

Estimating total magnetization direction using equivalent-layer technique

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Running head: **Determining total magnetization direction**

ABSTRACT

We have developed a new method for estimating the total magnetization direction of magnetic sources based on equivalent layer technique using total field anomaly data. In this approach, we do not have to impose a strong information about the shape and the depth of the sources, and do not require a regularly spaced data. Usually, this technique is used for processing potential data estimating a 2D magnetic moment distribution over a fictitious layer composed by dipoles below the observation plane. In certain conditions, when the magnetization direction of equivalent sources is almost the same of true body, the estimated magnetic property over the layer is all positive. The methodology uses a positivity constraint to estimate a set of magnetic moment over the layer and a magnetization direction of the layer through a iterative process. Mathematically, the algorithm solve a least squares problem in two steps: the first one solve a linear problem for estimating a magnetic moment and the second solve a non-linear problem for magnetization direction of the layer. We test the methodology applying to synthetic data for a complicated scenarios and

geometries of sources. Moreover, we applied the method to field data from Goias Alkaline Province (GAP), center of Brazil, over Montes Claros complex. The result suggests the area is composed by intrusions with remarkable strong remanent magnetization component, being in agreement with the current literature for this region.

METHODOLOGY

Fundamentals of magnetic equivalent layer and the positive magnetic-moment distribution

Considering a Cartesian coordinate system with x -, y - and z -axis being oriented to north, east and downward, respectively. Let $\Delta T_i \equiv \Delta T(x_i, y_i, z_i)$ be the total-field anomaly, at the i th position (x_i, y_i, z_i) , produced by a continuous layer located below the observation plane at a depth equal to z_c , where $z_c > z_i$, and $p(x', y', z_c)$ is the distribution of magnetic dipoles moment per unit area over the layer. The total-field anomaly produced by this continuous layer is given by

$$\Delta T_i = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} p(x', y', z_c) [\gamma_m \hat{\mathbf{F}}_0^T \mathbf{M}(x_i, y_i, z_i, x', y', z_c) \hat{\mathbf{m}}(\mathbf{q})] dx' dy', \quad (1)$$

where γ_m is a constant proportional to the vacuum permeability, $\hat{\mathbf{F}}_0$ is a unit vector with the same direction of the main geomagnetic field given by

$$\hat{\mathbf{F}}_0 = \begin{bmatrix} \cos I \cos D \\ \cos I \sin D \\ \sin I \end{bmatrix}, \quad (2)$$

where I and D are, respectively, the inclination and declination and $\mathbf{M}(x_i, y_i, z_i, x', y', z_c)$ is a 3×3 dimensional matrix (Oliveira Jr et al., 2015) equal to

$$\mathbf{M}(x_i, y_i, z_i, x', y', z_c) = \begin{bmatrix} \partial_{xx}\phi & \partial_{xy}\phi & \partial_{xz}\phi \\ \partial_{yx}\phi & \partial_{yy}\phi & \partial_{yz}\phi \\ \partial_{zx}\phi & \partial_{zy}\phi & \partial_{zz}\phi \end{bmatrix}, \quad (3)$$

where $\partial_{\alpha\beta}\phi$, $\alpha = x, y, z$ and $\beta = x, y, z$, is the second derivative of the scalar function

$$\phi(x_i, y_i, z_i, x', y', z_c) = \frac{1}{[(x_i - x')^2 + (y_i - y')^2 + (z_i - z_c)^2]^{\frac{1}{2}}}. \quad (4)$$

with respect to the Cartesian coordinates x_i , y_i and z_i of the observation points. The $\hat{\mathbf{m}}(\mathbf{q})$ is a unit vector with the magnetization direction of the dipoles over layer given by

$$\hat{\mathbf{m}}(\mathbf{q}) = \begin{bmatrix} \cos \tilde{\mathbf{i}} \cos \tilde{d} \\ \cos \tilde{\mathbf{i}} \sin \tilde{d} \\ \sin \tilde{\mathbf{i}} \end{bmatrix} \quad (5)$$

and \mathbf{q} is a 2×1 vector with components given by

$$\mathbf{q} = \begin{bmatrix} \tilde{\mathbf{i}} \\ \tilde{d} \end{bmatrix}, \quad (6)$$

where $\tilde{\mathbf{i}}$ and \tilde{d} are the inclination and declination of the magnetization direction of the dipoles on the layer, respectively. We can also notice that the vector defined in equation 5 has a single and uniform magnetization direction of all dipoles on the layer. For convenience, this unit vector can be rewritten as follows

