Least Squares Adjustment of High Degree Spherical Harmonics

Wolf-Dieter Schuh

Technical University Graz, Mathematical Geodesy and Geoinformatics,
A-8010 Graz, Steyrergasse 30, Austria

1 Introduction

In spite of new developments in computer design, the standard least squares procedure for the estimation of spherical harmonic coefficients for high degree gravitational fields exceeds present capabilities. Only gridded data can be computed, because of orthogonality relations a sparse normal equation system results. In general, observations can not be performed on a regular grid and especially in connection with orbit dependent measurements, where an area between two parallels is well covered, no gridded data set is established. This is the reason why in this case the least squares harmonic analysis results in a dense normal equation system. The knowledge about the sparse structure of gridded data can be used for tailored preconditioning strategies. Therefore an optimal reordering of the sparse normal equation system brings benefit for gridded data in a direct approach as well as for well covered, but not gridded data in an iterative approach. This paper reports on an optimal reordering scheme for high degree spherical harmonic analysis. Two different scenarios, only gridded data and combined systems with not gridded low order (dense) and gridded high order (sparse) measurements are investigated. In both cases an optimal reordering strategy brings about the possibility to decompose (e.g. Cholesky-factorization) the normal equations without any fill-in.

The mathematical representation of earth's gravity potential is conveniently done with normalized spherical harmonics,

$$V(r,\theta,\lambda) = \frac{GM}{r}\left\{1+\sum_{\ell=1}^{\ell_{max}}\sum_{m=0}^{\ell}\left(\frac{a}{r}\right)^{\ell}\bar{P}_{\ell m}(\cos\theta)\left(\bar{C}_{\ell m}\cos m\lambda+\bar{S}_{\ell m}\sin m\lambda\right)\right\}\ . \tag{1}$$

GM	... geocentric gravitational constant	ℓ	... degree
a	... semimajor axis	m	... order
r	... radius vector	ℓ_{max}	... maximum degree
θ	... polar distance (colatitude)	$\bar{P}_{\ell m}$	... fully normalized associated Legendre functions of the first kind
λ	... longitude	$\bar{C}_{\ell m}$, $\bar{S}_{\ell m}$	... harmonic coefficients

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All groups of observations can be expressed with the help of the zero, first or second order derivative of the potential. Since the early 1980s a growing number of spherical harmonic models of the earth's gravity field has become available up to very high degrees and orders. Expansions up to degree and order 180 or 360, the latter with more than 130 000 individual coefficients, are widely used for many purposes. All the applications of spherical harmonics can be divided into two tasks:

– determination of the harmonic coefficients $\bar{C}_{\ell m}$ and $\bar{S}_{\ell m}$ using observed quantities of the gravity potential (*'global spherical harmonic analysis'*) and
– computation of the gravity potential and/or derivatives thereof at a special point P $(r_P, \theta_P, \lambda_P)$ with known harmonic coefficients $\bar{C}_{\ell m}$ and $\bar{S}_{\ell m}$ (*'global spherical harmonic synthesis'*).

Due to types and accuracies of the observations, but also due to the point location and distribution of the measurements a more or less high degree expansion can be determined using least squares techniques or analytic approaches.

In the continuous case the global spherical harmonics have the nice property of orthogonality. In reality, in most of the cases only discrete function values are available and therefore, only orthogonalities in the discrete case are of interest. If we discretize the Legendre function the orthogonalities are lost, but this does not hold for the cosine and sine series under special assumptions. Therefore, if the data set meets these assumptions, orthogonalities between different orders m will occur and sparse normal equations are preserved. But these assumptions are very restrictive because all the data (along a parallel) should be

– of the same type,
– with homogeneous weights,
– on an equiangular grid,
– without any gap.

We denote such a data set as *'grid'* data. In addition the (anti-)symmetry

$$\bar{P}_{\ell m}(-\cos\theta) = (-1)^{(\ell-m)}\bar{P}_{\ell m}(\cos\theta) \tag{2}$$

of the Legendre function can be used if the data set is symmetric with respect to the equator. Orthogonalities appear between even and odd degree elements within the same order.

Ungridded data of satellite missions essentially cause new investigations. Due to high sampling rates quite a number of measurements with a good coverage can be collected. But this data sets are not gridded, because the measurements can only be performed along the orbit. On the other side, low orbit satellites bring about a lot of information to the higher order coefficients of the gravity potential also. In future missions it will be intended to use the satellite gravity gradiometry (SGG) technique to gain better information of the high frequency part of the gravity field. This technique brings about only poor information on the low frequency part and therefore it will be completed by a satellite-to-satellite tracking (SST) system. This allows to determine a high precision orbit as well as the low frequency part of the gravity field. The standard least squares procedure for the estimation of high degree spherical harmonic coefficients with these data sets exceeds present computer capabilities. Therefore, special techniques have to be developed to accomplish this task. Tailored procedures must be developed with the help of orthogonality considerations, special numbering schemes and optimized preconditioning strategies. Also the use of parallel resources and robust statistical methods have to be investigated.

This paper gives a report about orthogonality considerations in connection with numbering schemes. Especially the combination of gridded data for the high frequency part with ungridded informations within the low frequency part is of interest. Due to the orthogonality relations of gridded data sets a sparse normal equation system can be expected. Therefore an optimal numbering scheme allows an efficient storage and computation of these sparse systems. This knowledge can be used in two directions: First, if gridded data are available high degree spherical harmonic analysis can be performed very efficient (Colombo 1981) and secondly if the data sets are not gridded but cover the whole region between two parallels very regularly, then the information of the idealized sparse systems allows to find tailored preconditioning strategies to speed up iterative procedures very well (Schuh 1995).

2 Gridded Data: Orthogonalities and Numbering Schemes

The commutativity law of addition in Eq. (1) allows different choices for the ordering of the summation sequences. Fig. 1 illustrates the pattern of all the

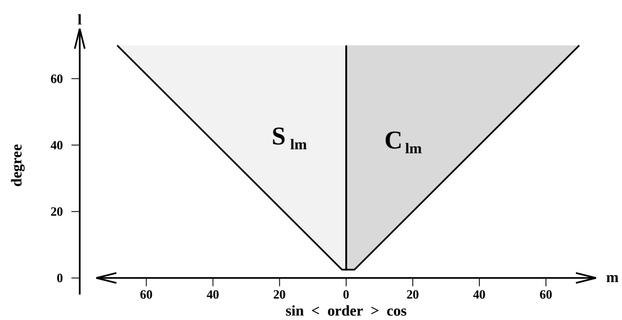


Fig. 1. Triangular scheme with information about the coefficients of the spherical harmonics.

spherical harmonic coefficients. This triangular scheme can be divided into two sub-triangles. The left triangle contains the sine coefficients and the right triangle contains the cosine coefficients. The degree ℓ increases from bottom to top, and the order increases from the center to the left (right) for the sine (cosine) coefficients.

The elements within a horizontal line contain coefficients of the same degree, for example $\bar{C}_{\ell,*}$ or $\bar{S}_{\ell,*}$, whereas vertical lines contain coefficients of the same order, $\bar{C}_{*,m}$ or $\bar{S}_{*,m}$.

To find short and terse key words for the numbering schemes we identify the sums only by their indices ($\ell \ldots$ sum over all degrees, $m \ldots$ sum over all orders). The sequence of the sums from the left to the right is reflected by the sequence of the indices (first (outer) sum ... first character, second (nested) sum ... second character, and so on). The key words carry no information about the limits, the direction and the spacing step of the sum. Only increasing loops with step '1' are used. It is only necessary to restrict the indices to even and odd numbers. This is done with the subscript 'e' or 'o'. For example ℓ_e means only even degrees. Upper letters C and S symbolically stand for the $\bar{C}_{\ell m}$ and $\bar{S}_{\ell m}$ coefficients. Brackets are used to emphasize the processing sequence.

The numbering schemes can be divided into two groups. The first group, **organized per degree**, is characterized by an outer loop over all degrees ℓ and an inner loop with increasing order m. The cosine and sine coefficients may alternate or not. Two members of this group are:

$$\mathcal{NUM}\,\{\ell m(C+S)\} \quad \Longrightarrow \quad \sum_{\ell=2}^{\ell_{max}} \left(\bar{C}_{\ell 0} + \sum_{m=1}^{\ell} \left(\bar{C}_{\ell m} + \bar{S}_{\ell m} \right) \right)$$

$$\mathcal{NUM}\,\{\ell m(C)+\ell m(S)\} \quad \Longrightarrow \quad \sum_{\ell=2}^{\ell_{max}} \sum_{m=0}^{\ell} \bar{C}_{\ell m} + \sum_{\ell=2}^{\ell_{max}} \sum_{m=1}^{\ell} \bar{S}_{\ell m} \quad .$$

These two schemes are widely used because they allow a simple management of the coefficients, an easy assignment of the proper storage place for each element and an easy truncation of the spherical harmonic series at a certain degree and order.

The second group of numbering schemes, **organized per order**, is characterized by an outer loop over all orders m and an inner loop with increasing degree ℓ. Within each order first all cosine coefficients and then all sine coefficients are arranged. These numbering schemes reflect the sparsity of the normals due to the orthogonalities in a block-diagonal structure. Depending on the utilization of the symmetry with respect to the equator two schemes are used:

$$\mathcal{NUM}\,\{m(\ell C+\ell S)\} \quad \Longrightarrow \quad \sum_{\ell=2}^{\ell_{max}} \bar{C}_{\ell 0} + \sum_{m=1}^{\ell_{max}} \left(\sum_{\ell=\max(2,m)}^{\ell_{max}} \bar{C}_{\ell m} + \sum_{\ell=\max(2,m)}^{\ell_{max}} \bar{S}_{\ell m} \right)$$

$$\mathcal{NUM}\,\{m(\ell_e C+\ell_o C+\ell_e S+\ell_o S)\} \quad \Longrightarrow \sum_{\ell=1}^{\mathrm{Int}(\ell_{max}/2)} \bar{C}_{2\ell,0} + \sum_{\ell=1}^{\mathrm{Int}(\ell_{max}/2)} \bar{C}_{2\ell+1,0} +$$
$$+ \sum_{m=1}^{\ell_{max}} \left(\sum_{\ell=m}^{\mathrm{Int}(\ell_{max}/2)} \bar{C}_{2\ell,m} + \sum_{\ell=m}^{\mathrm{Int}(\ell_{max}/2)} \bar{C}_{2\ell+1,m} + \sum_{\ell=m}^{\mathrm{Int}(\ell_{max}/2)} \bar{S}_{2\ell,m} + \sum_{\ell=m}^{\mathrm{Int}(\ell_{max}/2)} \bar{S}_{2\ell+1,m} \right) \quad .$$

The resulting structure of the normal equations using gridded data distribution is a block-diagonal structure. In the first case the size of the block starts form $(\ell_{max}-1) \times (\ell_{max}-1)$ and ends by 1×1. In the second case each large block is represented by two blocks with half the size.

If we use gridded data we can use the last two numbering schemes to assemble block-diagonal structured normal equations and perform a high degree spherical analysis. This technique is based on a work by Colombo (1981).

3 Numbering Schemes for Combined Data Sets

Because of the poor performance of satellite gravity gradiometry (SGG) with respect to long wavelength, it is important to combine these data with other informations. Especially satellite-to-satellite tracking (SST) data build a nice supplementation, because they provide strong information at exactly those frequencies where SGG is poor. The low degree/order system coming from SST depends on the configuration of the tracking satellites. The configuration changes from situation to situation. This irregularity results in a dense normal equation system. Therefore the combination of a full low degree/order system with a block-diagonal high degree/order system is required. If the usual numbering scheme $\mathcal{NUM}\,\{m(\ell_e C + \ell_o C + \ell_e S + \ell_o S)\}$ is used, the full low degree/order system produces a *chess-board pattern* outside the block-diagonal structure. Fig. 2a illustrates this behaviour and in addition, Fig. 2b shows the fill-in elements which are generated during the reduction step (e.g. Cholesky-factorization).

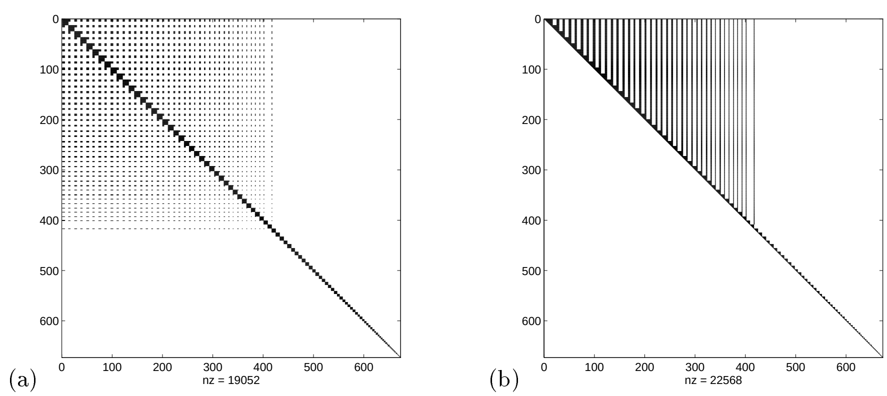


Fig. 2. Sparsity of the (reduced) normal equations, numbering scheme $\mathcal{NUM}\,\{m(\ell_e C + \ell_o C + \ell_e S + \ell_o S)\}$. Block-diagonal structure up to degree 25, full system up to degree 10. (a) normal equations (b) reduced normal equations.

An appropriate organization scheme to store the normals and to manage the fill-in is a profile structure (variable bandwidth). Unfortunately the storage requirements increase quadratically with respect to lower degrees as well as with respect to the higher degree field. Balmino (1993) and Bosch (1993) introduce a numbering scheme which works with different regions within the pattern of spherical harmonic coefficients. The first region is defined by the full

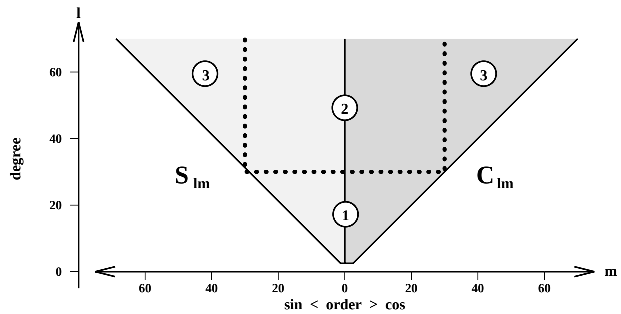


Fig. 3. Numbering scheme *block* $\mathcal{NUM}\,\{m(\ell_e C + \ell_o C + \ell_e S + \ell_o S)\}$.

low degree/order model (cf. Fig. 3). After these coefficients all coefficients with higher order are arranged. At last the coefficients with higher degree and order are numbered. Fig. 4a illustrates the normal equations based on this particular

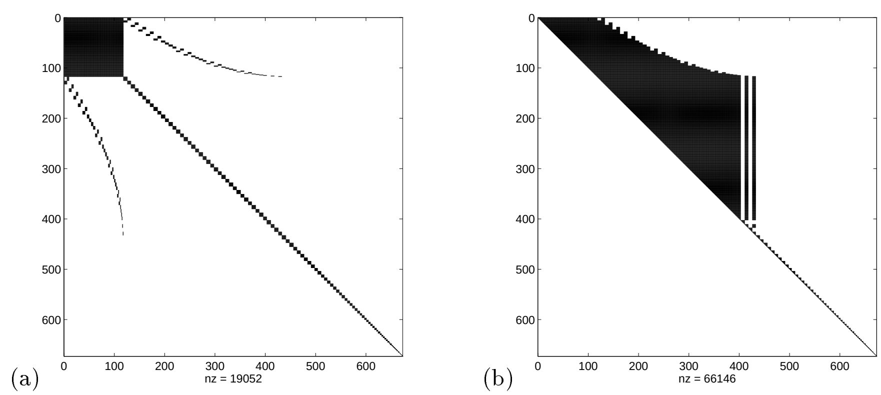


Fig. 4. Sparsity of the (reduced) normal equations, numbering scheme *block* $\mathcal{NUM}\,\{m(\ell_e C + \ell_o C + \ell_e S + \ell_o S)\}$. Block-diagonal structure up to degree 25, full system up to degree 10. (a) normal equations (b) reduced normal equations.

blocked numbering scheme. The non-zero elements are packed in the first part of the normals. Two thin lines, like the tails of a kite, represent the correlations between low and high degree coefficients within the same order. Unfortunately, during a factorization step the region below this tail is filled up with non-zero elements. Fig. 4b shows the result of this factorization step. This numbering scheme doesn't preserve the symmetry with respect to the equator and produces a lot of fill-in elements. The advantage of this method is the concentration of the fill-in elements to the first part of the normal equations.

It's not necessary to compute and compare the number of fill-in elements of the above numbering schemes, just because another numbering scheme can be employed which produces **no fill-in** elements during the whole factorization process.

The main idea behind the new numbering scheme is the reversal of the ordering. Not the figure of an ascending but of a descending kite should appear. Therefore first the high degree and high order elements are numbered. Next the high degree and low order elements are arranged and the full block of low degree and order comes at the end (cf. Fig. 5). After a first look to this structure we

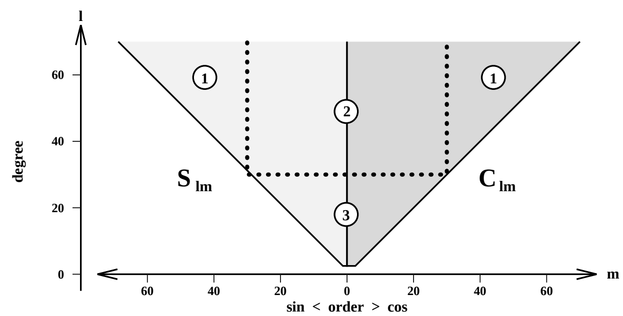
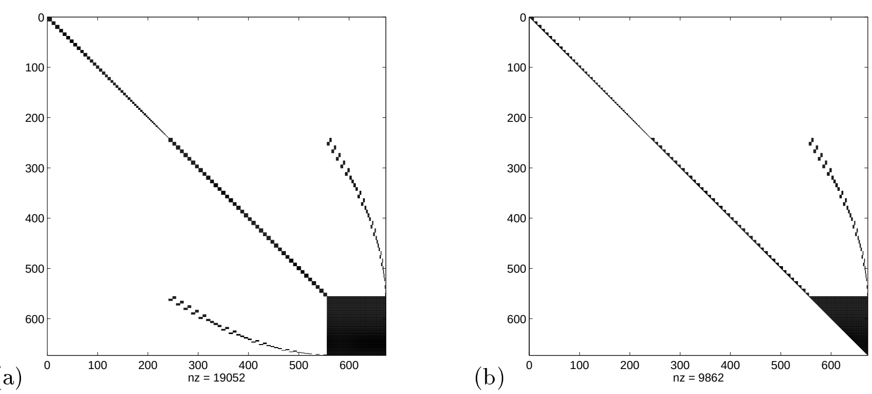


Fig. 5. Numbering scheme *reverse block* $\mathcal{NUM}\,\{m(\ell_e C + \ell_o C + \ell_e S + \ell_o S)\}$.



(a) (b)

Fig. 6. Sparsity of the (reduced) normal equations employing *reverse block* numbering scheme $\mathcal{NUM}\,\{m(\ell_e C + \ell_o C + \ell_e S + \ell_o S)\}$. Block-diagonal structure up to degree 25, full system up to degree 10. (a) normal equations (b) reduced normal equations.

would expect only few fill-in elements in the area below the lateral tails of the kite. But an exact analysis shows, that in each column and row of this lateral tail region only one nonzero block exists. Therefore the typical scalar product of two columns during the factorization step vanishes and no fill-in elements are produced.

Just by reversing the order of block numbering we achieve an arrangement of the normals such that during the factorization step no fill-in elements are generated (cf. Fig. 6). The normals can therefore be stored in a fixed structure. Parallelism within the factorization process can be easily exploited and the amount of process intercommunication is reduced dramatically.

4 Concluding Remarks

This newly developed numbering scheme, especially for the combination of dense low degree fields and block-structured high degree fields produce no fill-in during the factorization step. Therefore very efficient solutions can be performed:

- with a combined data set (ungridded low frequency data and gridded high frequency data) a very efficient direct solution can be determined and
- in the case of ungridded low frequency data and irregular distributed high frequency data, which densely cover the area between two parallels, the knowledge about the sparse structure can be used to find optimal preconditioning techniques.

The fast iterative solution mainly bases on the possibility to find a representative matrix, which can be easily computed, quickly solved and on the other side represents as close as possible all informations of the whole system. If the block structured high degree model combined with a dense low degree model is used as a mask for the representative matrix both facts are fulfilled, easiest computation and a close relation between the behaviour of the rigorous dense system and the sparse preconditioner.

Numerical simulations demonstrate that these iterative techniques are well tailored and ideally suited for the least squares solution of harmonic coefficients of high degree models based on satellite-to-satellite tracking data and satellite gravity gradiometry data. The very favorable convergence rate with a spectral radius up to 0.04 for the preconditioned conjugate gradient algorithm permits the solution of a system with $2,597$ unknowns within 3 to 5 iteration steps. The fast solution is based on the possibility to find a fit and proper preconditioner. This is possible because of the newly developed numbering scheme.

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