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Global spherical harmonic analysis by least-squares and numerical quadrature methods in historical perspective

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SUMMARY

Methods of global spherical harmonic analysis of discrete data on a sphere are placed in a historical context. The paper concentrates on the loss of orthogonality in the direction of latitude, due to the transition from continuous to discretized functions. Special attention is paid to Neumann's (1838) solution to this problem. By recasting the formulae of spherical harmonic analysis into matrix–vector notation, both least-squares solutions and quadrature methods are represented in a general framework of weighted least squares. It is also shown that the two-step formulation of global spherical harmonic computation was applied already by Neumann (1838) and Gauss (1839). Computational modifications to Neumann's method are reviewed as well.

Key words: global spherical harmonic analysis, least squares, Neumann quadrature, numerical integration.

1 INTRODUCTION

Since the early 1980s a growing number of spherical harmonic models of the earth's gravity field have become available up to very high degrees and orders (Wenzel 1985; Rapp, Wang & Pavlis 1991). Expansions up to degree and order 180 or 360, the latter with more than 130 000 individual coefficients, are widely used for many purposes. This development has been triggered by work of Rizos (1979), Colombo (1981), and Tscherning & Poder (1982). They showed that if in the case of global spherical harmonic *synthesis* (GSHS) proper care is taken in the sequence of summation over degree and order, the two can be treated independently. Application of efficient summation (Rizos 1979), FFT algorithms and block structure (Colombo 1981) or Clenshaw summation (Tscherning & Poder 1982) then results in an enormous increase of computer efficiency. Algorithms for GSHS, based on these methods have been compared, e.g. by Tscherning, Rapp & Goad (1983). Analogously, in the case of global spherical harmonic *analysis* (GSHA), the integration in the direction of longitude is separated from the one in the direction of latitude. The resulting efficient algorithms, both for synthesis and for analysis, are thus based on a two-step formulation of global spherical harmonic computation (GSHC).

It is the objective of this paper to draw the attention to old German literature in which the ideas of a two-step formalism were first explained, some 150 years ago†. These ideas evolved in a period of great mathematical flourishing: eminent mathematicians like Gauss and Neumann were engaged in global spherical harmonic computation. Apart from a purely mathematical interest, a great incentive came from the fact that global geomagnetic data became available (*cf.* Gauss 1839). Bearing in mind that all computations had to be done by hand, it seems only natural that algorithms in those days had to be efficient. Since the number of parameters in a spherical harmonic expansion goes with the square of its maximum degree, the need for such algorithms is still present nowadays, despite the availability of powerful computers.

The efficiency of the methods that will be described stems from a suitable ordering of the degree and order summations in the spherical harmonic series formulation. In the next section this specific ordering will be called order-degree summation swap. Almost at the same time Neumann (1838) and Gauss (1839) developed such two-step GSHA formulations. A common first step consisted of a Fourier transformation along parallels. As will be shown later, this first step can be performed easily for discrete data, due to the orthogonality properties of the trigonometric base functions. However, the two authors differ in

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† In this sense the words of the title should be understood. It is not intended to give a thorough review of past and present methods of global spherical harmonic analysis in this paper.

their treatment of the second analysis step: the computation of spherical harmonic coefficients from the obtained Fourier coefficients. A complication in this second step is the loss of orthogonality of Legendre functions at discrete points.

Gauss (1839) approached the second step by a least-squares inversion of the linear relationship between spherical harmonic and Fourier coefficients. In this work an expansion of geomagnetic point data up to degree and order 4 was performed. In the two-step formalism the maximum size of matrices to be inverted will then be 4, if zero-order terms are absent. It will be clear that this method was restricted to low maximum degree expansions in those days. More serious objections to Gauss's method of least squares are the dependence of the final spherical harmonic coefficients on the choice of maximum expansion degree L, and mutual dependence between coefficients of varying degree for a given order, due to the non-orthogonality of discretized Legendre functions.

Neumann's (1838) starting point was the numerical evaluation of an integral. In an elegant way he devised certain quadrature weights which preserve orthogonality of the Legendre functions, thus leading to exact quadrature formulae. Basically two versions of Neumann's method exist. In the first one, the number of parallels employed is roughly twice the maximum degree of expansion. Although this ratio is not so favourable, the distribution of the parallels may be chosen at will, for instance equi-angular. Neumann's second method requires only $L+1$ latitude circles, if L is the maximum degree. However, they must be situated in the roots of a certain Legendre polynomial. This second method appears to be equal to Gauss's quadrature method (1814), as Neumann himself had indicated. It seems, though, that Gauss did not apply this quadrature to spherical harmonic analysis, but favoured the least-squares approach instead. In numerical analysis the method is more specifically known as Gauss–Legendre quadrature (Stroud & Secrest 1966).

Unlike Gauss's method of least squares, Neumann's methods have not found widespread application. Prey (1922) developed the earth's topography into a spherical harmonic series up to degree and order 16 using Neumann's second method. This work was extended by Vening-Meinesz (1959) who developed the topography up to degree 31. The actual computations are described in Hofsommer (1957). Other applications may be found in the atmospheric sciences, e.g. Ellsaesser (1966), where both the first and second method are treated, and used to analyse hemispheric pressure data.

In geodesy only the second Neumann method is used or mentioned, though only implicitly, namely as Gauss–Legendre quadrature, *cf.* Payne (1971) or Colombo (1981). The non equi-angular distribution of parallels seems to be a major objection to the method. A geodetic reference to Neumann can be found in Pellinen (1966). For one reason or another the geodetic use of Gauss–Legendre quadrature was most popular in the former Eastern Block countries.

This paper recalls the basic formulae of GSHC, after which most attention is paid to the problematic second analysis step. The problem arises, as mentioned before, from the loss of orthogonality of Legendre functions after discretization. This *skewness*, and its reparation by Neumann, is most clearly seen in terms of point data discretizations. Moreover, stochasticity of the data and too high signal frequencies would ruin Neumann's quadrature methods. The scope of this paper is therefore limited to treating the rather academic question of GSHA of a point-gridded, non-stochastic function without signal beyond the Nyquist frequency. Although far from reality, these simplifications explain Neumann's and Gauss's ideas best, and do correspond to the underlying principles of GSHA.

Subsequently, Gauss's least-squares approach, approximate quadrature and Neumann's methods are treated. Furthermore, the equations of discrete GSHC are given in matrix–vector notation as well. As a result all three approaches fit into the general framework of a weighted least-squares formulation of GSHA.

