

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

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1 FUNDAMENTALS

- 2 Let 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

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

- 5 where, p_i 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

$$g_{ij} \equiv g(x_i - x_j, y_i - y_j, z_i - z_j), \quad z_i < \min\{z_j\}, \quad \forall i \in \{1 : D\},$$
 (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 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 p leading to a predicted data vector f (equation 3) sufficiently close to the observed data vector 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.,
- 17 Menke, 2018, p. 41). Because of that, almost all methods for determining 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
- 19 estimate \tilde{p} , it is then possible to compute a potential field transformation

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

where t is a $T \times 1$ vector with k-th element t_k representing the transformed potential field at the position

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$$(x_k, y_y, z_k), k \in \{1:T\}$$
, and

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

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

23 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
- 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 Uieda
- 29 (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.

49 **1.2 Matrix** G

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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) ,

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

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

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

53 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., 55 2017; Reis et al., 2020; Takahashi et al., 2020; Soler and Uieda, 2021; Takahashi et al., 2022). Another 56 common approach consists in not defining g_{ij} by using equations 6–8, but other harmonic functions 57 58 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 59 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 61 62 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} 63 (equation 2) is independent on the actual physical relationship between the observed potential field and 64 their true sources (e.g., Cordell, 1992; Guspí and Novara, 2009; Li et al., 2014). Hence, g_{ij} can be 65 defined according to the problem. The only condition imposed to this function is that it decays to zero 66 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. 67 However, several methods use a function g_{ij} that preserves the physical relationship between the observed 68 potential field and their true sources. For the case in which the observed potential field is gravity data, g_{ij} 69 is commonly defined as a component of the gravitational field produced at (x_i, y_i, z_i) by a point mass or 70 prism located at (x_j, y_j, z_j) , with unit density. On the other hand, g_{ij} is commonly defined as a component 71 of the magnetic induction field produced at (x_i, y_i, z_i) by a dipole or prism located at (x_i, y_i, z_i) , with unit magnetization intensity, when the observed potential field is magnetic data. 73

74 The main challenge in the equivalent-layer technique is the computational complexity associated with 75 handling large datasets. This complexity arises because the sensitivity matrix 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 G is not well-defined, regardless of the spatial distribution of the equivalent sources. 77 However, in a specific scenario where (i) each potential-field datum is directly associated with a single 78 equivalent source located directly below it, and (ii) both the data and sources are based on planar and 79 regularly spaced grids, Takahashi et al. (2020, 2022) demonstrate that G exhibits a block-Toeplitz Toeplitz-80 block (BTTB) structure. In such cases, the product of G and an arbitrary vector can be efficiently computed 81 using a 2D fast Fourier transform as a discrete convolution.

83 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 **H** is a $P \times Q$ matrix. The predicted data vector **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

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

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

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

94 and

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

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

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

- 99 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 $\Gamma(\mathbf{q})$,

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

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

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

105 where

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

$$\delta_d = \mathbf{d} - \mathbf{G} \mathbf{H} \,\bar{\mathbf{q}} \,, \tag{19}$$

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$$\mathbf{B} = \left(\mathbf{H}^{\top} \mathbf{G}^{\top} \mathbf{W}_{d} \mathbf{G} \mathbf{H} + \mu \mathbf{W}_{q}\right)^{-1} \mathbf{H}^{\top} \mathbf{G}^{\top} \mathbf{W}_{d},$$
(20)

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

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

- 109 Evidently, we have considered that all inverses exist in equations 20 and 21.
- The $Q \times D$ matrix 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
- 112 \tilde{q} is obtained by solving the following linear system for δ_q (equation 18):

$$\left(\mathbf{H}^{\top}\mathbf{G}^{\top}\mathbf{W}_{d}\mathbf{G}\mathbf{H} + \mu\mathbf{W}_{q}\right)\tilde{\boldsymbol{\delta}}_{q} = \mathbf{H}^{\top}\mathbf{G}^{\top}\mathbf{W}_{d}\boldsymbol{\delta}_{d}.$$
(22)

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

116 matrix-vector product as follows:

$$\left(\mathbf{G}\mathbf{H}\mathbf{W}_{q}^{-1}\mathbf{H}^{\top}\mathbf{G}^{\top} + \mu\mathbf{W}_{d}^{-1}\right)\mathbf{u} = \boldsymbol{\delta}_{d}$$

$$\tilde{\boldsymbol{\delta}}_{q} = \mathbf{W}_{q}^{-1}\mathbf{H}^{\top}\mathbf{G}^{\top}\mathbf{u}$$
(23)

- where u is a dummy vector. After obtaining $\tilde{\delta}_q$ (equations 22 and 23), the estimate \tilde{q} is computed with equation 18.
- 119 1.3.1 Classical approach
- The classical approach in the equivalent-layer technique consists in using $\mathbf{H} = \mathbf{I}_P$, so that P = Q, $\mathbf{p} = \mathbf{q}$
- 121 (equation 9), $\bar{\mathbf{p}} = \bar{\mathbf{q}}$ (equation 14) and $\tilde{\mathbf{p}} = \tilde{\mathbf{q}}$ (equation 15). In this case, the linear system (equations 22)
- 122 and 23) is directly solved for

$$\tilde{\boldsymbol{\delta}}_p = \tilde{\mathbf{p}} - \bar{\mathbf{p}} \,, \tag{24}$$

