MAG3D

A Program Library for Forward Modelling and Inversion of Magnetic Data over 3D Structures

Version 5.0

Developed under the consortium research project:

COOPERATIVE INVERSION OF GEOPHYSICAL AND GEOLOGICAL DATA

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1 Package overview

1.1 Description

MAG3D v5.0 is a program library for carrying out forward modelling and inversion of surface, airborne, and/or borehole magnetic data in the presence of a three dimensional Earth. The program library carries out the following functions:

1. Forward modelling of the magnetic field anomaly response to a 3D volume of susceptibility contrast. Data are assumed to be the anomalous magnetic response to buried susceptible material.
2. The model is specified in the mesh of rectangular cells, each with a constant value of susceptibility. Topography is included in the mesh. The magnetic response can be calculated anywhere within the model volume, including above the topography to simulate ground or airborne surveys. There is also a capability to simulate and invert data collected beneath the surface (e.g. borehole surveys) and combinations of ground and borehole surveys.
3. Assumptions:
   - This code assumes susceptibilities are small enough that the effects of self-demagnetization can be neglected.
   - Remanent magnetization is not directly accounted for, although anomaly projections can be included with the observations.
4. Inversion of surface, airborne, and/or borehole magnetic data to generate 3D models of susceptibility contrast:
   - The inversion is solved as an optimization problem with the simultaneous goals of (i) minimizing an objective function on the model and (ii) generating synthetic data that match observations to within a degree of misfit consistent with the statistics of those data.
   - To counteract the inherent lack of information about the distance between source and measurement, the formulation incorporates depth or distance weighting.
   - By minimizing the model objective function, distributions of subsurface susceptibility contrast are found that are both close to a reference model and smooth in three dimensions. The degree to which either of these two goals dominates is controlled by the user by incorporating a priori geophysical or geological information into the inversion. Explicit prior information may also take the form of upper and lower bounds on the susceptibility contrast in any cell.
   - The regularization parameter (controlling relative importance of objective function and misfit terms) is determined in either of three ways, depending upon how much is known about errors in the measured data.
5. The large size of 3D inversion problems is mitigated by the use of wavelet compression. Parameters controlling the implementation of this compression are available for advanced users.

The initial research underlying this program library was funded principally by the mineral industry consortium "Joint and Cooperative Inversion of Geophysical and Geological Data" (1991 - 1997) which was sponsored by NSERC (Canada's **N**ational **S**cience and **E**ngineering **R**esearch **C**ouncil) and the following 11 companies: BHP Minerals, CRA Exploration, Cominco Exploration, Falconbridge, Hudson Bay Exploration and Development, INCO Exploration & Technical Services, Kennecott Exploration Company, Newmont Gold Company, Noranda Exploration, Placer Dome, and WMC.

Since then, improvements have been implemented as time and resources permit.

1.2 MAG3D program library content

1. **Executable programs**. For performing 3D forward modelling and inversion of magnetic surveys. The MAG3D library (Windows or Linux platforms) consists of four major programs:
   - `MAGFOR3D`: performs forward modelling
   - `MAGSEN3D`: calculates sensitivity and the depth weighting function
   - `MAGPRE3D`: multiplies the sensitivity file by the model to get the predicted data
   - `MAGINV3D`: performs 3D magnetic inversion.
2. **A graphical user interface**. It is available for the Windows platforms **only**. Facilities include:
   - `GM-DATA-VIEWER`: a utility for viewing raw surface or airborne data (but not borehole data), error distributions, and for comparing observed to predicted data directly or as difference maps.
   - `MESHTOOLS3D`: a utility for displaying resulting 3D models as volume renderings. Susceptibility volumes can be sliced in any direction, or isosurface renderings can be generated.
3. **Documentation** is provided for MAG3D v5.0.
4. **Example data sets** are provided in "EXAMPLES" directory.

1.3 Licensing

A **constrained educational version** of the program is available with the IAG package (please visit UBC-GIF website for details). The educational version is fully functional so that users can learn how to carry out effective and efficient 3D inversions of magnetic data. **However, RESEARCH OR COMMERCIAL USE IS NOT POSSIBLE because the educational version will NOT work with more than 200 data points or 12,000 cells in the 3D mesh**.

Licensing for an unconstrained academic version is available - see the Licensing policy document.

NOTE: All academic licenses will be **time-limited to one year**. You can re-apply after that time. This ensures that everyone is using the most recent versions of codes.

Licensing for commercial use is managed by distributors, not by the UBC-GIF research group. Details are in the Licensing policy document.

1.4 Installing MAG3D v5.0

There is no automatic installer currently available for the MAG3D v5.0. Please follow the following steps in order to use the software:

1. Extract all files provided from the given zip-based archive and place them all together in a new folder such as `C:\ubcgif\mag3d\bin`
2. Add this directory as new path to your environment variables.
3. If you are running the software on a cluster of computers, please install the Message Pass Interface (MPI) on your computer and add it to your path in addition.
4. Make sure to create a separate directory for each new inversion, where all the associated files will be stored. Do not store anything in the "bin" directory other than executable applications and Graphical User Interface applications (GUIs).

1.5 MAG3D v5.0: Highlights of changes from version 4.0

The principal upgrades, described below, allow the new code to take advantage of current multi-core computers and also provide greater flexibility to incorporate the geological information.

Improvements since version 4.0 :

1. A new projected gradient algorithm is used to implement constraints.
2. Fully parallelized computational capability (for both sensitivity matrix calculations and inversion calculations).
3. An alternative version of the software compatible with Message Pass Interface (MPI) is available.
4. A facility to have active and inactive (i.e. fixed) cells is implemented
5. Additional flexibility is added when using the reference model in the model objective function

1.6 Notes on computation speed

- The execution time using MAG3D 4.0 and 5.0 are compared in Figure 1 for a moderately complicated problem. This was a synthetic example involving 3,600 data points and 131,072 cells in the model, and moderate topography.
- The version 5.0 code is significantly faster in all cases due to parallelization of sensitivity matrix computation and inversion calculations.

- Speed is dependent upon the computer. It is strongly recommended to use multicore processors for running the `magsen3d` and `mag3d`. The calculation of the sensitivity matrix ($\mathbf{G}$) is directly proportional to the number of data. The parallelization of $\mathbf{G}$ calculation splits the calculation of n rows between p processors. By default, all available processors are used. There is a feature to limit p to user-defined number of processors.

- In the parallelized inversion calculation, $\mathbf{G}^T\mathbf{G}$ is multiplied by a vector, therefore each parallel process uses only a submatrix of $\mathbf{G}$ and then the calculations are summed. Since there is a lot of communication between the CPUs, the speedup may be less than directly proportional to the number of processors, however when running the same inversion under MPI environment on multiple computers the advantage is that a single computer does not have to store the entire sensitivity matrix.

- Using a single thread for running the parallelized version resulted in sensitivity matrix calculation slowdown exactly proportional to the reduction in number of threads, while the slowdown in inversion calculation was insignificant (21.7 seconds with 1 thread vs 18.18 seconds with 12 threads).

- The implementation of the "projected gradient" algorithm in version 5.0 versus the "logarithmic barrier" algorithm in version 4.0results in faster convergence (11 iterations versus 33 iterations, respectively) with almost identical result (the recovered susceptibility models have been compared and their mismatch is under 0.4%).

- The complexity of the problem also affects computation times. More complex problems include topography, complicated distributions of susceptibility, weighting functions, reference models, bounds, etc.

- These results are presented for illustration only. The time to compute any given problem is strongly dependent upon the number of data points, the size of the mesh, and how all the parameters for the inversion are set, including data, constraints, regularization, wavelet compression, etc.

