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1

The computation aspects of the equivalent-layer technique: review and perspective

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1 FUNDAMENTALS

Let $\mathbf{d}$ be a $D \times 1$ vector, whose i-th element d_i is the observed potential field at the position (x_i, y_i, z_i), $i \in \{1 : D\}$, of a topocentric Cartesian system with x, y and z axes pointing to north, east and down, respectively. Consider that d_i can be satisfactorily approximated by a harmonic function

$$f_i = \sum_{j=1}^{P} g_{ij}\, p_j \,, \quad i \in \{1 : D\} \,, \tag{1}$$

where, p_j represents the scalar physical property of a virtual source (i.e., monopole, dipole, prism) located at (x_j, y_j, z_j), $j \in \{1 : P\}$ and

$$g_{ij} \equiv g(x_i - x_j, y_i - y_j, z_i - z_j) \,, \quad z_i < \min\{z_j\} \,, \quad \forall i \in \{1 : D\} \,, \tag{2}$$

is a harmonic function, where $\min\{z_j\}$ denotes the minimum z_j, or the vertical coordinate of the shallowest virtual source. These virtual sources are called *equivalent sources* and they form an *equivalent layer*. In matrix notation, the potential field produced by all equivalent sources at all points (x_i, y_i, z_i), $i \in \{1 : D\}$, is given by:

$$\mathbf{f} = \mathbf{G}\mathbf{p} \,, \tag{3}$$

where $\mathbf{p}$ is a $P \times 1$ vector with j-th element p_j representing the scalar physical property of the j-th equivalent source and $\mathbf{G}$ is a $D \times P$ matrix with element g_{ij} given by equation 2.

The equivalent-layer technique consists in solving a linear inverse problem to determine a parameter vector $\mathbf{p}$ leading to a predicted data vector $\mathbf{f}$ (equation 3) *sufficiently close to* the observed data vector $\mathbf{d}$, whose i-th element d_i is the observed potential field at (x_i, y_i, z_i). The notion of *closeness* is intrinsically related to the concept of *vector norm* (e.g., Golub and Van Loan, 2013, p. 68) or *measure of length* (e.g., Menke, 2018, p. 41). Because of that, almost all methods for determining $\mathbf{p}$ actually estimate a parameter vector $\tilde{\mathbf{p}}$ minimizing a length measure of the difference between $\mathbf{f}$ and $\mathbf{d}$ (see subsection 1.3). Given an estimate $\tilde{\mathbf{p}}$, it is then possible to compute a potential field transformation

$$\mathbf{t} = \mathbf{A}\tilde{\mathbf{p}} \,, \tag{4}$$

where $\mathbf{t}$ is a $T \times 1$ vector with k-th element t_k representing the transformed potential field at the position (x_k, y_y, z_k), $k \in \{1 : T\}$, and

$$a_{kj} \equiv a(x_k - x_j, y_k - y_j, z_k - z_j) \,, \quad z_k < \min\{z_j\} \,, \quad \forall k \in \{1 : T\} \,, \tag{5}$$

is a harmonic function representing the kj-th element of the $T \times P$ matrix $\mathbf{A}$.

1.1 Spatial distribution and total number of equivalent sources

There is no well-established criteria to define the optimum number P or the spatial distribution of the equivalent sources. We know that setting an equivalent layer with more (less) sources than potential-field data usually leads to an underdetermined (overdetermined) inverse problem (e.g., Menke, 2018, p. 52–53). Concerning the spatial distribution of the equivalent sources, the only condition is that they must rely on a surface that is located below and does not cross that containing the potential field data. Soler and Uieda (2021) present a practical discussion about this topic.

From a theoretical point of view, the equivalent layer reproducing a given potential field data set cannot cross the true gravity or magnetic sources. This condition is a consequence of recognizing that the equivalent layer is essentially an indirect solution of a boundary value problem of potential theory (e.g., Roy, 1962; Zidarov, 1965; Dampney, 1969; Li et al., 2014; Reis et al., 2020). In practical applications, however, there is no guarantee that this condition is satisfied. Actually, its is widely known from practical experience (e.g., Gonzalez et al., 2022) that the equivalent-layer technique works even for the case in which the layer cross the true sources.

Regarding the depth of the equivalent layer, Dampney (1969) proposed a criterion based on horizontal data sampling, suggesting that the equivalent-layer depth should be between two and six times the horizontal grid spacing, considering evenly spaced data. However, when dealing with a survey pattern that has unevenly spaced data, Reis et al. (2020) adopted an alternative empirical criterion. According to their proposal, the depth of the equivalent layer should range from two to three times the spacing between adjacent flight lines. The criteria of Dampney (1969) and Reis et al. (2020) are valid for planar equivalent layers. Cordell (1992) have proposed and an alternative criterion for scattered data that leads to an undulating equivalent layer. This criterion have been slightly modified by Guspí et al. (2004), Guspí and Novara (2009) and Soler and Uieda (2021), for example, and consists in setting one equivalent source below each datum at a depth proportional to the horizontal distance to the nearest neighboring data points. Soler and Uieda (2021) have compared different strategies for defining the equivalent sources depth for the specific problem of interpolating gravity data, but they have not found significant differences between them.

1.2 Matrix G

Generally, the harmonic function g_{ij} (equation 2) is defined in terms of the inverse distance between the observation point (x_i, y_i, z_i) and the j-th equivalent source at (x_j, y_j, z_j),

$$\frac{1}{r_{ij}} \equiv \frac{1}{\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}} \,, \tag{6}$$

or by its partial derivatives of first and second orders, respectively given by

$$\partial_\alpha \frac{1}{r_{ij}} \equiv \frac{-(\alpha_i - \alpha_j)}{r_{ij}^3} \,, \quad \alpha \in \{x, y, z\} \,, \tag{7}$$

and

$$\partial_{\alpha\beta} \frac{1}{r_{ij}} \equiv \begin{cases} \frac{3\,(\alpha_i - \alpha_j)^2}{r_{ij}^5} \,, & \alpha = \beta \,, \\ \frac{3\,(\alpha_i - \alpha_j)\,(\beta_i - \beta_j)}{r_{ij}^5} - \frac{1}{r_{ij}^3} \,, & \alpha \neq \beta \,, \end{cases} \quad \alpha, \beta \in \{x, y, z\} \,. \tag{8}$$

In this case, the equivalent layer is formed by punctual sources representing monopoles or dipoles (e.g., Dampney, 1969; Emilia, 1973; Leão and Silva, 1989; Cordell, 1992; Oliveira Jr. et al., 2013; Siqueira et al., 2017; Reis et al., 2020; Takahashi et al., 2020; Soler and Uieda, 2021; Takahashi et al., 2022). Another common approach consists in not defining g_{ij} by using equations 6–8, but other harmonic functions obtained by integrating them over the volume of regular prisms (e.g., Li and Oldenburg, 2010; Barnes and Lumley, 2011; Li et al., 2014; Jirigalatu and Ebbing, 2019). There are also some less common approaches defining the harmonic function g_{ij} (equation 2) as the potential field due to plane faces with constant physical property (Hansen and Miyazaki, 1984), doublets (Silva, 1986) or by computing the double integration of the inverse distance function with respect to z (Guspí and Novara, 2009).

A common assumption for most of the equivalent-layer methods is that the harmonic function g_{ij} (equation 2) is independent on the actual physical relationship between the observed potential field and their true sources (e.g., Cordell, 1992; Guspí and Novara, 2009; Li et al., 2014). Hence, g_{ij} can be defined according to the problem. The only condition imposed to this function is that it decays to zero as the observation point (x_i, y_i, z_i) goes away from the position (x_j, y_j, z_j) of the j-th equivalent source. However, several methods use a function g_{ij} that preserves the physical relationship between the observed potential field and their true sources. For the case in which the observed potential field is gravity data, g_{ij} is commonly defined as a component of the gravitational field produced at (x_i, y_i, z_i) by a point mass or prism located at (x_j, y_j, z_j), with unit density. On the other hand, g_{ij} is commonly defined as a component of the magnetic induction field produced at (x_i, y_i, z_i) by a dipole or prism located at (x_j, y_j, z_j), with unit magnetization intensity, when the observed potential field is magnetic data.

The main challenge in the equivalent-layer technique is the computational complexity associated with handling large datasets. This complexity arises because the sensitivity matrix $\mathbf{G}$ (equation 3) is dense regardless of the harmonic function g_{ij} (equation 2) employed. In the case of scattered potential-field data, the structure of $\mathbf{G}$ is not well-defined, regardless of the spatial distribution of the equivalent sources. However, in a specific scenario where (i) each potential-field datum is directly associated with a single equivalent source located directly below it, and (ii) both the data and sources are based on planar and regularly spaced grids, Takahashi et al. (2020, 2022) demonstrate that $\mathbf{G}$ exhibits a block-Toeplitz Toeplitz-block (BTTB) structure. In such cases, the product of $\mathbf{G}$ and an arbitrary vector can be efficiently computed using a 2D fast Fourier transform as a discrete convolution.

1.3 General formulation

A general formulation for almost all equivalent-layer methods can be achieved by first considering that the $P \times 1$ parameter vector $\mathbf{p}$ (equation 3) can be reparameterized into a $Q \times 1$ vector $\mathbf{q}$ according to:

$$\mathbf{p} = \mathbf{H}\,\mathbf{q}\,, \tag{9}$$

where $\mathbf{H}$ is a $P \times Q$ matrix. The predicted data vector $\mathbf{f}$ (equation 3) can then be rewritten as follows:

$$\mathbf{f} = \mathbf{G}\,\mathbf{H}\,\mathbf{q}\,. \tag{10}$$

Note that the original parameter vector $\mathbf{p}$ is defined in a P-dimensional space whereas the reparameterized parameter vector $\mathbf{q}$ (equation 9) lies in a Q-dimensional space. For convenience, we use the terms P-space and Q-space to designate them.

In this case, the problem of estimating a parameter vector $\tilde{\mathbf{p}}$ minimizing a length measure of the difference between $\mathbf{f}$ (equation 3) and $\mathbf{d}$ is replaced by that of estimating an auxiliary vector $\tilde{\mathbf{q}}$ minimizing the goal function

$$\Gamma(\mathbf{q}) = \Phi(\mathbf{q}) + \mu\,\Theta(\mathbf{q})\,, \tag{11}$$

which is a combination of particular measures of length given by

$$\Phi(\mathbf{q}) = (\mathbf{d} - \mathbf{f})^\top\,\mathbf{W}_d\,(\mathbf{d} - \mathbf{f})\;, \tag{12}$$

and

$$\Theta(\mathbf{q}) = (\mathbf{q} - \bar{\mathbf{q}})^\top\,\mathbf{W}_q\,(\mathbf{q} - \bar{\mathbf{q}})\;, \tag{13}$$

where the regularization parameter μ is a positive scalar controlling the trade-off between the data-misfit function $\Phi(\mathbf{q})$ and the regularization function $\Theta(\mathbf{q})$; $\mathbf{W}_d$ is a $D \times D$ symmetric matrix defining the relative importance of each observed datum d_i; $\mathbf{W}_q$ is a $Q \times Q$ symmetric matrix imposing prior information on $\mathbf{q}$; and $\bar{\mathbf{q}}$ is a $Q \times 1$ vector of reference values for $\mathbf{q}$ that satisfies

$$\bar{\mathbf{p}} = \mathbf{H}\,\bar{\mathbf{q}}\,, \tag{14}$$

where $\bar{\mathbf{p}}$ is a $P \times 1$ vector containing reference values for the original parameter vector $\mathbf{p}$.