123 instead of $\tilde{\delta}_q$ (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 d, for example, are specified by d[i], where i is a list of integer numbers that "pick out" the elements of d forming the subvector d[i]. For example, $\mathbf{i} = (1, 6, 4, 6)$ gives the subvector d[i] = $[d_1 \ d_6 \ d_4 \ d_6]^{\top}$. Note that the list 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 d. Sequential lists with increment of 1, if the starting index is smaller than the final index, or -1, if the starting index is greater than the final index, can be represented by using the colon notation. For example,

$$\mathbf{i} = (3:8) \Leftrightarrow \mathbf{d}[\mathbf{i}] = [d_3 \ d_4 \ \dots \ d_8]^{\top}$$

$$\mathbf{i} = (8:3) \Leftrightarrow \mathbf{d}[\mathbf{i}] = [d_8 \ d_7 \ \dots \ d_3]^{\top}$$

$$\mathbf{i} = (:8) \Leftrightarrow \mathbf{d}[\mathbf{i}] = [d_1 \ d_2 \ \dots \ d_8]^{\top}$$

$$\mathbf{i} = (3:) \Leftrightarrow \mathbf{d}[\mathbf{i}] = [d_3 \ d_4 \ \dots \ d_D]^{\top}$$

where D is the number of elements forming d.

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

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

Note that, in this case, the lists i and j "pick out", respectively, the rows and columns of G that form the submatrix G[i, j]. The *i*-th row of G is given by the $1 \times P$ vector G[i, :]. Similarly, the $D \times 1$ vector 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 G from rows 2 to 5 and from columns 3 to 7.

3 COMPUTATIONAL STRATEGIES

- 126 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
- 128 22 and 23). This, in turn, means to deal with some obstacles concerning large computational cost:
- 129 (i) the large computer memory to store large and full matrices;
- 130 (ii) the long computation time to multiply a matrix by a vector; and
- 131 (iii) the long computation time to solve a large linear system of equations.
- 132 Two important factors affecting the efficiency of a given matrix algorithm are the storage and amount of
- 133 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
- 135 strategies used by the selected methods.

136 3.1 Moving window

- The initial approach to enhance the computational efficiency of the equivalent-layer technique is
- 138 commonly denoted moving window and involves first splitting the observed data d_i , $i \in \{1 : D\}$, into
- 139 M overlapping subsets (or data windows) formed by D^m data each, $m \in \{1: M\}$. The data inside the
- 140 m-th window are usually adjacent to each other and have indices defined by an integer list \mathbf{i}^m having
- 141 D^m elements. The number of data D^m forming the data windows are not necessarily equal to each other.
- 142 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
- 143 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
- 145 m-th window have indices defined by an integer list \mathbf{j}^m having P^m elements. Each source window has a
- 146 $P^m \times 1$ parameter vector \mathbf{p}^m and is located right below the corresponding m-th data window. Then, each
- 147 $\mathbf{d}^m \equiv \mathbf{d}[\mathbf{i}^m]$ is approximated by

$$\mathbf{f}^m = \mathbf{G}^m \mathbf{p}^m \,, \tag{25}$$

- where $G^m \equiv G[i^m, j^m]$ is a submatrix of G (equation 3) formed by the elements computed with equation
- 149 2 using only the data and equivalent sources located inside the window m-th. The main idea of the moving-
- 150 window approach is using the $\tilde{\mathbf{p}}^m$ estimated for each window to obtain (i) an estimate $\tilde{\mathbf{p}}$ of the parameter
- 151 vector for the entire equivalent layer or (ii) a given potential-field transformation t (equation 4). The main
- advantages of this approach is that (i) the estimated parameter vector $\tilde{\mathbf{p}}$ or transformed potential field are
- 153 not obtained by solving the full, but smaller linear systems and (ii) the full matrix G (equation 3) is never
- 154 stored.

Leão and Silva (1989) presented a pioneer work using the moving-window approach. Their method 155 requires a regularly-spaced grid of observed data on a horizontal plane z_0 . The data windows are defined by 156 square local grids of $\sqrt{D'} \times \sqrt{D'}$ adjacent points, all of them having the same number of points D'. The 157 equivalent sources in the m-th data window are located below the observation plane, at a constant vertical 158 distance Δz_0 . They are arranged on a regular grid of $\sqrt{P'} \times \sqrt{P'}$ adjacent points following the same 159 grid pattern of the observed data. The local grid of sources for all data windows have the same number 160 of elements P'. Besides, they are vertically aligned, but expands the limits of their corresponding data 161 windows, so that D' < P'. Because of this spatial configuration of observed data and equivalent sources, 162 we have that $G^m = G'$ (equation 25) for all data windows (i.e., $\forall m \in \{1 : M\}$), where G' is a $D' \times P'$ 163 constant matrix. 164

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:

$$t_c^m = (\mathbf{a}')^\top \mathbf{B}' \mathbf{d}^m, \quad m \in \{1 : M\},$$
 (26)

where 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 and

$$\mathbf{B}' = \left(\mathbf{G}'\right)^{\top} \left[\mathbf{G}' \left(\mathbf{G}'\right)^{\top} + \mu \mathbf{I}_{D'}\right]^{-1}$$
(27)

is a particular case of matrix B associated with underdetermined problems (equation 21) 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. 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 26 combines the potential-field transformation (equation 4) with the solution of the undetermined problem (equation 23).