$$\hat{\mathbf{m}}(\mathbf{q}) = \mathbf{R} \hat{\mathbf{h}}, \quad (7)$$

where $\hat{\mathbf{h}}$ defines the uniform magnetization direction of an arbitrary magnetic source and \mathbf{R} is a 3×3 matrix obtained from Euler's rotation theorem. This theorem states that any rotation can be parametrized by using three parameters called Euler angles (H. Goldstein and Safko, 1980). That is, if all dipoles that set up the equivalent layer have the same magnetization direction $\hat{\mathbf{m}}(\mathbf{q})$ and this direction is the same as the true magnetic source $\hat{\mathbf{h}}$,

then the matrix \mathbf{R} (equation 7) is equal to identity. For this reason, the total-field anomaly produced by equivalent layer at the i th position (x_i, y_i, z_i) (equation 1) can be rewritten as

$$\Delta T_i = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} p(x', y', z_c) [\gamma_m \hat{\mathbf{F}}_0^T \mathbf{M}(x_i, y_i, z_i, x', y', z_c) \hat{\mathbf{h}}] dx' dy', \quad (8)$$

which represents the total-field anomaly produced by continuous layer with the same direction of the arbitrary magnetic source. Thus, the RTP field ΔT_i^{PL} produced by equivalent layer at the point (x_i, y_i, z_i) is equal to

$$\Delta T_i^{PL} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} p(x', y', z_c) [\gamma_m \partial_{zz} \phi(x_i, y_i, z_i, x', y', z_c)] dx' dy', \quad (9)$$

where $\partial_{zz} \phi(x_i, y_i, z_i, x', y', z_c)$ is the second derivative of the inverse of distance (equation 4) with respect of z_i , evaluated at the point (x_i, y_i, z_i) . However, by considering the RTP field ΔT_i^{PS} that would be produced by an arbitrary uniformly magnetized source at the pole, we have

$$\Delta T_i^{PS} = \gamma_m \partial_{zz} \Gamma(x_i, y_i, z_i) m, \quad (10)$$

where m is the magnetization intensity of the magnetic source. The $\partial_{zz} \Gamma(x_i, y_i, z_i)$ is the second derivative in relation to z_i of a scalar function $\Gamma(x_i, y_i, z_i)$

$$\Gamma(x_i, y_i, z_i) = \iiint_v \frac{dv}{[(x_i - \alpha)^2 + (y_i - \beta)^2 + (z_i - \gamma)^2]^{\frac{1}{2}}} \quad (11)$$

in which α , β and γ are the Cartesian coordinates of an infinitesimal element inside the volume v of the magnetic source. From equation 9 and 10, we obtain

$$m \partial_{zz} \Gamma(x_i, y_i, z_i) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} p(x', y', z_c) \partial_{zz} \phi(x_i, y_i, z_i, x', y', z_c) dx' dy'. \quad (12)$$

We can notice that equation 12 can be calculated differentiating the following equation

$$m \partial_z \Gamma(x_i, y_i, z_i) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{p(x', y', z_c)(z_c - z_i)}{[(x_i - x')^2 + (y_i - y')^2 + (z_i - z_c)^2]^{\frac{3}{2}}} dx' dy', \quad (13)$$

where $z_c > z_i$, with respect to the vertical component z_i .

From potential-field theory, we can highlight the classical upward continuation integral

$$U(x_i, y_i, z_i) = \frac{(z_c - z_i)}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{U(x', y', z_c)}{[(x_i - x')^2 + (y_i - y')^2 + (z_i - z_c)^2]^{\frac{3}{2}}} dx' dy', \quad (14)$$

where the function $U(x_i, y_i, z_i)$ is an hamornic function at all (x_i, y_i, z_i) and $U(x', y', z_c)$ is the same harmonic function ate (x', y', z_c) (Blakely, 1996). In this case, if this harmonic function represents the total-field anomaly at the point (x_i, y_i, z_i) , it can be mathematically interpreted as the convolution between its values $U(x', y', z_c)$ and the vertical derivative in relation to z_i of the equation 4, evaluated on the horizontal plane $z_i = z_c$. Therefore, according to the classical upward continuation function (equation 14), the magnetic-moment distribution $p(x', y', z_c)$ in equation 13 assumes the form

$$p(x', y', z_c) = \frac{m}{2\pi} \partial_z \Gamma(x', y', z_c), \quad (15)$$

where $\partial_z \Gamma(x', y', z_c)$ is the derivative of the scalar function 11 in relation to z_i evaluated over the equivalent layer. The most interesting aspect of equation 15 is that the magnetic-moment distribution is defined as the product of a positive constant $\frac{m}{2\pi}$ and the function $\partial_z \Gamma(x', y', z_c)$, which is all positive at all points (x', y', z_c) over the equivalent layer.