After obtaining an estimate $\tilde{\mathbf{q}}$ for the reparameterized parameter vector $\mathbf{q}$ (equation 9), the estimate $\tilde{\mathbf{p}}$ for the original parameter vector (equation 3) is computed by

$$\tilde{\mathbf{p}} = \mathbf{H}\,\tilde{\mathbf{q}}\,. \tag{15}$$

The reparameterized vector $\tilde{\mathbf{q}}$ is obtained by first computing the gradient of $\Gamma(\mathbf{q})$,

$$\boldsymbol{\nabla}\Gamma(\mathbf{q}) = -2\,\mathbf{H}^\top\mathbf{G}^\top\mathbf{W}_d\,(\mathbf{d} - \mathbf{f}) + 2\,\mu\,\mathbf{W}_q\,(\mathbf{q} - \bar{\mathbf{q}})\;. \tag{16}$$

Then, by considering that $\boldsymbol{\nabla}\Gamma(\tilde{\mathbf{q}}) = \mathbf{0}$ (equation 16), where $\mathbf{0}$ is a vector of zeros, as well as adding and subtracting the term $\left(\mathbf{H}^\top\mathbf{G}^\top\mathbf{W}_d\mathbf{G}\,\mathbf{H}\right)\bar{\mathbf{q}}$, we obtain

$$\tilde{\boldsymbol{\delta}}_q = \mathbf{B}\,\boldsymbol{\delta}_d\,, \tag{17}$$

where

$$\tilde{\boldsymbol{\delta}}_q = \tilde{\mathbf{q}} - \bar{\mathbf{q}}\,, \tag{18}$$

$$\boldsymbol{\delta}_d = \mathbf{d} - \mathbf{G}\,\mathbf{H}\,\bar{\mathbf{q}}\,, \tag{19}$$

$$\mathbf{B} = \left(\mathbf{H}^\top\mathbf{G}^\top\mathbf{W}_d\,\mathbf{G}\,\mathbf{H} + \mu\,\mathbf{W}_q\right)^{-1}\mathbf{H}^\top\mathbf{G}^\top\mathbf{W}_d\,, \tag{20}$$

or, equivalently (Menke, 2018, p. 62),

$$\mathbf{B} = \mathbf{W}_q^{-1}\,\mathbf{H}^\top\mathbf{G}^\top\left(\mathbf{G}\,\mathbf{H}\,\mathbf{W}_q^{-1}\,\mathbf{H}^\top\mathbf{G}^\top + \mu\mathbf{W}_d^{-1}\right)^{-1}\;. \tag{21}$$

Evidently, we have considered that all inverses exist in equations 20 and 21.

The $Q \times D$ matrix $\mathbf{B}$ defined by equation 20 is commonly used for the case in which $D > Q$, i.e., when there are more data than parameters (overdetermined problems). In this case, we consider that the estimate $\tilde{\mathbf{q}}$ is obtained by solving the following linear system for $\tilde{\boldsymbol{\delta}}_q$ (equation 18):

$$\left(\mathbf{H}^\top\mathbf{G}^\top\mathbf{W}_d\,\mathbf{G}\,\mathbf{H} + \mu\,\mathbf{W}_q\right)\tilde{\boldsymbol{\delta}}_q = \mathbf{H}^\top\mathbf{G}^\top\mathbf{W}_d\,\boldsymbol{\delta}_d\,. \tag{22}$$

On the other hand, for the cases in which $D < Q$ (underdetermined problems), matrix $\mathbf{B}$ is usually defined according to equation 21. In this case, the general approach involves estimating $\tilde{\mathbf{q}}$ in two steps. The first consists in solving a linear system for a dummy vector, which is subsequently used to compute $\tilde{\mathbf{q}}$ by a

matrix-vector product as follows:

$$\begin{aligned} \left(\mathbf{G}\,\mathbf{H}\,\mathbf{W}_q^{-1}\,\mathbf{H}^\top\mathbf{G}^\top + \mu\mathbf{W}_d^{-1}\right)\mathbf{u} &= \boldsymbol{\delta}_d \\ \tilde{\boldsymbol{\delta}}_q &= \mathbf{W}_q^{-1}\,\mathbf{H}^\top\mathbf{G}^\top\mathbf{u} \end{aligned} \quad , \tag{23}$$

where $\mathbf{u}$ is a dummy vector. After obtaining $\tilde{\boldsymbol{\delta}}_q$ (equations 22 and 23), the estimate $\tilde{\mathbf{q}}$ is computed with equation 18.

1.3.1 Optional normalization strategy

Setting the regularization parameter μ (equation 11) can be very difficult due to scale differences between $\mathbf{G}$ and $\mathbf{p}$ (equation 3) or $\mathbf{GH}$ and $\mathbf{q}$ (equation 9. When faced with this scenario, a popular strategy (e.g., Li and Oldenburg, 2010; Soler and Uieda, 2021) involves creating the linear system (equations 22 and 23) by substituting $\mathbf{GH}$ and $\mathbf{q}$ with

$$\mathbf{G}_n = \mathbf{G}\,\mathbf{H}\,\mathbf{N}\,, \quad \mathbf{q}_n = \mathbf{N}^{-1}\mathbf{q}\,, \tag{24}$$

and then finding the solution $\tilde{\mathbf{q}}_n$ for the normalized parameter vector $\mathbf{q}_n$. The estimate $\tilde{\mathbf{q}}$ for the reparameterized parameter vector $\mathbf{q}$ (equation 9) is subsequently obtained by removing the normalization as follows:

$$\tilde{\mathbf{q}} = \mathbf{N}\,\tilde{\mathbf{q}}_n\,, \tag{25}$$

where $\mathbf{N}$ is an invertible normalization matrix. This strategy usually constrains the practical range of the regularization parameter μ (equation 11).

1.3.2 Classical approach

The classical approach in the equivalent-layer technique consists in using $\mathbf{H} = \mathbf{I}_P$, so that $P = Q$, $\mathbf{p} = \mathbf{q}$ (equation 9), $\bar{\mathbf{p}} = \bar{\mathbf{q}}$ (equation 14), $\tilde{\mathbf{p}} = \tilde{\mathbf{q}}$ (equation 15), $\mathbf{p}_n = \mathbf{q}_n$ (equation 24) and $\tilde{\mathbf{p}}_n = \tilde{\mathbf{q}}_n$ (equation 25). In this case, the linear system (equations 22 and 23) is directly solved for

$$\tilde{\boldsymbol{\delta}}_p = \tilde{\mathbf{p}} - \bar{\mathbf{p}}\,, \tag{26}$$

instead of $\tilde{\boldsymbol{\delta}}_q$ (equation 18).

2 NOTATION FOR SUBVECTORS AND SUBMATRICES

Here, we use a notation inspired on that presented by (Van Loan, 1992, p. 4) to represent subvectors and submatrices. Subvectors of $\mathbf{d}$, for example, are specified by $\mathbf{d}[\mathbf{i}]$, where $\mathbf{i}$ is a list of integer numbers that "pick out" the elements of $\mathbf{d}$ forming the subvector $\mathbf{d}[\mathbf{i}]$. For example, $\mathbf{i} = (1, 6, 4, 6)$ gives the subvector $\mathbf{d}[\mathbf{i}] = [d_1 \;\; d_6 \;\; d_4 \;\; d_6]^\top$. Note that the list $\mathbf{i}$ of indices may be sorted or not and it may also have repeated indices. For the particular case in which the list has a single element $\mathbf{i} = (i)$, then it can be used to extract the i-th element $d_i \equiv \mathbf{d}[i]$ of $\mathbf{d}$. Regular lists can be represented by using the colon notation. For example,

$$\begin{aligned} \mathbf{i} = (3:8) &\Leftrightarrow \mathbf{d}[\mathbf{i}] = [d_3 \;\; d_4 \;\; \ldots \;\; d_8]^\top \\ \mathbf{i} = (:8) &\Leftrightarrow \mathbf{d}[\mathbf{i}] = [d_1 \;\; d_2 \;\; \ldots \;\; d_8]^\top \\ \mathbf{i} = (3:) &\Leftrightarrow \mathbf{d}[\mathbf{i}] = [d_3 \;\; d_4 \;\; \ldots \;\; d_D]^\top \end{aligned} \quad ,$$

where D is the number of elements forming $\mathbf{d}$.

The notation above can also be used to define submatrices of the $D \times P$ matrix $\mathbf{G}$. For example, $\mathbf{i} = (2, 7, 4, 6)$ and $\mathbf{j} = (1, 3, 8)$ lead to the submatrix

$$\mathbf{G}[\mathbf{i}, \mathbf{j}] = \begin{bmatrix} g_{21} & g_{23} & g_{28} \\ g_{71} & g_{73} & g_{78} \\ g_{41} & g_{43} & g_{48} \\ g_{61} & g_{63} & g_{68} \end{bmatrix} .$$

Note that, in this case, the lists $\mathbf{i}$ and $\mathbf{j}$ "pick out", respectively, the rows and columns of $\mathbf{G}$ that form the submatrix $\mathbf{G}[\mathbf{i}, \mathbf{j}]$. The i-th row of $\mathbf{G}$ is given by the $1 \times P$ vector $\mathbf{G}[i, :]$. Similarly, the $D \times 1$ vector $\mathbf{G}[:, j]$ represents the j-th column. Finally, we may use the colon notation to define the following submatrix:

$$\mathbf{i} = (2:5), \mathbf{j} = (3:7) \Leftrightarrow \mathbf{G}[\mathbf{i}, \mathbf{j}] = \begin{bmatrix} g_{23} & g_{24} & g_{25} & g_{26} & g_{27} \\ g_{33} & g_{34} & g_{35} & g_{36} & g_{37} \\ g_{43} & g_{44} & g_{45} & g_{46} & g_{47} \\ g_{53} & g_{54} & g_{55} & g_{56} & g_{57} \end{bmatrix} ,$$

which contains the contiguous elements of $\mathbf{G}$ from rows 2 to 5 and from columns 3 to 7.

3 COMPUTATIONAL STRATEGIES

Here, we review some strategies for reducing the computational cost of equivalent-layer technique. Typically, estimating a parameter vector $\tilde{\mathbf{p}}$ or $\tilde{\mathbf{q}}$ requires to solve a large-scale linear inversion (equations 22 and 23). This, in turn, means to deal with some obstacles concerning large computational cost:

(i) the large computer memory to store large and full matrices;

(ii) the long computation time to multiply a matrix by a vector; and

(iii) the long computation time to solve a large linear system of equations.

Two important factors affecting the efficiency of a given matrix algorithm are the storage and amount of required arithmetic. Here, we quantify this last factor by counting *flops*, which are floating point additions, subtractions, multiplications or divisions (Golub and Van Loan, 2013, p. 12–14). We focus on the overall strategies used by the selected methods.