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 25). 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 182 data on an undulating surface. A direct consequence of this generalization is that a different submatrix 183 $G^m \equiv G[i^m, j^m]$ (equation 25) must be computed for each window. Differently from Leão and Silva 184 (1989), Soler and Uieda (2021) store the computed \tilde{p}^m for all windows and subsequently use them to obtain 185 a desired potential-field transformation (equation 4) as the superposed effect of all windows. The estimated 186 $\tilde{\mathbf{p}}^m$ for all windows are combined to form a single $P \times 1$ vector $\tilde{\mathbf{p}}$, which is an estimate for original 187 parameter vector p (equation 3). For each data window, Soler and Uieda (2021) solve an overdetermined 188 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 189 a diagonal matrix of weights for the data inside the m-th window and $\bar{p} = 0$ (equation 14), so that

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

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

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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 the matrix \mathbf{B}' (equation 27);

7 Compute the vector (\mathbf{a}')^{\top} \mathbf{B}';

8 m = 1;

9 while m < M do

10 | Compute t_c^m (equation 26);

11 | m \leftarrow m + 1;

12 end
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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). Note that this algorithm starts with a residuals vector r that is iteratively updated. The iterative algorithm in Soler and Uieda (2021) estimates a solution ($\tilde{\mathbf{p}}^m$ in equation 28) 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 G (equation 3) is calculated iteratively.

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 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

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

```
Initialization:
 1 Set the indices i^m for each data window, m \in \{1 : M\};
 2 Set the indices 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};
 5 Set a P \times 1 vector \tilde{\mathbf{p}} = \mathbf{0};
 6 m = 1;
    while m < M do
          Set the matrix \mathbf{W}_d^m;
          Compute the matrix G^m
 9
          Compute \tilde{\mathbf{p}}^m (equation 28);
10
          \tilde{\mathbf{p}}[\mathbf{j}^m] \leftarrow \tilde{\mathbf{p}}[\mathbf{j}^m] + \tilde{\mathbf{p}}^m;
11
          \mathbf{r} \leftarrow \mathbf{r} - \mathbf{G}[:, \mathbf{j}^m] \, \tilde{\mathbf{p}}^m \; ;
12
         m \leftarrow m + 1;
13
14 end
```

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 $G[:, i_{max}]$ of the $D \times D$ matrix G (equation 3) is used per iteration, where i_{max} is the index of the maximum absolute value in 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_{max} in 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 G (equation 3) is calculated per iteration.

3.3 Row-action update

We call the computational strategy *row-action update* because a single row of the sensitivity matrix G (equation 3) is calculated iteratively. Hence, the equivalent-layer solution is updated by processing a

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

Initialization:

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1 Compute a D \times 1 vector \Delta z whose i-th element \Delta z_i is a vertical distance controlling the depth of
      the i-th equivalent source, i \in \{1 : D\};
 2 Set a tolerance \epsilon;
    Set a maximum number of iterations 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_{\text{max}} in r;
    while (r_{\text{max}} > \epsilon) and (m < \text{ITMAX}) do
          Define the coordinates (x_{\text{max}}, y_{\text{max}}, z_{\text{max}}) and index i_{\text{max}} of the observation point associated with
          \tilde{\mathbf{p}}[i_{\text{max}}] \leftarrow \tilde{\mathbf{p}}[i_{\text{max}}] + (r_{\text{max}} \Delta \mathbf{z}[i_{\text{max}}]);
10
          \mathbf{r} \leftarrow \mathbf{r} - (\mathbf{G}[:, i_{\text{max}}] \, \tilde{\mathbf{p}}[i_{\text{max}}]) ;
11
          Define the new r_{\text{max}} in \mathbf{r};
12
13
          m \leftarrow m + 1;
14 end
```

new datum (one matrix row) at each iteration. To reduce the total processing time and memory usage of 248 249 equivalent-layer technique, Mendonça and Silva (1994) proposed a strategy called *equivalent data concept*. 250 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, 251 called equivalent data, that contributes effectively to the final solution and fits the remaining observations 252 253 (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 254 at a time. 255

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{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 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

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

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 29) for the particular case in which $\mathbf{H} = \mathbf{W}_p = \mathbf{I}_P$ (equations 9 and 13), $\mathbf{W}_d = \mathbf{I}_{D_e}$

272 (equation 12) and $\bar{p} = 0$ (equation 14), which results in

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

273 where ${f F}$ is a computationally-efficient $D_e imes D_e$ matrix that approximates ${f G}_e {f G}_e^ op$. Mendonça and Silva

274 (1994) presume that the estimated parameter vector $\tilde{\mathbf{p}}$ obtained from equation 30 leads to a $D_r \times 1$ residuals

275 vector

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

276 having a maximum absolute value $r_{\text{max}} \leq \epsilon$, 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 30 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.

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 \epsilon;
 3 Set a D \times 1 residuals vector \mathbf{r} = \mathbf{d};
 4 Define the maximum absolute value r_{\text{max}} in r;
 5 Define the index i_{\max} of r_{\max};
6 Define the list of indices i_r of the remaining data in r;
 7 Define \mathbf{d}_e = \mathbf{d}[i_{\mathtt{max}}];
    Compute (\mathbf{F} + \mu \mathbf{I}_{D_e}) and \mathbf{G}_e;
    Compute \tilde{\mathbf{p}} (equation 30);
10 Compute \mathbf{r} = \mathbf{d}[\mathbf{i}_r] - \mathbf{G}[\mathbf{i}_r,:] \tilde{\mathbf{p}};
    Define the maximum absolute value r_{\text{max}} in \mathbf{r};
     while (r_{\text{max}} > \epsilon) do
           Define the index i_{max} of r_{max};
Define the list of indices i_r of the remaining elements in r;
13
14
           \mathbf{d}_e \leftarrow egin{bmatrix} \mathbf{d}_e \ \mathbf{d}[i_{	exttt{max}}] \end{bmatrix};
15
           Update (\mathbf{F} + \mu \mathbf{I}_{D_e}) and \mathbf{G}_e;
16
           Update \tilde{\mathbf{p}} (equation 30);
17
           Update \mathbf{r} = \mathbf{d}[\mathbf{i}_r] - \mathbf{G}[\mathbf{i}_r,:] \tilde{\mathbf{p}};
18
           Define the maximum absolute value r_{\text{max}} in \mathbf{r};
19
20 end
```

3.4 Reparameterization

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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

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system dimension from the original P-space to a lower-dimensional subspace (the Q-space). An estimate 288 289 $\tilde{\mathbf{q}}$ for the reparameterized parameter vector \mathbf{q} is obtained in the Q-space and subsequently used to obtain an estimate \tilde{p} for the parameter vector p (equation 3) in the P-space by using equation 9. Hence, the key 290 291 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). 292

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.

