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

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1 FUNDAMENTALS

2 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),
3 $i \in \{1 : D\}$, of a topocentric Cartesian system with x, y and z axes pointing to north, east and down,
4 respectively. Consider that d_i can be satisfactorily approximated by a harmonic function

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

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

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

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

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

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

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

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

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

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

22 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

24 There is no well-established criteria to define the optimum number P or the spatial distribution of the
25 equivalent sources. We know that setting an equivalent layer with more (less) sources than potential-field
26 data usually leads to an underdetermined (overdetermined) inverse problem (e.g., Menke, 2018, p. 52–53).
27 Concerning the spatial distribution of the equivalent sources, the only condition is that they must rely on a
28 surface that is located below and does not cross that containing the potential field data. Soler and Ueda
29 (2021) present a practical discussion about this topic.

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

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38   DO GRID) E REIS (ESPAÇAMENTO DAS LINHAS)

39 **1.2 Matrix** G

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

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

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

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

43   and

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

44 In this case, the equivalent layer is formed by punctual sources representing monopoles or dipoles (e.g.,
45 Dampney, 1969; Emilia, 1973; Leão and Silva, 1989; Cordell, 1992; Oliveira Jr. et al., 2013; Siqueira et al.,
46 2017; Reis et al., 2020; Takahashi et al., 2020; Soler and Uieda, 2021; Takahashi et al., 2022). Another
47 common approach consists in not defining g_{ij} by using equations 6–8, but other harmonic functions
48 obtained by integrating them over the volume of regular prisms (e.g., Li and Oldenburg, 2010; Barnes and
49 Lumley, 2011; Li et al., 2014; Jirigalatu and Ebbing, 2019). There are also some less common approaches
50 defining the harmonic function g_{ij} (equation 2) as the potential field due to plane faces with constant
51 physical property (Hansen and Miyazaki, 1984), doublets (Silva, 1986) or by computing the double
52 integration of the inverse distance function with respect to z (Guspí and Novara, 2009).

53   A common assumption for most of the equivalent-layer methods is that the harmonic function g_{ij}
54 (equation 2) is independent on the actual physical relationship between the observed potential field and
55 their true sources (e.g., Cordell, 1992; Guspí and Novara, 2009; Li et al., 2014). Hence, g_{ij} can be
56 defined according to the problem. The only condition imposed to this function is that it decays to zero
57 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.
58 However, several methods use a function g_{ij} that preserves the physical relationship between the observed
59 potential field and their true sources. For the case in which the observed potential field is gravity data, g_{ij}
60 is commonly defined as a component of the gravitational field produced at (x_i, y_i, z_i) by a point mass or
61 prism located at (x_j, y_j, z_j), with unit density. On the other hand, g_{ij} is commonly defined as a component

62 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
63 magnetization intensity, when the observed potential field is magnetic data.

64   For all harmonic functions discussed above, the sensitivity matrix $\mathbf{G}$ (equation 3) is always dense. For
65 scattered potential-field data, $\mathbf{G}$ does not have a well-defined structure, regardless of whether the spatial
66 distribution of the equivalent sources is set. Nevertheless, for the particular case in which (i) there is a
67 single equivalent source right below each potential-field datum and (ii) both data and sources rely on
68 planar and regularly spaced grids, Takahashi et al. (2020, 2022) show that $\mathbf{G}$ assumes a block-Toeplitz
69 Toeplitz-block (BTTB) structure. In this case, the product of $\mathbf{G}$ and an arbitrary vector can be efficiently
70 computed via 2D fast Fourier transform as a discrete convolution.

1.3 General formulation

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

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

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

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

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

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

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

81 which is a combination of particular measures of length given by

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

82 and

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

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

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

87 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.

Matrix $\mathbf{B}$ defined by equation 20 is commonly used for the cases in which $D > P$, 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 $D < P$ (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:

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

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.

107 1.3.1 Optional normalization strategy

108 Setting the regularization parameter μ (equation 11) can be very difficult due to scale differences between
109 $\mathbf{G}$ and $\mathbf{p}$ (equation 3) or $\mathbf{GH}$ and $\mathbf{q}$ (equation 9. When faced with this scenario, a popular strategy (e.g., Li
110 and Oldenburg, 2010; Soler and Uieda, 2021) involves creating the linear system (equations 22 and 23) by
111 substituting $\mathbf{GH}$ and $\mathbf{q}$ with

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

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

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

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

2 COMPUTATIONAL STRATEGIES

117 COMEÇAR EXPLICANDO AS LIMITAÇÕES DA SOLUÇÃO OBTIDA PELA FORMULAÇÃO
118 GERAL

119 Two important factors affecting the efficiency of a given matrix algorithm are the storage and amount of
120 required arithmetic. Here, we quantify this last factor by counting flops. A flop is a floating point addition,
121 subtraction, multiplication or division (Golub and Van Loan, 2013, p. 12–14).

122 To investigate the efficiency of equivalent-layer methods, we consider how they:

123 (i) set up the linear system (equations 22 and 23);

124 (ii) solve the linear system (equations 22 and 23);

125 (iii) perform potential-field transformations (equation 4).

126 We focus on the overall strategies used by the selected methods.

2.1 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,

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

128 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:

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

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

130 **2.2 Moving window**

131 The initial approach to enhance the computational efficiency of the equivalent-layer technique is
132 commonly denoted *moving window* and involves first splitting the observed data d_i, $i \in \{1 : D\}$, into
133 M overlapping subsets (or data windows) formed by D^m data each, $m \in \{1 : M\}$. The data inside the
134 m-th window are usually adjacent to each other and have indices defined by an integer list $\mathbf{i}^m$ having
135 D^m elements. The number of data D^m forming the data windows are not necessarily equal to each other.
136 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
137 a set of P equivalent sources with scalar physical property p_j, $j \in \{1 : P\}$, and also split them into M
138 overlapping subsets (or source windows) formed by P^m data each, $m \in \{1 : M\}$. The sources inside the
139 m-th window have indices defined by an integer list $\mathbf{j}^m$ having P^m elements. Each source window has a
140 $P^m \times 1$ parameter vector $\mathbf{p}^m$ and is located right below the corresponding m-th data window. Then, each
141 $\mathbf{d}^m \equiv \mathbf{d}[\mathbf{i}^m]$ is approximated by

$$\mathbf{f}^m = \mathbf{G}^m \mathbf{p}^m , \tag{26}$$

142 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
143 2 using only the data and equivalent sources located inside the window m-th. The main idea of the moving-
144 window approach is using the $\tilde{\mathbf{p}}^m$ estimated for each window to obtain (i) an estimate $\tilde{\mathbf{p}}$ of the parameter
145 vector for the entire equivalent layer or (ii) a given potential-field transformation $\mathbf{t}$ (equation 4). The main
146 advantages of this approach is that (i) the estimated parameter vector $\tilde{\mathbf{p}}$ or transformed potential field are
147 not obtained by solving the full, but smaller linear systems and (ii) the full matrix $\mathbf{G}$ (equation 3) is never
148 stored.

149 Leão and Silva (1989) presented a pioneer work using the moving-window approach. Their method
150 requires a regularly-spaced grid of observed data on a horizontal plane z_0. The data windows are defined by
151 square local grids of $\sqrt{D'} \times \sqrt{D'}$ adjacent points, all of them having the same number of points D'. The
152 equivalent sources in the m-th data window are located below the observation plane, at a constant vertical
153 distance Δz_0. They are arranged on a regular grid of $\sqrt{P'} \times \sqrt{P'}$ adjacent points following the same
154 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 26) 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:

$$t_c^m = \left(\mathbf{G}'\mathbf{a}'\right)^\top \left[\mathbf{G}' \left(\mathbf{G}'\right)^\top + \mu \, \mathbf{I}_{D'}\right]^{-1} \mathbf{d}^m, \quad m \in \{1 : M\}, \tag{27}$$

where $\mathbf{I}_{D'}$ is the identity matrix of order D' and $\mathbf{a}'$ is a $P' \times 1$ vector with elements computed by equation 5 by using all equivalent sources in the m-th subset 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, $\mathbf{a}'$ is the same for all data windows. Note that equation 27 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), $\bar{p} = \mathbf{0}$ (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 26). 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.

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

Initialization :
1 Set the indices $\mathbf{i}^m$ for each data window, $m \in \{1 : M\}$;
2 Set the indices $\mathbf{j}^m$ for each source window, $m \in \{1 : M\}$;
3 Set the constant depth $z_0 + \Delta z_0$ for all equivalent sources ;
4 Compute the vector $\mathbf{a}'$ associated with the desired potential-field transformation ;
5 Compute the matrix $\mathbf{G}'$;
6 Compute $\left(\mathbf{G}'\mathbf{a}'\right)^\top \left[\mathbf{G}' \left(\mathbf{G}'\right)^\top + \mu \, \mathbf{I}_{D'}\right]^{-1}$;
7 $m = 1$;
8 **while** $m < M$ **do**
9 $\quad$ Compute t_c^m (equation 27) ;
10 $\quad$ $m \leftarrow m + 1$;
11 **end**

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 26) 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 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

182 a diagonal matrix of weights for the data inside the m-th window and $\bar{p} = \mathbf{0}$ (equation 14), so that

$$\left[(\mathbf{G}^m)^\top \, \mathbf{W}_d^m \, \mathbf{G}^m + \mu \, \mathbf{I}_{P'} \right] \tilde{\mathbf{p}}^m = (\mathbf{G}^m)^\top \, \mathbf{W}_d^m \, \mathbf{d}^m \ . \tag{28}$$

183 It is important to stress here that Soler and Uieda (2021) used the normalization strategy described in
184 section 1.3.1, but we have conveniently omitted here. The overall steps of their method are defined by the
185 Algorithm 2. Note that this algorithm starts with a residuals vector $\mathbf{r}$ that is iteratively updated. At each
186 iteration, the potential field predicted a source window is computed at all observation points and removed
187 from the residuals vector $\mathbf{r}$.

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

   Initialization :
1   Set the indices $\mathbf{i}^m$ for each data window, $m \in \{1 : M\}$;
2   Set the indices $\mathbf{j}^m$ for each source window, $m \in \{1 : M\}$;
3   Set the depth of all equivalent sources ;
4   Set a $D \times 1$ residuals vector $\mathbf{r} = \mathbf{d}$;
5   Set a $P \times 1$ vector $\tilde{\mathbf{p}} = \mathbf{0}$;
6   $m = 1$;
7   **while** $m < M$ **do**
8   Set the matrix $\mathbf{W}_d^m$;
9   Compute the matrix $\mathbf{G}^m$;
10   Compute $\tilde{\mathbf{p}}^m$ (equation 28) ;
11      $\tilde{\mathbf{p}}[\mathbf{j}^m] \leftarrow \tilde{\mathbf{p}}[\mathbf{j}^m] + \tilde{\mathbf{p}}^m$;
12      $\mathbf{r} \leftarrow \mathbf{r} - \mathbf{G}[:, \mathbf{j}^m] \, \tilde{\mathbf{p}}^m$;
13      $m \leftarrow m + 1$;
14   **end**

2.3 Column update

189   Cordell (1992) proposed a computational strategy that was later used by Guspí and Novara (2009) and
190 relies on first defining one equivalent source located right below each observed data d_i, $i \in \{1 : D\}$, at
191 a vertical coordinate $z_i + \Delta z_i$, where Δz_i is proportional to the distance from the i-th observation point
192 (x_i, y_i, z_i) to its closest neighbor. The second step consists in updating the physical property p_j of a given
193 equivalent source, $j \in \{1 : D\}$ and remove its predicted potential field from the observed data vector $\mathbf{d}$,
194 producing a residuals vector $\mathbf{r}$. Then, the same procedure is repeated for other sources with the purpose of
195 iteratively updating $\mathbf{r}$ and the $D \times 1$ parameter vector $\mathbf{p}$ containing the physical property of all equivalent
196 sources. At the end, the algorithm produces an estimate $\tilde{\mathbf{p}}$ for the parameter vector yielding a predicted
197 potential field $\mathbf{f}$ (equation 3) satisfactorily fitting the observed data $\mathbf{d}$ according to a given criterion. Note
198 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 $\mathbf{G}$.
199 At each iteration, only a single column of $\mathbf{G}$ (equation 3) is used. An advantage of this *column-update*
200 *approach* is that the full matrix $\mathbf{G}$ is never stored.

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

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206 in $\mathbf{r}$ decreases robustly at the beginning and oscillates within a narrowing envelope for the subsequent
207 iterations.

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

Initialization :
1   Compute a $D \times 1$ vector $\boldsymbol{\Delta z}$ whose i-th element Δz_i is a vertical distance controlling the depth of
    the i-th equivalent source, $i \in \{1 : D\}$;
2   Set a tolerance ϵ ;
3   Set a maximum number of iteration `ITMAX` ;
4   Set a $D \times 1$ residuals vector $\mathbf{r} = \mathbf{d}$;
5   Set a $D \times 1$ vector $\tilde{\mathbf{p}} = \mathbf{0}$;
6   Define the maximum absolute value r_{max} in $\mathbf{r}$;
7   $m = 1$;
8   **while** $(r_{\text{max}} > \epsilon)$ **and** $(m < \texttt{ITMAX})$ **do**
9   $\quad$ Define the coordinates $(x_{\text{max}}, y_{\text{max}}, z_{\text{max}})$ and index i_{max} of the observation point associated with
    $\quad \quad r_{\text{max}}$;
10 $\quad \tilde{\mathbf{p}}[i_{\text{max}}] \leftarrow \tilde{\mathbf{p}}[i_{\text{max}}] + (a_{\text{max}} \boldsymbol{\Delta z}[i_{\text{max}}])$;
11 $\quad \mathbf{r} \leftarrow \mathbf{r} - (\mathbf{G}[:, i_{\text{max}}] \, \tilde{\mathbf{p}}[i_{\text{max}}])$;
12 $\quad$ Define the new r_{max} in $\mathbf{r}$;
13 $\quad m \leftarrow m + 1$;
14 **end**

2.4 Row update

209 Mendonça and Silva (1994) proposes an algebraic reconstruction technique (ART) (e.g., van der Sluis
210 and van der Vorst, 1987, p. 58) to estimate a parameter vector $\tilde{\mathbf{p}}$ for a regular grid of P equivalent sources
211 on a horizontal plane z_0. Such methods iterate on the linear system rows to estimate corrections for the
212 parameter vector, which may substantially save computer time and memory required to compute and store
213 the full linear system matrix along the iterations. The convergence of such *row-update methods* depends on
214 the linear system condition. The main advantage of such methods is not computing and storing the full
215 linear system matrix, but iteratively using its rows. The particular ART method proposed by Mendonça and
216 Silva (1994) considers that

$$\mathbf{d} = \begin{bmatrix} \mathbf{d}_e \\ \mathbf{d}_r \end{bmatrix} , \quad \mathbf{G} = \begin{bmatrix} \mathbf{G}_e \\ \mathbf{R}_r \end{bmatrix} , \tag{29}$$

217 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,
218 respectively. Mendonça and Silva (1994) designate $\mathbf{d}_e$ and $\mathbf{d}_r$ as, respectively, *equivalent* and *redundant*
219 data. With the exception of a normalization strategy, Mendonça and Silva (1994) calculate a $P \times 1$ estimated
220 parameter vector $\tilde{\mathbf{p}}$ by solving an underdetermined problem (equation 23) involving only the equivalent
221 data $\mathbf{d}_e$ (equation 29) for the particular case in which $\mathbf{H} = \mathbf{W}_p = \mathbf{I}_P$ (equations 9 and 13), $\mathbf{W}_d = \mathbf{I}_{D_e}$
222 (equation 12) and $\bar{p} = \mathbf{0}$ (equation 14), which results in

$$\begin{aligned} (\mathbf{F} + \mu \, \mathbf{I}_{D_e}) \, \mathbf{u} &= \mathbf{d}_e \\ \tilde{\mathbf{p}} &= \mathbf{G}_e^\top \mathbf{u} \end{aligned} , \tag{30}$$

223 where $\mathbf{F}$ is a $P \times P$ matrix that replaces $\mathbf{G}_e \mathbf{G}_e^\top$. Mendonça and Silva (1994) presume that the estimated
224 parameter vector $\tilde{\mathbf{p}}$ obtained from equation 30 leads to a $D_r \times 1$ residuals vector

$$\mathbf{r} = \mathbf{d}_r - \mathbf{G}_r \tilde{\mathbf{p}} \tag{31}$$

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

226   The overall method of Mendonça and Silva (1994) is defined by Algorithm 4. It is important noting
227 that the number D_e of equivalent data in $\mathbf{d}_e$ increases by one per iteration, which means that the order
228 of the linear system in equation 30 also increases by one at each iteration. Those authors also propose
229 a computational strategy based on Cholesky factorization (e.g., Golub and Van Loan, 2013, p. 163) for
230 efficiently updating $(\mathbf{F} + \mu \mathbf{I}_{D_e})$ at a given iteration (line 16 in Algorithm 4) by computing only its new
231 elements with respect to those computed in the previous iteration.

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

Initialization :
1 Set a regular grid of P equivalent sources at a horizontal plane z_0 ;
2 Set a tolerance ϵ ;
3 Set a $D \times 1$ residuals vector $\mathbf{r} = \mathbf{d}$;
4 Define the maximum absolute value $r_{\texttt{max}}$ in $\mathbf{r}$;
5 Define the index $i_{\texttt{max}}$ of $r_{\texttt{max}}$;
6 Define the list of indices $\mathbf{i}_r$ of the remaining data in $\mathbf{r}$;
7 Define $\mathbf{d}_e = \mathbf{d}[i_{\texttt{max}}]$;
8 Compute $(\mathbf{F} + \mu \mathbf{I}_{D_e})$ and $\mathbf{G}_e$;
9 Compute $\tilde{\mathbf{p}}$ (equation 30) ;
10 Compute $\mathbf{r} = \mathbf{d}[\mathbf{i}_r] - \mathbf{G}[\mathbf{i}_r, :] \tilde{\mathbf{p}}$;
11 Define the maximum absolute value $r_{\texttt{max}}$ in $\mathbf{r}$;
12 **while** $(r_{\texttt{max}} > \epsilon)$ **do**
13   Define the index $i_{\texttt{max}}$ of $r_{\texttt{max}}$;
14   Define the list of indices $\mathbf{i}_r$ of the remaining elements in $\mathbf{r}$;
15     $\mathbf{d}_e \leftarrow \begin{bmatrix} \mathbf{d}_e \\ \mathbf{d}[i_{\texttt{max}}] \end{bmatrix}$;
16   Update $(\mathbf{F} + \mu \mathbf{I}_{D_e})$ and $\mathbf{G}_e$;
17   Update $\tilde{\mathbf{p}}$ (equation 30) ;
18   Update $\mathbf{r} = \mathbf{d}[\mathbf{i}_r] - \mathbf{G}[\mathbf{i}_r, :] \tilde{\mathbf{p}}$;
19   Define the maximum absolute value $r_{\texttt{max}}$ in $\mathbf{r}$;
20 **end**

2.5 Reparameterization

233   Another approach for improving the computational performance of equivalent-layer technique consists
234 in setting a $P \times Q$ reparameterization matrix $\mathbf{H}$ (equation 9) with $Q << P$. This strategy has been used
235 in applied geophysics for decades (e.g., Skilling and Bryan, 1984; Kennett et al., 1988; Oldenburg et al.,
236 1993; Barbosa et al., 1997) and is known as *subspace method*. The main idea relies in reducing the linear
237 system dimension from the original P-space to a lower-dimensional subspace (the Q-space). An estimate
238 $\tilde{\mathbf{q}}$ for the reparameterized parameter vector $\mathbf{q}$ is obtained in the Q-space and subsequently used to obtain
239 an estimate $\tilde{\mathbf{p}}$ for the parameter vector $\mathbf{p}$ (equation 3) in the P-space by using equation 9. Hence, the key
240 aspect of this *reparameterization approach* is solving an appreciably smaller linear inverse problem for $\tilde{\mathbf{q}}$
241 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 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

$$\left(\mathbf{H}^\top \mathbf{G}^\top \mathbf{G} \mathbf{H} + \mu \mathbf{W}_q\right) \tilde{\mathbf{q}} = \mathbf{H}^\top \mathbf{G}^\top \mathbf{d}, \tag{32}$$

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 $\mathbf{G}\mathbf{H}$ (equation 10) is notably sparse. Barnes and Lumley (2011) explore this sparsity in solving the overdetermined problem for $\tilde{\mathbf{q}}$ (equation 32) via conjugate-gradient method (e.g., Golub and Van Loan, 2013, sec. 11.3).

2.6 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

$$\mathbf{d}_w \approx \mathbf{G}_s \, \mathbf{p}_w, \tag{33}$$

281 where

$$\mathbf{d}_w = \boldsymbol{\mathcal{W}}\,\mathbf{d}\,, \quad \mathbf{p}_w = \boldsymbol{\mathcal{W}}\,\mathbf{p}\,, \tag{34}$$

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

$$\mathbf{G}_w = \boldsymbol{\mathcal{W}}\,\mathbf{G}\,\boldsymbol{\mathcal{W}} \tag{35}$$

284 with absolute value smaller than a given threshold.

285 Li and Oldenburg (2010) apply the normalization strategy defined in section 1.3.1 to equation 33 by using
286 a diagonal normalization matrix $\mathbf{N}$ (equation 24) and then formulate an overdetermined problem (equation
287 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
288 that

$$\left(\mathbf{G}_n^{\top}\mathbf{G}_n\right)\tilde{\mathbf{p}}_n = \mathbf{G}_n^{\top}\mathbf{d}_w\,, \tag{36}$$

289 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 33).
290 They solve this linear system (equation 36) with the conjugate-gradient method (e.g., Golub and Van Loan,
291 2013, sec. 11.3) and use it to obtain an estimate $\tilde{\mathbf{p}}$ for the parameter vector given by

$$\tilde{\mathbf{p}} = \boldsymbol{\mathcal{W}}^{\top}\left(\mathbf{N}\,\tilde{\mathbf{p}}_n\right)\,, \tag{37}$$

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

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

295 In the context of equivalent-layer technique, there are methods (e.g., Li and Oldenburg, 2010; Barnes
296 and Lumley, 2011) that modify the original linear system and then iteratively solve this modified system
297 by using the well-established conjugate gradient method (e.g., Golub and Van Loan, 2013, sec. 11.3).
298 Xia and Sprowl (1991) also proposed an iterative method for estimating a parameter vector $\tilde{\mathbf{p}}$ (equation
299 3). Their method, however, uses the original matrix $\mathbf{G}$ without previously computing a compression
300 or reparameterization, for example. More than two decades later, Siqueira et al. (2017) have deduced
301 essentially the same method presented by Xia and Sprowl (1991), but by following a more theoretical
302 approach based on the Gauss' theorem (e.g., Kellogg, 1967, p. 43) and the total excess of mass (e.g.,
303 Blakely, 1996, p. 60). Besides, Siqueira et al. (2017) have shown that this method produces very stable
304 solutions, even for noise-corrupted potential-field data.

305 The iterative method proposed by Xia and Sprowl (1991) and Siqueira et al. (2017) is outlined in
306 Algorithm 5, presumes an equivalent layer formed by monopoles (point masses) and can be applied to
307 irregularly-spaced data on an undulating surface. Note that the residuals $\mathbf{r}$ are used to compute a correction
308 $\Delta\mathbf{p}$ for the parameter vector at each iteration (line 11), which requires a matrix-vector product involving
309 the full matrix $\mathbf{G}$. Interestingly, this approach for estimating the physical property distribution on an
310 equivalent layer is the same originally proposed by Bott (1960) for estimating the basement relief under
311 sedimentary basins. The method of Xia and Sprowl (1991) and Siqueira et al. (2017) was originally
312 proposed for processing gravity data, but can be potentially applied to any harmonic function because it
313 actually represents an iterative solution of the classical *Dirichlet's problem* or the *first boundary value*
314 *problem of potential theory* (Kellogg, 1967, p. 236) on a plane.

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

324   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 "∘" 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      $\Delta\mathbf{p} = \mathbf{s} \circ \mathbf{r}$;
10     $\tilde{\mathbf{p}} \leftarrow \tilde{\mathbf{p}} + \Delta\mathbf{p}$;
11     $\mathbf{r} \leftarrow \mathbf{r} - \mathbf{G}\,\Delta\mathbf{p}$;
12   Compute $\|\mathbf{r}\|$;
13 **end**

2.8 Discrete convolution

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

331   Takahashi et al. (2020, 2022) consider a regular grid of D potential-field data at points (x_i, y_i, z_0),
332   $i \in \{1 : D\}$, on a horizontal plane z_0. The data indices i may be ordered along the $x-$ or $y-$direction,
333   which results in an $x-$ or $y-$oriented grid, respectively. They also consider a single equivalent source
334   located right below each datum, at a constant vertical coordinate $z_0 + \Delta z$, $\Delta z > 0$. In this case, the number
335   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
336   formed by $D_B \times D_B$ blocks, where each block has $D_b \times D_b$ elements, with $D = D_B\,D_b$.

337   Let $\mathcal{D}$ be a $2D_B \times 2D_b$ matrix formed by four blocks of $D_B \times D_b$ elements. All blocks have null
338   elements, except the first block in the first quadrant, which has the observed data d_i, $i \in \{1 : D\}$ arranged
339   along its rows or columns if the data grid has a $x-$ or $y-$oriented pattern, respectively. Let us also consider

340   a $2D_B \times 2D_b$ matrix $\mathcal{P}$ having the same structure of $\mathcal{D}$, but containing the elements p_j of the parameter
341   vector $\mathbf{p}$, $j \in \{1 : P\}$.

342   The first block (in the first quadrant) contains

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

350   Takahashi et al. (2020)

351   Takahashi et al. (2022)

3   TEXTO ANTIGO

3.0.1   The wavelet compression and lower-dimensional subspace

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

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

$$\tilde{\mathbf{A}} = \mathbf{W_2}\, \mathbf{A}\, \mathbf{W_2}^\top \,, \tag{38}$$

360   where $\tilde{\mathbf{A}}$ is the expanded original sensitivity matrix in the wavelet bases with many elements zero or close
361   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
362   is obtained by retaining only the large elements of the $\tilde{\mathbf{A}}$. Thus, the elements of $\tilde{\mathbf{A}}$ whose amplitudes
363   fall below a relative threshold are discarded. In **?**, the original sensitivity matrix $\mathbf{A}$ is high compressed
364   resulting in a sparce matrix $\tilde{\mathbf{A}}_{\mathbf{s}}$ with a few percent of nonzero elements and the the inverse problem is
365   solved in the wavelet domain by using $\tilde{\mathbf{A}}_{\mathbf{s}}$ and a incomplete conjugate gradient least squares, without an
366   explicit regularization parameter and a limited number of iterations. The solution is obtained by solving the
367   following linear system

$$\tilde{\mathbf{A}}_{\mathbf{L}}^\top\, \tilde{\mathbf{A}}_{\mathbf{L}}\, \tilde{\mathbf{p}}_{\mathbf{L}}^* = \tilde{\mathbf{A}}_{\mathbf{L}}^\top\, \tilde{\mathbf{d}}^o \,, \tag{39}$$

368   where $\tilde{\mathbf{p}}_{\mathbf{L}}^*$ is obtained by solving the linear system given by equation 39,

$$
\begin{aligned}
\tilde{\mathbf{A}}_{\mathbf{L}} &= \tilde{\mathbf{A}}_{\mathbf{s}}\, \tilde{\mathbf{L}}^{-1}, &\tag{40a}\\
\tilde{\mathbf{p}}_{\mathbf{L}} &= \tilde{\mathbf{L}}\tilde{\mathbf{p}}, &\tag{40b}\\
\tilde{\mathbf{d}}^o &= \mathbf{W_2}\, \mathbf{d}^o, &\tag{40c}
\end{aligned}
$$

369   where $\tilde{\mathbf{L}}$ is a diagonal and invertible weighting matrix representing the finite-difference approximation in
370   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.:

$$\tilde{\mathbf{p}} = \tilde{\mathbf{L}}^{-1}\,\tilde{\mathbf{p}}_{\mathbf{L}}^{*}\,, \tag{41}$$

and

$$\mathbf{p} = \mathbf{W_2}\,\tilde{\mathbf{p}}\,. \tag{42}$$

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

$$\mathbf{p} = \mathbf{V}\,\boldsymbol{\alpha}\,, \tag{43}$$

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 43, 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.:

$$\mathbf{V}^{\top}\,\mathbf{A}^{\top}\,\mathbf{A}\,\mathbf{V}\,\boldsymbol{\alpha}^{*}\,=\,\mathbf{V}^{\top}\,\mathbf{d}^{o}\,. \tag{44}$$

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 44) 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 43. The choice of the Q basis vectors $\mathbf{v}_i = 1, ..., Q$ (equation 43) 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.

3.0.2 The quadtree discretization

To make the equivalent-layer technique tractable, **?** also transformed the dense sensitivity matrix **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.

3.0.3 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

$$\mathbf{p}^k = \mathbf{B}^k\,\mathbf{c}^k\,, \qquad k\,=\,1\dots Q\,, \tag{45}$$

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

$$\left(\mathbf{B}^\top\,\mathbf{A}^\top\,\mathbf{A}\,\mathbf{B}\,+\,\mu\mathbf{I}\right)\,\mathbf{c}^* \,=\, \mathbf{B}^\top\,\mathbf{A}^\top\,\mathbf{d}^o\,, \tag{46}$$

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 45) and all off-diagonal blocks are zero matrices. For ease of the explanation of equation 46, 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 46), 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 46) 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.

3.0.4 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.:

$$\tilde{\mathbf{A}} = 2\,\pi\,\gamma\,\mathbf{\Delta S^{-1}}\,, \tag{47}$$

where γ is Newton's gravitational constant and $\mathbf{\Delta S^{-1}}$ 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:

$$\tilde{\mathbf{A}}^\top \tilde{\mathbf{A}} \mathbf{\Delta}\,\hat{\mathbf{p}}^k = \tilde{\mathbf{A}}^\top \mathbf{r}^k\,, \tag{48}$$

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

$$r_i^k = d_i^o \ - \ d_i^k \ . \tag{49}$$

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

480 Because $\tilde{\tilde{\mathbf{A}}}$, in equation 48, is a diagonal matrix (equation 47), the parameter correction estimate is
481 directly calculated without solving system of linear equations, and thus, an ith element of $\mathbf{\Delta} \, \hat{\mathbf{p}}^k$ is directly
482 calculated by

$$\Delta \hat{p}^k{}_i = \frac{\Delta s_i \, r_i^k}{2 \, \pi \, \gamma} \ . \tag{50}$$

483 The mass distribution over the equivalent layer is updated by:

$$\hat{p}_i^{k+1} = \hat{p}_i^k \ + \ \Delta \hat{p}^k{}_i \ . \tag{51}$$

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

$$p_i^o = \frac{\Delta s_i \, d_i^o}{2 \, \pi \, \gamma} \ . \tag{52}$$

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

488 For jointly process two gravity gradient components, Jirigalatu and Ebbing (2019) used the Gauss-FFT
489 for forward calculation of potential fields in the wavenumber domain combined with Landweber's iteration
490 coupled with a mask matrix $\mathbf{M}$ to reduce the edge effects without increasing the computation cost. The
491 mask matrix $\mathbf{M}$ is defined in the following way: if the corresponding pixel does not contain the original
492 data, the element of $\mathbf{M}$ is set to zero; otherwise, it is set to one. The kth Landweber iteration is given by

$$\mathbf{p}_{k+1} = \mathbf{p}_k + \omega \left[\mathbf{A_1}^\top (\mathbf{d_1} - \mathbf{M}\mathbf{A_1}\mathbf{p}_k) + \mathbf{A_2}^\top (\mathbf{d_2} - \mathbf{M}\mathbf{A_2}\mathbf{p}_k) \right] \ , \tag{53}$$

493 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
494 corresponding gravity gradient kernels. Jirigalatu and Ebbing (2019) applied their method for processing
495 two horizontal curvature components of Falcon airborne gravity gradient.

3.0.5 The convolutional equivalent layer with BTTB matrices

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

499 **?** demonstrated that the sensitivity matrix $\mathbf{A}$ (equation 3) associated with a planar equivalent layer formed
500 by a set of point masses, each one directly beneath each observation point and considering a regular grid of
501 observation points at a constant height has a symmetric block-Toeplitz Toeplitz-block (BTTB) structure. A
502 symmetric BTTB matrix has, at least, two attractive properties. The first one is that it can be defined by
503 using only the elements forming its first column (or row). The second attractive property is that any BTTB
504 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

$$\mathbf{w} = \mathbf{C}\mathbf{v} \,, \tag{54}$$

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

$$\mathbf{C} = \left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right)^{*} \mathbf{\Lambda} \left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right) \,, \tag{55}$$

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 54) can be rewritten by using equation 55 and premultiplying both sides of the result by $\left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right)$, i.e.,

$$\mathbf{\Lambda} \left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right) \mathbf{v} = \left(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}\right) \mathbf{w} \,. \tag{56}$$

By applying the vec-operator (**?**) to both sides of equation 56, by premultiplying both sides of the result by $\mathbf{F}_{2Q}^{*}$ and then postmultiplying both sides of the result by $\mathbf{F}_{2P}^{*}$

$$\mathbf{F}_{2Q}^{*} \left[\mathbf{L} \circ \left(\mathbf{F}_{2Q} \, \mathbf{V} \, \mathbf{F}_{2P}\right)\right] \mathbf{F}_{2P}^{*} = \mathbf{W} \,, \tag{57}$$

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 57 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 55) and can be efficiently computed by using only the first column of the BCCB matrix $\mathbf{C}$ (equation 54).

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.

3.0.6 The deconvolutional equivalent layer with BTTB matrices

To avoid the iterations of the conjugate gradient method in **?**, we can employ the deconvolution process. Equation 57 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 57, the matrix $\mathbf{V}$ can be obtain by deconvolution, i.e.

$$\mathbf{V} \;=\; \mathbf{F}_{2Q}^{*} \left[\frac{\left(\mathbf{F}_{2Q} \mathbf{W} \, \mathbf{F}_{2P} \right)}{\mathbf{L}} \right] \mathbf{F}_{2P}^{*} \,. \tag{58}$$

Equation 58 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 58 requires regularization to be useful. We usede wiener deconvolution to obtain a stable solution, i.e.,

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

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

3.1 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 $\mathbf{d}_{\ell}^{\mathrm{o}}$, $\ell = 1, ..., D$. From each $\mathbf{d}_{\ell}^{\mathrm{o}}$, we estimate a physical-property distribution $\hat{\mathbf{p}}_{\ell}$ within the equivalent layer.

574   Next, for each noise-corrupted data $\mathbf{d}_\ell^{\mathrm{o}}$ and estimated solution $\hat{\mathbf{p}}_\ell$, the ℓth model perturbation δp_ℓ and the
575   ℓth data perturbation δd_ℓ are, respectively, evaluated by

$$\delta p_\ell = \frac{\parallel \hat{\mathbf{p}}_\ell - \mathbf{p} \parallel_2}{\parallel \mathbf{p} \parallel_2}, \quad \ell = 1, ..., D, \tag{60}$$

576   and

$$\delta d_\ell = \frac{\parallel \mathbf{d}_\ell^{\mathrm{o}} - \mathbf{d} \parallel_2}{\parallel \mathbf{d} \parallel_2}, \quad \ell = 1, ..., D. \tag{61}$$

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

$$\delta p_\ell \leq \kappa \, \delta d_\ell, \quad \ell = 1, ..., D, \tag{62}$$

578   where κ is the constant of proportionality between the model perturbation δp_ℓ (equation 60) and the data
579   perturbation δd_ℓ (equation 61). The constant κ acts as the condition number of an invertible matrix in a
580   given inversion, and thus measures the instability of the solution. The larger (smaller) the value of κ the
581   more unstable (stable) is the estimated solution.

582   Equation 62 shows a linear relationship between the model perturbation and the data perturbation. By
583   plotting δp_ℓ (equation 60) against δd_ℓ (equation 61) produced by a set of D estimated solution obtained by
584   applying a given equivalent-layer method, we obtain a straight line behaviour described by equation 62.
585   By applying a linear regression, we obtain a fitted straight line whose estimated slope (κ in equation 62)
586   quantifies the solution stability.

587   Here, the analysis of solution stability is numerically conducted by applying the classical equivalent-
588   layer technique with zeroth-order Tikhonov regularization, the convolutional method for gravimetric and
589   magnetic data, the deconvolutional method (equation 58) and the deconvolutional method with different
590   values for the Wiener stabilization (equation 59).

4 NUMERICAL SIMULATIONS

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

4.1 Floating-point operations calculation

598 To measure the computational effort of the different algorithms to solve the equivalent layer linear system,
599 a non-hardware dependent method can be useful because allow us to do direct comparison between them.
600 Counting the floating-point operations (*flops*), i.e., additions, subtractions, multiplications and divisions
601 is a good way to quantify the amount of work of a given algorithm (Golub and Van Loan, 2013). For
602 example, the number of *flops* necessary to multiply two vectors $\mathbb{R}^N$ is $2N$. A common matrix-vector
603 multiplication with dimension $\mathbb{R}^{N \times N}$ and $\mathbb{R}^N$, respectively, is $2N^2$ and a multiplication of two matrices
604 $\mathbb{R}^{N \times N}$ is $2N^3$. Figure **??** shows the total flops count for the different methods presented in this review
605 with a crescent number of data, ranging from $10,000$ to $1,000,000$ for the gravity equivalent layer and
606 figure **??** for magnetic data.

4.1.1 Normal equations using Cholesky decomposition

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

$$f_{classical} = \frac{5}{6}N^3 + 4N^2 \tag{63}$$

4.1.2 Window method (Leão and Silva, 1989)

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

$$f_{window} = N\frac{5}{6}M_w N_w^2 + 4N_w M_w \tag{64}$$

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

619 The polynomial equivalent layer uses a simliar approach od moving windows from Leão and Silva (1989).
620 For this operations calculation (equation 46) we used a first degree polynomial (two variables) and each
621 window contains $N_s = 1,000$ observed data and $M_s = 1,000$ equivalent sources. Following the steps
622 given in (Oliveira Jr. et al., 2013) the total *flops* becomes

$$f_{pel} = \frac{1}{3}H^3 + 2H^2 + 2NM_sH + H^2N + 2HN + 2NP \tag{65}$$

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

4.1.4 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 ($12N$) (**?**)

$$f_{cgls} = 2N^2 + it(4N^2 + 12N) \tag{66}$$

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

For the wavelet method (equation 39) 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 38 and 40c), with its inverse also using the same number of operations (equation 42). Combined with the conjugate gradient least square necessary steps and iterations, the number of *flops* are

$$f_{wavelet} = 2NC_r + 4N\log_2(N) + it(4N\log_2(N) + 4NC_r + 12C_r) \tag{67}$$

4.1.6 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 48,49, 50 and 51)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)

$$f_{siqueira} = it(3N + 2N^2) \tag{68}$$

4.1.7 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 57). Considering that the first column of our BCCB matrix has $4N$ elements, the flops count of this method is

$$f_{convgrav} = \kappa 4N\log_2(4N) + it(27N + \kappa 8N\log_2(4N)) \tag{69}$$

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 69 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.

4.1.8   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 57), 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 66.

$$f_{convmag} = \kappa 16N \log_2(4N) + 24N + it(\kappa 16N \log_2(4N) + 60N) \tag{70}$$

4.1.9   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 58 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 ($\kappa 4N \log_2(4N)$).

$$f_{deconv} = \kappa 12N \log_2(4N) + 24N \tag{71}$$

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 59

$$f_{deconvwiener} = \kappa 12N \log_2(4N) + 76N \tag{72}$$

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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