3.1 Moving window

The initial approach to enhance the computational efficiency of the equivalent-layer technique is commonly denoted *moving window* and involves first splitting the observed data d_i, $i \in \{1 : D\}$, into M overlapping subsets (or data windows) formed by D^m data each, $m \in \{1 : M\}$. The data inside the m-th window are usually adjacent to each other and have indices defined by an integer list $\mathbf{i}^m$ having D^m elements. The number of data D^m forming the data windows are not necessarily equal to each other. Each data window has a $D^m \times 1$ observed data vector $\mathbf{d}^m \equiv \mathbf{d}[\mathbf{i}^m]$. The second step consists in defining a set of P equivalent sources with scalar physical property p_j, $j \in \{1 : P\}$, and also split them into M overlapping subsets (or source windows) formed by P^m data each, $m \in \{1 : M\}$. The sources inside the m-th window have indices defined by an integer list $\mathbf{j}^m$ having P^m elements. Each source window has a $P^m \times 1$ parameter vector $\mathbf{p}^m$ and is located right below the corresponding m-th data window. Then, each

$\mathbf{d}^m \equiv \mathbf{d}[\mathbf{i}^m]$ is approximated by

$$\mathbf{f}^m = \mathbf{G}^m \mathbf{p}^m \,, \tag{27}$$

where $\mathbf{G}^m \equiv \mathbf{G}[\mathbf{i}^m, \mathbf{j}^m]$ is a submatrix of $\mathbf{G}$ (equation 3) formed by the elements computed with equation 2 using only the data and equivalent sources located inside the window m-th. The main idea of the moving-window approach is using the $\tilde{\mathbf{p}}^m$ estimated for each window to obtain (i) an estimate $\tilde{\mathbf{p}}$ of the parameter vector for the entire equivalent layer or (ii) a given potential-field transformation $\mathbf{t}$ (equation 4). The main advantages of this approach is that (i) the estimated parameter vector $\tilde{\mathbf{p}}$ or transformed potential field are not obtained by solving the full, but smaller linear systems and (ii) the full matrix $\mathbf{G}$ (equation 3) is never stored.

Leão and Silva (1989) presented a pioneer work using the moving-window approach. Their method requires a regularly-spaced grid of observed data on a horizontal plane z_0. The data windows are defined by square local grids of $\sqrt{D'} \times \sqrt{D'}$ adjacent points, all of them having the same number of points D'. The equivalent sources in the m-th data window are located below the observation plane, at a constant vertical distance Δz_0. They are arranged on a regular grid of $\sqrt{P'} \times \sqrt{P'}$ adjacent points following the same grid pattern of the observed data. The local grid of sources for all data windows have the same number of elements P'. Besides, they are vertically aligned, but expands the limits of their corresponding data windows, so that $D' < P'$. Because of this spatial configuration of observed data and equivalent sources, we have that $\mathbf{G}^m = \mathbf{G}'$ (equation 27) for all data windows (i.e., $\forall\, m \in \{1 : M\}$), where $\mathbf{G}'$ is a $D' \times P'$ constant matrix.

By omitting the normalization strategy used by Leão and Silva (1989), their method consists in directly computing the transformed potential field t_c^m at the central point $(x_c^m, y_c^m, z_0 + \Delta z_0)$ of each data window as follows:

$$t_c^m = \mathbf{U}\, \mathbf{d}^m \,, \quad m \in \{1 : M\} \,, \tag{28}$$

where

$$\mathbf{U} = \left(\mathbf{G}'\mathbf{a}'\right)^\top \left[\mathbf{G}' \left(\mathbf{G}'\right)^\top + \mu\, \mathbf{I}_{D'}\right]^{-1} \tag{29}$$

and $\mathbf{a}'$ is a $P' \times 1$ vector with elements computed by equation 5 by using all equivalent sources in the m-th window and only the coordinate of the central point in the m-th data window. Due to the presumed spatial configuration of the observed data and equivalent sources, $\mathbf{a}'$ and $\mathbf{G}'$ are the same for all data windows. Hence, only the data vector $\mathbf{d}^m$ is modified according to the position of the data window. Note that equation 28 combines the potential-field transformation (equation 4) with the solution of the undetermined problem (equation 23) for the particular case in which $\mathbf{H} = \mathbf{W}_q = \mathbf{I}_{P'}$ (equations 9 and 13), $\mathbf{W}_d = \mathbf{I}_{D'}$ (equation 12), $\bar{\mathbf{p}} = \mathbf{0}$ (equation 14), where $\mathbf{I}_{P'}$ and $\mathbf{I}_{D'}$ are identity matrices of order P' and D', respectively, and $\mathbf{0}$ is a vector of zeros.

The method proposed by Leão and Silva (1989) can be outlined by the Algorithm 1. Note that Leão and Silva (1989) directly compute the transformed potential t_c^m at the central point of each data window without explicitly computing and storing an estimated for $\mathbf{p}^m$ (equation 27). It means that their method allows computing a single potential-field transformation. A different transformation or the same one evaluated at different points require running their moving-data window method again.

Soler and Uieda (2021) generalized the method proposed by Leão and Silva (1989) for irregularly spaced data on an undulating surface. A direct consequence of this generalization is that a different submatrix $\mathbf{G}^m \equiv \mathbf{G}[\mathbf{i}^m, \mathbf{j}^m]$ (equation 27) must be computed for each window. Differently from Leão and Silva (1989), Soler and Uieda (2021) store the computed $\tilde{\mathbf{p}}^m$ for all windows and subsequently use them to obtain

Algorithm 1: Generic pseudo-code for the method proposed by Leão and Silva (1989).

Initialization :

Set the indices $\mathbf{i}^m$ for each data window, $m \in \{1 : M\}$;
Set the indices $\mathbf{j}^m$ for each source window, $m \in \{1 : M\}$;
Set the constant depth $z_0 + \Delta z_0$ for all equivalent sources ;
Compute the vector $\mathbf{a}'$ associated with the desired potential-field transformation ;
Compute the matrix $\mathbf{G}'$;
Compute the matrix $\mathbf{U}$ (equation 29) ;
$m = 1$;
while $m < M$ **do**
    Compute t_c^m (equation 28) ;
    $m \leftarrow m + 1$;
end

a desired potential-field transformation (equation 4) as the superposed effect of all windows. The estimated $\tilde{\mathbf{p}}^m$ for all windows are combined to form a single $P \times 1$ vector $\tilde{\mathbf{p}}$, which is an estimate for original parameter vector $\mathbf{p}$ (equation 3). For each data window, Soler and Uieda (2021) solve an overdetermined problem (equation 22) for $\tilde{\mathbf{p}}^m$ by using $\mathbf{H} = \mathbf{W}_q = \mathbf{I}_{P^m}$ (equations 9 and 13), $\mathbf{W}_d^m$ (equation 12) equal to a diagonal matrix of weights for the data inside the m-th window and $\bar{p} = \mathbf{0}$ (equation 14), so that

$$\left[(\mathbf{G}^m)^\top \mathbf{W}_d^m \mathbf{G}^m + \mu \mathbf{I}_{P'} \right] \tilde{\mathbf{p}}^m = (\mathbf{G}^m)^\top \mathbf{W}_d^m \mathbf{d}^m \, . \tag{30}$$

Unlike Leão and Silva (1989), Soler and Uieda (2021) do not adopt a sequential order of the data windows; rather, they adopt a randomized order of windows in their iterations. The overall steps of the method proposed by Soler and Uieda (2021) are defined by the Algorithm 2. For convenience, we have omitted the details about the randomized window order and the normalization strategy employed by Soler and Uieda (2021) which was described in section 1.3.1 Note that this algorithm starts with a residuals vector $\mathbf{r}$ that is iteratively updated. The iterative algorithm in Soler and Uieda (2021) estimates a solution ($\tilde{\mathbf{p}}^m$ in equation 30) using the data and the equivalent sources that fall within a moving-data window; however, it calculates the predicted data and the residual data in the whole survey data. Next, the residual data that fall within a new position of the data window is used as input data to estimate a new solution within the data window which, in turn, is used to calculated a new predicted data and a new residual data in the whole survey data. Regarding the equivalent-source layout, Soler and Uieda (2021) proposed the block-averaged sources locations in which the survey area is divided into horizontal blocks and one single equivalent source is assigned to each block. Each single source per block is placed over the layer with its horizontal coordinates given by the average horizontal positions of observation points. According to Soler and Uieda (2021), the block-averaged sources layout may prevent aliasing of the interpolated values, specially when the observations are unevenly sampled. This strategy also reduces the number of equivalent sources without affecting the accuracy of the potential-field interpolation. This reduction reduces the computational load for estimating the physical property on the equivalent layer. This block-averaged sources layout is not included in the Algorithm 2.

3.2 Column-action update

We call the computational strategy *column-action update* because a single source is used to calculate the predicted data and the residual data in the whole survey data. Hence, a single column of the sensitivity matrix $\mathbf{G}$ (equation 3) is calculated iteratively.

Algorithm 2: Generic pseudo-code for the method proposed by Soler and Uieda (2021).

Initialization :
Set the indices $\mathbf{i}^m$ for each data window, $m \in \{1 : M\}$;
Set the indices $\mathbf{j}^m$ for each source window, $m \in \{1 : M\}$;
Set the depth of all equivalent sources ;
Set a $D \times 1$ residuals vector $\mathbf{r} = \mathbf{d}$;
Set a $P \times 1$ vector $\tilde{\mathbf{p}} = \mathbf{0}$;
$m = 1$;
while $m < M$ **do**
    Set the matrix $\mathbf{W}_d^m$;
    Compute the matrix $\mathbf{G}^m$;
    Compute $\tilde{\mathbf{p}}^m$ (equation 30) ;
    $\tilde{\mathbf{p}}[\mathbf{j}^m] \leftarrow \tilde{\mathbf{p}}[\mathbf{j}^m] + \tilde{\mathbf{p}}^m$;
    $\mathbf{r} \leftarrow \mathbf{r} - \mathbf{G}[:, \mathbf{j}^m]\, \tilde{\mathbf{p}}^m$;
    $m \leftarrow m + 1$;
end

Cordell (1992) proposed a computational strategy that was later used by Guspí and Novara (2009) and relies on first defining one equivalent source located right below each observed data d_i, $i \in \{1 : D\}$, at a vertical coordinate $z_i + \Delta z_i$, where Δz_i is proportional to the distance from the i-th observation point (x_i, y_i, z_i) to its closest neighbor. The second step consists in updating the physical property p_j of a single equivalent source, $j \in \{1 : D\}$ and remove its predicted potential field from the observed data vector $\mathbf{d}$, producing a residuals vector $\mathbf{r}$. At each iteration, the single equivalent source is the one located vertically beneath the observation station of the maximum data residual. Next, the predicted data produced by this single source is calculated over all of the observation points and a new data residual $\mathbf{r}$ and the $D \times 1$ parameter vector $\mathbf{p}$ containing the physical property of all equivalent sources are updated iteratively. During each subsequent iteration, Cordell's method either incorporates a single equivalent source or adjusts an existing equivalent source to match the maximum amplitude of the current residual field. The convergence occurs when all of the residuals are bounded by an envelope of prespecified expected error. At the end, the algorithm produces an estimate $\tilde{\mathbf{p}}$ for the parameter vector yielding a predicted potential field $\mathbf{f}$ (equation 3) satisfactorily fitting the observed data $\mathbf{d}$ according to a given criterion. Note that the method proposed by Cordell (1992) iteratively solves the linear $\mathbf{G}\tilde{\mathbf{p}} \approx \mathbf{d}$ with a $D \times D$ matrix $\mathbf{G}$. At each iteration, only a single column of $\mathbf{G}$ (equation 3) is used. An advantage of this *column-action update approach* is that the full matrix $\mathbf{G}$ is never stored.

Algorithm 3 delineates the Cordell's method. Note that a single column $\mathbf{G}[:, i_{\texttt{max}}]$ of the $D \times D$ matrix $\mathbf{G}$ (equation 3) is used per iteration, where $i_{\texttt{max}}$ is the index of the maximum absolute value in $\mathbf{r}$. As pointed out by Cordell (1992), the method does not necessarily decrease monotonically along the iterations. Besides, the method may not converge depending on how the vertical distances Δz_i, $i \in \{1 : D\}$, controlling the depths of the equivalent sources are set. According to Cordell (1992), the maximum absolute value $r_{\texttt{max}}$ in $\mathbf{r}$ decreases robustly at the beginning and oscillates within a narrowing envelope for the subsequent iterations.