301 The method proposed by Oliveira Jr. et al. (2013) consists in solving an overdetermined problem (equation 302 22) for estimating the polynomial coefficients $\tilde{\bf q}$ with ${\bf W}_d={\bf I}_D$ (equation 12) and $\bar{q}={\bf 0}$ (equation 14), so 303 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 304 regularization (e.g., Aster et al., 2019, p. 103). Note that, in this case, the prior information is defined in the 305 306 P-space for the original parameter vector 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. 307

308 Mendonça (2020) also proposed a reparameterization approach for the equivalent-layer technique. Their 309 approach, however, consists in setting 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 310 method of Mendonça (2020) requires a regular grid of potential-field data on horizontal plane. Another 311 difference is that these authors uses $W_q = I_Q$ (equation 13), which means that the regularization is defined 312 directly in the Q-space. 313

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 315 difference, however, is that Barnes and Lumley (2011) did not set a $P \times Q$ reparameterization matrix H 316 (equation 9) with $Q \ll P$. Instead, they used a matrix **H** with $Q \approx 1.7 P$. Their central idea is setting a 317 reparameterization scheme that groups distant equivalent sources into blocks by using a bisection process. 318 This scheme leads to a quadtree representation of the physical-property distribution on the equivalent layer, 319 so that matrix GH (equation 10) is notably sparse. Barnes and Lumley (2011) explore this sparsity in 320 solving the overdetermined problem for \tilde{q} (equation 32) via conjugate-gradient method (e.g., Golub and 321 Van Loan, 2013, sec. 11.3). 322

Wavelet compression

Previously to Barnes and Lumley (2011), the idea of transforming the dense matrix G (equation 3) into a 324 325 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 326 matrix G. Those authors approximate a planar grid of potential-field data by a regularly-spaced grid of 327 equivalent sources, so that the number of data D and sources P is the same, i.e., D = P. Specifically, Li 328

- and Oldenburg (2010) proposed a method that applies the wavelet transform to the original dense matrix G 329
- 330 and sets to zero the small coefficients that are below a given threshold, which results in an approximating
- sparse representation of G in the wavelet domain. They first consider the following approximation 331

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

332 where

$$\mathbf{d}_w = \mathbf{W} \, \mathbf{d} \,, \quad \mathbf{p}_w = \mathbf{W} \, \mathbf{p} \,,$$
 (34)

- are the observed data and parameter vector in the wavelet domain; $\boldsymbol{\mathcal{W}}$ is a $D \times D$ orthogonal matrix 333
- defining a discrete wavelet transform; and G_s is a sparse matrix obtained by setting to zero the elements of 334

$$G_w = \mathcal{W} G \mathcal{W}^{\top} \tag{35}$$

- 335 with absolute value smaller than a given threshold.
- 336 Li and Oldenburg (2010) solve a normalized inverse problem in the wavelet domain. Specifically, they
- 337 first define a matrix

$$\mathbf{G}_L = \mathbf{G}_s \, \mathbf{L}^{-1} \tag{36}$$

338 and a normalized parameter vector

$$\mathbf{p}_L = \mathbf{L} \, \mathbf{p}_w \,, \tag{37}$$

- where L is a diagonal and invertible matrix representing an approximation of the first-order Tikhonov 339
- regularization in the wavelet domain. Then they solve an overdetermined problem (equation 22) to obtain 340
- an estimate $\tilde{\mathbf{p}}_L$ for \mathbf{p}_L (equation 37), with \mathbf{G}_L (equation 36), $\mathbf{H} = \mathbf{I}_P$ (equations 9), $\mu = 0$ (equation 11),
- $\mathbf{W}_d = \mathbf{I}_D$ (equation 12) and $\bar{p} = \mathbf{0}$ (equation 14) via conjugate-gradient method (e.g., Golub and Van
- Loan, 2013, sec. 11.3). Finally, Li and Oldenburg (2010) compute an estimate \tilde{p} for the original parameter
- vector given by

$$\tilde{\mathbf{p}} = \mathbf{W}^{\top} \left(\mathbf{L}^{-1} \, \tilde{\mathbf{p}}_L \right) \,, \tag{38}$$

- where the term within parenthesis is an estimate $\tilde{\mathbf{p}}_w$ of the parameter vector \mathbf{p}_w (equation 34) in the wavelet
- domain and matrix $\boldsymbol{\mathcal{W}}^{\top}$ represents an inverse wavelet transform.