This relation is similar to that presented by Pedersen (1991) and Li et al. (2014). In the wavenumber domain, these authors determined the magnetic-moment distribution within a continuous equivalent layer with the same magnetization direction as the local-geomagnetic field at the pole. They also considered a planar equivalent layer located below and parallel to a horizontal plane containing the observed total-field anomaly. They assume a magnetic source having a purely induced magnetization. Under these assumptions, Pedersen (1991) and Li et al. (2014) concluded that the magnetic-moment distribution within the continuous equivalent layer is proportional to the pseudogravity anomaly produced by the source on the plane of the equivalent layer. By following different approaches using magnetic microscopy data, Baratchart et al. (2013) and Lima and Weiss (2016) pointed out by imposing a non-negativity constraint, the solution to the inverse problem is a unique magnetic-moment distribution. Here we do not follow the same wavenumber-domain reasoning used by all these authors. Moreover, equation 15 generalizes this positivity condition because (1) it holds true for all cases in which the magnetization of the equivalent layer has the same direction as the true magnetization of the sources, regardless it is purely induced or not, (2) does not require that the observed total-field anomaly data be on a plane and, (3) does not require a planar equivalent layer.

Parametrization and forward problem

In practical situations, its not possible to determine a continuous magnetic-moment distribution $p(x', y', z_c)$ over the layer as shown in equation 1. For this reason, the layer has to be approximated by a discrete set of dipoles with unit volume located at a constant depth $z = z_c$. By discretizing the integrand of equation 1, the predicted total-field anomaly at the point (x_i, y_i, z_i) is given by

$$\Delta T_i = f_i(\mathbf{s}), \quad (16)$$

where ΔT_i is the i th element of the N -dimensional vector of predicted total-field anomaly $\Delta \mathbf{T}(\mathbf{s})$. The function f_i maps the unknown parameters onto the data, in which the parameter vector \mathbf{s} is formed by an M -dimensional vector \mathbf{p} whose j th element p_j is the magnetic moment of the j th dipole with a single magnetization direction \mathbf{q} (equation 6) assigned to all dipoles (figure 1). Explicitly, the function f_i is described as

$$f_i(\mathbf{s}) = \sum_{j=1}^M p_j g_{ij}(\mathbf{q}) = \mathbf{p}^T \mathbf{g}_i(\mathbf{q}), \quad (17)$$

where

$$g_{ij}(\mathbf{q}) = \gamma_m \hat{\mathbf{F}}_0^T \mathbf{M}_{ij} \hat{\mathbf{m}}(\mathbf{q}) \quad (18)$$

is an harmonic function representing the total-field anomaly at the i th position (x_i, y_i, z_i) yielded by a j th dipole located at (x_j, y_j, z_c) with unit magnetic-moment intensity. The matrix \mathbf{M}_{ij} is formed by the second derivatives of a function ϕ_{ij} that depends on the inverse of the scalar function $r_{ij} = [(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_c)^2]^{1/2}$, analogously to equations 3 and 4. From equations 16-18, we can notice that the predicted total-field anomaly $\Delta \mathbf{T}(\mathbf{s})$ has a linear relation with the magnetic moment \mathbf{p} and a nonlinear relation with the magnetization direction \mathbf{q} .

Inverse problem

Let $\Delta \mathbf{T}^o$ be an N -dimensional vector whose i th element ΔT_i^o is the total-field anomaly observation produced by a magnetic source at the point (x_i, y_i, z_i) , $i = 1, \dots, N$. In order to

estimate the magnetization direction, we have to formulate an inverse problem by imposing a positivity constraint on the magnetic-moment distribution. It can be performed minimizing the difference between the observed data $\Delta \mathbf{T}^o$ and the predicted data $\Delta \mathbf{T}(\mathbf{s})$ by solving the following constrained problem of

$$\text{minimizing} \quad \Psi(\mathbf{s}) = \|\Delta \mathbf{T}^o - \Delta \mathbf{T}(\mathbf{s})\|_2^2 + \mu f_0 \|\mathbf{p}\|_2^2 \quad (19a)$$

$$\text{subject to} \quad \mathbf{p} \geq 0. \quad (19b)$$

On the right side of equation 19a the first and second terms are the data-misfit function and the zeroth-order Tikhonov regularization function, μ is the regularizing parameter, $\|\cdot\|_2^2$ represents the squared Euclidean norm and f_0 is a normalizing factor. In the inequality 19b, $\mathbf{0}$ is a null vector and the inequality sign is applied element by element. This inequality imposes positivity constraints on the estimated magnetic moments of all dipoles, which is solved by using the nonnegative least squares (NNLS) proposed by Lawson and Hanson (1974).