Guspí and Novara (2009) generalized Cordell's method to perform reduction to the pole and other transformations on scattered magnetic observations by using two steps. The first step involves computing the vertical component of the observed field using equivalent sources while preserving the magnetization direction. In the second step, the vertical observation direction is maintained, but the magnetization direction is shifted to the vertical. The main idea employed by both Cordell (1992) and Guspí and Novara

(2009) is an iterative scheme that uses a single equivalent source positioned below a measurement station to compute both the predicted data and residual data for all stations. This approach entails a computational strategy where a single column of the sensitivity matrix $\mathbf{G}$ (equation 3) is calculated per iteration.

Algorithm 3: Generic pseudo-code for the method proposed by Cordell (1992).

Initialization :

Compute a $D \times 1$ vector $\mathbf{\Delta z}$ whose i-th element Δz_i is a vertical distance controlling the depth of the i-th equivalent source, $i \in \{1 : D\}$;
Set a tolerance ϵ ;
Set a maximum number of iteration ITMAX ;
Set a $D \times 1$ residuals vector $\mathbf{r} = \mathbf{d}$;
Set a $D \times 1$ vector $\tilde{\mathbf{p}} = \mathbf{0}$;
Define the maximum absolute value $r_{\mathtt{max}}$ in $\mathbf{r}$;
$m = 1$;
while $(r_{\mathtt{max}} > \epsilon)$ **and** $(m < \mathtt{ITMAX})$ **do**
    Define the coordinates $(x_{\mathtt{max}}, y_{\mathtt{max}}, z_{\mathtt{max}})$ and index $i_{\mathtt{max}}$ of the observation point associated with $r_{\mathtt{max}}$;
    $\tilde{\mathbf{p}}[i_{\mathtt{max}}] \leftarrow \tilde{\mathbf{p}}[i_{\mathtt{max}}] + (r_{\mathtt{max}}\, \mathbf{\Delta z}[i_{\mathtt{max}}])$;
    $\mathbf{r} \leftarrow \mathbf{r} - (\mathbf{G}[:, i_{\mathtt{max}}]\, \tilde{\mathbf{p}}[i_{\mathtt{max}}])$;
    Define the new $r_{\mathtt{max}}$ in $\mathbf{r}$;
    $m \leftarrow m + 1$;
end

3.3 Row-action update

We call the computational strategy *row-action update* because a single row of the sensitivity matrix $\mathbf{G}$ (equation 3) is calculated iteratively. Hence, the equivalent-layer solution is updated by processing a new datum (one matrix row) at each iteration. To reduce the total processing time and memory usage of equivalent-layer technique, Mendonça and Silva (1994) proposed a strategy called *equivalent data concept*. The equivalent data concept is grounded on the principle that there is a subset of redundant data that does not contribute to the final solution and thus can be dispensed. Conversely, there is a subset of observations, called equivalent data, that contributes effectively to the final solution and fits the remaining observations (redundant data). Iteratively, Mendonça and Silva (1994) selected the subset of equivalent data that is substantially smaller than the original dataset. This selection is carried out by incorporating one data point at a time.

Mendonça and Silva (1994) proposes an algebraic reconstruction technique (ART) (e.g., van der Sluis and van der Vorst, 1987, p. 58) to estimate a parameter vector $\tilde{\mathbf{p}}$ for a regular grid of P equivalent sources on a horizontal plane z_0. Such methods iterate on the linear system rows to estimate corrections for the parameter vector, which may substantially save computer time and memory required to compute and store the full linear system matrix along the iterations. The convergence of such *row-update methods* depends on the linear system condition. The main advantage of such methods is not computing and storing the full linear system matrix, but iteratively using its rows. In contrast to ART-type algorithms, the rows in Mendonça and Silva (1994) are not processed sequentially. Instead, in Mendonça and Silva (1994), the rows are introduced according to their residual magnitudes (maximum absolute value in $\mathbf{r}$), which are computed based on the estimate over the equivalent layer from the previous iteration. The particular ART

method proposed by Mendonça and Silva (1994) considers that

$$\mathbf{d} = \begin{bmatrix} \mathbf{d}_e \\ \mathbf{d}_r \end{bmatrix} \;, \quad \mathbf{G} = \begin{bmatrix} \mathbf{G}_e \\ \mathbf{R}_r \end{bmatrix} \;, \tag{31}$$

where $\mathbf{d}_e$ and $\mathbf{d}_r$ are $D_e \times 1$ and $D_r \times 1$ vectors and $\mathbf{G}_e$ and $\mathbf{G}_r$ are $D_e \times P$ and $D_r \times P$ matrices, respectively. Mendonça and Silva (1994) designate $\mathbf{d}_e$ and $\mathbf{d}_r$ as, respectively, *equivalent* and *redundant* data. With the exception of a normalization strategy, Mendonça and Silva (1994) calculate a $P \times 1$ estimated parameter vector $\tilde{\mathbf{p}}$ by solving an underdetermined problem (equation 23) involving only the equivalent data $\mathbf{d}_e$ (equation 31) for the particular case in which $\mathbf{H} = \mathbf{W}_p = \mathbf{I}_P$ (equations 9 and 13), $\mathbf{W}_d = \mathbf{I}_{D_e}$ (equation 12) and $\bar{p} = \mathbf{0}$ (equation 14), which results in

$$\begin{aligned} (\mathbf{F} + \mu\, \mathbf{I}_{D_e})\, \mathbf{u} &= \mathbf{d}_e \\ \tilde{\mathbf{p}} &= \mathbf{G}_e^\top \mathbf{u} \end{aligned} \;, \tag{32}$$

where $\mathbf{F}$ is a computationally-efficient $D_e \times D_e$ matrix that approximates $\mathbf{G}_e\, \mathbf{G}_e^\top$. Mendonça and Silva (1994) presume that the estimated parameter vector $\tilde{\mathbf{p}}$ obtained from equation 32 leads to a $D_r \times 1$ residuals vector

$$\mathbf{r} = \mathbf{d}_r - \mathbf{G}_r \tilde{\mathbf{p}} \tag{33}$$

having a maximum absolute value $r_{\texttt{max}} \leq \epsilon$, where ϵ is a predefined tolerance.

The overall method of Mendonça and Silva (1994) is defined by Algorithm 4. It is important noting that the number D_e of equivalent data in $\mathbf{d}_e$ increases by one per iteration, which means that the order of the linear system in equation 32 also increases by one at each iteration. Those authors also propose a computational strategy based on Cholesky factorization (e.g., Golub and Van Loan, 2013, p. 163) for efficiently updating $(\mathbf{F} + \mu\, \mathbf{I}_{D_e})$ at a given iteration (line 16 in Algorithm 4) by computing only its new elements with respect to those computed in the previous iteration.

3.4 Reparameterization

Another approach for improving the computational performance of equivalent-layer technique consists in setting a $P \times Q$ reparameterization matrix $\mathbf{H}$ (equation 9) with $Q << P$. This strategy has been used in applied geophysics for decades (e.g., Skilling and Bryan, 1984; Kennett et al., 1988; Oldenburg et al., 1993; Barbosa et al., 1997) and is known as *subspace method*. The main idea relies in reducing the linear system dimension from the original P-space to a lower-dimensional subspace (the Q-space). An estimate $\tilde{\mathbf{q}}$ for the reparameterized parameter vector $\mathbf{q}$ is obtained in the Q-space and subsequently used to obtain an estimate $\tilde{\mathbf{p}}$ for the parameter vector $\mathbf{p}$ (equation 3) in the P-space by using equation 9. Hence, the key aspect of this *reparameterization approach* is solving an appreciably smaller linear inverse problem for $\tilde{\mathbf{q}}$ than that for the original parameter vector $\tilde{\mathbf{p}}$ (equation 3).

Oliveira Jr. et al. (2013) have used this approach to describe the physical property distribution on the equivalent layer in terms of piecewise bivariate polynomials. Specifically, their method consists in splitting a regular grid of equivalent sources into source windows inside which the physical-property distribution is described by bivariate polynomial functions. The key aspect of their method relies on the fact that the total number of coefficients required to define the bivariate polynomials is considerably smaller than the original number of equivalent sources. Hence, they formulate a linear inverse problem for estimating the

Algorithm 4: Generic pseudo-code for the method proposed by Mendonça and Silva (1994).

Initialization :

Set a regular grid of P equivalent sources at a horizontal plane z_0 ;
Set a tolerance ϵ ;
Set a $D \times 1$ residuals vector $\mathbf{r} = \mathbf{d}$;
Define the maximum absolute value $r_{\texttt{max}}$ in $\mathbf{r}$;
Define the index $i_{\texttt{max}}$ of $r_{\texttt{max}}$;
Define the list of indices $\mathbf{i}_r$ of the remaining data in $\mathbf{r}$;
Define $\mathbf{d}_e = \mathbf{d}[i_{\texttt{max}}]$;
Compute $(\mathbf{F} + \mu\,\mathbf{I}_{D_e})$ and $\mathbf{G}_e$;
Compute $\tilde{\mathbf{p}}$ (equation 32) ;
Compute $\mathbf{r} = \mathbf{d}[\mathbf{i}_r] - \mathbf{G}[\mathbf{i}_r, :]\,\tilde{\mathbf{p}}$;
Define the maximum absolute value $r_{\texttt{max}}$ in $\mathbf{r}$;
while $(r_{\texttt{max}} > \epsilon)$ **do**
    Define the index $i_{\texttt{max}}$ of $r_{\texttt{max}}$;
    Define the list of indices $\mathbf{i}_r$ of the remaining elements in $\mathbf{r}$;
    $\mathbf{d}_e \leftarrow \begin{bmatrix} \mathbf{d}_e \\ \mathbf{d}[i_{\texttt{max}}] \end{bmatrix}$;
    Update $(\mathbf{F} + \mu\,\mathbf{I}_{D_e})$ and $\mathbf{G}_e$;
    Update $\tilde{\mathbf{p}}$ (equation 32) ;
    Update $\mathbf{r} = \mathbf{d}[\mathbf{i}_r] - \mathbf{G}[\mathbf{i}_r, :]\,\tilde{\mathbf{p}}$;
    Define the maximum absolute value $r_{\texttt{max}}$ in $\mathbf{r}$;
end

polynomial coefficients and use them later to compute the physical property distribution on the equivalent layer.

The method proposed by Oliveira Jr. et al. (2013) consists in solving an overdetermined problem (equation 22) for estimating the polynomial coefficients $\tilde{\mathbf{q}}$ with $\mathbf{W}_d = \mathbf{I}_D$ (equation 12) and $\bar{q} = \mathbf{0}$ (equation 14), so that

$$\left(\mathbf{H}^\top \mathbf{G}^\top \mathbf{G}\,\mathbf{H} + \mu\,\mathbf{W}_q\right) \tilde{\mathbf{q}} = \mathbf{H}^\top \mathbf{G}^\top\,\mathbf{d}\,, \tag{34}$$

where $\mathbf{W}_q = \mathbf{H}^\top \mathbf{W}_p\,\mathbf{H}$ is defined by a matrix $\mathbf{W}_p$ representing the zeroth- and first-order Tikhonov regularization (e.g., Aster et al., 2019, p. 103). Note that, in this case, the prior information is defined in the P-space for the original parameter vector $\mathbf{p}$ and then transformed to the Q-space. Another characteristic of their method is that it is valid for processing irregularly-spaced data on an undulating surface.

Mendonça (2020) also proposed a reparameterization approach for the equivalent-layer technique. Their approach, however, consists in setting $\mathbf{H}$ as a truncated singular value decomposition (SVD) (e.g., Aster et al., 2019, p. 55) of the observed potential field. Differently from Oliveira Jr. et al. (2013), however, the method of Mendonça (2020) requires a regular grid of potential-field data on horizontal plane. Another difference is that these authors uses $\mathbf{W}_q = \mathbf{I}_Q$ (equation 13), which means that the regularization is defined directly in the Q-space.

Before Oliveira Jr. et al. (2013) and Mendonça (2020), Barnes and Lumley (2011) also proposed a computationally efficient method for equivalent-layer technique based on reparameterization. A key difference, however, is that Barnes and Lumley (2011) did not set a $P \times Q$ reparameterization matrix $\mathbf{H}$ (equation 9) with $Q << P$. Instead, they used a matrix $\mathbf{H}$ with $Q \approx 1.7\,P$. Their central idea is setting a reparameterization scheme that groups distant equivalent sources into blocks by using a bisection process.

This scheme leads to a quadtree representation of the physical-property distribution on the equivalent layer, so that matrix $\mathbf{GH}$ (equation 10) is notably sparse. Barnes and Lumley (2011) explore this sparsity in solving the overdetermined problem for $\tilde{\mathbf{q}}$ (equation 34) via conjugate-gradient method (e.g., Golub and Van Loan, 2013, sec. 11.3).

3.5 Wavelet compression

Previously to Barnes and Lumley (2011), the idea of transforming the dense matrix $\mathbf{G}$ (equation 3) into a sparse one has already been used in the context of equivalent-layer technique. Li and Oldenburg (2010) proposed a method that applies the discrete wavelet transform to introduce sparsity into the original dense matrix $\mathbf{G}$. Those authors approximate a planar grid of potential-field data by a regularly-spaced grid of equivalent sources, so that the number of data D and sources P is the same , i.e., $D = P$. Specifically, Li and Oldenburg (2010) proposed a method that applies the wavelet transform to the original dense matrix $\mathbf{G}$ and sets to zero the small coefficients that are below a given threshold, which results in an approximating sparse representation of $\mathbf{G}$ in the wavelet domain. They first consider the following approximation

$$\mathbf{d}_w \approx \mathbf{G}_s \, \mathbf{p}_w \;, \tag{35}$$

where

$$\mathbf{d}_w = \boldsymbol{\mathcal{W}} \, \mathbf{d} \;, \quad \mathbf{p}_w = \boldsymbol{\mathcal{W}} \, \mathbf{p} \;, \tag{36}$$

are the observed data and parameter vector in the wavelet domain; $\boldsymbol{\mathcal{W}}$ is a $D \times D$ orthogonal matrix defining a discrete wavelet transform; and $\mathbf{G}_s$ is a sparse matrix obtained by setting to zero the elements of

$$\mathbf{G}_w = \boldsymbol{\mathcal{W}} \, \mathbf{G} \, \boldsymbol{\mathcal{W}} \tag{37}$$

with absolute value smaller than a given threshold.

Li and Oldenburg (2010) apply the normalization strategy defined in section 1.3.1 to equation 35 by using a diagonal normalization matrix $\mathbf{N}$ (equation 24) and then formulate an overdetermined problem (equation 22) with $\mathbf{H} = \mathbf{I}_P$ (equations 9), $\mu = 0$ (equation 11), $\mathbf{W}_d = \mathbf{I}_D$ (equation 12) and $\bar{p} = \mathbf{0}$ (equation 14) so that

$$\left(\mathbf{G}_n^\top \mathbf{G}_n \right) \tilde{\mathbf{p}}_n = \mathbf{G}_n^\top \mathbf{d}_w \;, \tag{38}$$

where $\mathbf{G}_n$ and $\tilde{\mathbf{p}}_n$ are defined according to equation 24 in terms of the sparse matrix $\mathbf{G}_s$ (equation 35). They solve this linear system (equation 38) with the conjugate-gradient method (e.g., Golub and Van Loan, 2013, sec. 11.3) and use it to obtain an estimate $\tilde{\mathbf{p}}$ for the parameter vector given by

$$\tilde{\mathbf{p}} = \boldsymbol{\mathcal{W}}^\top \left(\mathbf{N} \, \tilde{\mathbf{p}}_n \right) \;, \tag{39}$$

where the term within parentheses removes the normalization (equation 25) and matrix $\boldsymbol{\mathcal{W}}^\top$ applies an inverse wavelet transform.

3.6 Iterative methods using the full matrix $\mathbf{G}$

In the context of equivalent-layer technique, there are methods (e.g., Li and Oldenburg, 2010; Barnes and Lumley, 2011) that modify the original linear system and then iteratively solve this modified system by using the well-established conjugate gradient method (e.g., Golub and Van Loan, 2013, sec. 11.3). Xia and Sprowl (1991) also proposed an iterative method for estimating a parameter vector $\tilde{\mathbf{p}}$ (equation

3). Their method, however, uses the original matrix $\mathbf{G}$ without previously computing a compression or reparameterization, for example. More than two decades later, Siqueira et al. (2017) have deduced essentially the same method presented by Xia and Sprowl (1991), but by following a more theoretical approach based on the Gauss' theorem (e.g., Kellogg, 1967, p. 43) and the total excess of mass (e.g., Blakely, 1996, p. 60). Besides, Siqueira et al. (2017) have shown that this method produces very stable solutions, even for noise-corrupted potential-field data.

The iterative method proposed by Xia and Sprowl (1991) and Siqueira et al. (2017) is outlined in Algorithm 5, presumes an equivalent layer formed by monopoles (point masses) and can be applied to irregularly-spaced data on an undulating surface. Note that the residuals $\mathbf{r}$ are used to compute a correction $\boldsymbol{\Delta}\mathbf{p}$ for the parameter vector at each iteration (line 11), which requires a matrix-vector product involving the full matrix $\mathbf{G}$. Interestingly, this approach for estimating the physical property distribution on an equivalent layer is the same originally proposed by Bott (1960) for estimating the basement relief under sedimentary basins. The method of Xia and Sprowl (1991) and Siqueira et al. (2017) was originally proposed for processing gravity data, but can be potentially applied to any harmonic function because it actually represents an iterative solution of the classical *Dirichlet's problem* or the *first boundary value problem of potential theory* (Kellogg, 1967, p. 236) on a plane.

Recently, Jirigalatu and Ebbing (2019) presented another iterative method for estimating a parameter vector $\tilde{\mathbf{p}}$ (equation 3). With the purpose of combining different potential-field data, their method basically modifies that shown in Algorithm 5 by changing the initial approximation and the iterative correction for the parameter vector. Specifically, Jirigalatu and Ebbing (2019) replace line 3 by $\tilde{\mathbf{p}} = \mathbf{0}$, where $\mathbf{0}$ is a vector of zeros, and line 8 by $\boldsymbol{\Delta}\mathbf{p} = \omega\,\mathbf{G}^{\top}\mathbf{r}$, where ω is a positive scalar defined by trial and error. Note that this modified approach requires two matrix-vector products involving the full matrix $\mathbf{G}$ per iteration. To overcome the high computational cost of these two products, Jirigalatu and Ebbing (2019) set an equivalent layer formed by prisms and compute their predicted potential field in the wavenumber domain by using the Gauss-FFT technique Zhao et al. (2018).

INCLUIMOS Xia et al. (1993) - FOURIER - OU NÃO?

Algorithm 5: Generic pseudo-code for the iterative methods proposed by Xia and Sprowl (1991) and Siqueira et al. (2017). The symbol "$\circ$" denotes the entrywise or Hadamard product (e.g., Horn and Johnson, 1991, p. 298) and $\mathbf{s}$ is a $P \times 1$ vector whose j-th element is a predefined element of area centered at the j-th equivalent source.

Initialization :
1 Set P equivalent sources on a horizontal plane z_0 ;
2 Set the auxiliary vector $\mathbf{s}$;
3 Set a tolerance ϵ ;
4 Compute $\tilde{\mathbf{p}} = \mathbf{s} \circ \mathbf{d}$;
5 Compute $\mathbf{G}$;
6 Compute $\mathbf{r} = \mathbf{d} - \mathbf{G}\,\tilde{\mathbf{p}}$;
7 Compute $\|\mathbf{r}\|$;
8 **while** $(\|\mathbf{r}\| > \epsilon)$ **do**
9 $\quad \boldsymbol{\Delta}\mathbf{p} = \mathbf{s} \circ \mathbf{r}$;
10 $\quad \tilde{\mathbf{p}} \leftarrow \tilde{\mathbf{p}} + \boldsymbol{\Delta}\mathbf{p}$;
11 $\quad \mathbf{r} \leftarrow \mathbf{r} - \mathbf{G}\,\boldsymbol{\Delta}\mathbf{p}$;
12 $\quad$ Compute $\|\mathbf{r}\|$;
13 **end**

3.7 Discrete convolution

Recently, Takahashi et al. (2020, 2022) have shown that $\mathbf{G}$ assumes a *doubly block Toeplitz* (Jain, 1989, p. 28) or *block-Toeplitz Toeplitz-block* (BTTB) (Chan and Jin, 2007, p. 67) structure for the particular case in which (i) there is a single equivalent source right below each potential-field datum and (ii) both data and sources rely on planar and regularly spaced grids. This structure allows formulating the product of $\mathbf{G}$ and an arbitrary vector as a *fast discrete convolution* (Van Loan, 1992, section 4.2).

Takahashi et al. (2020, 2022) consider a regular grid of D potential-field data at points (x_i, y_i, z_0), $i \in \{1 : D\}$, on a horizontal plane z_0. The data indices i may be ordered along the $x-$ or $y-$direction, which results in an $x-$ or $y-$oriented grid, respectively. They also consider a single equivalent source located right below each datum, at a constant vertical coordinate $z_0 + \Delta z$, $\Delta z > 0$. In this case, the number of data and equivalent sources are equal to each other (i.e., $D = P$) and $\mathbf{G}$ (equation 3) is a $D \times D$ matrix formed by $D_B \times D_B$ blocks, where each block has $D_b \times D_b$ elements, with $D = D_B\, D_b$.

Let $\boldsymbol{\mathcal{D}}$ be a $2D_B \times 2D_b$ matrix formed by four blocks of $D_B \times D_b$ elements. All blocks have null elements, except the first block in the first quadrant, which has the observed data d_i, $i \in \{1 : D\}$ arranged along its rows or columns if the data grid has a $x-$ or $y-$oriented pattern, respectively. Let us also consider a $2D_B \times 2D_b$ matrix $\boldsymbol{\mathcal{P}}$ having the same structure of $\boldsymbol{\mathcal{D}}$, but containing the elements p_j of the parameter vector $\mathbf{p}$, $j \in \{1 : P\}$.

The first block (in the first quadrant) contains

The conjugate gradient (CG) is a very popular iterative method for solving linear systems. This method was originally developed to solve systems having a square and positive definite matrix. There are two adapted versions of the CG method. The first is called *conjugate gradient normal equation residual* (CGNR) Golub and Van Loan (2013, sec. 11.3) or *conjugate gradient least squares* (CGLS) (Aster et al., 2019, p. 165) and is used to solve overdetermined problem (equation 22). The second is called *conjugate gradient normal equation error* (CGNE) method Golub and Van Loan (2013, sec. 11.3) and is used to solve the underdetermined problem (equation 23).

Takahashi et al. (2020)

Takahashi et al. (2022)

4 TEXTO ANTIGO

4.0.1 The wavelet compression and lower-dimensional subspace

For large data sets, the sensitivity matrix $\mathbf{A}$ (equation 3) is a drawback in applying the equivalent-layer technique because it is a large and dense matrix.