Iterative methods using the full matrix G 347

- Xia and Sprowl (1991) introduced an iterative method for estimating the parameter vector $\tilde{\mathbf{p}}$ (equation 3), 348
- which was subsequently adapted to the Fourier domain by Xia et al. (1993). Their method uses the full 349
- 350 and dense sensitivity matrix G (equation 3) (without applying any compression or reparameterization, for
- example) to compute the predicted data at all observation points per iteration. More than two decades later, 351
- Siqueira et al. (2017) have proposed an iterative method similar to that presented by Xia and Sprowl (1991). 352
- The difference is that Siqueira et al.'s algorithm was deduced from the Gauss' theorem (e.g., Kellogg, 1967, 353
- p. 43) and the total excess of mass (e.g., Blakely, 1996, p. 60). Besides, Siqueira et al. (2017) have included 354
- a numerical analysis showing that their method produces very stable solutions, even for noise-corrupted 355
- potential-field data. 356
- The iterative method proposed by Siqueira et al. (2017) is outlined in Algorithm 5, presumes an equivalent 357
- layer formed by monopoles (point masses) and can be applied to irregularly-spaced data on an undulating 358
- surface. Note that the residuals r are used to compute a correction Δp for the parameter vector at each 359
- iteration (line 11), which requires a matrix-vector product involving the full matrix G. Interestingly, this 360

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 methods of Xia and Sprowl (1991) and Siqueira et al. (2017) were originally proposed for processing gravity data, but can be potentially applied to any harmonic function because they actually represent iterative solutions 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 367 vector $\tilde{\mathbf{p}}$ (equation 3). With the purpose of combining different potential-field data, their method basically 368 modifies that shown in Algorithm 5 by changing the initial approximation and the iterative correction for 369 the parameter vector. Specifically, Jirigalatu and Ebbing (2019) replace line 4 by $\tilde{\mathbf{p}} = \mathbf{0}$, where $\mathbf{0}$ is a vector 370 of zeros, and line 9 by $\Delta p = \omega G^{T} r$, where ω is a positive scalar defined by trial and error. Note that 371 this modified approach requires two matrix-vector products involving the full matrix G per iteration. To 372 overcome the high computational cost of these two products, Jirigalatu and Ebbing (2019) set an equivalent 373 layer formed by prisms and compute their predicted potential field in the wavenumber domain by using the 374 375 Gauss-FFT technique Zhao et al. (2018).

Algorithm 5: Generic pseudo-code for the iterative method proposed by Siqueira et al. (2017). The symbol " \circ " denotes the entrywise or Hadamard product (e.g., Horn and Johnson, 1991, p. 298) and σ is a $P \times 1$ vector whose j-th element is the ratio of a predefined element of area centered at the j-th equivalent source and the term $2\pi\gamma$, where γ is the gravitational constant.

```
Initialization:
```

```
Set P equivalent sources on a horizontal plane z_0;
 2 Set a tolerance \epsilon;
 3 Set an auxiliary vector \sigma;
 4 Compute \tilde{\mathbf{p}} = \boldsymbol{\sigma} \circ \mathbf{d};
    Compute G (equation 3);
 6 Compute \mathbf{r} = \mathbf{d} - \mathbf{G}\,\tilde{\mathbf{p}};
    Compute \delta = \|\mathbf{r}\|/D;
     while (\delta > \epsilon) do
           Compute \Delta \mathbf{p} = \boldsymbol{\sigma} \circ \mathbf{r};
 9
           Update \tilde{\mathbf{p}} \leftarrow \tilde{\mathbf{p}} + \Delta \mathbf{p};
10
           Compute \nu = G \Delta p;
11
           Update \mathbf{r} \leftarrow \mathbf{r} - \boldsymbol{\nu};
12
           Compute \delta = \|\boldsymbol{\nu}\|/D;
13
14 end
```

3.7 Discrete convolution

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Recently, Takahashi et al. (2020, 2022) proposed the *convolutional equivalent-layer method*, which explores the structure of the sensitivity matrix G (equation 3) 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. Specifically, they 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 G (equation 3) assumes a *doubly block Toeplitz* (Jain, 1989, p. 28) or *block-Toeplitz Toeplitz-block* (BTTB) (Chan and

- 386 Jin, 2007, p. 67) structure formed by $D_B \times D_B$ blocks, where each block has $D_b \times D_b$ elements, with
- 387 $D = D_B D_b$. This particular structure allows formulating the product of G and an arbitrary vector as a fast
- 388 2D discrete convolution via Fast Fourier Transform (FFT) (Van Loan, 1992, section 4.2).

Consider, for example, the particular case in which $D_B = 4$, $D_b = 3$ and D = 12. In this case, G (equation 3) is 12×12 block matrix given by

$$\mathbf{G} = \begin{bmatrix} \mathbf{G}^{0} & \mathbf{G}^{1} & \mathbf{G}^{2} & \mathbf{G}^{3} \\ \mathbf{G}^{-1} & \mathbf{G}^{0} & \mathbf{G}^{1} & \mathbf{G}^{2} \\ \mathbf{G}^{-2} & \mathbf{G}^{-1} & \mathbf{G}^{0} & \mathbf{G}^{1} \\ \mathbf{G}^{-3} & \mathbf{G}^{-2} & \mathbf{G}^{-1} & \mathbf{G}^{0} \end{bmatrix}_{D \times D},$$
(39)

391 where each block \mathbf{G}^{ℓ} , $\ell \in \{(1 - D_B) : (D_B - 1)\}$, is a 3×3 Toeplitz matrix.

392 Consider the product

$$\mathbf{G}\,\mathbf{v} = \mathbf{w}\,\,,\tag{40}$$

393 where

$$\mathbf{v} = \begin{bmatrix} \mathbf{v}^0 \\ \vdots \\ \mathbf{v}^{D_B - 1} \end{bmatrix}_{D \times 1}, \quad \mathbf{w} = \begin{bmatrix} \mathbf{w}^0 \\ \vdots \\ \mathbf{w}^{D_B - 1} \end{bmatrix}_{D \times 1}, \tag{41}$$

are arbitrary partitioned vectors formed by D_B sub-vectors \mathbf{v}^{ℓ} and \mathbf{w}^{ℓ} , $\ell \in \{0 : (D_B - 1)\}$, all of them having D_b elements. The matrix-vector product given by equation 40 can be efficiently computed in terms of

$$\mathbf{G}_c \, \mathbf{v}_c = \mathbf{w}_c \,, \tag{42}$$

397 where

$$\mathbf{v}_{c} = \begin{bmatrix} \mathbf{v}_{c}^{0} \\ \vdots \\ \mathbf{v}_{c}^{D_{B}-1} \\ \mathbf{0}_{2D\times1} \end{bmatrix}_{4D\times1}, \quad \mathbf{w}_{c} = \begin{bmatrix} \mathbf{w}_{c}^{0} \\ \vdots \\ \mathbf{w}_{c}^{D_{B}-1} \\ \mathbf{0}_{2D\times1} \end{bmatrix}_{4D\times1}, \quad (43)$$