Minimizing the goal function shown in equation 19a starts with an initial approximation \mathbf{s}^k to the parameter vector and then solving a sequence of linear problem of estimating a correction $\Delta \mathbf{s}^k$ at each k th iteration. The procedure is repeated until a minimum of goal function (equation 19a) is reached. This procedure is determined by using a gradient-based iterative optimization method like Gauss-Newton (Aster et al., 2005). Mathematically, the correction $\Delta \mathbf{s}^k$ is expressed as a second-order expansion of the goal function given by

$$\Psi(\mathbf{s}^k + \Delta \mathbf{s}^k) \approx \Psi(\mathbf{s}^k) + \mathbf{J}^{kT}(\mathbf{s}^k) \Delta \mathbf{s}^k + \frac{1}{2} \Delta \mathbf{s}^{kT} \mathbf{H}^k(\mathbf{s}^k) \Delta \mathbf{s}^k \quad (20)$$

in which $\mathbf{J}^k(\mathbf{s}^k)$ and $\mathbf{H}^k(\mathbf{s}^k)$ are, respectively, the gradient vector and the Hessian matrix

of equation 19a. Thus, taking the gradient of the function 20, the parameter perturbation vector $\Delta \mathbf{s}^k$ at the k th iteration is obtained by solving the linear system

$$\mathbf{H}^k(\mathbf{s}^k) \Delta \mathbf{s}^k = -\mathbf{J}^k(\mathbf{s}^k), \quad (21)$$

where the estimate $\Delta \mathbf{s}^k$ is a single step of the Gauss-Newton method required to attain the minimum of the expanded function (equation 20). The linear system given by equation 21 can be rewritten as

$$\left[\begin{array}{c|c} \mathbf{H}_{pp}^k & \mathbf{H}_{pq}^k \\ \hline \mathbf{H}_{qp}^k & \mathbf{H}_{qq}^k \end{array} \right] \left[\begin{array}{c} \Delta \mathbf{p}^k \\ \Delta \mathbf{q}^k \end{array} \right] = - \left[\begin{array}{c} \mathbf{J}_p^k \\ \mathbf{J}_q^k \end{array} \right], \quad (22)$$

in which \mathbf{J}_α^k and $\mathbf{H}_{\alpha\beta}^k$, where $\alpha = p, q$ and $\beta = p, q$, are the gradient vector and the Hessian matrix calculated in relation to each component of the magnetic-moment vector \mathbf{p} and the magnetization direction vector \mathbf{q} , respectively. Besides, in order to simplify the linear system 22, we consider null cross-derivatives.

However, the gradient vector and the Hessian matrix relative to the part of magnetic moments are, respectively,

$$\mathbf{J}_p^k = -2\mathbf{G}_p^{kT} [\Delta \mathbf{T}^o - \Delta \mathbf{T}(\mathbf{s}^k)] + 2\mu f_0^k \mathbf{p}^k \quad (23)$$

and

$$\mathbf{H}_{pp}^k = 2\mathbf{G}_p^{kT} \mathbf{G}_p^k + 2\mu f_0^k \mathbf{I} \quad (24)$$

where \mathbf{G}_p^k is the $N \times M$ sensitivity matrix at the k th iteration, whose elements are composed by the derivative of equation 19a in relation of j th element of the vector \mathbf{p}^k , \mathbf{I} is an identity

matrix and the normalizing factor f_0^k is equal to

$$f_0^k = \frac{\text{tr}(\mathbf{G}_p^{kT} \mathbf{G}_p^k)}{M}, \quad (25)$$

where tr is denotated as the trace of the matrix $\mathbf{G}_p^{kT} \mathbf{G}_p^k$ and M is the total number of dipoles composing the layer. From the correction $\Delta \mathbf{p}^k = \mathbf{p}^{k+1} - \mathbf{p}^k$, we can conclude that the linear system to be solved is given by

$$\left[\mathbf{G}_p^{kT} \mathbf{G}_p^k + \mu f_0^k \mathbf{I} \right] \mathbf{p}^{k+1} = \mathbf{G}_p^{kT} \Delta \mathbf{T}^o. \quad (26)$$

Owing to nonlinear relation of the magnetization direction \mathbf{q}^k with the predicted total-field anomaly, the gradient vector and the Hessian matrix for this case are, respectively,

$$\mathbf{J}_q^k = -2\mathbf{G}_q^{kT} [\Delta \mathbf{T}^o - \Delta \mathbf{T}(\mathbf{s}^k)] \quad (27)$$

and

$$\mathbf{H}_{qq}^k = 2\mathbf{G}_q^{kT} \mathbf{G}_q^k \quad (28)$$

in which \mathbf{G}_q^k is a $N \times 2$ sensitivity matrix, whose elements are composed by derivative of equation 19 in relation of each component of the vector \mathbf{q}^k , that are the inclination and declination, respectively. Nevertheless, in order to calculate the correction $\Delta \mathbf{q}^k$ at the k th iteration, we use the Levenberg-Marquardt method (Aster et al., 2005) by solving the linear system

$$\left[\mathbf{G}_q^{kT} \mathbf{G}_q^k + \lambda^k \mathbf{I} \right] \Delta \mathbf{q}^k = \mathbf{G}_q^{kT} [\Delta \mathbf{T}^o - \Delta \mathbf{T}(\mathbf{s}^k)], \quad (29)$$

where λ is the Marquardt parameter that is updated along the iterative process and \mathbf{I} is an identity matrix.