? transformed a large and full sensitivity matrix into a sparse one by using fast wavelet transforms. In the wavelet domain, **?** applyied a 2D wavelet transform to each row and column of the original sensitivity matrix $\mathbf{A}$ to expand it in the wavelet bases. This operation can be done by premultiplying the original sensitivity matrix $\mathbf{A}$ by a matrix representing the 2D wavelet transform $\mathbf{W_2}$ and then the resulting is postmultiplied by the transpose of $\mathbf{W_2}$ (i.e., $\mathbf{W_2}^\top$).

$$\tilde{\mathbf{A}} = \mathbf{W_2}\, \mathbf{A}\, \mathbf{W_2}^\top , \tag{40}$$

where $\tilde{\mathbf{A}}$ is the expanded original sensitivity matrix in the wavelet bases with many elements zero or close to zero. Next, the matrix $\tilde{\mathbf{A}}$ is replaced by its sparse version $\tilde{\mathbf{A}}_\mathbf{s}$ in the wavelet domain which in turn is obtained by retaining only the large elements of the $\tilde{\mathbf{A}}$. Thus, the elements of $\tilde{\mathbf{A}}$ whose amplitudes fall below a relative threshold are discarded. In **?**, the original sensitivity matrix $\mathbf{A}$ is high compressed resulting in a sparce matrix $\tilde{\mathbf{A}}_\mathbf{s}$ with a few percent of nonzero elements and the the inverse problem is solved in the wavelet domain by using $\tilde{\mathbf{A}}_\mathbf{s}$ and a incomplete conjugate gradient least squares, without an explicit regularization parameter and a limited number of iterations. The solution is obtained by solving the following linear system

$$\tilde{\mathbf{A}}_\mathbf{L}^\top \, \tilde{\mathbf{A}}_\mathbf{L} \, \tilde{\mathbf{p}}_\mathbf{L}^* \, = \tilde{\mathbf{A}}_\mathbf{L}^\top \, \tilde{\mathbf{d}}^o \, , \tag{41}$$

where $\tilde{\mathbf{p}}_\mathbf{L}^*$ is obtained by solving the linear system given by equation 41,

$$\tilde{\mathbf{A}}_\mathbf{L} \;=\; \tilde{\mathbf{A}}_\mathbf{s} \, \tilde{\mathbf{L}}^{-\mathbf{1}}, \tag{42a}$$

$$\tilde{\mathbf{p}}_\mathbf{L} \;=\; \tilde{\mathbf{L}}\tilde{\mathbf{p}}, \tag{42b}$$

$$\tilde{\mathbf{d}}^o \;=\; \mathbf{W_2} \, \mathbf{d}^o, \tag{42c}$$

where $\tilde{\mathbf{L}}$ is a diagonal and invertible weighting matrix representing the finite-difference approximation in the wavelet domain. Finally, the distribution over the equivalent layer in the space domain $\mathbf{p}$ is obtained by applying an inverse wavelet transform in two steps, i.e.:

$$\tilde{\mathbf{p}} = \tilde{\mathbf{L}}^{-1} \, \tilde{\mathbf{p}}_\mathbf{L}^* \, , \tag{43}$$

and

$$\mathbf{p} = \mathbf{W_2} \, \tilde{\mathbf{p}} \, . \tag{44}$$

Although the data misfit quantifying the difference between the observed and predicted data by the equivalent source is calculated in the wavelet domain, we understand that the desired transformation is calculated via equation **??** which uses a full matrix of Green's functions $\mathbf{T}$.

? used the equivalent-layer technique with a wavelet compression to perform an upward continuation of total-field anomaly between uneven surfaces. For regularly spaced grid of data, **?** reported that high compression ratios are achived with insignificant loss of accuracy. As compared to the upward-continued total-field anomaly by equivalent layer using the dense matrix, **?**'s (**?**) approach, using the Daubechies wavelet, decreased CPU (central processing unit) time by up to two orders of magnitude.

? overcame the solution of intractable large-scale equivalent-layer problem by using the subspace method (e.g., Skilling and Bryan, 1984; Kennett et al., 1988; Oldenburg et al., 1993; Barbosa et al., 1997). The subspace method reduces the dimension of the linear system of equations to be solved. Given a higher-dimensional space (e.g., M-dimensional model space, $\mathbb{R}^M$), there exists many lower-dimensional subspaces (e.g., Q-dimensional subspace) of $\mathbb{R}^M$. The linear inverse problem related to the equivalent-layer technique consists in finding an M-dimension parameter vector $\mathbf{p} \in \mathbb{R}^M$ which adequately fits the potential-field data. The subspace method looks for a parameter vector who lies in a Q-dimensional subspace of $\mathbb{R}^M$ which, in turn, is spanned by a set of Q vectors $\mathbf{v}_i = 1, ..., Q$, where $\mathbf{v}_i \in \mathbb{R}^M$ In matrix notation, the parameter vector in the subspace method can be written as

$$\mathbf{p} = \mathbf{V} \, \boldsymbol{\alpha} \, , \tag{45}$$

where $\mathbf{V}$ is an $M \times Q$ matrix whose columns $\mathbf{v}_i = 1, ..., Q$ form a basis vectors for a subspace Q of $\mathbb{R}^M$. In equation 45, the parameter vector $\mathbf{p}$ is defined as a linear combination in the space spanned by Q basis vectors $\mathbf{v}_i = 1, ..., Q$ and $\boldsymbol{\alpha}$ is a Q-dimensional unknown vector to be determined. The main advantage of the subspace method is that the linear system of M equations in M unknowns to be originally solved is reduced to a new linear system of Q equations in Q unknowns which requires much less computational effort since $Q << M$, i.e.:

$$\mathbf{V}^\top \, \mathbf{A}^\top \, \mathbf{A} \, \mathbf{V} \, \boldsymbol{\alpha}^* \; = \; \mathbf{V}^\top \, \mathbf{d}^o \, . \tag{46}$$

To avoid the storage of matrices $\mathbf{A}$ and $\mathbf{V}$, **?** evaluates an element of the matrix $\mathbf{AV}$ by calculating the dot product between the row of matrix $\mathbf{A}$ and the column of the matrix $\mathbf{B}$. After estimating $\boldsymbol{\alpha}^*$ (equation 46) belonging to a Q-dimensional subspace of $\mathbb{R}^M$, the distribution over the equivalent layer $\mathbf{p}$ in the $\mathbb{R}^M$ is obtained by applying equation 45. The choice of the Q basis vectors $\mathbf{v}_i = 1, ..., Q$ (equation 45) in the subspace method is not strict. **?**, for example, chose the eigenvectors yielded by applying the singular value decomposition of the matrix containing the gridded data set. The number of eigenvectors used to form basis vectors will depend on the singular values.

The proposed subspace method for solving large-scale equivalent-layer problem by **?** was applied to estimate the mass excess or deficiency caused by causative gravity sources.

4.0.2 The quadtree discretization

To make the equivalent-layer technique tractable, **?** also transformed the dense sensitivity matrix $\mathbf{A}$ (equation 3) into a sparse matrix. In **?**, a sparce version of the sensitivity matrix is achived by grouping equivalent sources (e.g., they used prisms) distant from an observation point together to form a larger prism or larger block. Each larger block has averaged physical properties and averaged top- and bottom-surfaces of the grouped smaller prisms (equivalent sources) that are encompassed by the larger block. The authors called it the 'larger averaged block' and the essence of their method is the reduction in the number of equivalent sources, which means a reduction in the number of parameters to be estimated implying in model dimension reduction.

The key of the **?**'s (**?**) method is the algorithm for deciding how to group the smaller prisms. In practice, these authors used a recursive bisection process that results in a quadtree discretization of the equivalent-layer model.

By using the quadtree discretization, **?** were able to jointly process multiple components of airborne gravity-gradient data using a single layer of equivalent sources. To our knowledge, **?** are the pioneers on processing full-tensor gravity-gradient data jointly. In addition to computational feasibility, **?**'s (**?**) method reduces low-frequency noise and can also remove the drift in time-domain from the survey data. Those authors stressed that the $G_{zz}-$component calculated through the single estimated equivalent-layer model projected on a grid at a constant elevation by inverting full gravity-gradient data has the low-frequency error reduced by a factor of 2.4 as compared to the inversion of an individual component of the gravity-gradient data.

4.0.3 The reparametrization of the equivalent layer

Oliveira Jr. et al. (2013) reparametrized the whole equivalent-layer model by a piecewise bivariate-polynomial function defined on a set of Q equivalent-source windows. In Oliveira Jr. et al.'s (2013) approach, named polynomial equivalent layer (PEL), the parameter vector within the kth equivalent-source

window $\mathbf{p}^k$ can be written in matrix notation as

$$\mathbf{p}^k = \mathbf{B}^k \, \mathbf{c}^k \, , \qquad k \, = \, 1 \, ... \, Q \, , \tag{47}$$

where $\mathbf{p}^k$ is an M_w-dimensional vector containing the physical-property distribution within the kth equivalent-source window, $\mathbf{c}^k$ is a P-dimensional vector whose lth element is the lth coefficient of the αth-order polynomial function and $\mathbf{B}^k$ is an $M_w \times P$ matrix containing the first-order derivative of the αth-order polynomial function with respect to one of the P coefficients.

By using a regularized potential-field inversion, Oliveira Jr. et al. (2013) estimates the polynomial coefficients for each equivalent-source window by solving the following linear system

$$\left(\mathbf{B}^\top \, \mathbf{A}^\top \, \mathbf{A} \, \mathbf{B} \, + \, \mu \mathbf{I}\right) \, \mathbf{c}^* \, = \, \mathbf{B}^\top \, \mathbf{A}^\top \, \mathbf{d}^o \, , \tag{48}$$

where μ is a regularizing parameter, $\mathbf{c}^*$ is an estimated H-dimensional vector containing all coefficients describing all polynomial functions within all equivalent-source windows which compose the entire equivalent layer, $\mathbf{I}$ is an identity matrix of order $H (H = P\dot{Q})$ and $\mathbf{B}$ is an $M \times H$ block diagonal matrix such that the main-diagonal blocks are $\mathbf{B}^k$ matrices (equation 47) and all off-diagonal blocks are zero matrices. For ease of the explanation of equation 48, we keep only the zeroth-order Tikhonov regularization and omitting the first-order Tikhonov regularization (**?**) which was also used by Oliveira Jr. et al. (2013).

The main advantage of the PEL is solve H-dimensional system of equations (equation 48), where H totalizes the number of polynomial coefficients composing all equivalent-source windows, requiring a lower computational effort since $H <<< N$. To avoid the storage of matrices $\mathbf{A}$ and $\mathbf{B}$, Oliveira Jr. et al. (2013) evaluate an element of the matrix $\mathbf{AB}$ by calculating the dot product between the row of matrix $\mathbf{A}$ and the column of the matrix $\mathbf{B}$. After estimating all polynomial coefficients of all windows, the estimated coefficients ($\mathbf{c}^*$ in equation 48) are transformed into a single physical-property distribution encompassing the entire equivalent layer.

As stated by Oliveira Jr. et al. (2013), the computational efficiency of PEL approach stems from the fact that the total number of polynomial coefficients H required to depict the physical-property distribution within the equivalent layer is generally much smaller than the number of equivalent sources. Consequently, this leads to a considerably smaller linear system that needs to be solved. Hence, the main strategy of polynomial equivalent layer is the model dimension reduction.

The polynomial equivalent layer was applied to perform upward continuations of gravity and magnetic data and reduction to the pole of magnetic data.