398 are partitioned vectors formed by $2D_b \times 1$ sub-vectors

$$\mathbf{v}_{c}^{\ell} = \begin{bmatrix} \mathbf{v}^{\ell} \\ \mathbf{0}_{D_{b} \times 1} \end{bmatrix}_{2D_{c} \times 1}, \quad \mathbf{w}_{c}^{\ell} = \begin{bmatrix} \mathbf{w}^{\ell} \\ \mathbf{0}_{D_{b} \times 1} \end{bmatrix}_{2D_{c} \times 1}, \tag{44}$$

399 and G_c is a $4D \times 4D$ doubly block circulant (Jain, 1989, p. 28) or block-circulant circulant-block (BCCB)

- 400 (Chan and Jin, 2007, p. 76) matrix. Matrix G_c is formed by $2D_B \times 2D_B$ blocks, where each block is a
- 401 $2D_b \times 2D_b$ circulant matrix. By considering the example defined by equation 39, the first column of blocks

402 forming the BCCB matrix G_c assumes the form

$$\mathbf{G}_{c}[:,:6] = \begin{bmatrix} \mathbf{G}_{c}^{0} \\ \mathbf{G}_{c}^{-1} \\ \mathbf{G}_{c}^{-2} \\ \mathbf{G}_{c}^{-3} \\ \mathbf{0}_{6 \times 6} \\ \mathbf{G}_{c}^{3} \\ \mathbf{G}_{c}^{2} \\ \mathbf{G}_{c}^{1} \end{bmatrix}_{D \times 2D_{b}}$$

$$(45)$$

- 403 The complete matrix G_c is obtained by properly downshifting G_c :,: 6] to form its remaining columns of
- 404 blocks. Because a BCCB matrix is diagonalized by the 2D unitary discrete Fourier transform (DFT), G_c
- 405 can be written as

$$\mathbf{G}_{c} = \left(\boldsymbol{\mathcal{F}}_{2D_{B}} \otimes \boldsymbol{\mathcal{F}}_{2D_{b}} \right)^{*} \boldsymbol{\Lambda} \left(\boldsymbol{\mathcal{F}}_{2D_{B}} \otimes \boldsymbol{\mathcal{F}}_{2D_{b}} \right) , \tag{46}$$

- 406 where the symbol " \otimes " denotes the Kronecker product (e.g., Horn and Johnson, 1991, p. 243), \mathcal{F}_{2D_B} and
- 407 \mathcal{F}_{2D_b} are the $2D_B \times 2D_B$ and $2D_b \times 2D_b$ unitary DFT matrices (e.g., Davis, 1979, p. 31), respectively,
- 408 the superscritpt "*" denotes the complex conjugate and Λ is a $4D \times 4D$ diagonal matrix containing the
- 409 eigenvalues of G_c . Due to the diagonalization of the matrix G_c , equation 42 can be rewritten by using
- 410 equation 46 and premultiplying both sides of the result by $(\mathcal{F}_{2D_B} \otimes \mathcal{F}_{2D_b})$, i.e.,

$$\Lambda \left(\mathcal{F}_{2D_B} \otimes \mathcal{F}_{2D_b} \right) \mathbf{v}_c = \left(\mathcal{F}_{2D_B} \otimes \mathcal{F}_{2D_b} \right) \mathbf{w}_c . \tag{47}$$

411 By following Takahashi et al. (2020), we rearrange equation 47 as follows

$$\mathcal{L} \circ (\mathcal{F}_{2D_B} \mathcal{V}_c \mathcal{F}_{2D_b}) = \mathcal{F}_{2D_B} \mathcal{W}_c \mathcal{F}_{2D_b}$$
(48)

- 412 where " \circ " denotes the Hadamard product (e.g., Horn and Johnson, 1991, p. 298) and \mathcal{L} , \mathcal{V}_c and \mathcal{W}_c are
- 413 $2D_B \times 2D_b$ matrices obtained by rearranging, along their rows, the elements forming the diagonal of Λ ,
- 414 vector \mathbf{v}_c and vector \mathbf{w}_c , respectively. Then, by premultiplying both sides of equation 48 by $\mathcal{F}_{2D_B}^*$ and
- 415 then postmultiplying both sides by $\mathcal{F}_{2D_b}^*$, we obtain

$$\mathcal{F}_{2D_{B}}^{*} \left[\mathcal{L} \circ \left(\mathcal{F}_{2D_{B}} \mathcal{V}_{c} \mathcal{F}_{2D_{b}} \right) \right] \mathcal{F}_{2D_{b}}^{*} = \mathcal{W}_{c}. \tag{49}$$

- 416 The left side of equation 49 represents the 2D Inverse Discrete Fourier Transform (IDFT) of the term in
- 417 brackets. Finally, we get from equation 46 that matrix \mathcal{L} can be efficiently computed by using only the first
- 418 column $G_c[:, 1]$ of the BCCB matrix G_c (equation 42) according to (Takahashi et al., 2020)

$$\mathcal{L} = \sqrt{4D} \, \mathcal{F}_{2D_B} \, \mathcal{C} \, \mathcal{F}_{2D_b} \,, \tag{50}$$

419 where C is a $2D_B \times 2D_b$ matrix obtained by rearranging, along its rows, the elements of $G_c[:, 1]$. PAREI

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4 SOLUTION STABILITY

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

Algorithm 6: Generic pseudo-code for the convolutional equivalent-layer method proposed by Takahashi et al. (2020, 2022).

Initialization:

- 1 Set the regular grid of P equivalent sources on a horizontal plane z_0 ;
- 2 Set a tolerance ϵ and a maximum number of iterations ITMAX;
- 3 Compute the first column G[:, 1] of the sensitivity matrix G (equation 3) for the particular case in which it has a BTTB structure (equation 39);
- 4 Rearrange the elements of G[:, 1] into the first column $G_c[:, 1]$ of the BCCB matrix G_c (equation 46);
- 5 Rearrange $G_c[:,1]$ to obtain \mathcal{C} (equation 50);
- 6 Compute $\mathcal{F}_{2D_B} \mathcal{C} \mathcal{F}_{2D_b}$ by using a 2D Fast Fourier Transform (2D-FFT) and multiply by $\sqrt{4D}$ to obtain \mathcal{L} (equation 50);

```
7 Set \tilde{\mathbf{p}} = \mathbf{0};
 8 Set \mathbf{r} = \mathbf{d} and compute \delta = \|\mathbf{r}\|/D;
     Compute \boldsymbol{\vartheta} = \mathbf{G}^{\top} \mathbf{r} (Algorithm 7) and \rho_0 = \boldsymbol{\vartheta}^{\top} \boldsymbol{\vartheta};
     Set \tau = 0 and \eta = 0;
11 m = 1;
     while (\delta > \epsilon) and (m < ITMAX) do
            Update \eta \leftarrow \vartheta + \tau \eta;
```

```
13
               Compute \nu = \mathbf{G} \, \boldsymbol{\eta} (Algorithm 7);
14
               Compute v = \rho_0/(\nu^{\top}\nu);
15
               Update \tilde{\mathbf{p}} \leftarrow \tilde{\mathbf{p}} + v \boldsymbol{\eta};
16
               Update \mathbf{r} \leftarrow \mathbf{r} - \upsilon \, \boldsymbol{\nu} and compute \delta \leftarrow \|\upsilon \, \boldsymbol{\nu}\|/D;
17
               Compute \boldsymbol{\vartheta} = \mathbf{G}^{\top} \mathbf{r} (Algorithm 7) and \rho = \boldsymbol{\vartheta}^{\top} \boldsymbol{\vartheta};
18
               Compute \tau = \rho/\rho_0;
19
               Update \rho_0 \leftarrow \rho;
20
```

 $m \leftarrow m + 1$; 21 22 end

Algorithm 7: Pseudo-code for computing the generic matrix-vector product given by equation 40 via fast 2D discrete convolution.

- 1 Rearrange v (equations 40 and 41) into v_c (equations 42–44);
- 2 Rearrange \mathbf{v}_c into $\mathbf{\mathcal{V}}_c$, compute $\mathbf{\mathcal{F}}_{2D_B}$ $\mathbf{\mathcal{V}}_c$ $\mathbf{\mathcal{F}}_{2D_b}$ via 2D-FFT and evaluate its Hadamard product with matrix \mathcal{L} to define an auxiliary matrix $\mathcal{A} = \mathcal{L} \circ (\mathcal{F}_{2D_B} \mathcal{V}_c \mathcal{F}_{2D_b});$
- 3 Compute $\mathcal{F}_{2D_B}^* \mathcal{A} \mathcal{F}_{2D_b}^*$ via 2D-FFT inverse to evaluate \mathcal{W}_c (equation 49); 4 Retrieve \mathbf{w}_c (equations 42–44) from \mathcal{W}_c (equation 49);
- 5 Retrieve w (equations 40 and 41) from \mathbf{w}_c (equations 42–44);
- 423 Let us assume noise-free potential-field data d, we estimate a physical-property distribution p (estimated
- solution) within the equivalent layer. Then, the noise-free data d are contaminated with additive D different 424
- sequences of pseudorandom Gaussian noise, creating different noise-corrupted potential-field data d_ℓ, 425
- $\ell = 1, ..., D$. From each $\mathbf{d}_{\ell}^{\mathbf{o}}$, we estimate a physical-property distribution $\hat{\mathbf{p}}_{\ell}$ within the equivalent layer.
- 427 Next, for each noise-corrupted data $\mathbf{d}_{\ell}^{\mathbf{o}}$ and estimated solution $\hat{\mathbf{p}}_{\ell}$, the ℓ th model perturbation δp_{ℓ} and the 428 ℓ th data perturbation δd_{ℓ} are, respectively, evaluated by

$$\delta p_{\ell} = \frac{\parallel \hat{\mathbf{p}}_{\ell} - \mathbf{p} \parallel_2}{\parallel \mathbf{p} \parallel_2}, \quad \ell = 1, ..., D,$$
(51)

429 and

$$\delta d_{\ell} = \frac{\parallel \mathbf{d}_{\ell}^{\mathbf{o}} - \mathbf{d} \parallel_2}{\parallel \mathbf{d} \parallel_2}, \quad \ell = 1, ..., D.$$
 (52)

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

$$\delta p_{\ell} \le \kappa \, \delta d_{\ell}, \quad \ell = 1, ..., D,$$
 (53)

- 431 where κ is the constant of proportionality between the model perturbation δp_{ℓ} (equation 51) and the data
- 432 perturbation δd_{ℓ} (equation 52). The constant κ acts as the condition number of an invertible matrix in a
- 433 given inversion, and thus measures the instability of the solution. The larger (smaller) the value of κ the
- 434 more unstable (stable) is the estimated solution.
- Equation 53 shows a linear relationship between the model perturbation and the data perturbation. By
- 436 plotting δp_{ℓ} (equation 51) against δd_{ℓ} (equation 52) produced by a set of D estimated solution obtained by
- 437 applying a given equivalent-layer method, we obtain a straight line behaviour described by equation 53.
- 438 By applying a linear regression, we obtain a fitted straight line whose estimated slope (κ in equation 53)
- 439 quantifies the solution stability.
- Here, the analysis of solution stability is numerically conducted by applying the classical equivalent-
- 441 layer technique with zeroth-order Tikhonov regularization, the convolutional method for gravimetric and
- 442 magnetic data, the deconvolutional method (equation ??) and the deconvolutional method with different
- 443 values for the Wiener stabilization (equation ??).

5 NUMERICAL SIMULATIONS

- 444 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
- 446 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
- 448 number of observation points, ranging from 10,000 up to 1,000,000. The results generated when using
- 449 iterative methods are set to it = 50 for the number of iterations.

450 5.1 Floating-point operations calculation

- To measure the computational effort of the different algorithms to solve the equivalent layer linear system,
- 452 a non-hardware dependent method can be useful because allow us to do direct comparison between them.
- 453 Counting the floating-point operations (flops), i.e., additions, subtractions, multiplications and divisions
- 454 is a good way to quantify the amount of work of a given algorithm (Golub and Van Loan, 2013). For
- 455 example, the number of *flops* necessary to multiply two vectors \mathbb{R}^N is 2N. A common matrix-vector
- 456 multiplication with dimension $\mathbb{R}^{N\times N}$ and \mathbb{R}^N , respectively, is $2N^2$ and a multiplication of two matrices
- 457 $\mathbb{R}^{N \times N}$ is $2N^3$. Figure ?? shows the total flops count for the different methods presented in this review
- 458 with a crescent number of data, ranging from 10,000 to 1,000,000 for the gravity equivalent layer and
- 459 figure ?? for magnetic data.

460 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
- 463 the lower triangule of A^TA (1/2N³), the Cholesky factor (1/3N³), a matrix-vector multiplication (2N²)
- 464 and finally solving the triangular system $(2N^2)$, totalizing

$$f_{classical} = \frac{5}{6}N^3 + 4N^2 \tag{54}$$

465 5.1.2 Window method (Leão and Silva, 1989)

- 466 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
- 468 presented in theirs work ($N_w = 49$) and the same number of equivalent sources ($M_w = 225$). We are doing
- 469 this process for all the other techniques to standardize the resolution of our problem. Using the Cholesky
- 470 decomposition with this method the *flops* are

$$f_{window} = N\frac{5}{6}M_w N_w^2 + 4N_w M_w (55)$$

471 5.1.3 PEL method (Oliveira Jr. et al., 2013)

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

$$f_{pel} = \frac{1}{3}H^3 + 2H^2 + 2NM_sH + H^2N + 2HN + 2NP$$
 (56)

- where H is the number of constant coefficients for the first degree polynomial (P=3) times the number of windows ($P \times N/N_s$).
- 478 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) (?)

$$f_{cals} = 2N^2 + it(4N^2 + 12N) (57)$$

- 482 5.1.5 Wavelet compression method with CGLS (?)
- 483 For the wavelet method (equation ??) we have calculated a coompression rate of 98% ($C_r = 0.02$)
- 484 for the threshold as the authors used in ? and the wavelet transformation requiring $\log_2(N)$ flops each
- 485 (equations ?? and ??c), with its inverse also using the same number of operations (equation ??). Combined
- 486 with the conjugate gradient least square necessary steps and iterations, the number of *flops* are

$$f_{wavelet} = 2NC_r + 4N\log_2(N) + it(4N\log_2(N) + 4NC_r + 12C_r)$$
(58)

- 487 5.1.6 Fast equivalent layer for gravity data (Siqueira et al., 2017)
- 488 The fast equivalent layer from Siqueira et al. (2017) solves the linear system in *it* iterations. The main
- 489 cost of this method (equations ??,??, ?? and ??)is the matrix-vector multiplication to asses the predicted
- 490 data $(2N^2)$ and three simply element by element vector sum, subtraction and division (3N total)

$$f_{siqueira} = it(3N + 2N^2) \tag{59}$$

- 491 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 $\ref{equation}$). Considering that the first column of our BCCB matrix has 4N elements,
- 495 the flops count of this method is

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

$$\tag{60}$$

- In the resultant count we considered a *radix-2* algorithm for the fast Fourier transform and its inverse,
- 497 which has a κ equals to 5 and requires $\kappa 4N\log_2(4N)$ flops each. The Hadarmard product of two matrices
- 498 of 4N elements with complex numbers takes 24N flops. Note that equation 60 is different from the one
- 499 presented in ? because we also added the flops necessary to calculate the eigenvalues in this form. It does

500 not differentiate much in order of magnitude because the iterative part is the most costful.

501 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 ??), 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 57.

$$f_{convmag} = \kappa 16N \log_2(4N) + 24N + it(\kappa 16N \log_2(4N) + 60N)$$
(61)

506 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 ?? 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 ($\kappa 4N \log_2(4N)$).

$$f_{deconv} = \kappa 12N \log_2(4N) + 24N \tag{62}$$

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 ??

$$f_{deconvwiener} = \kappa 12N \log_2(4N) + 76N \tag{63}$$

CONFLICT OF INTEREST STATEMENT

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

AUTHOR CONTRIBUTIONS

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

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DATA AVAILABILITY STATEMENT

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

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