Iterative process for magnetization estimation

The estimation of the magnetic moments $\mathbf{p}^\#$ and the magnetization direction $\mathbf{q}^\#$ is formulated as an inverse problem of minimizing the difference between the observed data $\Delta\mathbf{T}^o$ and the predicted data $\Delta\mathbf{T}(\mathbf{s})$. As we can notice, the solution of the inversion is given by solving two linear systems, one shown in equation 26 and other in equation 29. For this reason, we propose a nested algorithm for solving the inverse problem in two steps.

Our iterative algorithm starts with an initial guess for the magnetization direction \mathbf{q}_0 . At the k th iteration, we calculated a set of magnetic moment \mathbf{p}^k by imposing a positivity constraint on equation 26. After estimating the magnetic-moment distribution \mathbf{p}^k at the k th iteration using the previous estimate \mathbf{q}^k for the magnetization direction, we estimate a new vector \mathbf{q}^{k+1} by solving an unconstrained nonlinear inverse problem and applying the correction $\Delta\mathbf{q}^k$ using the equation 29. The iterative process stops when the minimum of the goal function (equation 19a) is reached. An overview of the algorithm is shown in figure 2 and in the algorithm 1.

Algorithm 1: Nested NNLS and Levenberg-Marquardt method

Input : $\Delta \mathbf{T}^o, \mathbf{q}_0$

Output: $\mathbf{p}^\sharp, \mathbf{q}^\sharp$

```
while (not converge) or ( $i < i_{max}$ ) do
    step 1: Solve equation 26 using NNLS ;
    step 2: Compute goal function (19) ;
    while (not converge) or ( $j < j_{max}$ ) do
        step 3: Initialize the Levenberg-Marquardt algorithm ;
        step 4: Compute goal function (19);
        while  $k < k_{marq}$  do
            step 5: Solve equation 29 ;
            step 6: Apply the correction for magnetization direction ;
            step 7: Compute goal function (19);
        end
        step 8: Analysis of convergence for inner loop.
    end
    step 9: Analysis of convergence for outer loop.
end
```

The choice of layer depth z_c and regularization parameter μ

The procedure for the use of our methodology for estimating the total magnetization require the choice of two main parameters. The first one is the layer depth z_c as shown in figure 1 and the second is the regularization parameter μ shown in equation 26.

The method of the choice of layer is based on a classical approach proposed by Dampney

(1969). The author pointed out that the layer depth should satisfy an interval from 2.5 to 6 times the grid spacing. It should be notice that this rule was applied on an evenly spaced data. However, the choice for applying our method should correspond to an interval from 2 to 3 times the greater grid spacing. It is necessarily to point out that this range of values was found empirically due to the application on a irregular grid data.

To solve the equation 26 we have to choose a reliable regularization parameter μ . For this purpose, we use the L-curve method (Hansen and OLeary, 1993). This approach is widely used in the literature to find a regularizing parameter, which filtering out enough noise whithout loosing to much information in the final solution. The procedure of finding the parameter is basically to plot a curve of optimal values between the solution norm and residual norm. The corner of the curve is the final result which gives a threshold between the regularization function and the data misfit.

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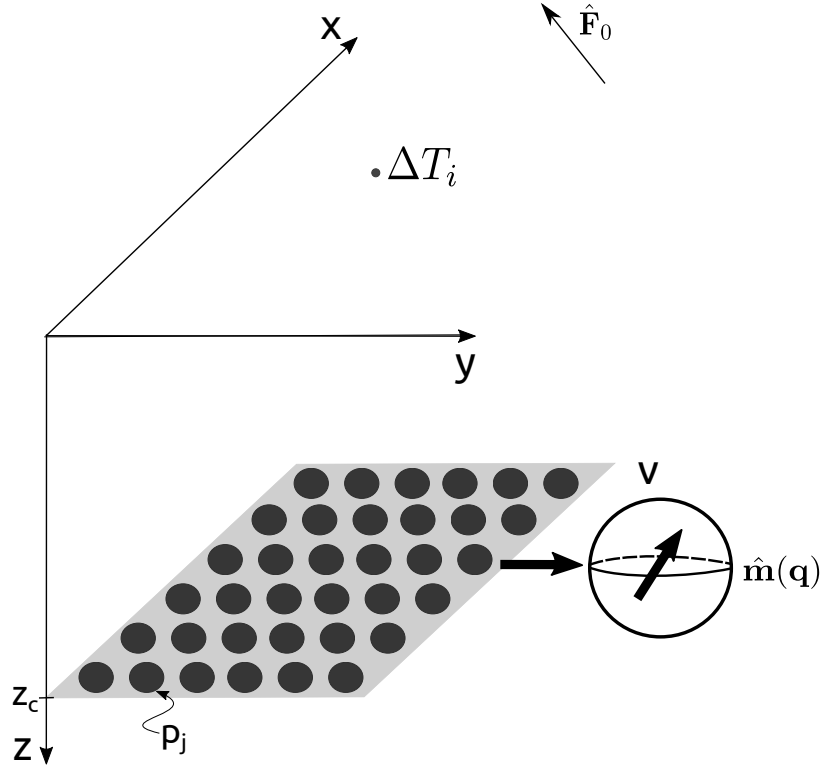