4.0.4 The iterative scheme without solving a linear system

There exists a class of methods that iteratively estimate the distribution of physical properties within an equivalent layer without the need to solve linear systems. The method initially introduced by Cordell (1992) and later expanded upon by Guspí and Novara (2009) updates the physical property of sources, located beneath each potential-field data, by removing the maximum residual between the observed and fitted data. In addition, Xia and Sprowl (1991) and Xia et al. (1993) have developed efficient iterative algorithms for updating the distribution of physical properties within the equivalent layer in the wavenumber and space domains, respectively. Specifically, in Xia and Sprowl's (1991) method the physical-property distribution is updated by using the ratio between the squared depth to the equivalent source and the gravitational constant

multiplied by the residual between the observed and predicted observation at the measurement station. Neither of these methods solve linear systems.

Following this class of methods of iterative equivalent-layer technique that does not solve linear systems, Siqueira et al. (2017) developed a fast iterative equivalent-layer technique for processing gravity data in which the sensitivity matrix $\mathbf{A}$ (equation 3) is replaced by a diagonal matrix $N \times N$, i.e.:

$$\tilde{\tilde{\mathbf{A}}} = 2\,\pi\,\gamma\,\boldsymbol{\Delta}\mathbf{S}^{-\mathbf{1}}\,, \tag{49}$$

where γ is Newton's gravitational constant and $\boldsymbol{\Delta}\mathbf{S}^{-\mathbf{1}}$ is a diagonal matrix of order N whose diagonal elements Δs_i, $i = 1, ..., N$ are the element of area centered at the ith horizontal coordinates of the ith observation point. The physical foundations of Siqueira et al.'s (2017) method rely on two constraints: i) the excess of mass; and ii) the positive correlation between the gravity observations and the mass distribution over the equivalent layer.

Although Siqueira et al.'s (2017) method does not solve any linear system of equations, it can be theoretically explained by solving the following linear system at the kth iteration:

$$\tilde{\tilde{\mathbf{A}}}^{\top}\,\tilde{\tilde{\mathbf{A}}}\boldsymbol{\Delta}\,\hat{\mathbf{p}}^{k} \;=\; \tilde{\tilde{\mathbf{A}}}^{\top}\,\mathbf{r}^{k}\,, \tag{50}$$

where $\mathbf{r}^k$ is an N-dimensional residual vector whose ith element is calculated by subtracting the ith observed data d_i^o from the ith fitted data d_i^k at the kth iteration, i.e.,

$$r_i^k = d_i^o \;-\; d_i^k\,. \tag{51}$$

and $\boldsymbol{\Delta}\,\hat{\mathbf{p}}^k$ is an estimated N-dimensional vector of parameter correction.

Because $\tilde{\tilde{\mathbf{A}}}$, in equation 50, is a diagonal matrix (equation 49), the parameter correction estimate is directly calculated without solving system of linear equations, and thus, an ith element of $\boldsymbol{\Delta}\,\hat{\mathbf{p}}^k$ is directly calculated by

$$\Delta\hat{p}^{k}{}_{i} = \frac{\Delta s_i\; r_i^k}{2\,\pi\,\gamma}\,. \tag{52}$$

The mass distribution over the equivalent layer is updated by:

$$\hat{p}_i^{k+1} = \hat{p}_i^k \;+\; \Delta\hat{p}^{k}{}_{i}\,. \tag{53}$$

Siqueira et al.'s (2017) method starts from a mass distribution on the equivalent layer, whose ith mass p_i^o is proportional to the ith observed data d_i^o, i.e.,

$$p_i^o = \frac{\Delta s_i\; d_i^o}{2\,\pi\,\gamma}\,. \tag{54}$$

Siqueira et al. (2017) applied their fast iterative equivalent-layer technique to interpolate, calculate the horizontal components, and continue upward (or downward) gravity data.

For jointly process two gravity gradient components, Jirigalatu and Ebbing (2019) used the Gauss-FFT for forward calculation of potential fields in the wavenumber domain combined with Landweber's iteration coupled with a mask matrix $\mathbf{M}$ to reduce the edge effects without increasing the computation cost. The

mask matrix $\mathbf{M}$ is defined in the following way: if the corresponding pixel does not contain the original data, the element of $\mathbf{M}$ is set to zero; otherwise, it is set to one. The kth Landweber iteration is given by

$$\mathbf{p}_{k+1} = \mathbf{p}_k + \omega \left[\mathbf{A_1}^\top (\mathbf{d_1} - \mathbf{M}\mathbf{A_1}\mathbf{p}_k) + \mathbf{A_2}^\top (\mathbf{d_2} - \mathbf{M}\mathbf{A_2}\mathbf{p}_k) \right] , \tag{55}$$

where ω is a relaxation factor, $\mathbf{d_1}$ and $\mathbf{d_2}$ are the two gravity gradient components and $\mathbf{A_1}$ and $\mathbf{A_2}$ are the corresponding gravity gradient kernels. Jirigalatu and Ebbing (2019) applied their method for processing two horizontal curvature components of Falcon airborne gravity gradient.

4.0.5 The convolutional equivalent layer with BTTB matrices

? (**?**, **?**) introduced the convolutional equivalent layer for gravimetric and magnetic data processing, respectively.

? demonstrated that the sensitivity matrix $\mathbf{A}$ (equation 3) associated with a planar equivalent layer formed by a set of point masses, each one directly beneath each observation point and considering a regular grid of observation points at a constant height has a symmetric block-Toeplitz Toeplitz-block (BTTB) structure. A symmetric BTTB matrix has, at least, two attractive properties. The first one is that it can be defined by using only the elements forming its first column (or row). The second attractive property is that any BTTB matrix can be embedded into a symmetric Block-Circulat Circulant-Block (BCCB) matrix. This means that the full sensitivity matrix $\mathbf{A}$ (equation 3) can be completely reconstruct by using the first column of the BCCB matrix only. In what follows, **?** computed the forward modeling by using only a single equivalent source. Specifically, it is done by calculating the eigenvalues of the BCCB matrix that can be efficiently computed by using only the first column of the BCCB matrix via 2D fast Fourier transform (2D FFT). By comparing with the classic approach in the Fourier domain, the convolutional equivalent layer for gravimetric data processing proposed by **?** performed upward- and downward-continue gravity data with a very small border effects and noise amplification.

By using the original idea of the convolutional equivalent layer proposed by **?** for gravimetric data processing, **?** developed the convolutional equivalent layer for magnetic data processing. By assuming a regularly spaced grid of magnetic data at a constant height and a planar equivalent layer of dipoles, **?** proved that the sensitivity matrix linked with this layer possess a BTTB structure in the specific scenario where each dipole is exactly beneath each observed magnetic data point. **?** used a conjugate gradient least-squares (CGLS) algorithm which does not require an inverse matrix or matrix-matrix multiplication. Rather, it only requires matrix-vector multiplications per iteration, which can be effectively computed using the 2D FFT as a discrete convolution. The matrix-vector product only uses the elements that constitute the first column of the associated BTTB matrix, resulting in computational time and memory savings. **?** (**?**) showed the robustness of the convolutional equivalent layer in processing magnetic survey that violates the requirement of regular grids in the horizontal directions and flat observation surfaces.

The matrix-vector product in **?** (**?**, **?**) (e.g., $\mathbf{d} = \mathbf{A}\mathbf{p}$, such as in equation 3) is the main issue to be solved. To solve it efficiently, these authors involked the auxiliary linear system

$$\mathbf{w} = \mathbf{C}\mathbf{v} , \tag{56}$$

where $\mathbf{w}$ and $\mathbf{v}$ are, respectively, vectors of data and parameters completed by zeros and $\mathbf{C}$ is a BCCB matrix formed by $2Q \times 2Q$ blocks, where each block $\mathbf{C}_q$, $q = 0, \ldots, Q-1$, is a $2P \times 2P$ circulant matrix. The first column of $\mathbf{C}$ is obtained by rearranging the first column of the sensitivity matrix $\mathbf{A}$ (equation 3).

Because a BCCB matrix is diagonalized by the 2D unitary discrete Fourier transform (DFT), $\mathbf{C}$ can be written as

$$\mathbf{C} = \left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right)^{*} \mathbf{\Lambda} \left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right) \ , \tag{57}$$

where the symbol "$\otimes$" denotes the Kronecker product (**?**), $\mathbf{F}_{2Q}$ and $\mathbf{F}_{2P}$ are the $2Q \times 2Q$ and $2P \times 2P$ unitary DFT matrices (**?**, p. 31), respectively, the superscritpt "$*$" denotes the complex conjugate and $\mathbf{\Lambda}$ is a $4QP \times 4QP$ diagonal matrix containing the eigenvalues of $\mathbf{C}$. Due to the diagonalization of the matrix $\mathbf{C}$, the auxiliary system (equation 56) can be rewritten by using equation 57 and premultiplying both sides of the result by $\left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right)$, i.e.,

$$\mathbf{\Lambda} \left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right) \mathbf{v} = \left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right) \mathbf{w} \ . \tag{58}$$

By applying the vec-operator (**?**) to both sides of equation 58, by premultiplying both sides of the result by $\mathbf{F}_{2Q}^{*}$ and then postmultiplying both sides of the result by $\mathbf{F}_{2P}^{*}$

$$\mathbf{F}_{2Q}^{*} \left[\mathbf{L} \circ \left(\mathbf{F}_{2Q}\, \mathbf{V}\, \mathbf{F}_{2P}\right)\right] \mathbf{F}_{2P}^{*} = \mathbf{W} \ , \tag{59}$$

where "$\circ$" denotes the Hadamard product (**?**, p. 298) and $\mathbf{L}$, $\mathbf{V}$ and $\mathbf{W}$ are $2Q \times 2P$ matrices obtained by rearranging, along their rows, the elements forming the diagonal of matrix $\mathbf{\Lambda}$, vector $\mathbf{v}$ and vector $\mathbf{w}$, respectively. The left side of equation 59 contains the 2D Inverse Discrete Fourier Transform (IDFT) of the term in brackets, which in turn represents the Hadamard product of matrix $\mathbf{L}$ and the 2D DFT of matrix $\mathbf{V}$. Matrix $\mathbf{L}$ contains the eigenvalues of $\mathbf{\Lambda}$ (equation 57) and can be efficiently computed by using only the first column of the BCCB matrix $\mathbf{C}$ (equation 56).

Actually, in **?** (**?**, **?**) a fast 2D discrete circular convolution (Van Loan, 1992) is used to process very large gravity and magnetic datasets efficiently. The convolutional equivalent layer was applied to perform upward continuation of large magnetic datasets. Compared to the classical Fourier approach, **?**'s (**?**) method produces smaller border effects without using any padding scheme.

Without taking advantage of the symmetric BTTB structure of the sensitivity matrix (**?**, **?**) that arises when gravimetric observations are measured on a horizontally regular grid, on a flat surface and considering a regular grid of equivalent sources whithin a horizontal layer, **?** explored the symmetry of the gravity kernel to reduce the number of forward model evaluations. By exploting the symmetries of the gravity kernels and redundancies in the forward model evaluations on a regular grid and combining the subspace solution based on eigenvectors of the gridded dataset, **?** estimated the mass excess or deficiency produced by anomalous sources with positive or negative density contrast.

4.0.6 The deconvolutional equivalent layer with BTTB matrices

To avoid the iterations of the conjugate gradient method in **?**, we can employ the deconvolution process. Equation 59 shows that estimate the matrix $\mathbf{V}$, containing the elements of parameter vector $\mathbf{p}$, is a inverse problem that could be solved by deconvolution. From equation 59, the matrix $\mathbf{V}$ can be obtain by deconvolution, i.e.

$$\mathbf{V} \ = \ \mathbf{F}_{2Q}^{*} \left[\frac{\left(\mathbf{F}_{2Q} \mathbf{W}\, \mathbf{F}_{2P}\right)}{\mathbf{L}}\right] \mathbf{F}_{2P}^{*} \ . \tag{60}$$

Equation 60 shows that the parameter vector (in matrix $\mathbf{V}$) can be theoretically obtain by dividing each potential-field observations (in matrix $\mathbf{W}$) by each eigenvalues (in matrix $\mathbf{L}$). Hence, the parameter vector is constructed by element-by-element division of data by eigenvalues.

However, the deconvolution often is extremely unstable. This means that a small change in data can lead to an enormous change in the estimated parameter. Hence, equation 60 requires regularization to be useful. We usede wiener deconvolution to obtain a stable solution, i.e.,

$$\mathbf{V} \;=\; \mathbf{F}_{2Q}^{*}\left[\left(\mathbf{F}_{2Q}\mathbf{W}\,\mathbf{F}_{2P}\right)\frac{\mathbf{L}^{*}}{(\mathbf{L}\,\mathbf{L}^{*}+\mu)}\right]\mathbf{F}_{2P}^{*}\,, \tag{61}$$

where the matrix $\mathbf{L}^{*}$ contains the complex conjugate eigenvalues and μ is a parameter that controls the degree of stabilization.

4.1 Solution stability

The solution stability of the equivalent-layer methods is rarely addressed. Here, we follow the numerical stability analysis presented in Siqueira et al. (2017).

Let us assume noise-free potential-field data $\mathbf{d}$, we estimate a physical-property distribution $\mathbf{p}$ (estimated solution) within the equivalent layer. Then, the noise-free data $\mathbf{d}$ are contaminated with additive D different sequences of pseudorandom Gaussian noise, creating different noise-corrupted potential-field data $\mathbf{d}_{\ell}^{\mathbf{o}}$, $\ell = 1, ..., D$. From each $\mathbf{d}_{\ell}^{\mathbf{o}}$, we estimate a physical-property distribution $\hat{\mathbf{p}}_{\ell}$ within the equivalent layer.

Next, for each noise-corrupted data $\mathbf{d}_{\ell}^{\mathbf{o}}$ and estimated solution $\hat{\mathbf{p}}_{\ell}$, the ℓth model perturbation δp_{ℓ} and the ℓth data perturbation δd_{ℓ} are, respectively, evaluated by

$$\delta p_{\ell} = \frac{\parallel \hat{\mathbf{p}}_{\ell} - \mathbf{p} \parallel_2}{\parallel \mathbf{p} \parallel_2}, \quad \ell = 1, ..., D, \tag{62}$$

and

$$\delta d_{\ell} = \frac{\parallel \mathbf{d}_{\ell}^{\mathbf{o}} - \mathbf{d} \parallel_2}{\parallel \mathbf{d} \parallel_2}, \quad \ell = 1, ..., D. \tag{63}$$

Regardless of the particular method used, the following inequality (**?**, p. 66) is applicable:

$$\delta p_{\ell} \leq \kappa\, \delta d_{\ell}, \quad \ell = 1, ..., D, \tag{64}$$

where κ is the constant of proportionality between the model perturbation δp_{ℓ} (equation 62) and the data perturbation δd_{ℓ} (equation 63). The constant κ acts as the condition number of an invertible matrix in a given inversion, and thus measures the instability of the solution. The larger (smaller) the value of κ the more unstable (stable) is the estimated solution.

Equation 64 shows a linear relationship between the model perturbation and the data perturbation. By plotting δp_{ℓ} (equation 62) against δd_{ℓ} (equation 63) produced by a set of D estimated solution obtained by applying a given equivalent-layer method, we obtain a straight line behaviour described by equation 64. By applying a linear regression, we obtain a fitted straight line whose estimated slope (κ in equation 64) quantifies the solution stability.

Here, the analysis of solution stability is numerically conducted by applying the classical equivalent-layer technique with zeroth-order Tikhonov regularization, the convolutional method for gravimetric and magnetic data, the deconvolutional method (equation 60) and the deconvolutional method with different values for the Wiener stabilization (equation 61).

5 NUMERICAL SIMULATIONS

We investigated different computational algorithms for inverting gravity disturbances and total-field anomalies. To test the capability of the fast equivalent-layer technique for processing that potential field data we measure of the computational effort by counting the number of floating-point operations (*flops*), such as additions, subtractions, multiplications, and divisions (Golub and Van Loan, 2013) for different number of observation points, ranging from $10,000$ up to $1,000,000$. The results generated when using iterative methods are set to $it = 50$ for the number of iterations.

5.1 Floating-point operations calculation

To measure the computational effort of the different algorithms to solve the equivalent layer linear system, a non-hardware dependent method can be useful because allow us to do direct comparison between them. Counting the floating-point operations (*flops*), i.e., additions, subtractions, multiplications and divisions is a good way to quantify the amount of work of a given algorithm (Golub and Van Loan, 2013). For example, the number of *flops* necessary to multiply two vectors $\mathbb{R}^N$ is $2N$. A common matrix-vector multiplication with dimension $\mathbb{R}^{N\times N}$ and $\mathbb{R}^N$, respectively, is $2N^2$ and a multiplication of two matrices $\mathbb{R}^{N\times N}$ is $2N^3$. Figure **??** shows the total flops count for the different methods presented in this review with a crescent number of data, ranging from $10,000$ to $1,000,000$ for the gravity equivalent layer and figure **??** for magnetic data.

5.1.1 Normal equations using Cholesky decomposition

The equivalent sources can be estimated directly from solving the normal equations 3. In this work we will use the Cholesky decompositions method to calculate the necessary *flops*. In this method it is calculated the lower triangule of $\mathbf{A}^T\mathbf{A}$ $(1/2N^3)$, the Cholesky factor $(1/3N^3)$, a matrix-vector multiplication $(2N^2)$ and finally solving the triangular system $(2N^2)$, totalizing

$$f_{classical} = \frac{5}{6}N^3 + 4N^2 \tag{65}$$

5.1.2 Window method (Leão and Silva, 1989)

The moving data-window scheme (Leão and Silva, 1989) solve N linear systems with much smaller sizes (equation **??**). For our results we are considering a data-window of the same size of wich the authors presented in theirs work ($N_w = 49$) and the same number of equivalent sources ($M_w = 225$). We are doing this process for all the other techniques to standardize the resolution of our problem. Using the Cholesky decomposition with this method the *flops* are

$$f_{window} = N\frac{5}{6}M_w N_w^2 + 4N_w M_w \tag{66}$$

5.1.3 PEL method (Oliveira Jr. et al., 2013)

The polynomial equivalent layer uses a simliar approach od moving windows from Leão and Silva (1989). For this operations calculation (equation 48) we used a first degree polynomial (two variables) and each window contains $N_s = 1,000$ observed data and $M_s = 1,000$ equivalent sources. Following the steps given in (Oliveira Jr. et al., 2013) the total *flops* becomes

$$f_{pel} = \frac{1}{3}H^3 + 2H^2 + 2NM_sH + H^2N + 2HN + 2NP \tag{67}$$

where H is the number of constant coefficients for the first degree polynomial ($P = 3$) times the number of windows ($P \times N/N_s$).

5.1.4 Conjugate gradient least square (CGLS)

The CGLS method is a very stable and fast algorithm for solving linear systems iteratively. Its computational complexity envolves a matrix-vector product outside the loop ($2N^2$), two matrix-vector products inside the loop ($4N^2$) and six vector products inside the loop ($12N$) (**?**)

$$f_{cgls} = 2N^2 + it(4N^2 + 12N) \tag{68}$$

5.1.5 Wavelet compression method with CGLS (**?**)

For the wavelet method (equation 41) we have calculated a coompression rate of 98% ($C_r = 0.02$) for the threshold as the authors used in **?** and the wavelet transformation requiring $\log_2(N)$ ***flops*** each (equations 40 and 42c), with its inverse also using the same number of operations (equation 44). Combined with the conjugate gradient least square necessary steps and iterations, the number of ***flops*** are

$$f_{wavelet} = 2NC_r + 4N\log_2(N) + it(4N\log_2(N) + 4NC_r + 12C_r) \tag{69}$$

5.1.6 Fast equivalent layer for gravity data (Siqueira et al., 2017)

The fast equivalent layer from Siqueira et al. (2017) solves the linear system in *it* iterations. The main cost of this method (equations 50,51, 52 and 53)is the matrix-vector multiplication to asses the predicted data ($2N^2$) and three simply element by element vector sum, subtraction and division ($3N$ total)

$$f_{siqueira} = it(3N + 2N^2) \tag{70}$$

5.1.7 Convolutional equivalent layer for gravity data (**?**)

This methods replaces the matrix-vector multiplication of the iterative fast-equivalent technique (Siqueira et al., 2017) by three steps, involving a Fourier transform, an inverse Fourier transform, and a Hadamard product of matrices (equation 59). Considering that the first column of our BCCB matrix has $4N$ elements, the flops count of this method is

$$f_{convgrav} = \kappa 4N\log_2(4N) + it(27N + \kappa 8N\log_2(4N)) \tag{71}$$

In the resultant count we considered a *radix-2* algorithm for the fast Fourier transform and its inverse, which has a κ equals to 5 and requires $\kappa 4N\log_2(4N)$ flops each. The Hadarmard product of two matrices of $4N$ elements with complex numbers takes $24N$ flops. Note that equation 71 is different from the one presented in **?** because we also added the flops necessary to calculate the eigenvalues in this form. It does not differentiate much in order of magnitude because the iterative part is the most costful.

5.1.8 Convolutional equivalent layer for magnetic data (**?**)

The convolutional equivalent layer for magnetic data uses the same flops count of the main operations as in the gravimetric case (equation 59), the difference is the use of the conjugate gradient algorithm to solve the inverse problem. It requires a Hadamard product outside of the iterative loop and the matrix-vector and vector-vector multiplications inside the loop as seem in equation 68.

$$f_{convmag} = \kappa 16N \log_2(4N) + 24N + it(\kappa 16N \log_2(4N) + 60N) \tag{72}$$

5.1.9 Deconvolutional method

The deconvolution method does not require an iterative algorithm, rather it solves the estimative of the physical properties in a single step using the $4N$ eigenvalues of the BCCB matrix as in the convolutional method. From equation 60 it is possible to deduce this method requires two fast Fourier transform ($\kappa 4N \log_2(4N)$), one for the eigenvalues and another for the data transformation, a element by element division ($24N$) and finally, a fast inverse Fourier transform for the final estimative ($\kappa 4N \log_2(4N)$).

$$f_{deconv} = \kappa 12N \log_2(4N) + 24N \tag{73}$$

Using the deconvolutional method with a Wiener stabilization adds two multiplications of complex elements of the conjugates eigenvalues ($24N$ each) and the sum of $4N$ elements with the stabilization parameter μ as shown in equation 61

$$f_{deconvwiener} = \kappa 12N \log_2(4N) + 76N \tag{74}$$

CONFLICT OF INTEREST STATEMENT

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

AUTHOR CONTRIBUTIONS

The Author Contributions section is mandatory for all articles, including articles by sole authors. If an appropriate statement is not provided on submission, a standard one will be inserted during the production process. The Author Contributions statement must describe the contributions of individual authors referred to by their initials and, in doing so, all authors agree to be accountable for the content of the work. Please see here for full authorship criteria.

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DATA AVAILABILITY STATEMENT

The datasets generated for this study can be found in the frontiers-paper Github repository link: https://github.com/DiegoTaka/frontiers-paper.

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