapter VII, section 5.3].

DERIVATIVES OF THE POTENTIAL

In geomagnetism the purpose of obtaining an expression for the scalar potential is simply to satisfy the curl and divergence constraints on the geomagnetic field. Because these constraints are satisfied, the field components can then be expressed as derivatives of the potential.

Differentiation of an infinite series is not always valid, however, since the derivative of an infinite sum does not necessarily converge to the infinite sum of the term-wise derivatives, unless this latter sum is uniformly convergent. The north component B_N , for example, is not zero at $\theta_0 \neq \pi$ and so could not be represented only by derivatives which have been forced to be zero at θ_0 by the boundary condition (10). Similarly, the vertical component B_V could not be represented only by functions satisfying (11).

Including the two boundary conditions (10) and (11), however, permits both the potential, through (8), and its derivative with respect to θ , through (9), to be represented arbitrarily closely on the boundary and by virtue of the Sturm-Liouville theorem throughout the whole domain of θ . The derivative of expansion (12) with respect to θ is therefore uniformly convergent, and the geographic north component can be expressed as

$$B_{N} = -\frac{1}{r} \frac{\partial V(r, \theta, \lambda)}{\partial \theta} = -\sum_{m=0}^{\infty} \sum_{k=m}^{\infty} \left(\frac{a}{r}\right)^{n_{k}(m)+2} \cdot \frac{dP_{n_{k}(m)}^{m}(\cos \theta)}{d\theta} \left\{g_{k}^{m} \cos (m\lambda) + h_{k}^{m} \sin (m\lambda)\right\}$$
(13)

Similarly, since $V(r, \theta, \lambda)$ is a continuous periodic function in λ , it can be differentiated term by term [e.g., Tolstov, 1962, chapter 5, section 8] to give the geographic east component:

$$B_{E} = \frac{1}{r \sin \theta} \frac{\partial V(r, \theta, \lambda)}{\partial \lambda} = \sum_{m=1}^{\infty} \sum_{k=m}^{\infty} m \left(\frac{a}{r}\right)^{n_{k}(m)+2} \cdot \frac{P_{n_{k}(m)}^{m}(\cos \theta)}{\sin \theta} \left\{-g_{k}^{m} \sin (m\lambda) + h_{k}^{m} \cos (m\lambda)\right\}$$
(14)

assuming λ to be east longitude. The sin θ is not an essential singularity at $\theta = 0$ since $P^m_{n_k(m)}(\cos \theta)$ has sin θ as a factor when $m \neq 0$.

Differentiating the potential with respect to r, to give the vertical component B_{ν} , presents no difficulty:

$$B_{V} = -\frac{\partial V(r, \theta, \lambda)}{\partial r} = \sum_{m=0}^{\infty} \sum_{k=m}^{\infty} (n_{k}(m) + 1) \left(\frac{a}{r}\right)^{n_{k}(m) + 2} \cdot P^{m}_{n_{k}(m)}(\cos \theta) \left\{g^{m}_{k} \cos (m\lambda) + h^{m}_{k} \sin (m\lambda)\right\}$$
(15)

The solution in θ for V and $\partial V/\partial\theta$ may involve up to four linearly independent boundary conditions [Coddington and Levinson, 1955, chapter 11, section 2]. Here, for $\theta_0 \neq \pi$, there are three boundary conditions in θ for the simultaneous formulation: Equations (4), (10), and (11) for m=0 and (5), (10), and (11) for $m\neq 0$. One boundary condition at $\theta=0$ is not required because of the natural continuity of the field resulting from the spherical geometry. For $\theta_0=\pi$, only two boundary conditions are required: Equations (4) and (6) for m=0 and (5) and (7) for $m\neq 0$. Here, another boundary condition can be dispensed with because of the field continuity at $\theta=\pi$.

Each zonal (m=0) term is associated with one coefficient (g^o_k) , while each nonzonal term is associated with two (g^m_k, h^m_k) . The total number of coefficients required in a representation of maximum index K is $(K+1)^2$ when solving for B_N , B_E , and B_V simultaneously (or for the potential without the constant term). Solving for B_V , B_N , or B_E separately requires $(K+1)^2$, K(K+2), or K(K+1) coefficients, respectively. This is analogous to the case of ordinary spherical harmonics, except that the n=0, m=0 (monopole) term is frequently omitted, giving the same number of coefficients for both B_V and B_N .

Including only the functions with k - m = even (for a potential not differentiable in θ) would require only (K + 1)(K + 2)/2 coefficients for B_V rather than $(K + 1)^2$.