Figure 1: Schematic representation of an equivalent layer. The layer is positioned over the horizontal plane at a depth of $z = z_c$. $\Delta T_i = f_i(\mathbf{s})$ is the predicted total-field anomaly at the point (x_i, y_i, z_i) produced by the set of M equivalent sources (black dots). Each source is located at the point (x_j, y_j, z_c) , $j = 1, \dots, M$, and represented by a dipole with unity volume v with magnetization direction $\hat{\mathbf{m}}(\mathbf{q})$ and magnetic moment p_j .

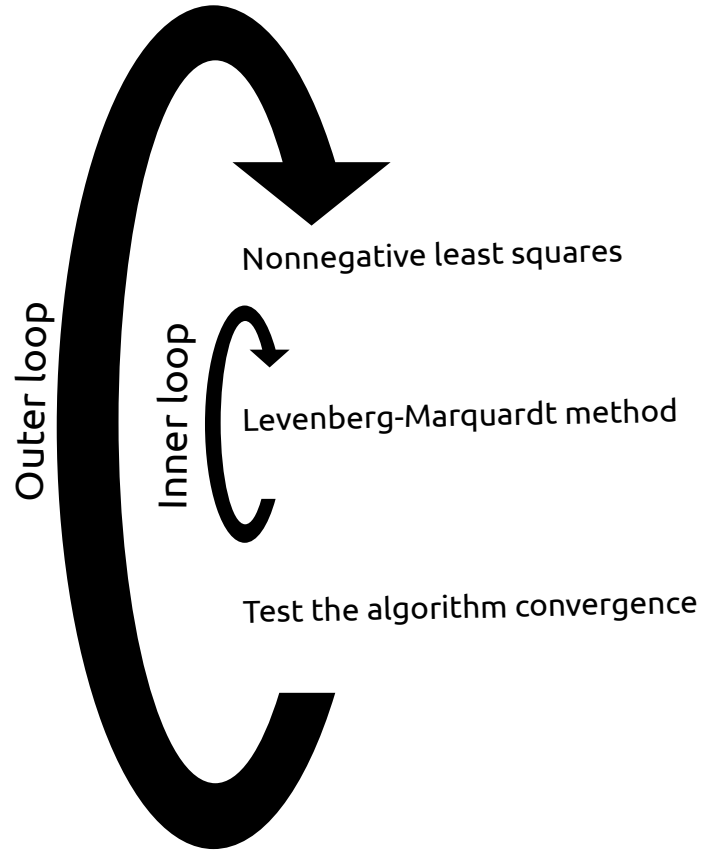


Figure 2: Iterative scheme overview for NNLS and Levenberg-Marquardt method for estimating magnetization direction. The outer loop is the nonnegative solution for magnetic-moment distribution and the inner loop calculates the magnetization direction correction using Levenberg-Marquardt method.