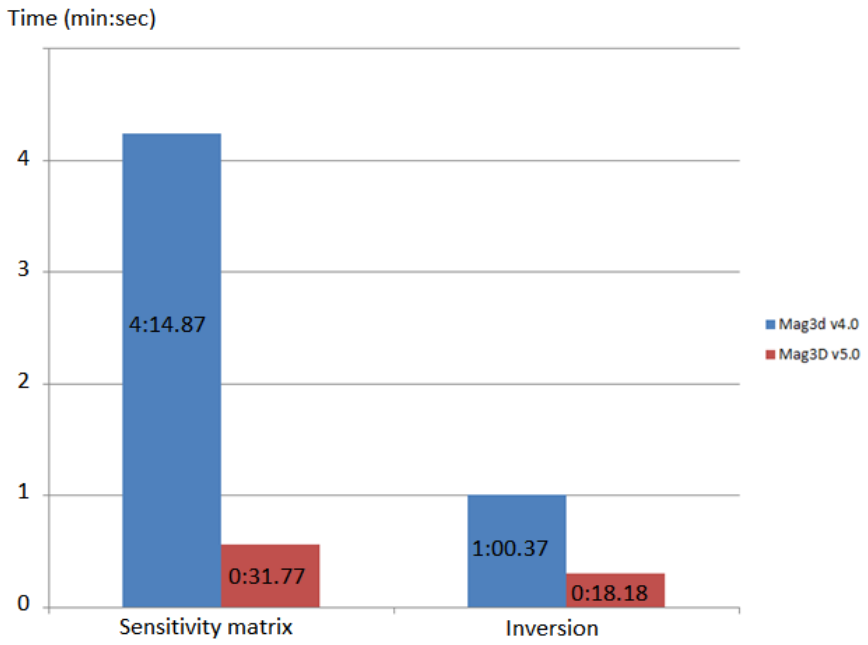

Figure 1: CPU time on 3.20 GHz 6 core i7 Intel processor with 16 Gb of RAM installed. Twelve parallel OpenMP threads were used for the calculations in version 5.0.

2 Background theory

2.1 Introduction

This manual presents theoretical background, numerical examples, and explanation for implementing the program library MAG3D v5.0. This suite of algorithms, developed at the UBC-Geophysical Inversion Facility, is needed to invert magnetic responses over a three-dimensional susceptibility distribution. The manual is designed so that a geophysicist who is familiar with the magnetic experiment, but who is not necessarily versed in the details of inverse theory, can use the codes and invert his or her data.

A magnetic experiment involves measuring the anomalous magnetic field produced by magnetically susceptible materials beneath the surface, which have been magnetized by the earth's main magnetic field. The material with susceptibility $\kappa(x, y, z)$ is magnetized when the earth's main field with flux intensity $\mathbf{B}_o$ impinges upon the subsurface formation. The magnetized material gives rise to a magnetic field, $\mathbf{B}_a$, which is superimposed on the inducing field to produce a total, or resultant, field. By measuring the resultant field and removing the inducing field from the measurements through numerical processing, one obtains the distribution of the anomalous field due to the susceptible material. Very often, the susceptible materials underground possess a certain amount of natural remanent magnetization. In this program library, however, we make the assumption that no remanent magnetization is present and restrict our attention to induced magnetization.

The data from a typical magnetic survey is a set of magnetic field measurements acquired over a 2D grid above the surface or along a number of boreholes within the volume of interest. These data are first processed to yield an estimate of the anomalous field due to the susceptible material in the area. The goal of the magnetic inversion is to obtain, from the extracted anomaly data, quantitative information about the distribution of the magnetic susceptibility in the ground. Thus it is assumed that the input data to the inversion program is the extracted residual anomaly and the programs in the library are developed accordingly.

2.2 Forward modelling

2.2.1 General formulation

For a given inducing field $\mathbf{B}_o$, the magnetization $\mathbf{J}$ depends upon the susceptibility through a differential equation. However, to the first order approximation when the actual susceptibility is very small, as is most often the case with material encountered in mineral explorations, the magnetization is proportional to the susceptibility and is given by the product of susceptibility with inducing magnetic field $\mathbf{H}_o$,

$$\mathbf{J} = \boldsymbol{\kappa}\mathbf{H}_o, \tag{1}$$

where $\mathbf{H}_o = \mathbf{B}_o/\mu_o$ and μ_o is the free-space magnetic permeability. This essentially ignores the self-demagnetization effect by which the secondary field reduces the total inducing field within the susceptible region and results in a weaker magnetization than that given by equation 1.

The anomalous field produced by the distribution of magnetization $\mathbf{J}$ given by the following integral equation with a dyadic Green's function:

$$\mathbf{B}_a(\mathbf{r}) = \frac{\mu_0}{4\pi} \int_V \nabla\nabla \frac{1}{|\mathbf{r} - \mathbf{r}_o|} \cdot \mathbf{J} dv, \tag{2}$$

where $\mathbf{r}$ is the position of the observation point and V represents the volume of magnetization. The above equation is valid for observation locations above the earth's surface. It is also valid in the boreholes provided we assume that the magnetic permeability is μ_o.

When the susceptibility is constant within a volume of source region, the above equation can be written in matrix form as:

$$\mathbf{B}_a = \mu_o \begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} \kappa \mathbf{H}_o \equiv \mu_o \kappa \mathbf{T} \mathbf{H}_o. \tag{3}$$

The tensor $\mathbf{T}_{ij}$ is given by

$$\mathbf{T}_{ij} = \frac{1}{4\pi} \int_V \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \frac{1}{|\mathbf{r} - \mathbf{r}_o|} dv, \text{ for } i = 1, 3; j = 1, 3, \tag{4}$$

and where x_1, x_2, and x_3 represent $x-$, $y-$, and $z-$directions, respectively. The expressions of $\mathbf{T}_{ij}$ for a cuboidal source volume can be found in Bhattacharyya (1964) and Sharma (1966) (here we assume that the effect of borehole cavity can be neglected). Since $\mathbf{T}$ is symmetric and its trace is equal to -1 when the observation is inside the cell and is 0 when the observation is outside the cell, only five independent elements need to be calculated.

Once $\mathbf{T}$ is formed, the magnetic anomaly $\mathbf{B}_a$ and its projection onto any direction of measurement are easily obtained by the inner product with the directional vector. The projection of the field $\mathbf{B}_a$ onto different directions yields different anomalies commonly obtained in the magnetic survey. For instance, the vertical anomaly is simply B_{az}, the vertical component of $\mathbf{B}_a$, whereas the total field anomaly is, to first order, the projection of $\mathbf{B}_a$ onto the direction of the inducing field $\mathbf{B}_o$.

2.2.2 Borehole data

In a borehole experiment, the three components are measured in the directions of local coordinate axes (l_1, l_2, l_3) defined according to the borehole orientation. Assuming that the borehole dip θ is measured downward from the horizontal surface and azimuth φ is measured eastward from the North; a commonly used convention has the l_3-axis pointing downward along borehole, l_1-axis pointing perpendicular to the borehole in the direction of the azimuth. The l_2-axis completes the right-handed coordinate system and is 90° clockwise from the azimuth and perpendicular to the borehole. Based upon the above definition the rotation matrix that transforms three components

of a vector in the global coordinate system to the components in the local coordinates is given by

$$\mathbf{R} = \begin{pmatrix} \cos\varphi\sin\theta & \sin\varphi\sin\theta & -\cos\theta \\ -\sin\varphi & \cos\varphi & 0 \\ \cos\varphi\cos\theta & \sin\varphi\cos\theta & \sin\theta \end{pmatrix} \tag{5}$$

If a vector is defined in local coordinates as $(l_1, l_2, l_3)^T$, and in global coordinates as $(g_1, g_2, g_3)^T$, then the following two relations hold:

$$\begin{aligned} (l_1, l_2, l_3)^T &= \mathbf{R}(g_1, g_2, g_3)^T \\ (g_1, g_2, g_3)^T &= \mathbf{R}^T(l_1, l_2, l_3)^T \end{aligned} \tag{6}$$

The rotation matrix $\mathbf{R}$ therefore allows measured components in local coordinates to be rotated into global coordinate, or the components of the regional field to be rotated into local coordinates for use in regional removal.

2.2.3 Numerical implementation of forward modelling

We divide the region of interest into a set of 3D cuboidal cells by using a 3D orthogonal mesh and assume a constant susceptibility within each cell. By equation 1, we have a uniform magnetization within each cell and its field anomaly can be calculated using equations 3 and 6. The actual anomaly that would be measured at an observation point is the sum of field produced by all cells having a non-zero susceptibility value. The calculation involves the evaluation of equation 3 in a 3D rectangular domain define by each cell. The program that performs this calculation is MAGFOR3D. As input parameters, the coordinates of the observation points and the inclination and declination of the anomaly direction must be specified for each datum. For generality, each component in a multi-component data set is specified as a separate datum with its own location and direction of projection.

2.3 Inversion methodology

Let the set of extracted anomaly data be $\mathbf{d} = (d_1, d_2, ..., d_N)^T$ and the susceptibility of cells in the model be $\boldsymbol{\kappa} = (\kappa_1, \kappa_2, ..., \kappa_M)^T$. The two are related by the sensitivity matrix

$$\mathbf{d} = \mathbf{G}\boldsymbol{\kappa}. \tag{7}$$

The matrix has elements g_{ij} which quantify the contribution to the i^{th} datum due to a unit susceptibility in the j^{th} cell. The program MAGSEN3D performs the calculation of the sensitivity matrix, which is to be used by the subsequent inversion. The sensitivity matrix provides the forward mapping from the model to the data during the entire inverse process. We will discuss its efficient representation via the wavelet transform in a separate section.

The inverse problem is formulated as an optimization problem where an objective function of the model is minimized subject to the constraints in equation 7. For magnetic inversion the first question that arises concerns definition of the "model". We choose magnetic susceptibility κ as the

model since the anomalous field is directly proportional to the susceptibility. This is the choice for the inversion program MAGINV3D. For generality, we introduce the generic symbol m for the model element. Having define a "model" we next construct an objective function which, when minimized, produces a model that is geophysically interpretable. The details of the objective function are problem dependent but generally we need the flexibility to be close to a reference model m_o and also require that the model be relatively smooth in three spatial directions. Here we adopt a right handed Cartesian coordinate system with positive north and positive down. Let the model objective function be

$$\begin{aligned} \phi_m(m) &= \alpha_s \int_V w_s \left\{ w(\mathbf{r})[m(\mathbf{r}) - m_o] \right\}^2 dv + \alpha_x \int_V w_x \left\{ \frac{\partial w(\mathbf{r})[m(\mathbf{r}) - m_o]}{\partial x} \right\}^2 dv \\ &+ \alpha_y \int_V w_y \left\{ \frac{\partial w(\mathbf{r})[m(\mathbf{r}) - m_o]}{\partial y} \right\}^2 dv + \alpha_z \int_V w_z \left\{ \frac{\partial w(\mathbf{r})[m(\mathbf{r}) - m_o]}{\partial z} \right\}^2 dv, \end{aligned} \tag{8}$$

where the functions w_s, w_x, w_y and w_z are spatially dependent, while α_s, α_x, α_y and α_z are coefficients, which affect the relative importance of different components in the objective function. Here the function $w(\mathbf{r})$ is a generalized depth weighting function. The purpose of this function is to counteract the geometrical decay of the sensitivity with the distance from the observation location so that the recovered susceptibility is not concentrated near the observation locations. The details of the depth weighting function will be discussed in the next section.

The objective function in equation 8 has the flexibility to construct many different models. The reference model m_o may be a general background model that is estimated from previous investigations or it could be a zero model. The reference model would generally be included in the first component of the objective function but it can be removed if desired from the remaining terms; often we are more confident in specifying the value of the model at a particular point than in supplying an estimate of the gradient. The choice of whether or not to include m_o in the derivative terms can have significant effect on the recovered model. The relative closeness of the final model to the reference model at any location is controlled by the function w_s. For example, if the interpreter has high confidence in the reference model at a particular region, he can specify w_s to have increased amplitude there compared to other regions of the model. The weighting functions w_x, w_y, and w_z can be designed to enhance or attenuate structures in various regions in the model domain. If geology suggests a rapid transition zone in the model, then a decreased weighting for flatness can be put there and the constructed model will exhibit higher gradients provided that this feature does not contradict the data.

To perform a numerical solution, we discretize the model objective function in equation 8 using a finite difference approximation on the mesh defining the susceptibility model. This yields:

$$\begin{aligned} \phi_m(\mathbf{m}) = (\mathbf{m} - \mathbf{m}_o)^T (\alpha_s \mathbf{W}_s^T \mathbf{W}_s + \alpha_x \mathbf{W}_x^T \mathbf{W}_x + \alpha_y \mathbf{W}_y^T \mathbf{W}_y + \alpha_z \mathbf{W}_z^T \mathbf{W}_z)(\mathbf{m} - \mathbf{m}_o), \\ \equiv (\mathbf{m} - \mathbf{m}_o)^T (\mathbf{W}_m^T \mathbf{W}_m)(\mathbf{m} - \mathbf{m}_o), \\ = \left\| \mathbf{W}_m (\mathbf{m} - \mathbf{m}_o) \right\|^2, \end{aligned} \tag{9}$$

where $\mathbf{m}$ and $\mathbf{m}_o$ are M-length vectors. The individual matrices $\mathbf{W}_s$, $\mathbf{W}_x$, $\mathbf{W}_y$, and $\mathbf{W}_z$ are straight-forwardly calculated once the model mesh and the weighting functions $w(\mathbf{r})$ and w_s , w_x, w_y, w_z are defined. The cumulative matrix $\mathbf{W}_m^T\mathbf{W}_m$ is then formed.

The next step in setting up the inversion is to define a misfit measure. Here we use the l_2-norm measure

$$\phi_d = \|\mathbf{W}_d(\mathbf{Gm} - \mathbf{d})\|^2 . \tag{10}$$

For the work here we assume that the contaminating noise on the data is independent and Gaussian with zero mean. Specifying $\mathbf{W}_d$ to be a diagonal matrix whose i^{th} element is $1/\sigma_i$, where σ_i is the standard deviation of the i^{th} datum, makes ϕ_d a chi-squared variable distributed with N degrees of freedom. Accordingly $E[\chi^2] = N$ provides a target misfit for the inversion.

The inverse problem is solved by finding a model m which minimizes ϕ_m and misfits the data by a pre-determined amount. Since the susceptibility is positive by definition we also need to impose the constraint that all model elements be positive. More generally, we can require that the recovered model (m) lies between imposed lower (m^l) and upper (m^u) bounds. Thus the solution is obtained by the following minimization problem of a global objective function ϕ,

$$\begin{aligned} \min \phi &= \phi_d + \beta\phi_m \\ \text{s. t. } & m^l \leq m \leq m^u, \end{aligned} \tag{11}$$

where β is a trade off parameter that controls the relative importance of the model norm and data misfit. When the standard deviations of data errors are known, the acceptable misfit is given by the expected value ϕ_d and we will search for the value of β via an L-curve criterion (Hansen, 2000) that produces the expected misfit. Otherwise, an estimated value of β can be obtained using a generalized cross validation (GCV) estimate (Golub et al., 1979) or by providing a user-defined β.

To solve the optimization problem when constraints are imposed we use the projected gradients method (Calamai and Moré, 1987; Vogel, 2002). Previous versions of MAG3Dhave used the logarithmic barrier method (Wright, 1997; Nocedal and Wright, 1999), however the projected gradient method is considerably faster.

This methodology provides a basic framework for solving 3D magnetic inversion with arbitrary observation locations. The basic components are the forward modelling, a model objective function that incorporates a depth weighting and information about the reference model, a data misfit function, a trade off parameter that ultimately determines how well the data will be fit and an optimization algorithm that minimizes an objective function, subject to bound constraints.

The weighting function is directly incorporated in the sensitivity file generated by program MAGSEN3D. This program allows user to specify whether to use the depth weighting or the distance weighting for surface data. When borehole data are present, however, distance weighting must be used.

2.4 Depth Weighting and Distance Weighting

It is a well-known fact that static magnetic data have no inherent depth resolution. A numerical consequence of this is that when an inversion is performed, which minimizes $\int m(\mathbf{r})^2 dv$, subject to fitting the data, the constructed susceptibility is concentrated close to the observation locations. This is a direct manifestation of the kernel's decay with the distance between the cell and observation locations. Because of the rapidly diminishing amplitude, the kernels of magnetic data are not sufficient to generate a function, which possess significant structure at locations that are far away from observations. In order to overcome this, the inversion needs to introduce a weighting to counteract this natural decay. Intuitively, such a weighting will approximately cancel the decay and give cells at different locations equal probability to enter into the solution with a non-zero susceptibility.

2.4.1 Depth weighting for surface or airborne data

For surface data, the sensitivity decays predominantly in the depth direction. Numerical experiments indicate that the function of the form $(z + z_o)^{-3}$ closely approximates the kernel's decay directly under the observation point provided that a reasonable value is chosen for z_o. The value of 3 in the exponent is consistent with the fact that, to first order, a cuboidal cell acts like a dipole source whose magnetic field decays as inverse distance cubed. The value of z_o can be obtained by matching the function $1/(z + z_o)^3$ with the field produced at an observation point by a column of cells. Thus we use a depth weighting function of the form

$$w(\mathbf{r}_j) = \left[\frac{1}{\Delta z_j} \int\limits_{\Delta z_{ij}} \frac{dz}{(z + z_o)^{\alpha}} \right]^{1/2}, \quad j = 1, ..., M. \tag{12}$$

For the inversion of surface data, where $\alpha = 3.0$, $\mathbf{r}_j$ is used to identify the j^{th} cell, and Δz_j is its thickness. This weighting function is first normalized so that the maximum value is unity. Numerical tests indicate that when this weighting is used, the susceptibility model constructed by minimizing a model objective function in equation 8, subject to fitting the data, places the recovered anomaly at approximately the correct depth.

If the data set involves highly variable observation heights the normal depth weighting function might not be most suitable. Distance weighting used for borehole data may be more appropriate as explained in the next section.

2.4.2 Distance weighting for borehole data

For data sets that contain borehole measurements, the sensitivities do not have a predominant decay direction, therefore a weighting function that varies in three dimensions is needed. We generalize the depth weighting used in surface data inversion to form such a 3D weighting function called distance weighting:

$$w(\mathbf{r}_j) = \frac{1}{\sqrt{\Delta V_j}} \left\{ \sum_{i=1}^{N} \left[\int_{\Delta V_j} \frac{dv}{(R_{ij} + R_o)^{\alpha}} \right]^2 \right\}^{1/4}, \quad j = 1, ..., M, \tag{13}$$

where $\alpha = 3.0$, V_j is the volume of j^{th} cell, R_{ij} is the distance between a point within the source volume and the i^{th} observation, and R_o is a small constant used to ensure that the integral is well-defined (chosen to be a quarter of the smallest cell dimension). Similarly, this weighting function is normalized to have a maximum value of unity. For inversion of borehole data, it is necessary to use this more general weighting. This weighting function is also advantageous if surface data with highly variable observation heights are inverted.

2.5 Wavelet Compression of Sensitivity Matrix

The two major obstacles to the solution of large scale magnetic inversion problem are the large amount of memory required for storing the sensitivity matrix and the CPU time required for the application of the sensitivity matrix to model vectors. The MAG3D v5.0 program library overcomes these difficulties by forming a sparse representation of the sensitivity matrix using a wavelet transform based on compactly supported, orthonormal wavelets. For more details, the users are referred to Li and Oldenburg (2003, 2010). In the following, we give a brief description of the method necessary for the use of the MAG3D v5.0 library.

Each row of the sensitivity matrix in a 3D magnetic inversion can be treated as a 3D image and a 3D wavelet transform can be applied to it. By the properties of the wavelet transform, most transform coefficients are nearly or identically zero. When coefficients of small magnitudes are discarded (the process of thresholding), the remaining coefficients still contain much of the necessary information to reconstruct the sensitivity accurately. These retained coefficients form a sparse representation of the sensitivity in the wavelet domain. The need to store only these large coefficients means that the memory requirement is reduced. Further, the multiplication of the sensitivity with a vector can be carried out by a sparse multiplication in the wavelet domain. This greatly reduces the CPU time. Since the matrix-vector multiplication constitutes the core computation of the inversion, the CPU time for the inverse solution is reduced accordingly. The use of this approach increases the size of solvable problems by nearly two orders of magnitude.

Let $\mathbf{G}$ be the sensitivity matrix and $\mathcal{W}$ be the symbolic matrix-representation of the 3D wavelet transform. Then applying the transform to each row of $\mathbf{G}$ and forming a new matrix consisting of rows of transformed sensitivity is equivalent to the following operation:

$$\widetilde{\mathbf{G}} = \mathbf{G}\mathcal{W}^T, \tag{14}$$

where $\widetilde{\mathbf{G}}$ is called the transformed matrix. The thresholding is applied to individual rows of $\mathbf{G}$ by the following rule to form the sparse representation $\widetilde{\mathbf{G}}^S$,

$$\widetilde{g}_{ij}^s = \begin{cases} \widetilde{g}_{ij} & \text{if } |\widetilde{g}_{ij}| \geq \delta_i \\ 0 & \text{if } |\widetilde{g}_{ij}| < \delta_i \end{cases}, \quad i = 1, \ldots, N, \tag{15}$$

where δ_i is the threshold level, and $\widetilde{g}_{ij}$ and $\widetilde{g}^s_{ij}$ are the elements of $\widetilde{\mathbf{G}}$ and $\widetilde{\mathbf{G}}^S$, respectively. The threshold level δ_i are determined according to the allowable error of the reconstructed sensitivity, which is measured by the ratio of norm of the error in each row to the norm of that row, $r_i(\delta_i)$. It can be evaluated directly in the wavelet domain by the following expression:

$$r_i(\delta_i) = \sqrt{\frac{\sum\limits_{|\widetilde{g}_{ij}|<\delta_i} \widetilde{g}^2_{ij}}{\sum\limits_j \widetilde{g}^2_{ij}}}, \quad i = 1, \ldots, N, \tag{16}$$

Here the numerator is the norm of the discarded coefficients. For each row we choose δ_i such that $r_i(\delta_i) = r^*$, where r^* is the prescribed reconstruction accuracy. However, this is a costly process. Instead, we choose a representative row, i_o, and calculate the threshold level δ_{i_o}. This threshold is then used to define a relative threshold $\epsilon = \delta_{i_o} / \max\limits_j |\widetilde{g}_{ij}|$. The absolute threshold level for each row is obtained by

$$\delta_i = \epsilon \max_j |\widetilde{g}_{ij}|, \quad i = 1, \ldots, N. \tag{17}$$

The program that implements this compression procedure is `MAGSEN3D`. The user is asked to specify the relative error r^* and the program will determine the relative threshold level δ_i. Usually a value of a few percent is appropriate for r^*. When both surface and borehole data are present, two different relative threshold levels are calculated by choosing a representative row for surface data and another for borehole data. For experienced users, the program also allows the direct input of the relative threshold level.

3 Elements of the program MAG3D

3.1 Introduction

The MAG3D v5.0 program library consists of four major programs:

1. MAGFOR3D: performs forward modelling.
2. MAGSEN3D: calculates sensitivity and the depth weighting function.
3. MAGINV3D: performs 3D magnetic inversion.
4. MAGPRE3D: multiplies the sensitivity file by the model to get the predicted data. This rarely used utility multiplies a model by the sensitivity matrix in maginv3d.mtx to produce the predicted data. This program is included so that users who are not familiar with the wavelet transform and the structure of maginv3d.mtx can utilize the available sensitivity matrix to carry out model studies.

Each of the above programs requires input files, as well as the specification of parameters, in order to run. However, some files are used by a number of programs. Before detailing the procedures for running each of the above programs, we first present information about these general files.

3.2 General files for MAG3D v5.0 programs

There are eight general files which are used in MAG3D v5.0. All are in ASCII text format. **Input** files can have any user-defined name. Only program **output** files have restricted file names. Also the filename extensions are not important. Many prefer to use the *.txt filename convention so that files are more easily read and edited in the Windows environment. The files contain components of the inversion:

1. mesh: 3D mesh defining the discretization of the 3D model region.
2. topography: specifies the surface topography
3. location: specifies the inducing field parameters, anomaly type, and data locations, and is typically used for forward modelling
4. observation: specifies the inducing field parameters, anomaly type, observation locations, and the observed magnetic anomalies with estimated standard deviation, and is used for the inversion
5. model: model file structure for forward, initial, reference, and recovered models
6. weighting: file that contains user-supplied 3D weighting functions
7. bounds: optional file that contains values for upper and lower bounds
8. active: Contains location information about active/inactive cells

3.2.1 Mesh file

This file contains the 3D mesh, for example mesh.msh, which defines the model region. Mesh file has the following structure:

NE	NN	NV	
E_o	N_o	Z_o	
ΔE_1	ΔE_2	$\cdots$	ΔE_{NE}
ΔN_1	ΔN_2	$\cdots$	ΔN_{NN}
ΔV_1	ΔV_2	$\cdots$	ΔV_{NV}

NE Number of cells in the East direction.

NN Number of cells in the North direction

NV Number of cells in the vertical direction

E_o N_o V_o Coordinates, in meters, of the southwest top corner, specified in (Easting, Northing, Elevation). The elevation can be relative to a reference elevation other than the sea level, but it needs to be consistent with the elevation used to specify the locations, observations, and topography files (see the relevant file descriptions).

ΔE_n n^{th} cell width in the easting direction (ordered W to E).

ΔN_n n^{th} cell width in the northing direction (ordered S to N).

ΔV_n n^{th} cell thickness (ordered top to bottom).

The mesh can be designed in accordance with the area of interest and the spacing of the data available in the area. In general, the mesh consists of a core region which is directly beneath the area of available data, and a padding zone surrounding this core mesh. Within the core mesh, the size of the cells should be comparable with the spacing of the data. There is no restriction on the relative position of data location and nodal points in horizontal direction. The cell width in this area is usually uniform.

The maximum depth of the mesh used for inversion should be large enough so that no magnetic material below that depth would produce a noticeable anomaly with the length scale covered by the data area. A rule of thumb is that the maximum depth should be at least half of the longest side of the data area. Based upon the user's knowledge of the survey area, one may adjust the maximum depth as necessary. The cell thickness in vertical direction usually increases slightly with depth. In the shallow region, the ratio of thickness to width of about half is good, especially when surface topography is present. At depth, a cell thickness close to the cell width is advisable. Once this core mesh is designed, it can be extended laterally by padding with a few cells, possibly of variable width. This padding is necessary when the extracted anomalies are close to the boundary of the core mesh or if there are influences from anomalies outside the area which cannot be easily removed. Problems with more than 1,000,000 model cells, and/or more than a few thousand data points

would be considered large, and can be expected to require a considerable amount of computing memory and time.

The vertical position of the mesh is specified in elevation. This is to accommodate the inversion of a data set acquired over a topographic surface. When there is strong topographic relief, which the user wishes to incorporate it into the inversion, special care should be taken to design the mesh. A conceptually simple approach is first to design a rectangular mesh whose top (specified by Z_o) is just below the highest elevation point, and then to strip off cells that are above the topographic surface. This is the approach taken in MAG3D v5.0. The number of cells to be stripped off in each column is determined by the user-supplied topography file. Only the remaining cells will be used in the forward modelling or included in the inversion as model parameters.

Example of mesh file

This example shows a mesh that consists of 26 cells in easting, 27 cells in the northing, and 23 cells in the vertical directions. The top of the mesh is located at 0 m of elevation and the southwest corner is at -350 m easting and -400 m northing. The cells in the core portion of the mesh are all 50 m $\times$ 50 m $\times$ 25 m. There are three cells in the padding zone in every direction.

```
26          27     23
-350       -400    0
200         100    50    21*50.0   50   100   200
200         100    50    20*50.0   50   100   200
20*25.0     50     100     200
```

3.2.2 Topography file

This optional file is used to define the surface topography of the 3D model by the elevation at different locations. The topography file has the following structure:

```
!     comment
npt
E1        N1        ELEV1
E2        N2        ELEV2
⋮         ⋮          ⋮
En        Nn        ELEVn
```

Parameter definitions:

`!` Top lines starting with ! are comments.

`npt` Number of points defining the topographic surface.

$\texttt{E}_i$ Easting of the i^{th} point on the surface.

N_j Northing of the j^{th} point on the surface.

$ELEV_n$ Elevation of the n^{th} point on the profile.

The lines in this file can be in any order as long as the total number is equal to npt. The topographic data need not be supplied on a regular grid. MAG3D v5.0 assumes a set of scattered points for generality and uses triangulation-based interpolation to determine the surface elevation above each column of cells. To ensure the accurate discretization of the topography, it is important that the topographic data be supplied over the entire area above the model and that the supplied elevation data points are not too sparse.

Example of topography file

The following is an example of a topography file:

```
2007
12300.00   9000.00   0.109411E+04
12300.00   9025.00   0.109545E+04
12300.00   9050.00   0.109805E+04
12300.00   9075.00   0.110147E+04
12300.00   9100.00   0.110555E+04
12300.00   9125.00   0.111011E+04
12300.00   9150.00   0.111490E+04
12300.00   9175.00   0.111971E+04
```

NOTE: Although the cells above the topographic surface are removed from the model, they must still be included in the model file as if they are a part of the model. For input model files these cells can be assigned any value. The recovered model produced by inversion program also includes the cells that are excluded from the model, but these cells will have unrealistic values as an identifier (e.g. -100).

3.2.3 Locations file

This file is used to specify the inducing field parameters, anomaly type, and observation locations specifically for the forward modelling of magnetic data. The following is the file structure:

```
!       comment
incl     decl     geomag
aincl    adecl     idir
ndat
E1         N1       ELEV1      [aincl1      adecl1]
E2         N2       ELEV2      [aincl2      adecl2]
⋮          ⋮          ⋮          ⋮           ⋮
Endat      Nndat    ELEVndat   [ainclndat   adeclndat]
```

Parameter definitions:

`!` Lines starting with ! are comments.

`incl/decl` Inclination and declination of the inducing magnetic field. The declination is specified positive east with respect to the northing used in the mesh. These value should be the same in the observations file.

`geomag` Strength of the inducing field in nanoTesla (nT).

`aincl/adecl/idir` Inclination and declination of the anomaly projection. Set `idir=0` for a multi-component dataset and `idir=1` for a single component dataset where all the observations have the same inclination and declination of the anomaly projection.

`ndat` Number of observations. When single component data are specified the number of observations is equal to the number of data locations. When multi-component data are specified the number of observations will exceed the number of data locations. For example, if three-component data are specified at N locations, the number of observations is $3N$.

$\texttt{E}_n\texttt{,N}_n\texttt{,Elev}_n$ Easting, northing and elevation of the observation, measured in meters. Elevation should be above the topography for surface data, and below the topography for borehole data. The observation locations can be listed in any order.

$\texttt{ainc}_n\texttt{/adec}_n$ Inclination and declination of the anomaly projection for the nth observation. This is used only when `idir = 0`. The brackets "$[\cdots]$" indicate that these two field are optional depending on the value of `idir`.

The total field anomaly is calculated when `aincl` equals `incl` and `adecl` equals `decl`. The vertical field anomaly is calculated when `aincl`=90° and `adecl`=0°. The user can specify other (`aincl`, `adecl`) pairs to calculate the anomaly component in those directions. Easting, northing and elevation information should be in the same coordinate system as defined in the mesh.

Examples of a locations file

We provide two example files below. The first file is for calculating total field anomaly at 441 stations. The inducing field has an inclination of 45^o and a declination of 45°. The second file is for calculating multi-component anomalies in boreholes and each datum is specified by its own inclination and declination of anomaly projection.

Example of single-component data:

```
  !                          surface data
 45.0      45.0     50000   !!  Incl        Decl   geomag
 45.0      45.0       0     !!  AIncl       Adecl  idir
 441                        !!  # of data
 0.00      0.00     1.00
 0.00     50.00     1.00
 0.00    100.00     1.00
  ⋮         ⋮        ⋮
1000.00   900.00    1.00
1000.00   950.00    1.00
1000.00  1000.00    1.00
```

Example of multi-component data:

```
  !                                                  borehole data
 45.0      45.0      50000    !!  Incl    Decl      geomag
 45.0      45.0        0      !!  AIncl   Adecl     idir
 441                                                !!  # of data
-12.50   -137.50   -12.50        0.0       0.0
-12.50   -137.50   -37.50        0.0       0.0
-12.50   -137.50   -62.50        0.0       0.0
  ⋮         ⋮         ⋮          ⋮         ⋮
-237.50   -12.50   -337.50       90.0      0.0
-237.50   -12.50   -362.50       90.0      0.0
-237.50   -12.50   -387.50       90.0      0.0
```

3.2.4 Observations file

This file is used to specify the inducing field parameters, anomaly type, observation locations, and the observed magnetic anomalies with estimated standard deviation. The values of parameters specifying the inducing field anomaly type and observation locations are identical to those in locations file. The output of the forward modelling program MAGFOR3D has the same structure except that the column of standard deviations for the error is omitted. The following is the file structure of the observations file:

```
  !     comment
 Incl     Decl     geomag
AIncl    Adecl      idir
 ndat
  E1       N1       ELEV1      [aincl1      adecl1]      Mag1      Err1
  E2       N2       ELEV2      [aincl2      adecl2]      Mag2      Err2
  ⋮        ⋮         ⋮           ⋮            ⋮           ⋮         ⋮
 Endat    Nndat    ELEVndat   [ainclndat   adecclndat]  Magndat   Errndat
```

Parameter definitions:

`!` Lines starting with ! are comments.

`incl/decl` Inclination and declination of the inducing magnetic field. The declination is specified positive east with respect to the northing used in the mesh and locations files.

`geomag` Strength of the inducing field in nanoTesla (nT).

`aincl/adecl/idir` Inclination and declination of the anomaly projection. Set `idir=0` for a multi-component dataset and `idir=1` for a single component dataset where all the observations have the same inclination and declination of the anomaly projection.

`ndat` Number of observations. When single component data are specified the number of observations is equal to the number of data locations. When multi-component data are specified the number of observations will exceed the number of data locations. For example, if three-component data are specified at N locations, the number of observations is $3N$.

$\texttt{E}_n\texttt{,N}_n\texttt{,Elev}_n$ Easting, northing and elevation of the observation, measured in meters. Elevation should be above the topography for surface data, and below the topography for borehole data. The observation locations can be listed in any order.

$\texttt{ainc}_n\texttt{/adec}_n$ Inclination and declination of the anomaly projection for observation n. This is used only when `idir = 0`. The brackets "$[\cdots]$" indicate that these two field are optional depending on the value of `idir`.

$\texttt{Mag}_n$ Magnetic anomaly data, measured in nT.

$\texttt{Err}_n$ Standard deviation of Mag_n. This represents the absolute error. It CANNOT be zero or negative.

NOTE: It should be noted that the data are **extracted anomalies** which are derived by removing the regional from the field measurements. Furthermore, the inversion program assumes that the anomalies are produced by a positive susceptibility (contrast) distribution. It is crucial that the data be prepared as such.

Examples of obs.mag file

The following are two examples of data files. The first example file specifies a set of total field anomaly data, and the second example file provides a set of multi-component borehole data.

Example 1: single-component data

```
   !                          surface data
  45.0      45.0     50000      !!  Incl         Decl       geomag
  45.0      45.0       0        !!  AIncl        Adecl      direction of anomaly (idir)
   144                                                      !!  Number of data
  0.00      0.00     1.00    0.174732E+02   0.598678E+01
  0.00     50.00     1.00    0.265550E+02   0.613890E+01
  0.00     100.00    1.00    0.311366E+02   0.629117E+01
   ⋮         ⋮        ⋮          ⋮              ⋮
1000.00   900.00    1.00   -0.109595E+01   0.530682E+01
1000.00   950.00    1.00   -0.902209E+01   0.523738E+01
1000.00   1000.00   1.00   -0.397501E+01   0.518496E+01
```

Example 2: Multi-component data

```
   !                                                    borehole data
  45.0      45.0      50000     !!  Incl    Decl    geomag
  45.0      45.0        0       !!  AIncl   Adecl   direction of anomaly (idir)
   144                                              !!  Number of data
 -12.50   -137.50   -12.50       0.0      0.0      0.134759E+03  0.200000E+01
 -12.50   -137.50   -37.50       0.0      0.0      0.162606E+03  0.200000E+01
 -12.50   -137.50   -62.50       0.0      0.0      0.165957E+03  0.200000E+01
   ⋮         ⋮         ⋮          ⋮        ⋮
-237.50   -12.50   -337.50      90.0      0.0      0.662445E+02  0.200000E+01
-237.50   -12.50   -362.50      90.0      0.0      0.693134E+02  0.200000E+01
-237.50   -12.50   -387.50      90.0      0.0      0.608605E+02  0.200000E+01
```

3.2.5 Model file

This file contains the cell values of the susceptibility model. The susceptibility must have values in SI units. The initial, reference, and forward models must be in this format. Likewise, the recovered model files will be in this format. The following is the file structure of the model file

$\kappa_{1,1,1}$
$\kappa_{1,1,2}$
⋮
$\kappa_{1,1,NV}$
$\kappa_{1,2,1}$
⋮
$\kappa_{1,j,k}$
⋮
$\kappa_{NN,NE,NV}$

Each $\kappa_{i,j,k}$ is susceptibility at location $[i, j, k]$.

$\kappa_{i,j,k}$ Susceptibility in cell $[i, j, k]$. The susceptibility is always in SI units and always positive. There are no a priori bound constraints set on recovered susceptibility, however it is recommended that positivity condition to be enforced during the inversion.

$[i, j, k] = [1, 1, 1]$ is defined as the cell at the top, south-west corner of the model. The total number of lines in this file should equal $NN \times NE \times NV$, where NN is the number of cells in the north direction, NE is the number of cells in the east direction, and NV is the number of cells in the vertical direction.

3.2.6 Weights file

This file supplies the user-based weights that acts upon the model objective function. The following is the file structure is for the weights file:

$\texttt{W.S}_{1,1,1}$	$\cdots$	$\texttt{W.S}_{NN,NE,NV}$
$\texttt{W.E}_{1,1,1}$	$\cdots$	$\texttt{W.E}_{NN,NE-1,NV}$
$\texttt{W.N}_{1,1,1}$	$\cdots$	$\texttt{W.N}_{NN-1,NE,NV}$
$\texttt{W.Z}_{1,1,1}$	$\cdots$	$\texttt{W.Z}_{NN,NE,NV-1}$

Parameter definitions:

$\texttt{W.S}_{i,j,k}$ Cell weights for the smallest model.

$\texttt{W.E}_{i,j,k}$ Cell weights for the interface perpendicular to the easting direction.

$\texttt{W.N}_{i,j,k}$ Cell weights for the interface perpendicular to the northing direction.

$\texttt{W.Z}_{i,j,k}$ Cell weights for the interface perpendicular to the vertical direction.

Within each part, the values are ordered in the same way as in model file, however, they can be all on one line, or broken up over several lines. Since the weights for a derivative term are applied to the boundary between cells, the weights have one fewer value in that direction. For instance, the weights for the derivative in easting direction has $(NE - 1) \times NN \times NV$ values, whereas the number of cells is $NE \times NN \times NV$.

If the surface topography file is supplied, the cell weights above the surface will be ignored. It is recommended that these weights be assigned a value of -1.0 to avoid confusion. If `null` is entered instead of the weights file, then all of the cell weights will be set equal (1.0).

3.2.7 Bounds file

This file contains the cell values of the lower and upper bounds on the sought model. It is an optional for the inversion program. The bounds have the same dimension as the model. The following is the file structure of a bounds file:

$$\begin{array}{cc} \mathtt{b}^l_{1,1,1} & \mathtt{b}^u_{1,1,1} \\ \mathtt{b}^l_{1,1,2} & \mathtt{b}^u_{1,1,2} \\ \vdots & \vdots \\ \mathtt{b}^l_{1,1,NV} & \mathtt{b}^u_{1,1,NV} \\ \mathtt{b}^l_{1,2,1} & \mathtt{b}^u_{1,2,1} \\ \vdots & \vdots \\ \mathtt{b}^l_{i,j,k} & \mathtt{b}^u_{i,j,k} \\ \vdots & \vdots \\ \mathtt{b}^l_{NN,NE,NV} & \mathtt{b}^u_{NN,NE,NV} \end{array}$$

Parameter definitions:

$\mathtt{b}^l_{i,j,k}$ Is the lower bound on cell $[i, j, k]$.

$\mathtt{b}^u_{i,j,k}$ Is the upper bound on cell $[i, j, k]$.

The ordering of the cells is the same as that for model cells: $[i, j, k] = [1, 1, 1]$ is defined as the cell at the top, south-west corner of the model. The total number of lines in this file should equal $NN \times NE \times NV$, where `NN` is the number of cells in the North direction, `NE` is the number of cells in the East direction, and `NV` is the number of cells in the vertical direction. The lines must be ordered so that k changes the quickest (from 1 to `NV`), followed by j (from 1 to `NE`), then followed by i (from 1 to `NN`). If the surface topography file is supplied, the bounds for cells above the surface will be ignored. It is recommended that these values be assigned a negative value (e.g. `-1.0`) to avoid confusion.

3.2.8 Active cells file

This file is optional. It has exact same format as the model file, and thus must be the same size. The active cells file contains information about the cells that will be incorporated into the inversion. By default all cells below the earth's surface are active and incorporated into the inversion. If the active cells file is provided, then zeros will mark the inactive cells (will NOT be included in the inversion), and cells set to 1, will define active cells. Any inactive cells will not influence the minimization in equation 11. The cells will remain the user given value (via the reference models) and do not factor into the model objective function calculation. The following is an example of an active cells file:

```
0
0  !  inactive cell
⋮
0
1  !  active cell
⋮
0
⋮
1
```

4 Running the programs

The software package MAG3Duses four general codes:

`MAGFOR3D` performs forward modelling.

`MAGSEN3D` calculates sensitivity and the depth weighting function.

`MAGINV3D` performs 3D magnetic inversion.

`MAGPRE3D` multiplies the sensitivity file by the model to get the predicted data.

This section discusses the use of these codes individually using.

4.1 Introduction

All programs in the package can be executed under Windows or Linux environments. They can be run by typing the program name followed by a control file in the "command prompt" (Windows) or "terminal" (Linux). They can be executed directly on the command line or in a shell script or batch file. When a program is executed without any arguments, it will print the usage to screen.

4.1.1 Execution on a single computer

The command format and the control file format on a single machine are described below. Within the command prompt or terminal, any of the programs can be called using:

$$\texttt{program arg}_1\ [\texttt{arg}_2\ \cdots\ \texttt{arg}_i]$$

where:

`program` is the name of the executable

$\texttt{arg}_i$ is a command line argument, which can be a name of corresponding required or optional file. Typing `-inp` as the control file, serves as a help function and returns an example input file. Some executables do not require control files and should be followed by multiple arguments instead. This will be discussed in more detail later in this section.

Each control file contains a formatted list of arguments, parameters and filenames in a combination and sequence specific for the executable, which requires this control file. Different control file formats will be explained further in the document for each executable.

4.1.2 Execution on a local network or commodity cluster

The MAG3D v5.0program library's main programs have been parallelized with Message Pass Interface (MPI). This allows running these codes on more than one computer in parallel. MPI installation package can be downloaded from `http://www.mcs.anl.gov/research/projects/mpich2/`. The following are the requirements for running an MPI job on a local network or cluster:

- An identical version of MPI must be installed on all participating machines
- The user must create an identical network account with matching "username" and "password" on every machine
- Both the executable folder and the working directory should be "shared" and visible on every participating computer
- Before the MPI job is executed, the firewall should be turned off on every participating computer
- The path should be defined to the executable directory

The following is an example of a command line executing an MPI process:

```
C:\Program Files\MPICH2\bin\mpiexec.exe -machinefile machine.txt nproc -priority
                                    0 maginv3d
```

An explanation of the arguments used in this command line are:

`PATH` Properly defined path to the `mpiexec.exe`.

`-machinefile` The list of participating machines will be read from a "machine file."

`machine.txt` Name of the machine file. This file lists the network names of the participating machines and number of processors to be allocated for the MPI job for each machine. The following is an example of a machine file:

```
machine01  16
machine02  16
```

In this simple example, there are two participating machines (named `machine01` and `machine02` and each is required to allocate 16 processors for the MPI job.

`nproc` The total number of allocated processors. This number should be equal to the sum of all processors listed for all machines in the machine file.

`-priority 0` Sets the priority of the process. Integer grades from -1 (lowest) to 4 (highest) follow. Higher priority means that RAM and processing resources will be primarily allocated for this process, at expense of lower priority processes. Generally, a large job should be assigned a lower priority, as selective resource allocation may slow down other important processes on the computer, including those needed for stable functioning of the operating system.

maginv3d.exe The name of the executable. In our case it is assumed that there is an existing path to the executable directory, otherwise proper path should be provided.

4.2 MAGFOR3D

This program performs forward modelling. Command line usage:

```
magfor3d mesh.msh obs.loc model.sus [topo.dat]
```

and will create a magfor3d.mag file.

4.2.1 Input files

All files are in ASCII text format - they can be read with any text editor. Input files can have any name the user specifies. Details for the format of each file can be found in Section 3. The files associated with magfor3d are:

mesh.msh The 3D mesh.

obs.loc The inducing field parameters, anomaly type and observation locations.

model.sus The susceptibility model.

topo.dat Surface topography (optional). If omitted, the surface will be treated as being flat.

4.2.2 Output file

The file created by MAGFOR3D is magfor3d.mag. The file format is that of the data file without the associated standard deviations.

magfor3d.mag The computed magnetic anomaly data. Since the data in this file are accurate, the column of the standard deviations for the error is not included.

4.3 MAGSEN3D

This program performs the sensitivity and depth weighting function calculations. Command line usage:

```
magsen3d magsen3d.inp
```

For a sample input file type: magsen3d -inp

4.3.1 Input files

Format of the control file magsen3d.inp:

```
mesh.msh      !  mesh file
obs.mag       !  observations file
topo.dat      !  topography file | null
iwt           !  weighting type
alpha, znot   !  weighting parameters | null
wvlt          !  wavelet type | null
itol, eps     !  wavelet parameters | null
```

The input parameters for the control file are:

mesh.msh Name of 3D mesh file.

obs.mag The data file that contains the inducing field parameters, anomaly type, observation locations, and the observed magnetic anomalies with estimated standard deviation.

topo.dat Surface topography (optional). If `null` is entered, the surface will be treated as being flat.

iwt An integer identifying the type of generalized depth weighting to use in the inversion.
=1 for depth weighting (only for surface data);
=2 for distance weighting (surface and/or borehole).

alpha,znot Parameters defining the depth weighting function. When iwt=1, alpha and znot are used as α and z_0 to define the *depth* weighting according to equation 12.
When iwt=2, alpha and znot are used as α and (R_o) to define the *distance* weighting according to equation 13.
If null is entered on this line (line 5), then the program sets `alpha=3` and calculates the value of z_o based upon the mesh and data location. This is true for iwt=1 or iwt=2.
For most inversions, however, setting this input line to null is recommended. The option for inputing α and z_o is provided for experienced users who would like to investigate the effect of the generalized depth weighting for special purposes. The value of α should normally be close to 3.0. Smaller values of give rise to weaker weighting as distance increases from the observation locations.

wvlt A five-character string identifying the type of wavelet used to compress the sensitivity matrix. The types of wavelets available are Daubechies wavelet with 1 to 6 vanishing moments (daub1, daub2, and so on) and Symmlets with 4 to 6 vanishing moments (symm4, symm5, symm6). Note that daub1 is the Haar wavelet and daub2 is the Daubechies-4 wavelet. The Daubechies-4 wavelet is suitable for most inversions, while the others are provided for users' experimentation. If null is entered, the program uses the default wavelet compression (daub2).

itol,eps An integer and a real number that specify how the wavelet threshold level is to be determined. itol=1: program calculates the relative threshold and eps is the relative reconstruction error of the sensitivity. A reconstruction error of 0.05 is usually adequate.

itol=2: the user defines the threshold level and eps is the relative threshold to be used. If null is entered on this line, a default relative reconstruction error of 0.05 (e.g. 5%) is used and the relative threshold level is calculated (i.e., itol=1, eps=0.05).
The detailed explanation of threshold level and reconstruction error can be found in Section 2.5 of this manual.

Example of magsen3d.inp control file

```
mesh.msh          !  mesh file
obs_noise.mag     !  data file
null              !  topography | null
2                 !  iwt=1 depth, =2 distance
null              !  alpha, znot | null
daub2             !  wavelet type
1.0 0.05          !  itol, eps | null
```

4.3.2 Output files

The program `magsen3d` outputs three files. They are:

1. maginv3d.mtx The sensitivity matrix file to be used in the inversion. This file contains the sensitivity matrix, generalized depth weighting function, mesh, and discretized surface topography. It is produced by the program and it's name is not adjustable. It is very large and may be deleted once the work is completed.

2. sensitivity.txt Output after running `magsen3d`. It contains the average sensitivity for each cell. This file can be used for depth of investigation analysis or for use in designing special model objective function weighting.

3. dist_weighting.txt A file in the model.sus format, which contains weights for each cell, based on equations 12 and 13.

4.4 MAGINV3D

This program performs 3D magnetic inversion. Command line usage is:

```
maginv3d maginv3d.inp
```

For a sample input file type: `maginv3d -inp`

4.4.1 Input files

Input files can be any file name. If there are spaces in the path or file name, you MUST use quotes around the entire path (including the filename).

1. obs.mag Mandatory observations file.
2. mag3d.mtx Mandatory sensitivity matrix from `magsen3d`.
3. ini.sus Optional initial model file; can be substituted by a value maginv3d.inp control file. Mandatory if and existing inversion is restarted after termination
4. ref.sus Optional reference model file; can be substituted by a value in the maginv3d.inp control file.
5. active.txt Optional active model file
6. bounds.sus Optional bounds file
7. w.dat Optional weighting files
8. maginv3d.inp The control file used by `maginv3d`.

Format of the control file maginv3d.inp has been changed since previous version. It has been modified as follows:

```
mode
par,tolc
obs.mag
maginv3d.mtx
ini.sus          | [number]     | null
ref.sus          | [number]     | null
active.txt       | null
bounds.sus       | b^l b^u      | null
α_s, α_x, α_y, α_z | Le Ln Lz
SMOOTH_MOD_DIF   | SMOOTH_MOD
w.dat
```

The parameters within the control file are:

mode An integer specifying one of three choices for determining the trade-off parameter.

1. mode=1: the program chooses the trade off parameter by carrying out a line search so that the target value of data misfit is achieved (where $1 = N$).
2. mode=2: the user inputs the trade off parameter.

3. mode=3: the program calculates the trade off parameter by applying the GCV analysis to the inversion without positivity.

par,tolc Two real numbers that are dependent upon the value of mode.

1. mode=1: the target misfit value is given by the product of `par` and the number of data N, i.e.,. The second parameter, `tolc`, is the misfit tolerance. The target misfit is considered to be achieved when the relative difference between the true and target misfits is less than tolc. Normally, the value of par should be 1.0 if the correct standard deviation of error is assigned to each datum. When tolc=0, the program assumes a default value of tolc=0.02.
2. mode=2: par is the user-input value of trade off parameter. In this case, tolc is not used by the program.
3. mode=3: none of the two input values are used by the program. However, this line of input still needs to be there.

NOTE: When mode=1 both `par` and `tolc` are used. When mode=2 only `par` is used. When `mode=3`, neither par nor `tolc` are used. However, the third line should always have two values.

obs.mag Input data file. The file must specify the standard deviations of the error. By definition these values are greater than zero.

mag3d.mtx The binary file created by `MAGSEN3D`.

ini.sus The initial susceptibility model can be defined as a value (for uniform models), or by a filename.

ref.sus The reference susceptibility model can be defined as a value (for uniform models), or by a filename (for non-uniform reference models).

active.txt The file containing which cells in the model are be defined as active (`1`) or inactive (brown0). This file must be fully compatible with the mesh.msh and ref.sus. Use the null option for all cells being active.

bounds.sus There are three options regarding the bounds selection:

1. Have 2 values (b_l and b_u), defining the lower and upper bounds, as a constraint for the entire recovered model.
2. Provide the file bounds.sus containing individual $\mathtt{b}_l$ and $\mathtt{b}_u$ values for each cell or
3. null, defining "no bounds" option.

$\alpha_s, \alpha_x, \alpha_y, \alpha_z$ Coefficients for the each model component. α's is the smallest model component. Coefficient for the derivative in the easting direction. α_y is the coefficient for the derivative in the northing direction. The coefficient α_z is for the derivative in the vertical direction.

If null is entered on this line, then the above four parameters take the following default values: $\alpha_s = 0.0001, \alpha_x = \alpha_y = \alpha_z = 1.0$. None of the alpha's can be negative and they cannot be all equal to zero at the same time.

NOTE: The four coefficients α_s, α_x, α_y and α_z in line 9 of the control file can be substituted for three corresponding length scales L_x, L_y and L_z. To understand the meaning of the length scales, consider the ratios α_x/α_s, α_y/α_s and α_z/α_s. They generally define smoothness of the recovered model in each direction. Larger ratios result in smoother models, smaller ratios result in blockier models. The conversion from α's to length scales can be done by:

$$L_x = \sqrt{\frac{\alpha_x}{\alpha_s}};\ L_y = \sqrt{\frac{\alpha_y}{\alpha_s}};\ L_z = \sqrt{\frac{\alpha_z}{\alpha_s}} \tag{18}$$

where length scales are defined in meters. When user-defined, it is preferable to have length scales exceed the corresponding cell dimensions.

SMOOTH_MOD This option was not available in previous versions of the code and can be used to define the reference model in and out of the derivative terms. The options are: SMOOTH_MOD_DIF (reference model is defined in the derivative terms) and SMOOTH_MOD (reference model is defined in only the smallest term)

w.dat Name of the file containing weighting matrix. If null is entered, default values of unity are used.

Example of maginv3d.inp control file

Below is an example of a control file with comments:

```
1                !  mode
1.0 0.0          !  par, tolc
obs_noise.mag    !  observation file
maginv3d.mtx     !  sensitivity matrix file
1.E-07           !  initial model
1.E-07           !  reference model
NULL             !  active cells file
0.0 0.08         !  lower and upper bounds
null             !  α_s, α_x, α_y, α_z
SMOOTH_MOD_DIF   !  reference model in the derivative terms
null             !  weighting matrix
```

4.4.2 Output files

Five output files are created by the program `maginv3d`. They are:

1. maginv3d.log The log file containing more detailed information for each iteration and summary of the inversion.
2. maginv3d_iter.sus Susceptibility files output after each iteration (iter defines the iteration step).

3. maginv3d_iter.pre Predicted data files output after each iteration (iter defines the iteration step).

4. maginv3d.sus Final magnetic susceptibility model.

5. maginv3d.pre Final predicted data file.

4.5 MAGPRE3D

This utility multiplies a model by the stored sensitivity matrix in maginv3d.mtx to produce predicted data. This program is included so that users who are not familiar with the wavelet transform and the structure of maginv3d.mtx could utilize the available sensitivity matrix to carry out modelling exercises. The command line usage is:

```
magpre3d maginv3d.mtx obs.loc model.sus
```

4.5.1 Input files

1. maginv3d.mtx The sensitivity matrix file from `MAGSEN3D`.

2. obs.loc The inducing field parameters, anomaly type and observation locations.

3. model.sus The magnetic susceptibility model

4.5.2 Output file

The output file is in the same form as the observation file without the standard deviation and called magpre3d.mag, which is the predicted data file.

5 References

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