2 THEORETICAL BACKGROUND

We start with recapitulating the necessary formulae of GSHS and GSHA, both for the continuous and the discretized cases. For the latter, the formulae are also presented in a compact matrix algebra formulation.

2.1 Global spherical harmonic computation—continuous

A square integrable function $f(\theta, \lambda)$ on a sphere (θ colatitude, λ longitude) can be developed into harmonic coefficients $\bar{C}_{lm}$ and $\bar{S}_{lm}$, using the GSHA:

$$\left.\begin{matrix}\bar{C}_{lm}\\ \bar{S}_{lm}\end{matrix}\right\} = \frac{1}{4\pi}\iint_{\sigma} f(\theta,\lambda)\bar{P}_{lm}(\cos\theta)\left\{\begin{matrix}\cos m\lambda\\ \sin m\lambda\end{matrix}\right\} d\sigma, \tag{1}$$

with $d\sigma = \sin\theta\, d\theta\, d\lambda$. Vice versa, the function $f(\theta, \lambda)$ can be reconstructed by the GSHS:

$$f(\theta,\lambda) = \sum_{l=0}^{\infty}\sum_{m=0}^{l}\bar{P}_{lm}(\cos\theta)(\bar{C}_{lm}\cos m\lambda + \bar{S}_{lm}\sin m\lambda). \tag{2}$$

The overbars denote normalized quantities, where the following normalization factor has been adopted:

$$N_{lm} = \sqrt{(2-\delta_{m0})(2l+1)\frac{(l-m)!}{(l+m)!}},$$

with

$$\delta_{m0} = \begin{cases}1, & m = 0,\\ 0, & m \neq 0.\end{cases}$$

A major contribution of Rizos (1979) and Colombo (1981) in spherical harmonic computation consisted of the observation that the latitude and longitude information can be dealt with independently if the summation scheme is reordered:

$$\sum_{l=0}^{\infty}\sum_{m=0}^{l} \rightarrow \sum_{m=0}^{\infty}\sum_{l=m}^{\infty}.$$

This summation swap leads to a two-step analysis and synthesis formulation, which is optimally suited to efficient computer programming.

Two-step synthesis—continuous

$$\left.\begin{matrix} A_m(\theta) \\ B_m(\theta) \end{matrix}\right\} = \sum_{l=m}^{\infty} \bar{P}_{lm}(\cos\theta) \left\{\begin{matrix} \bar{C}_{lm} \\ \bar{S}_{lm} \end{matrix}\right., \tag{3a}$$

$$f(\theta, \lambda) = \sum_{m=0}^{\infty} [A_m(\theta) \cos m\lambda + B_m(\theta) \sin m\lambda]. \tag{3b}$$

Two-step analysis—continuous

$$\left.\begin{matrix} A_m(\theta) \\ B_m(\theta) \end{matrix}\right\} = \frac{1}{(1+\delta_{m0})\pi} \int_0^{2\pi} f(\theta, \lambda) \left\{\begin{matrix} \cos m\lambda \\ \sin m\lambda \end{matrix}\right. d\lambda, \tag{3c}$$

$$\left.\begin{matrix} \bar{C}_{lm} \\ \bar{S}_{lm} \end{matrix}\right\} = \frac{1+\delta_{m0}}{4} \int_0^{\pi} \left\{\begin{matrix} A_m(\theta) \\ B_m(\theta) \end{matrix}\right. \bar{P}_{lm}(\cos\theta) \sin\theta \, d\theta. \tag{3d}$$

The reasons for the greater efficiency of the two-step formulation is twofold. First, eqs (3b) and (3c) can be treated by Fourier transformations over single parallels. Secondly, the equations may be evaluated for separate orders m, leading to block diagonal structures in the discrete case. Eqs (3a)–(3d) may be summarized in the following scheme:

$$f(\theta, \lambda) \underset{\Sigma}{\overset{\int}{\rightleftharpoons}} A_m(\theta), B_m(\theta) \underset{\Sigma}{\overset{\int}{\rightleftharpoons}} \bar{C}_{lm}, \bar{S}_{lm}.$$

2.2 Global spherical harmonic computation—discrete

In reality, one has to deal with discretized function values, either point values or area means. Here, we restrict ourselves to the case where the function has been sampled at discrete points. The aliasing problem will be ignored, i.e. it is tacitly assumed that the function does not contain information above degree L. In Section 3 reference is made to more realistic situations. Also, the last section returns to this problem. First, one has to truncate the spectrum at a maximum degree and order, say L. Next the function $f(\theta, \lambda)$ must be sampled. Assuming an equi-angular discretization in longitudinal direction $\lambda_i = i\,\Delta\lambda$, $i = 0, 1, \ldots, 2L-1$, where

$$\Delta\lambda = \frac{2\pi}{2L} = \frac{\pi}{L},$$

it can be shown that orthogonality is preserved.

$$\int_0^{2\pi} \cos m\lambda \cos k\lambda \, d\lambda = (1+\delta_{m0})\pi \, \delta_{mk} \leftrightarrow$$

$$\sum_{i=0}^{2L-1} \cos m\lambda_i \cos k\lambda_i = (1+\delta_{m0}+\delta_{mL})L \, \delta_{mk},$$

$$\int_0^{2\pi} \sin m\lambda \sin k\lambda \, d\lambda = (1-\delta_{m0})\pi \, \delta_{mk} \leftrightarrow$$

$$\sum_{i=0}^{2L-1} \sin m\lambda_i \sin k\lambda_i = (1-\delta_{m0}-\delta_{mL})L \, \delta_{mk},$$

$$\int_0^{2\pi} \cos m\lambda \sin k\lambda \, d\lambda = 0 \leftrightarrow \sum_{i=0}^{2L-1} \cos m\lambda_i \sin k\lambda_i = 0.$$

So far, it has not yet been decided what the sampling in the direction of latitude should be. There is no way yet to establish rigorously orthogonality in the discrete case:

$$\int_{-1}^{1} \bar{P}_{l_1 m}(x) \bar{P}_{l_2 m}(x) \, dx = 2(2-\delta_{m0}) \, \delta_{l_1 l_2} \leftrightarrow$$

$$\sum_{i=1}^{N} \bar{P}_{l_1 m}(x_i) \bar{P}_{l_2 m}(x_i) \neq 2(2-\delta_{m0}) \, \delta_{l_1 l_2},$$

in which N denotes the number of parallels, not necessarily equal to L. The GSHC equations now reduce to the following set.

Two-step synthesis—discrete

$$\left.\begin{matrix} A_m(\theta_i) \\ B_m(\theta_i) \end{matrix}\right\} = \sum_{l=m}^{L} \bar{P}_{lm}(\cos\theta_i) \left\{\begin{matrix} \bar{C}_{lm} \\ \bar{S}_{lm} \end{matrix}\right., \tag{4a}$$

$$f(\theta_i, \lambda_j) = \sum_{m=0}^{L} A_m(\theta_i) \cos m\lambda_j + B_m(\theta_i) \sin m\lambda_j. \tag{4b}$$

Two-step analysis—discrete

$$\left.\begin{matrix} A_m(\theta_i) \\ B_m(\theta_i) \end{matrix}\right\} = \frac{1}{L(1+\delta_{m0}+\delta_{mL})} \sum_{j=0}^{2L-1} f(\theta_i, \lambda_j) \left\{\begin{matrix} \cos m\lambda_j \\ \sin m\lambda_j \end{matrix}\right., \tag{4c}$$

$$\left.\begin{matrix} \bar{C}_{lm} \\ \bar{S}_{lm} \end{matrix}\right\} = \text{to be determined.} \tag{4d}$$

The coefficients $A_m(\theta_i)$ in the upper line in eq. (4c) have an index range $m = 0, 1, \ldots, L$, whereas the index for the B_m coefficients run from $m = 1, \ldots, L-1$. Since the distribution of parallels has not been decided yet and since the problem of non-orthogonality of the discretized Legendre functions has not been resolved, the determination of the $\bar{C}_{lm}$- and $\bar{S}_{lm}$-coefficients remains an open question. It must be noted that the number of function values for each parallel equals the number of $A_m(\theta_i)$- plus $B_m(\theta_i)$-coefficients: $(L+1)+(L-1) = 2L$.

A preliminary conclusion can be drawn on the m-limits to the sine terms. It is a known fact that $B_m(\theta_i)$-terms with $m = 0$, and consequently all zonals $\bar{S}_{l,0}$ do not exist. However, the same holds true for the $m = L$-term. The Fourier coefficient $B_L(\theta_i)$ does not exist either, which leads to the conclusion that $\bar{S}_{LL}$ is unestimable also.

Because of the orthogonality properties of the sine and cosine functions and because of the periodicity of the function on each parallel, the forward and backward Fourier transformations can efficiently be performed by Fast Fourier Transforms (FFT). Eqs (4a)–(4d) may be summarized now in the following scheme:

$$f(\theta_i, \lambda_j) \underset{\text{FFT}}{\overset{\text{FFT}}{\rightleftharpoons}} A_m(\theta_i), B_m(\theta_i) \underset{\Sigma}{\overset{?}{\rightleftharpoons}} \bar{C}_{lm}, \bar{S}_{lm}$$

2.3 Matrix notation

The discrete analysis and synthesis formulae are recast now into matrix–vector equations. This transition yields compact equations, which are helpful when comparing least squares with quadrature solutions. With $x_i = \cos\theta_i$, we introduce

the following vectors and matrices:

$$\mathbf{a}=\begin{bmatrix} A_m(\theta_1)\\ A_m(\theta_2)\\ \vdots\\ A_m(\theta_N)\end{bmatrix},\qquad \mathbf{b}=\begin{bmatrix} B_m(\theta_1)\\ B_m(\theta_2)\\ \vdots\\ B_m(\theta_N)\end{bmatrix},$$

$$\mathbf{P}=\begin{bmatrix} \bar{P}_{mm}(x_1) & \bar{P}_{m+1,m}(x_1) & \cdots & \bar{P}_{Lm}(x_1)\\ \bar{P}_{mm}(x_2) & \ddots & & \vdots\\ \vdots & & \ddots & \vdots\\ \bar{P}_{mm}(x_N) & \cdots & \cdots & \bar{P}_{Lm}(x_N)\end{bmatrix},$$

$$\mathbf{c}=\begin{bmatrix} \bar{C}_{mm}\\ \bar{C}_{m+1,m}\\ \vdots\\ \bar{C}_{Lm}\end{bmatrix},\qquad \mathbf{s}=\begin{bmatrix} \bar{S}_{mm}\\ \bar{S}_{m+1,m}\\ \vdots\\ \bar{S}_{Lm}\end{bmatrix},$$

$$\mathbf{f}=\begin{bmatrix} f(\theta_i,\lambda_0)\\ f(\theta_i,\lambda_1)\\ \vdots\\ f(\theta_i,\lambda_{2L-1})\end{bmatrix},$$

$\mathbf{F}=2L\times 2L$ Fourier matrix (*cf.* Strang 1986)

with $[\mathbf{F}]_{rs}=\mathrm{e}^{i(rs\pi)/L}$, $r, s=0, 1, \ldots, 2L-1$.

In order to apply the Fourier matrix $\mathbf{F}$ properly one should also introduce a complex vector, say $\mathbf{d}$, of length $2L$ composed of $\mathbf{a}+i\mathbf{b}$ and $\mathbf{a}-i\mathbf{b}$. $\mathbf{F}$ has the property

$$\mathbf{F}^{-1}=\frac{1}{2L}\mathbf{F}^{\dagger}\quad\Leftrightarrow\quad \mathbf{F}\mathbf{F}^{\dagger}=2L\mathbf{I},$$

with $\mathbf{I}$ the identity matrix. This relationship expresses again the orthogonality relations of the trigonometric functions. The matrix $\mathbf{F}^{\dagger}$ denotes the Hermitean (complex conjugated and transposed) of $\mathbf{F}$.

Having introduced the above notation, we may now write the GSHC equations as follows.

Synthesis

$$\mathbf{a}=\mathbf{P}\mathbf{c},\qquad \mathbf{b}=\mathbf{P}\mathbf{s},\qquad \mathbf{a},\mathbf{b}\rightarrow\mathbf{d}, \tag{5a}$$

$$\mathbf{f}=\mathbf{F}\mathbf{d}. \tag{5b}$$

Analysis

$$\mathbf{d}=\mathbf{F}^{-1}\mathbf{f},\qquad \mathbf{d}\rightarrow\mathbf{a},\mathbf{b}, \tag{5c}$$

$$\mathbf{c}=\mathbf{P}^{-}\mathbf{a},\qquad \mathbf{s}=\mathbf{P}^{-}\mathbf{b}, \tag{5d}$$

in which $\mathbf{P}^{-}$ denotes some generalized inverse. It refers to the fact that the inversion of eq. (5a) is still to be determined. It is underlined again that the Fourier transformations eqs (5b) and (5c) apply to each parallel individually, and that the formulae involving the matrix $\mathbf{P}$ pertain to one specific order m. This splitting of information and unknowns, originating from the degree-order swap, is what makes the two-step method so powerful.

The size of a single matrix $\mathbf{P}$ is $N\times(L-m+1)$. In order to have an overdetermined systems (eq. 5a) one has to demand that the number of latitude circles (N) at least equals the maximum of $(L-m+1)$, which occurs when $m=0$. Thus, the only restriction on the sampling in the direction of latitude is $N\geq L+1$. Except for this restriction, nothing has been said about the latitudinal sampling so far.

3 LEAST SQUARES

It has been shown that the sine and cosine functions retain their orthogonality, provided that an equidistant sampling is applied along each parallel. In the sequel therefore we are no longer concerned with the Fourier transformations, but concentrate on the 'Legendre transformation'. Basically, two approaches exist for solving the second analysis step. The first originated from Gauss (1839) and results—unsurprisingly—in a *least-squares* solution of the linear systems (eq. 5a), i.e.:

$$\mathbf{c}=(\mathbf{P}^{\mathrm{T}}\mathbf{P})^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{a},\qquad \mathbf{s}=(\mathbf{P}^{\mathrm{T}}\mathbf{P})^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{b}. \tag{6}$$

The maximum normal matrix size will be $(L+1)\times(L+1)$. A specific column out of $\mathbf{P}$ represents a discretized Legendre polynomial $\bar{P}_{lm}(\cos\theta_i)$, $i=1, 2, \ldots, N$. The normal matrix $\mathbf{P}^{\mathrm{T}}\mathbf{P}$ is composed of inner products between these columns. Therefore, each normal matrix entry represents the level of (non-)orthogonality of discretized Legendre functions:

$$[\mathbf{P}^{\mathrm{T}}\mathbf{P}]_{ln}=\sum_{i=1}^{N}\bar{P}_{lm}(\cos\theta_i)\bar{P}_{nm}(\cos\theta_i).$$

Thus, orthogonality is shown to be equivalent to a diagonal normal matrix. Since orthogonality is lost $\mathbf{P}^{\mathrm{T}}\mathbf{P}$ will not be diagonal. From a simple example with $N=21$, $L=10$, $m=0$, using an equi-angular θ_i-grid (*cf.* Fig. 1), it may be clear that $\mathbf{P}^{\mathrm{T}}\mathbf{P}$ is even far from diagonal. The maximum diagonal value becomes about 45 instead of 2, whereas the off-diagonals exhibit substantial values.

The two-step GSHA approach using least squares leads to non-diagonal normal matrices with a maximum size of only $L\times L$. Even though matrices of this size, e.g. 360×360, do not present difficulties on present-day computers, one may want to avoid matrix inversions of this size. In this case one could approximate the normal matrix by a scaled identity matrix, say $\mathbf{P}^{\mathrm{T}}\mathbf{P}=\lambda\mathbf{I}$, thus ignoring non-orthogonality. The scale factor λ is not necessarily equal to $2(2-\delta_{m0})$. This approximation would lead to the solution $\mathbf{c}=\lambda^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{a}$, $\mathbf{s}=\lambda^{-1}\mathbf{P}^{\mathrm{T}}\mathbf{b}$, or:

$$\left.\begin{matrix}\bar{C}_{lm}\\ \bar{S}_{lm}\end{matrix}\right\}=\frac{1}{\lambda}\sum_{i=1}^{N}\bar{P}_{lm}(\cos\theta_i)\left\{\begin{matrix}A_m(\theta_i)\\ B_m(\theta_i),\end{matrix}\right. \tag{7}$$

which can be considered as a very crude quadrature approximation to eq. (3d).

A major reason for the widespread use of the least-squares method is its flexibility concerning data distribution. Eq. (2) may be regarded as an observation equation which could be used on a totally irregular data set in a one-step approach. Moreover, the flexibility in using data of different types is a great advantage of the least-squares method. It can, for instance, be used to combine satellite-derived models with terrestrial data (*cf.* the OSU91A model up to degree 50) (Rapp *et al.* 1991). But the most important advantage is the possibility of incorporating a stochastic model and *a priori* information (*cf.* Colombo 1981), leading to a least-squares collocation formulation. From a practical viewpoint Wenzel (1985)

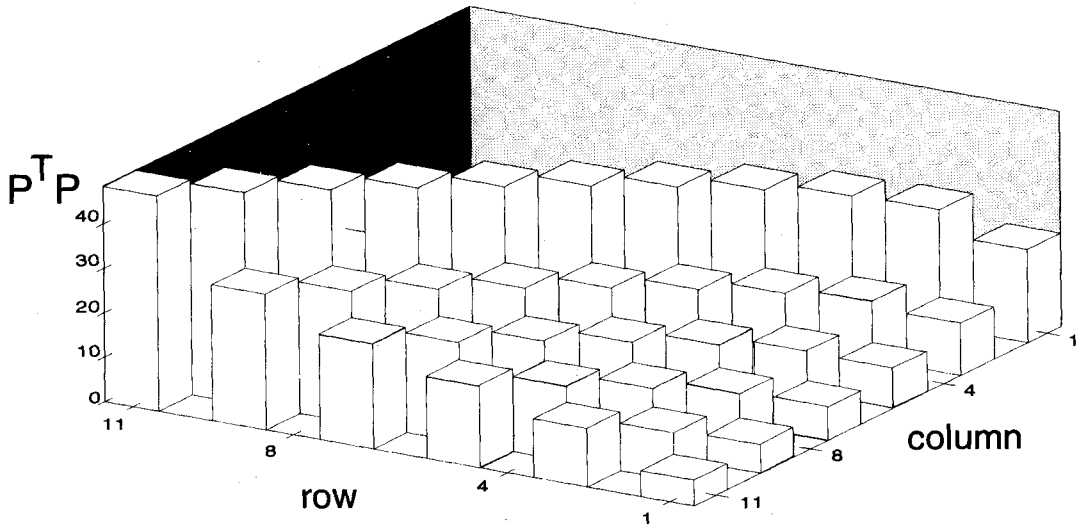

Figure 1. Normal matrix of least squares. $N = 21$, $L = 10$, $m = 0$.

considers quadrature methods as non-optimal as compared with least squares.

4 APPROXIMATE QUADRATURE

Comparing eq. (7) with eq. (3d) we notice the absence of a $\sin\theta\, d\theta$ term in the former. A direct discretization of eq. (3d) introduces such a term proportional to $\sin\theta_i$ into the solution, leading to the following *approximate quadrature* formula:

$$\left.\begin{matrix}\bar{C}_{lm}\\ \bar{S}_{lm}\end{matrix}\right\} = \tfrac{1}{4}(1+\delta_{m0}) \sum_{i=1}^{N} s_i \bar{P}_{lm}(\cos\theta_i) \left\{\begin{matrix}A_m(\theta_i)\\ B_m(\theta_i),\end{matrix}\right. \tag{8}$$

with either one of the following possibilities

$$s_i = \frac{\pi}{N}\sin\theta_i \tag{9a}$$

or

$$s_i = \frac{2}{\sum_{k=1}^{N}\sin\theta_k}\sin\theta_i, \tag{9b}$$

(*cf.* Ellsaesser 1966).

Thus, to each parallel θ_i there corresponds a weight s_i, proportional to the sine of the colatitude. As a generalization to the numerical quadrature (eq. 8) one could consider quadrature weights, not only depending on the colatitude, but on degree l and order m as well. The weights can be adapted to accommodate block averaging and desmoothing, and to minimize sampling and estimation error. In fact this type of quadrature can strictly be derived from a least-squares collocation formulation. The reader is referred to Colombo (1981), Hajela (1984) or Gleason (1989). A further discussion on 'real world harmonic analysis' is found, e.g. in Pavlis (1988), where a comparison between least-squares methods and quadratures is made (see also Wenzel 1985).

How good the approximate quadrature formula (8) is, may be assessed by writing down the equivalent matrix problem. Consider a diagonal weight matrix $\mathbf{S}$, whose diagonal is composed of the s_i weights. A weighted least-squares solution to the linear systems eq. (5a) now becomes:

$$\mathbf{c} = (\mathbf{P}^T\mathbf{S}\mathbf{P})^{-1}\mathbf{P}^T\mathbf{S}\mathbf{a}, \qquad \mathbf{s} = (\mathbf{P}^T\mathbf{S}\mathbf{P})^{-1}\mathbf{P}^T\mathbf{S}\mathbf{b}. \tag{10}$$

To a good approximation the normal matrix equals a scaled identity matrix, $\mathbf{P}^T\mathbf{S}\mathbf{P} \approx 2(2-\delta_{m0})\mathbf{I}$, resulting in:

$$\mathbf{c} \approx \tfrac{1}{4}(1+\delta_{m0})\mathbf{P}^T\mathbf{S}\mathbf{a}, \qquad \mathbf{s} \approx \tfrac{1}{4}(1+\delta_{m0})\mathbf{P}^T\mathbf{S}\mathbf{b}, \tag{11}$$

which is the matrix equivalent of eq. (8). Still the method of approximate quadrature suffers slightly from non-orthogonality. The lack of orthogonality of $\mathbf{P}^T\mathbf{S}\mathbf{P}$ is displayed in Fig. 2, where twice the identify matrix has been subtracted from the normal matrix. Again nothing has been said about θ_i-sampling. Its choice is still free, in principle, though the weights eq. (9a) suggest an equi-angular $\Delta\theta = \pi/N$ spacing already, which is used in Fig. 2 indeed.

5 NEUMANN'S EXACT METHODS

In 1838 Newmann showed that exact orthogonality can be attained in the discrete case by devising certain weights w_i. If stored in a diagonal weight matrix $\mathbf{W}$, these weights lead to the following weighted least-squares solution:

$$\begin{aligned}\mathbf{c} &= (\mathbf{P}^T\mathbf{W}\mathbf{P})^{-1}\mathbf{P}^T\mathbf{W}\mathbf{a} \equiv \tfrac{1}{4}(1+\delta_{m0})\mathbf{P}^T\mathbf{W}\mathbf{a},\\ \mathbf{s} &= (\mathbf{P}^T\mathbf{W}\mathbf{P})^{-1}\mathbf{P}^T\mathbf{W}\mathbf{b} \equiv \tfrac{1}{4}(1+\delta_{m0})\mathbf{P}^T\mathbf{W}\mathbf{b}.\end{aligned} \tag{12}$$

In this case the normal matrix is exactly diagonal.

$$\mathbf{P}^T\mathbf{W}\mathbf{P} = 2(2-\delta_{m0})\mathbf{I}. \tag{13}$$

Therefore, we may say that the analysis problem eq. (4d) has been solved by eq. (12), leading to the following exact quadrature formula:

$$\left.\begin{matrix}\bar{C}_{lm}\\ \bar{S}_{lm}\end{matrix}\right\} = \tfrac{1}{4}(1+\delta_{m0}) \sum_{i=1}^{N} w_i \bar{P}_{lm}(\cos\theta_i) \left\{\begin{matrix}A_m(\theta_i)\\ B_m(\theta_i).\end{matrix}\right. \tag{14}$$

In order to establish eq. (13), the Neumann weights w_i

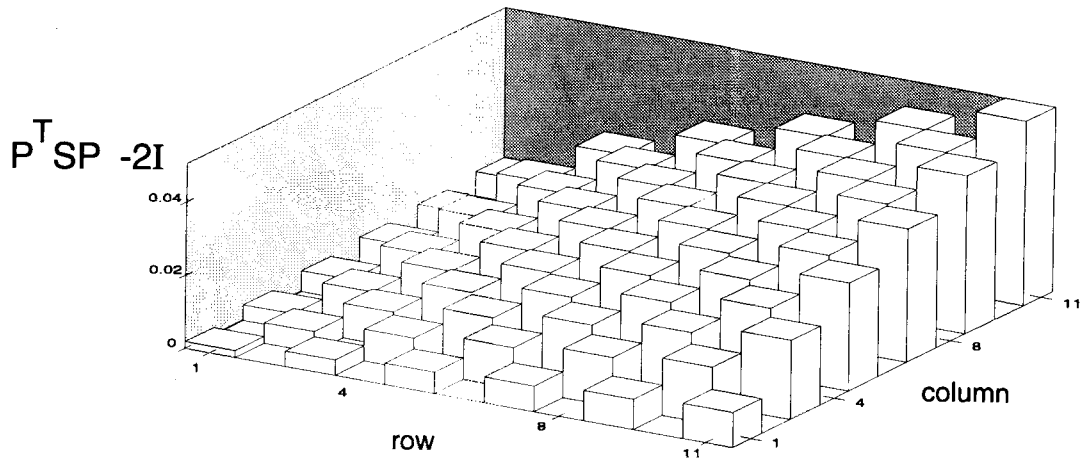

Figure 2. Normal matrix of approximate quadrature minus twice the identity matrix. $N = 21$, $L = 10$, $m = 0$.

must fulfil the following condition (*cf.* Neumann 1887):

$$\sum_{i=1}^{N} w_i x_i^n = \int_{-1}^{1} x^n \, dx = \begin{cases} \dfrac{2}{n+1}, & n \text{ even}, \\ 0, & n \text{ odd}, \end{cases} \tag{15}$$

in which n runs from $n = 0, 1, \ldots, N-1$, and x_i denotes $\cos\theta_i$. Though Neumann proves orthogonality himself, a very simple and elegant proof is given by Lense (1954). The product of two associated Legendre polynomials in x, $\bar{P}_{l_1 m}(x)$ and $\bar{P}_{l_2 m}(x)$, will be a polynomial in x of degree $l_1 + l_2$.

$$\bar{P}_{l_1 m}(x)\bar{P}_{l_2 m}(x) = \sum_{n=0}^{l_1+l_2} a_n x^n.$$

Its integral can be developed as:

$$\begin{aligned} \int_{-1}^{1} \bar{P}_{l_1 m}(x)\bar{P}_{l_2 m}(x)\, dx &= \sum_{n=0}^{l_1+l_2} a_n \int_{-1}^{1} x^n \, dx \\ &\overset{(15)}{=} \sum_{n=0}^{l_1+l_2} a_n \sum_{i=1}^{N} w_i x_i^n \\ &= \sum_{i=0}^{N} w_i \sum_{n=0}^{l_1+l_2} a_n x_i^n \\ &= \sum_{i=1}^{N} w_i \bar{P}_{l_1 m}(x_i)\bar{P}_{l_2 m}(x_i). \end{aligned}$$

Thus, discrete orthogonality has been proven:

$$\sum_{i=1}^{N} w_i \bar{P}_{l_1 m}(x_i)\bar{P}_{l_2 m}(x_i) = 2(2 - \delta_{m0})\, \delta_{l_1 l_2}, \tag{16}$$

which is equivalent to the matrix identity eq. (13). The normal matrix $\mathbf{P^T W P}$ is not displayed here since it does not show any deviation from $2\mathbf{I}$. The computational aspects of Neumann's quadrature weights w_i are treated in the following section. But first the θ-sampling question must be settled.

5.1. First Neumann method

The linear system eq. (15) may be written as the matrix–vector equation $\mathbf{Xw} = \mathbf{r}$, or:

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_1 & x_2 & x_3 & \cdots & x_N \\ x_1^2 & x_2^2 & \ddots & & x_N^2 \\ \vdots & \vdots & & \ddots & \vdots \\ x_1^{N-1} & x_2^{N-1} & \cdots & \cdots & x_N^{N-1} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_N \end{pmatrix} = \begin{pmatrix} 2/1 \\ 0 \\ 2/3 \\ 0 \\ \vdots \\ 2/N \end{pmatrix}. \tag{17}$$

Matrix $\mathbf{X}$ is a so-called Vandermonde matrix, known from Lagrangean interpolation, whose determinant has the analytic expression:

$$\begin{aligned} \det X = &(x_2 - x_1)(x_3 - x_1)(x_3 - x_2) \cdots (x_n - x_1) \\ &\cdot (x_n - x_2)(x_n - x_3) \cdots (x_N - x_{N-1}). \end{aligned}$$

It is clear that this determinant will only vanish when $x_i = x_j$, for $i \neq j$. Thus, the vector $\mathbf{w}$, containing the Neumann weights, is uniquely determined when parallels do not coincide. This is the only restriction to an arbitrary choice of the parallels. The number of them may be deduced from inspecting Lense's proof. We notice that the maximum power of x equals $\max(l_1 + l_2) = 2L$. Therefore, since the matrix $\mathbf{X}$ is square, the number of latitude circles must be $N = 2L + 1$.

In summary, the first Neumann method performs a GSHA up to degree and order L, which is exact if the function has been sampled on the following grid:

$$\begin{aligned} &\theta_i = \text{random but distinct}, \qquad i = 1, 2, \ldots, 2L+1, \\ &\lambda_j = j\,\Delta\lambda, \qquad j = 0, 1, \ldots, 2L-1, \\ &\Delta\lambda = \frac{\pi}{L}. \end{aligned}$$

The meridians have an equi-angular $\Delta\lambda$ spacing, whereas the parallels may be chosen freely without coinciding. One such choice could be an equi-angular $\Delta\theta$ spacing of course. The number of function values is roughly four times the number of spherical harmonic coefficients to be determined.

5.2 Second Neumann method

A special case of exact quadrature is achieved by restricting the θ-grid. Neumann (1887) showed that if one chooses the

latitude circles to coincide with the zeros of the Legendre polynomial of degree $L+1$, i.e.

$$P_{L+1}(x_i) = 0, \qquad i = 1, 2, \ldots, L+1$$

the number of parallels can be reduced to $N = L+1$. The order of precision of the numerical quadrature is doubled (*cf.* Lanczos 1956), and eq. (16) remains true with half the number of parallels as compared with the first method. The ratio of function values versus harmonic coefficients will roughly become two. In Section 2 it was noted that the number $L+1$ is the minimum number of parallels, required for having an overdetermined system (eq. 5a).

The specific θ-grid leads to the *Gaussian quadrature** method, well known form numerical analysis (*cf.* Lanczos 1956); Krylov 1962; Abramowitz & Stegun 1970, section 25.4). As such it is also known in geodesy (*cf.* Payne 1971; Colombo 1981). In Payne (1971) the specific θ-spacing is referred to as a Gauss grid. Summarizing Neumann's second method, an exact GSHA is performed up to degree L, making use of a Gauss–Neumann grid, defined by:

$$P_{L+1}(\cos\theta_i) = 0, \qquad i = 1, 2, \ldots, L+1,$$
$$\lambda_j = j\,\Delta\lambda, \qquad j = 0, 1, \ldots, 2L-1,$$
$$\Delta\lambda = \frac{\pi}{L}.$$

6 COMPUTATIONAL ASPECTS OF NEUMANN'S QUADRATURE WEIGHTS

For the computation of weights in the second Neumann's method, use can be made of the existing literature on Gauss quadrature. Nodes and corresponding quadrature weights have been tabulated (e.g. Krylov 1962; Stroud & Secrest 1966). If the zeros of $P_{L+1}(x)$ are available—they only have to be computed once—the weights may be calculated for instance from:

$$w_i = \frac{2}{(1-x_i^2)[P'_{L+1}(x_i)]^2} \tag{18a}$$

(*cf.* Krylov 1962), or

$$w_i = \frac{2(1-x_i^2)}{[(L+1)P_L(x_i)]^2}. \tag{18b}$$

The prime in the Krylov formula denotes the derivative with respect to x. Apart from these formulae, the w_i may be calculated from the matrix methods, to be treated next. Further numerical aspects of finding nodes and weights can be found, e.g. in Press *et al.* (1992).

As to the computation of weights in the first Neumann method, one will run into numerical problems in solving the linear system eq. (17). Suppose we have chosen a distribution of parallels which is symmetrical with respect to the equator, i.e. $x_i = -x_{N+1-i}$, or $\theta_i = \pi - \theta_{N+1-i}$, where $N = 2L+1$. The distribution is not necessarily equi-angular. Prey (1922) has shown that the quadrature weights are symmetrical as well: $w_i = w_{N+1-i}$. It turns out that the rows with odd powers of x_i may be removed, while the vector of unknowns $\mathbf{w}$ is reduced to the elements $w_1, \ldots, w_L$, which also implies that the corresponding columns are removed. Since $x_{L+1} = 0$, referring to the equator, the column corresponding to w_{L+1} would have zero entries and is also removed. In order to keep a square matrix the first row is eliminated. These operations leave the following reduced linear system $\mathbf{X}'\mathbf{w}' = \mathbf{r}'$:

$$\begin{pmatrix} x_1^2 & x_2^2 & \cdots & x_L^2 \\ x_1^4 & x_2^4 & \cdots & x_L^4 \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{2L} & x_2^{2L} & \cdots & x_L^{2L} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_L \end{pmatrix} = \begin{pmatrix} 1/3 \\ 1/5 \\ \vdots \\ 1/(2L+1) \end{pmatrix}. \tag{19}$$

This system may be solved either numerically by standard methods, or analytically by Lagrangean polynomials (*cf.* Lanczos 1956). The remaining weights $w_{L+2}, \ldots, w_{2L+1}$ come from the symmetry. Only the equator weight w_{L+1} is treated separately. It comes from the removed first row:

$$\sum_{i=1}^{2L+1} w_i = 2,$$

in which w_{L+1} is the only unknown.

However, the system (eq. 19) is extremely unstable. This fact is demonstrated in Fig. 3, where the condition numbers of the matrix $\mathbf{X}'$, in the case of an equi-angular distribution, have been plotted against the number of parallels, which is also the size of the matrix. Prey (1922) reports that in order to achieve six-digit accuracy for w_i the nodes x_i must be given with 10 digits. Prey applied the system (eq. 19) with $L = 16$ to Neumann's second method, thus having effectively an 8×8 matrix $\mathbf{X}'$. Test computations indicated that with double precision arithmetic $L = 35$ is somewhere the maximally attainable degree of expansion. In cases up to degree 360 for instance, applying eq. (19) is unthinkable.

A simple way out of this situation is setting $l_2 = m = 0$ and $l_1 = n$ in eq. (16), yielding the linear system:

$$\sum_{i=1}^{2L+1} w_i \bar{P}_n(x_i) = 2\delta_{n0}, \qquad n = 0, 1, \ldots, 2L$$

or in the case of a distribution, symmetrical with respect to the equator:

$$\sum_{i=1}^{L+1} \tfrac{1}{2}(2 - \delta_{L+1,i}) w_i \bar{P}_{2n}(x_i) = 2\delta_{n0}, \qquad n = 0, 1, \ldots, L.$$

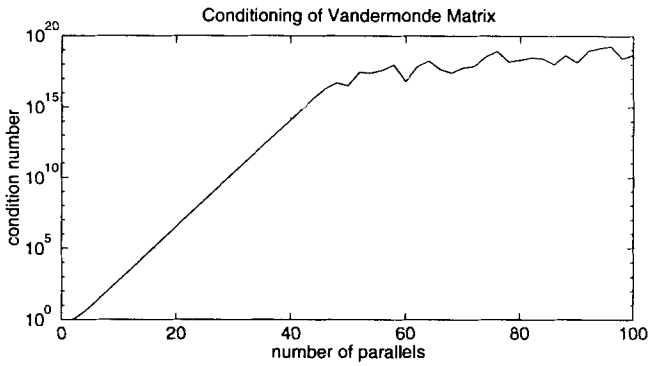

Figure 3. Conditioning of the linear system eq. (19).

* Gauss–Legendre quadrature to be more specific (*cf.* Stroud & Secrest 1966).

In matrix notation one would have:

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ \bar{P}_2(x_1) & \bar{P}_2(x_2) & \cdots & \bar{P}_2(x_{L+1}) \\ \bar{P}_4(x_1) & \ddots & \cdots & \bar{P}_4(x_{L+1}) \\ \vdots & \vdots & \ddots & \vdots \\ \bar{P}_{2L}(x_1) & \cdots & \cdots & \bar{P}_{2L}(x_{L+1}) \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_L \\ w'_{L+1} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad (20)$$

with $w'_{L+1} = \frac{1}{2}w_{L+1}$. This system is stable, due to the use of orthogonal polynomials. The powers x_i^n have been transformed into Legendre functions, which corresponds to forming linear combinations of the rows.

An alternative, which works even better in computational practice, is presented in Ellsaesser (1966), where the powers $(\cos\theta_i)^n$ are transformed into cosines of multiple angles $\cos n\theta_i$ instead. The result is

$$\sum_{i=1}^{2L+1} w_i \cos n\theta_i = -\int_0^{\pi} \cos n\theta \sin\theta \, d\theta = \begin{cases} \dfrac{-2}{n^2-1}, \\ 0 \end{cases}$$

with $n = 0, 2, \ldots, 2L$ for the upper line and $n = 1, 3, \ldots, 2L-1$ for the lower line. In case of a symmetrical distribution it would be:

$$\sum_{i=1}^{L+1} \tfrac{1}{2}(2-\delta_{L+1,i}) w_i \cos 2n\theta_i = \frac{-1}{4n^2-1}, \qquad n = 0, 1, \ldots, L.$$

In matrix notation we arrive at:

$$\begin{pmatrix} 1 & \cdots & 1 & 1 \\ \cos 2\theta_1 & \cdots & \cos 2\theta_L & -1 \\ \cos 4\theta_1 & \cdots & \cos 4\theta_L & 1 \\ \vdots & & \vdots & \vdots \\ \cos 2L\theta_1 & \cdots & \cos 2L\theta_L & \pm 1 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ w_L \\ w'_{L+1} \end{pmatrix} = \begin{pmatrix} 1 \\ -1/3 \\ -1/15 \\ \vdots \\ \dfrac{-1}{4L^2-1} \end{pmatrix}. \quad (21)$$

The conditioning of the matrices $\bar{P}_{2n}(x_i)$ and $\cos 2n\theta_i$ is displayed in Fig. 4. In the above figures an equi-angular grid without the poles has been assumed, i.e. $\theta_i = \frac{1}{2}(2i-1)\,\Delta\theta$ with $i = 1, 2, \ldots, 2L+1$ and

$$\Delta\theta = \frac{\pi}{2L+1}.$$

If the latitudinal distribution is more irregular, the conditioning of matrices above may become much poorer.

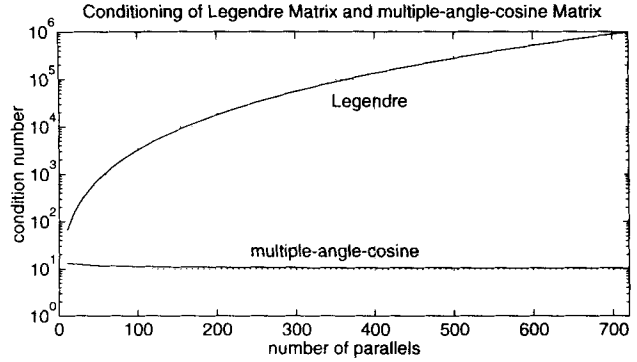

Figure 4. Conditioning of the linear systems eqs (20) and (21).

7 DISCUSSION AND CONCLUSIONS

7.1 A weighted least-squares framework of global spherical harmonic analysis

Global spherical harmonic analysis can be formulated as a two-step procedure, which assumes a certain gridding of data already. For instance irregularly distributed data cannot be analysed this way. The first step consists of a Fourier transformation along parallels. The second step is treated by least-squares and numerical quadrature, both approximate and exact. The latter subdivided again in the first Neumann method and the second Neumann method, also known as Gauss–Legendre quadrature. For each method the spherical harmonic coefficients are represented both as quadrature formulae and as a least-squares solution, either with or without weighting (*cf.* Table 1). Thus, all methods fit into a general framework of weighted least squares. The formal distinction between least-squares and quadrature methods in GSHA disappears.

Only specific weight matrices yield a diagonal normal matrix. The corresponding weights are the weights of exact quadrature. Consequently, other weight matrices will destroy orthogonality. Therefore, the incorporation of a stochastic model will not allow exact quadrature anymore.

7.2 Number of obtainable spherical harmonic coefficients

During the first step of discrete GSHA $2L$ Fourier coefficients $A_m(\theta_i)$ and $B_m(\theta_i)$ are retained for each latitude circle, which is equivalent to the number of data points, as shown in Section 2. The second step, though, does not show such a one-to-one relationship. The first Neumann method ($N = 2L+1$) requires a grid of $2L \times (2L+1)$ function samples in order to perform a GSHA up to degree L. The overall ratio between data points and *SH* coefficients becomes roughly 4 for Neumann's first method.

As to the second method, this ratio reduces to 2, due to the fact that roughly half the number of parallels is used ($N = L+1$). This much more favourable ratio of 2 only requires the data points to be given on a so-called Gauss-grid which is quite close to an equi-angular one. The difference $\Delta\phi$ between the equi-angular latitudes and the 'Gauss latitudes' is nearly equal to $\phi/2L$.

Owing to the orthogonality properties of discretized sine functions it has been shown that $B_0(\theta_i)$ and $B_L(\theta_i)$ Fourier coefficients cannot be determined. Therefore, not only the $\bar{S}_{l,0}$ coefficients are unestimable, but also $\bar{S}_{L,L}$.

7.3 Practical situation

It has been mentioned already that, in order to point out the ideas of Gauss and Neumann most clearly, our starting point

Table 1. Summary of equation numbers.

	Matrix form	Quadrature
Least squares	6	7
Approx. Quadr.	10/11	8
Neumann Quadr.	12	14

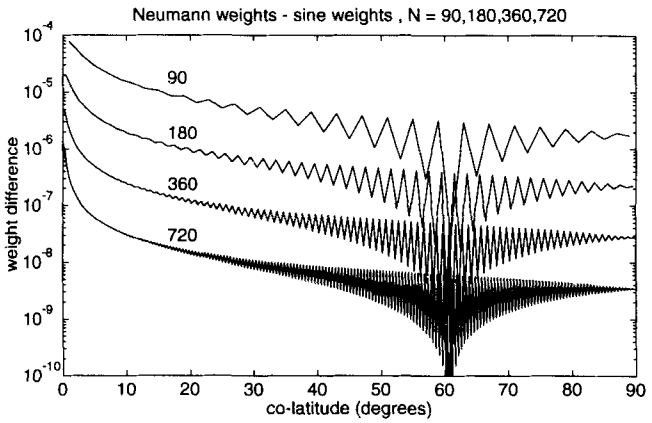

Figure 5. Logarithmic plot of the absolute differences between Neumann weights and sine weights, for the cases $N = 90$, 180, 360 and 720 parallels.

was a rather simple situation. The simplifications included assumptions on gridding (point data on some regular grid), band limitation (no signal beyond the Nyquist frequency) and stochasticity (no noise). These assumptions do not hold true in most practical situations. Data are mostly of area-mean type and corrupted with noise. Based on least-squares collocation, estimators can be found, which are optimal, in the sense of minimizing estimation and sampling errors, for more realistic situations. The basic reference for this is Colombo (1981). Hofsommer (1957) has shown furthermore that Neumann's methods may be extended to the use of block averages $\overline{f(\theta, \lambda)}$.

7.4 Comparison between the w_i and s_i weights

Though the w_i weights are determined in a purely numerical way, they do resemble a sine function, which is as they should be in the limit case. Compare them therefore with the sine weights in eq. (9b). These weights have the property that their sum equals 2, just like $\sum_i w_i = 2$, which makes them slightly more suitable for comparison than eq. (9a). The logarithm of the abolute difference between w_i and s_i is displayed in Fig. 5, for distributions of 90, 180, 360 and 720 equi-angular parallels.

7.5 Dual use of the name Gauss

As a result of his enormous oeuvre, both in terms of quantity and quality, the name of Gauss has been used widely in mathematics, physics and earth sciences. This paper makes a twofold use of the name of Gauss. On the one hand there is the *Gauss method of GSHA*, which refers to the combination of a two-step approach and application of least squares to the second step of GSHA. On the other hand there is the *Gauss quadrature*, equivalent to the second Neumann method, which requires data distribution on a *Gauss grid*.

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