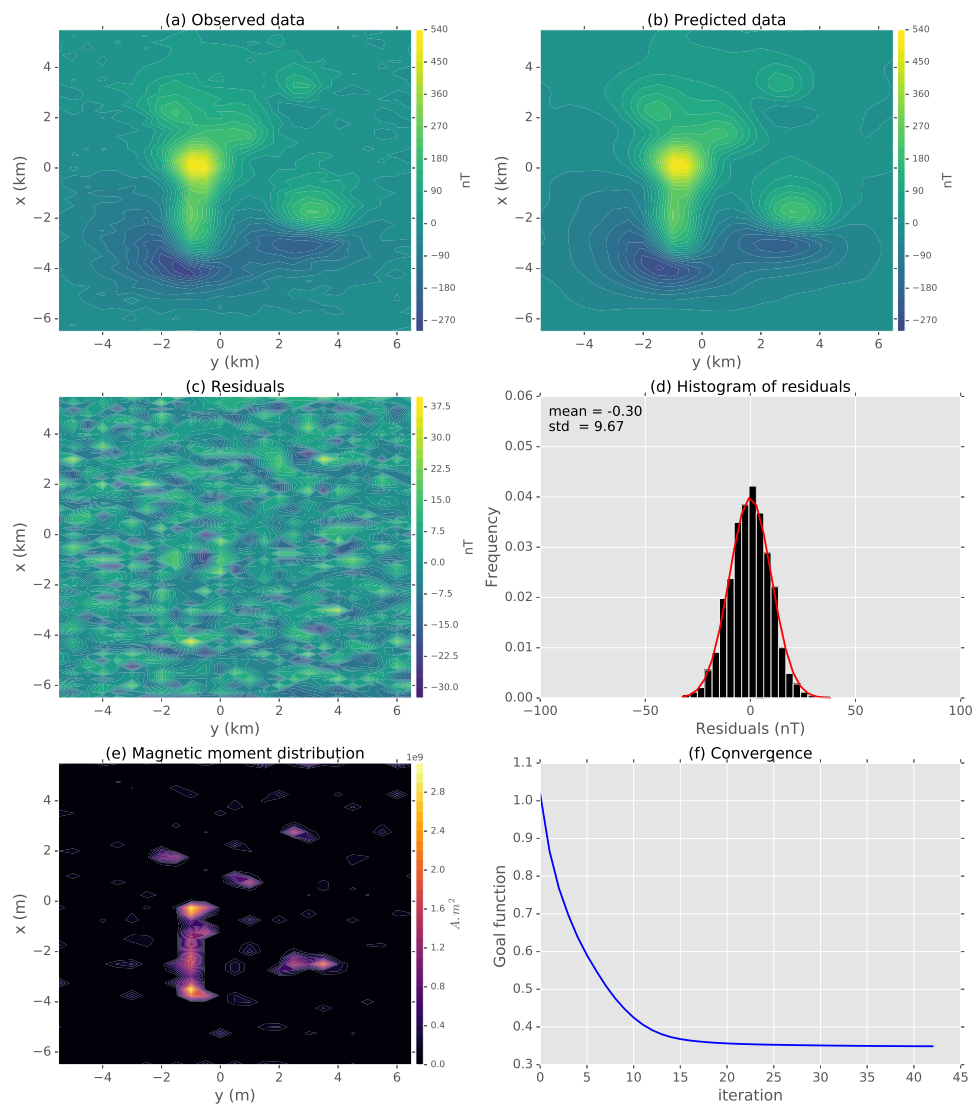


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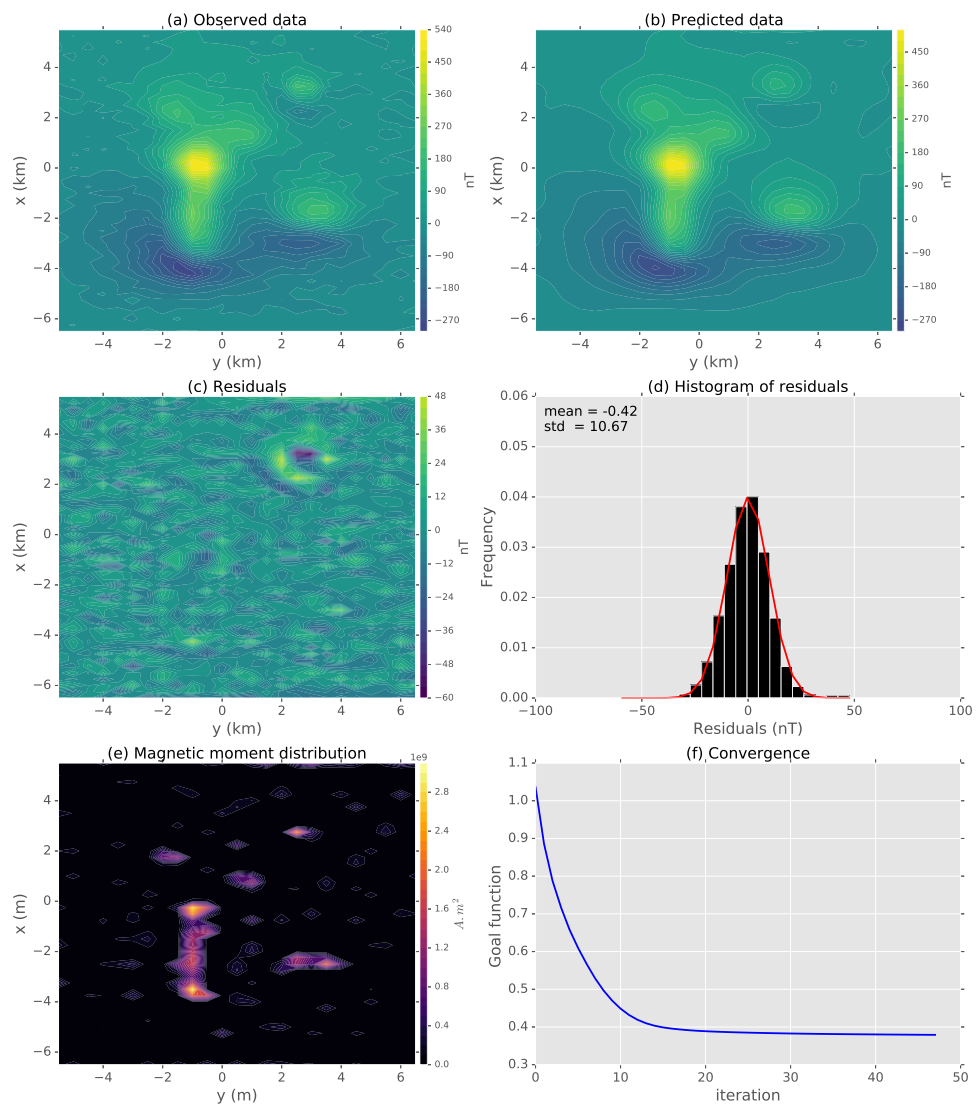