COMPUTATION OF THE LEGENDRE FUNCTION

The associated Legendre function $P^m_n(\cos \theta)$, when *n* is real and *m* is a positive integer, can be expressed for $-1 < \cos \theta \le 1$ [e.g., *Hobson*, 1931, section 230] as

$$P^{m}_{n}(\cos \theta) = K^{m}_{n} \sin^{m} \theta$$

$$F\left((m-n, n+m+1; 1+m; \frac{1-\cos\theta}{2}\right)$$

where F is the hypergeometric function:

$$F(\alpha, \beta; \gamma; x) = 1 + \frac{\alpha\beta}{1\gamma} x + \frac{\alpha(\alpha+1)\beta(\beta+1)}{1(2)\gamma(\gamma+1)} x^2 + \cdots$$

and the factor K_n^m is a constant depending on the type of normalization chosen. Using the terminology of *Chapman and Bartels* [1940, sections 17.3 and 17.4], the functions given by *Hobson* [1931] are Neuman-normalized; for Schmidtnormalized functions the normalizing factor for m = 0 is

$$K^m_n = 1$$

TABLE 1. $n_k(m)$ for $\theta_0 = 50^\circ$

k	0	1	2	3	4	5	6	7	8
0	0.00								
1	2.24	1.78							
2	3.92	3.92	3.27						
3	5.82	5.66	5.50	4.71					
4	7.56	7.56	7.30	7.02	6.12				
5	9.41	9.31	9.21	8.88	8.52	7.51			
6	11.17	11.17	11.00	10.82	10.42	9.99	8.90		
7	13.01	12.94	12.86	12.63	12.40	11.94	11.44	10.27	
8	14.78	14.78	14.65	14.52	14.24	13.95	13.44	12.89	11.64

and for $m \neq 0$ is

$$K^{m}_{n} = \frac{2^{1/2}}{2^{m}m!} \left[\frac{(n+m)!}{(n-m)!} \right]^{1/2}$$

where x! is the factorial function.

When n is not an integer (and since m is assumed to be integral), the hypergeometric series, like a sine or cosine series, has an infinite number of terms, and P_n^m is then called a Legendre function. When n is an integer, the series truncates after a finite number of terms, and P_n^m is then called a Legendre polynomial. In general, the degree n is nonintegral; for the hemisphere ($\theta_0 = \pi/2$), however, it is integral, and $n_k(m) = k$ for $k \ge m$. The above series for $P_n^m(\cos \theta)$, which involves a polynomial in $\sin^2(\theta/2)$, then converges to the usual $P_n^m(\cos \theta)$ that involves a polynomial in $\cos^2\theta$ [Hobson, 1931, section 58]. The ordinary spherical harmonic basis functions thus provide the solution to the boundary value problem for the hemisphere as well as for the whole sphere.

By using Stirling's formula for x! [e.g., Arfken, 1970, section 10.3], the K^m_n for n > m > 0 can be approximated by

$$K^{m}_{n} = \frac{2^{-m}}{(m\pi)^{1/2}} \left(\frac{n+m}{n-m}\right)^{(n/2)+(1/4)} p^{m/2} \exp\left(e_{1} + e_{2} + \cdots\right)$$

where

$$p = \left(\frac{n}{m}\right)^2 - 1$$

and the first two exponential terms are

$$e_1 = -\frac{1}{12m} \left\{ 1 + \frac{1}{p} \right\}$$

$$e_2 = \frac{1}{360m^3} \left\{ 1 + \frac{3}{p^2} + \frac{4}{p^3} \right\}$$

Normalization does not have to be exact, and the accuracy of the K^m_n approximation is not important in model fitting. It is of course necessary to use the same approximation when recomputing the field from the fitted model.

The hypergeometric function F can easily be computed by recursive methods. Thus if

$$P_{n}^{m}(\cos \theta) = \sum_{k=0}^{\infty} A_{k}(m, n) \left(\frac{1-\cos \theta}{2}\right)^{k}$$
 (16)

then

$$A_0(m, n) = K^m_n \sin^m \theta$$

and for k > 0,

$$A_k(m, n) = \frac{(k+m-1)(k+m) - n(n+1)}{k(k+m)} A_{k-1}(m, n)$$

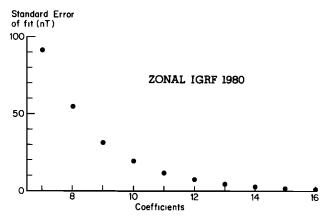


Fig. 2. Standard errors of fit from modeling zonal terms of IGRF 1980 by means of zonal spherical cap harmonic functions. A zonal expansion of maximum index K contains (K+1) coefficients.

The series can be truncated at any desired degree of accuracy, such as that governed by the word size of the computer. The terms can be seen to have a large range, however, and for large n, care must be taken not to lose too much accuracy in the summation. Asymptotic formulas are available for small m, large n [Hobson, 1931, section 194] and for large m, small n [Hobson, 1931, section 199], but generally, it is sufficient to use the above formulation (equation (16)) and do the computations in double precision.

The derivative of P_n^m is found simply by differentiating (16), with the computations being done recursively along with those for P_n^m .

CALCULATION OF THE $n_k(m)$

In order to represent the potential and its derivatives, values of n must be determined that separately satisfy (10) and (11) or, equivalently,

$$\frac{dP^m_n(\cos\,\theta_0)}{d\theta} = 0\tag{17}$$

$$P^{m}_{n}(\cos \theta_{0}) = 0 \tag{18}$$

Although analytical formulas have been developed for these purposes [Macdonald, 1900; Pal, 1919, 1920; Hobson, 1931, sections 238–241], it is a simple matter to solve for n numerically, by computer, using the formulations of the previous section. Since those formulations hold for any real n, they can be used to iteratively determine the roots $n_k(m)$ of (17) and (18), considered for each m to be equations in n. The computer program actually used was IBM Scientific Subroutine RTMI (form H20-0205-3, pp. 217–219), based on Mueller's iteration scheme of successive bisection and inverse parabolic interpolation. Solving for the roots in this way is more straightforward than utilizing the very complicated analytical equations.

The values of $n_k(m)$ up to K=8 for $\theta_0=50^\circ$ are given in Table 1. For the actual computations discussed in a later section, values to four decimal places were used, although the results were essentially the same (within a fraction of a nanotesla) when only two decimal places were used. Laplace's equation is satisfied for any value of n, of course, and the only way that a slight error in n affects the solution is that the relevant basis functions are then not precisely orthogonal.

The first, third, fifth, \cdots values in each column of Table 1 (i.e., those values for which k-m is even) are the values of n for which the derivative of the function is zero at $\theta = 50^{\circ}$

(satisfying (17)). The second, fourth, sixth, \cdots values in each column (k - m) is odd) are those values for which the function itself is zero at $\theta = 50^{\circ}$ (satisfying (18)).

Since P_n^1 can be expressed in terms of the derivative of P_n^0 [Hobson, 1931, section 55], those values of $n_k(0)$ giving a zero derivative at $\theta_0(k = \text{even})$ are the same as those values of $n_k(1)$ giving a zero function at θ_0 .

SUBTRACTION OF A KNOWN SPHERICAL HARMONIC POTENTIAL

For the whole sphere the ordinary spherical harmonic expansion is the natural and correct representation of the potential field. Because of the natural spherical geometry the potential and all its derivatives are periodic with period 2π , and there are no boundary discontinuities to affect convergence. The rate of convergence of the series depends only on the natural spectral decay of the field.

In fact, that representation, expressed in terms of a fundamental wavelength of 2π , is exactly what one would like, even over a spherical cap. The problem, as mentioned earlier, is in the numerically accurate solution of the least squares problem based on that representation. The spherical cap representation introduced in this paper provides better accuracy in the least squares solution but at the cost of introducing a boundary at $\theta = \theta_0$. At this boundary only the potential and its first derivative have been controlled in θ (equations (8) and (9)) and so the rate of convergence of the series (12) depends not only on the spectral decay of the field but also on the error at θ_0 in the higher derivatives. This is analogous to fitting Fourier series to nonperiodic functions [Lanczos, 1966, section 19].

Physically, this results from not considering data outside the spherical cap. It is therefore advantageous to substract a known spherical harmonic potential $V_{\rm SH}$, previously determined using data from the whole earth, from the total potential $V_{\rm TOT}$ and to compute spherical cap harmonic coefficients for a residual potential ΔV :

$$\Delta V = V_{\text{TOT}} - V_{\text{SH}}$$

The closer $V_{\rm SH}$ approximates $V_{\rm TOT}$, the more rapid will be the convergence of the fit to ΔV . Any existing model, such as the IGRF, should be adequate as $V_{\rm SH}$. Again, this is analogous to subtracting a linear trend (or, more generally, the Bernoulli polynomials) from data before fitting a Fourier series [Lanczos, 1966, section 16].

In the usual application of fitting the gradient of the potential rather than the potential itself, this procedure is still possible because of the linearity of the gradient operator.

DEMONSTRATION AND DISCUSSION OF THE METHOD

To demonstrate the method of fitting, over a spherical cap, the divergence-free and curl-free geomagnetic field resulting from internal sources, the International Geomagnetic Reference Field (IGRF) for 1980 [IAGA Division 1 Working Group 1, 1981] was modeled. No conversion to geodetic coordinates was made, and so the results apply only to a spherical earth. Values were computed on a latitude-longitude grid (or simply latitude for zonal fields) and these values used as input for a least squares solution of the coefficients of the spherical cap harmonic functions described in the previous sections of this paper. The effects of instrumental errors and of incomplete or improper reduction procedures, important in fitting real data, are ignored here. The resultant standard errors of estimation, or of fit, are thus caused solely by truncating the infinite series.

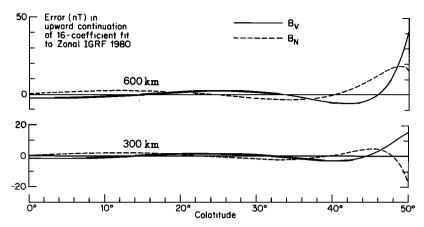


Fig. 3. Errors in upward continuations to 300 and 600 km altitudes of spherical cap harmonic fit to zonal terms of IGRF 1980 at earth's surface with K = 15. B_V and B_N are the vertical downward and horizontal north components, respectively.

This effect occurs in ordinary spherical harmonic analysis in fitting the earth's field, expressible as an infinite series, by a finite degree expansion. Here, on the other hand, it results from a change of basis functions, where even a finite degree expansion can only be expressed in a subinterval as an infinite series. This is analogous to fitting, over an interval of length l, a simple function such as $\sin \theta$ in terms of an infinite set of basis functions of fundamental period $2\pi/l$.

Values were first computed for the zonal (m=0) terms only. They were computed every $1/2^{\circ}$ from 0 to 50° in colatitude, at altitude 0. This region was chosen because of the interest, mentioned earlier, in analyzing Magsat data above 40° N. The mean square value of B_{ν} and B_{N} over the region is almost 40,000 nT. Individually, B_{ν} ranges from 42,000 to 56,000 nT, and B_{N} ranges from 0 to 24,000 nT. The standard error of the simultaneous fit to B_{ν} and B_{N} versus the number of coefficients in the expansion is shown in Figure 2. At 11 coefficients, the same number as are included in the zonal IGRF, the standard error of fit is 12 nT. At 16 coefficients the standard error is 1.2 nT. All coefficients are statistically significant.

Upward continuations of the fitted field agree very well with the zonal IGRF calculated at the corresponding altitudes. The standard errors of the fitted field upward continued to 300 and 600 km are 3.2 and 6.5 nT, respectively, for the 16-coefficient fit (K = 15). Figure 3 shows the differences (spherical harmonic minus spherical cap harmonic) versus colatitude for the two zonal components B_{ν} and B_{ν} , using this 16-coefficient fit computed at these two altitudes. Although at the boundary the fitted differences are only -4 nT in B_v and 3 nT in B_N at the earth's surface, these differences increase rapidly with altitude. It can be seen also, that the deterioration in the upward continuation spreads inward from the cap boundary with increasing continuation altitudes. This is to be expected because of the absence of any independent control at the boundary on derivatives in θ of the second order and higher. The errors in these higher derivatives affect the analytic continuation of the potential with respect to r, worsening with increasing r. Physically, this is again a consequence of ignoring data outside the cap. Even so, the differences are still quite small, over the 600-km continuation, especially when considered as a percentage of the mean square field value.

When data are available over a range of altitudes, as in the case of Magsat data, this continuation error does not apply over that range since the analysis provides the best least

squares fit over the entire region. The continuation error is only relevant when continuing the results to an altitude outside the range of observed altitudes for comparison with another data set.

Next, to demonstrate how the convergence can be improved by subtracting a known spherical harmonic potential field from the input data, only the nondipole part (terms with $n \ge 2$) of the zonal IGRF was modeled. The range of B_V is now from -3600 to 3700 nT, and that of B_N from -2500 to 1300 nT. The standard error of this fit is shown in Figure 4. The standard error reduces to 0.26 nT with 11 coefficients in the expansion and, in fact, is a mere 0.02 nT with 16 coefficients. Again, all the coefficients are statistically significant. The maximum error in upward continuation to 600 km, using 16 coefficients, is 0.3 nT in B_N and 0.7 nT in B_V .

Finally, values were computed for the nondipole part $(n \ge 2)$ of the IGRF 1980, zonal and nonzonal. Here values were computed at the earth's surface for every 5° of colatitude at increments in longitude of 5°/sin θ . Using a variable increment such as this for longitude avoids the high data density at the pole that would result from using a constant increment. Over the region, B_N varies from -9100 to 3800 nT, B_E from -7600 to 8600, and B_V from -7200 to 18,000. The reduction of the standard error of fit with the number of coefficients in the expansion is shown in Figure 5. The standard errors are

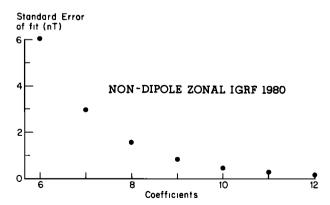


Fig. 4. Standard errors of fit from modeling nondipole zonal terms of IGRF 1980 by means of zonal spherical cap harmonic functions. Removal of the dipole term results in much faster convergence than in Figure 2.

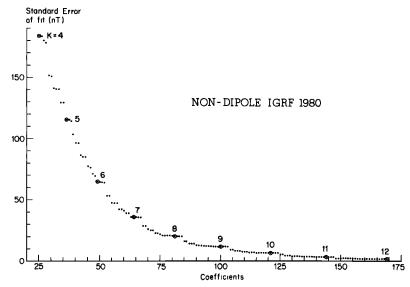


Fig. 5. Standard errors of fit from modeling nondipole terms of IGRF 1980 by means of spherical cap harmonic functions. Order of variable entry is g^m_k , h^m_k ; $m = 0, 1, \dots, k$; $k = 1, 2, \dots, K$. A full expansion of maximum index K contains $(K + 1)^2$ coefficients. Circled errors correspond to $K = 4, 5, \dots, 12$.

circled for each successive K from 4 to 12. At K=10, with the same number of coefficients as are included in the tenth degree IGRF, the standard error of fit is 6.8 nT. The small jumps occurring periodically throughout Figure 5 occur each time a g_n^2 is introduced into the regression. This is because the cos (2λ) terms are predominant in the geomagnetic potential and represent a feature that continues straight through the cap.

The top half of Figure 6 shows this feature at the boundary of the 50° spherical cap, at an altitude of 600 km. The lower half of Figure 6 shows the error in upward continuation to 600 km of the spherical cap harmonic fit with K = 12. The error is shown at the 50° boundary since this is where the main continuation error occurs. At $\theta = 45^{\circ}$, for example, the largest absolute error is 18.7 nT, and at $\theta = 40^{\circ}$ it is 9.3 nT. By comparing the top and bottom parts of Figure 6, it can be seen that the continuation error is, in this case, of the order of 1% of the field being represented. Of course, the fitted errors, at 0 km, are no worse at the boundary (here they are less than 1.5 nT) than elsewhere. For this fit, at 0 km altitude, the standard error of fit is 2.1 nT. At 300 km altitude the standard error (of continuation) is 6.1 nT, and at 600 km it is 9.3 nT. This is still an excellent agreement considering the mean square value of the fitted functions is over 5000 nT.

The spherical cap harmonic method has been applied to real data by fitting those functions with k-m= even and truncation at K=22 to Magsat vertical field anomaly data above $40^{\circ}N$ [Haines, this issue].

CONCLUSIONS

The method presented in this paper gives an excellent fit over a spherical cap to the derivatives of a potential function. The method provides a useful representation not only spatially over a spherical surface but also radially.

The method could be adapted to areas other than the polar regions by a simple rotation of the spherical coordinate system. Although it is theoretically possible to find similar solutions for other spherical surfaces (such as spherical sectors and tesserae, for example), the introduction of still more boundaries may not provide as satisfactory a result as the simple rotation of coordinates.

The spherical cap harmonic approach provides an excellent means of analysing satellite data over a spherical cap and throughout the radial region of satellite altitudes. However, in fact it can be readily applied to the construction of national charts of potential gradient (such as geomagnetic or gravity fields) or their secular variation. The potential constraints of

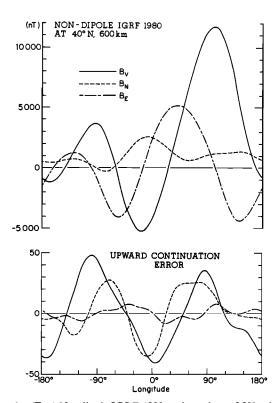


Fig. 6. (Top) Nondipole IGRF 1980 on boundary of 50° spherical cap, computed at 600 km. (Bottom) Error in upward continuation to 600 km altitude, at 50° colatitude, of spherical cap harmonic fit to nondipole IGRF 1980 at earth's surface with K=12. B_{ν} , B_{N} , and B_{E} are the vertical downward, horizontal north, and horizontal east components, respectively. Longitudes are positive east, negative west.

electromagnetic theory, that the curl and divergence of the field be zero, are automatically satisfied.

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