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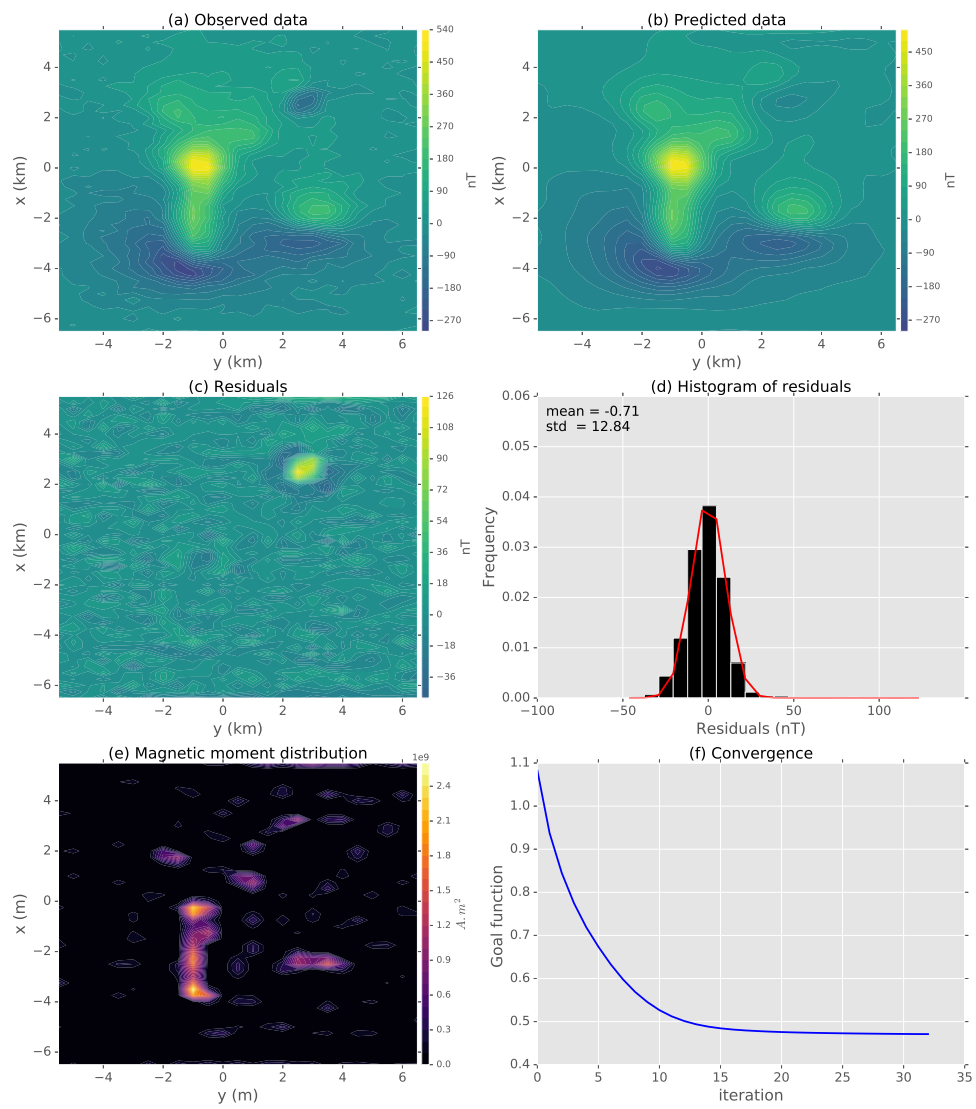


Figure 5: