

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

Diego Takahashi 1,* , André L. A. Reis 2 , Vanderlei C. Oliveira Jr. 1 and Valéria C. F. Barbosa 1

Correspondence*: Valéria C.F. Barbosa valcris@on.br

¹Observatório Nacional, Department of Geophysics, Rio de Janeiro, Brasil

² Universidade do Estado do Rio de Janeiro, Department of Applied Geology, Rio de Janeiro, Brasil

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 $i \in \{1:D\}$. 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)

- 4 where, p_i represents the scalar physical property of a virtual source (i.e., monopole, dipole, prism) located
- 5 at $(x_i, y_i, z_i), j \in \{1 : P\}$ 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)

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

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

- 10 where p is a $P \times 1$ vector with j-th element p_j representing the scalar physical property of the j-th
- 11 equivalent source and G is a $D \times P$ matrix with element g_{ij} given by equation 2.
- 12 The equivalent-layer technique consists in solving a linear inverse problem to determine a parameter
- 13 vector **p** leading to a predicted data vector **f** (equation 3) sufficiently close to the observed data vector **d**,
- 14 whose i-th element d_i is the observed potential field at (x_i, y_i, z_i) . The notion of closeness is intrinsically
- 15 related to the concept of vector norm (e.g., Golub and Van Loan, 2013, p. 68) or measure of length (e.g.,
- 16 Menke, 2018, p. 41). Because of that, almost all methods for determining p actually estimate a parameter
- 17 vector $\tilde{\mathbf{p}}$ minimizing a length measure of the difference between \mathbf{f} and \mathbf{d} (see subsection 1.3). Given an
- 18 estimate \tilde{p} , it is then possible to compute a potential field transformation

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

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

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

22 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
- 24 equivalent sources. We know that setting an equivalent layer with more (less) sources than potential-field
- 25 data usually leads to an underdetermined (overdetermined) inverse problem (e.g., Menke, 2018, p. 52–53).
- 26 Concerning the spatial distribution of the equivalent sources, the only condition is that they must rely on a
- 27 surface that is located below and does not cross that containing the potential field data. Soler and Uieda
- 28 (2021) present a practical discussion about this topic.

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

38 **1.2 Matrix** G

Generally, the harmonic function g_{ij} (equation 2) is defined in terms of the inverse distance between the

40 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)

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

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

42 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.,
- 14 Dampney, 1969; Emilia, 1973; Leão and Silva, 1989; Cordell, 1992; Oliveira Jr. et al., 2013; Siqueira et al.,
- 45 2017; Reis et al., 2020; Takahashi et al., 2020; Soler and Uieda, 2021; Takahashi et al., 2022). Another
- 46 common approach consists in not defining g_{ij} by using equations 6–8, but other harmonic functions
- 47 obtained by integrating them over the volume of regular prisms (e.g., Li and Oldenburg, 2010; Barnes and
- 48 Lumley, 2011; Li et al., 2014; Jirigalatu and Ebbing, 2019). There are also some less common approaches
- 49 defining the harmonic function g_{ij} (equation 2) as the potential field due to plane faces with constant
- 50 physical property (Hansen and Miyazaki, 1984), doublets (Silva, 1986) or by computing the double
- 51 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}
- 53 (equation 2) is independent on the actual physical relationship between the observed potential field and
- 54 their true sources (e.g., Cordell, 1992; Guspí and Novara, 2009; Li et al., 2014). Hence, g_{ij} can be
- 55 defined according to the problem. The only condition imposed to this function is that it decays to zero
- as the observation point (x_i, y_i, z_i) goes away from the position (x_j, y_j, z_j) of the j-th equivalent source.
- However, several methods use a function g_{ij} that preserves the physical relationship between the observed
- potential field and their true sources. For the case in which the observed potential field is gravity data, g_{ij}
- 59 is commonly defined as a component of the gravitational field produced at (x_i, y_i, z_i) by a point mass or
- prism located at (x_j, y_j, z_j) , with unit density. On the other hand, g_{ij} is commonly defined as a component

- of the magnetic induction field produced at (x_i, y_i, z_i) by a dipole or prism located at (x_j, y_j, z_j) , with unit magnetization intensity, when the observed potential field is magnetic data.
- For all harmonic functions discussed above, the sensitivity matrix G (equation 3) is always dense. For
- 64 scattered potential-field data, G does not have a well-defined structure, regardless of whether the spatial
- 65 distribution of the equivalent sources is set. Nevertheless, 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
- 67 planar and regularly spaced grids, Takahashi et al. (2020, 2022) show that G assumes a block-Toeplitz
- 68 Toeplitz-block (BTTB) structure. In this case, the product of G and an arbitrary vector can be efficiently
- 69 computed via 2D fast Fourier transform as a discrete convolution.

70 1.3 General formulation

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

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

73 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
- 76 and Q-space to designate them.
- 77 Then, the problem of estimating a parameter vector $\tilde{\mathbf{p}}$ minimizing a length measure of the difference
- 78 between f (equation 3) and d is replaced by that of estimating an auxiliary vector $\tilde{\mathbf{q}}$ minimizing the goal
- 79 function

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

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

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

81 and

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

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

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

- 85 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
- 87 the original parameter vector (equation 3) is computed by

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

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

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

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

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

91 where

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

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

93

92

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

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

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

- 95 Evidently, we have considered that all inverses exist in equations 20 and 21.
- Matrix B defined by equation 20 is commonly used for the cases in which D > P, i.e., when there are
- 97 more data than parameters (overdetermined problems). In this case, we consider that the estimate \tilde{q} is
- 98 obtained by solving the following linear system for $\tilde{\delta}_q$ (equation 18):

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

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

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

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

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

2 COMPUTATIONAL STRATEGIES

- 105 COMEÇAR EXPLICANDO AS LIMITAÇÕES DA SOLUÇÃO OBTIDA PELA FORMULAÇÃO 106 GERAL
- 107 Two important factors affecting the efficiency of a given matrix algorithm are the storage and amount of
- 108 required arithmetic. Here, we quantify this last factor by counting flops. A flop is a floating point addition,
- subtraction, multiplication or division (Golub and Van Loan, 2013, p. 12–14).

- To investigate the efficiency of equivalent-layer methods, we consider how they:
- 111 (i) set up the linear system (equations 22 and 23);
- 112 (ii) solve the linear system (equations 22 and 23);
- 113 (iii) perform potential-field transformations (equation 4).
- 114 We focus on the overall strategies used by the selected methods.

115 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 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 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. The list may also have a single element $\mathbf{i} = (i)$, which results in the i-th element $d_i \equiv \mathbf{d}[i]$ of \mathbf{d} . We may also define regular lists of indices by using the colon notation. For example,

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

$$\mathbf{i} = (:8) \Leftrightarrow \mathbf{d}[:8] = [d_1 \ d_2 \ \dots \ d_7]^{\top}$$

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

116 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

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

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:

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

which contains the contiguous elements of G from rows 2 to 5 and from columns 3 to 7.

118 2.2 Moving window

The initial approach to enhance the computational efficiency of the equivalent-layer technique is commonly denoted *moving window* and involves first splitting the observed data d_i , $i \in \{1 : D\}$, into M overlapping subsets (or data windows) formed by D^m data each, $m \in \{1 : M\}$. The data inside the M-th window are usually adjacent to each other and have indices defined by an integer list \mathbf{i}^m having

123 D^m elements. The number of data D^m forming the data windows are not necessarily equal to each other.

124 Each data window has a $D^m \times 1$ observed data vector $\mathbf{d}^m \equiv \mathbf{d}[\mathbf{i}^m]$. The second step consists in defining

- a set of P equivalent sources with scalar physical property p_j , $j \in \{1 : P\}$, and also split them into M
- overlapping subsets (or source windows) formed by P^m data each, $m \in \{1: M\}$. The sources inside the
- 127 m-th window have indices defined by an integer list j^m having P^m elements. Each source window has a
- 128 $P^m \times 1$ parameter vector \mathbf{p}^m and is located right below the corresponding m-th data window. Then, each
- 129 $\mathbf{d}^m \equiv \mathbf{d}[\mathbf{i}^m]$ is approximated by

$$\mathbf{f}^m = \mathbf{G}^m \mathbf{p}^m \,, \tag{24}$$

where $G^m \equiv G[i^m, j^m]$ is a submatrix of G (equation 3) formed by the elements computed with equation

- 131 2 using only the data and equivalent sources located inside the window m-th. The main idea of the moving-
- window approach is using the $\tilde{\mathbf{p}}^m$ estimated for each window to obtain (i) an estimate $\tilde{\mathbf{p}}$ of the parameter
- 133 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
- not obtained by solving the full, but smaller linear systems and (ii) the full matrix G (equation 3) is never
- 136 stored.
- Leão and Silva (1989) presented a pioneer work using the moving-window approach. Their method
- 138 requires a regularly-spaced grid of observed data on a horizontal plane z_0 . The data windows are defined by
- square local grids of $\sqrt{D'} \times \sqrt{D'}$ adjacent points, all of them having the same number of points D'. The
- 140 equivalent sources in the m-th data window are located below the observation plane, at a constant vertical
- 141 distance Δz_0 . They are arranged on a regular grid of $\sqrt{P'} \times \sqrt{P'}$ adjacent points following the same
- 142 grid pattern of the observed data. The local grid of sources for all data windows have the same number
- 143 of elements P'. Besides, they are vertically aligned, but expands the limits of their corresponding data
- 144 windows, so that D' < P'. Because of this spatial configuration of observed data and equivalent sources,
- 145 we have that $G^m = G'$ (equation 24) for all data windows (i.e., $\forall m \in \{1 : M\}$), where G' is a $D' \times P'$
- 146 constant matrix.
- By omitting the normalization strategy used by Leão and Silva (1989), their method consists in directly
- 148 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
- 149 as follows:

$$t_c^m = \left(\mathbf{G}'\mathbf{a}'\right)^{\top} \left[\mathbf{G}' \left(\mathbf{G}'\right)^{\top} + \mu \mathbf{I}_{D'}\right]^{-1} \mathbf{d}^m, \quad m \in \{1:M\},$$
(25)

- where $I_{D'}$ is the identity matrix of order D' and a' is a $P' \times 1$ vector with elements computed by equation
- 151 5 by using all equivalent sources in the m-th subset and only the coordinate of the central point in the
- 152 m-th data window. Due to the presumed spatial configuration of the observed data and equivalent sources,
- 153 a' is the same for all data windows. Note that equation 25 combines the potential-field transformation
- 154 (equation 4) with the solution of the undetermined problem (equation 23) for the particular case in which
- 155 $\mathbf{H} = \mathbf{W}_q = \mathbf{I}_{P'}$ (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 0 is a vector of zeros.
- 157 The method proposed by Leão and Silva (1989) can be outlined by the Algorithm 1. Note that Leão and
- 158 Silva (1989) directly compute the transformed potential t_c^m at the central point of each data window without
- 159 explicitly computing and storing an estimated for p^m (equation 24). It means that their method allows
- 160 computing a single potential-field transformation. A different transformation or the same one evaluated at
- 161 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 i^m for each data window, m \in \{1 : M\};
 2 Set the indices 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 a' associated with the desired potential-field transformation;
 5 Compute the matrix G';
6 Compute (\mathbf{G}'\mathbf{a}')^{\top} \left[ \mathbf{G}' \left( \mathbf{G}' \right)^{\top} + \mu \mathbf{I}_{D'} \right]^{-1};
 7 \ m = 1:
 8 while m < M do
        Compute t_c^m (equation 25); m \leftarrow m+1;
11 end
```

Soler and Uieda (2021) generalized the method proposed by Leão and Silva (1989) for irregularly spaced 162 data on an undulating surface. A direct consequence of this generalization is that a different submatrix 163 $G^m \equiv G[i^m, j^m]$ (equation 24) must be computed for each window. Differently from Leão and Silva 164 (1989), Soler and Uieda (2021) store the computed \tilde{p}^m for all windows and subsequently use them to obtain 165 a desired potential-field transformation (equation 4) as the superposed effect of all windows. The estimated 166 $\tilde{\mathbf{p}}^m$ for all windows are combined to form a single $P \times 1$ vector $\tilde{\mathbf{p}}$, which is an estimate for original 167 parameter vector p (equation 3). For each data window, Soler and Uieda (2021) solve an overdetermined 168 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 169 a diagonal matrix of weights for the data inside the m-th window and $\bar{p} = 0$ (equation 14), so that 170

$$\left[(\mathbf{G}^m)^\top \mathbf{W}_d^m \mathbf{G}^m + \mu \mathbf{I}_{P'} \right] \tilde{\mathbf{p}}^m = (\mathbf{G}^m)^\top \mathbf{W}_d^m \mathbf{d}^m.$$
 (26)

The overall steps of their method are defined by the Algorithm 2. Note that Algorithm 2 starts with a 171

residuals vector r that is iteratively updated. At each iteration, the potential field predicted a source window

is computed at all observation points and removed from the residuals vector r.

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

```
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};
    Set a P \times 1 vector \tilde{\mathbf{p}} = \mathbf{0};
   m = 1;
    while m < M do
          Set the matrix \mathbf{W}_d^m; Compute the matrix \mathbf{G}^m;
 8
 9
          Compute \tilde{\mathbf{p}}^m (equation 26);
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

2.3 Column update

175 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 176 177 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_i of a given 178 equivalent source, $j \in \{1 : D\}$ and remove its predicted potential field from the observed data vector d, 179 producing a residuals vector r. Then, the same procedure is repeated for other sources with the purpose of 180 iteratively updating r and the $D \times 1$ parameter vector p containing the physical property of all equivalent 181 sources. At the end, the algorithm produces an estimate \tilde{p} for the parameter vector yielding a predicted 182 potential field f (equation 3) satisfactorily fitting the observed data d according to a given criterion. Note 183 that the method proposed by Cordell (1992) iteratively solves the linear $G\tilde{p} \approx d$ with a $D \times D$ matrix G. 184 185 At each iteration, only a single column of G (equation 3) is used. An advantage of this *column-update* approach is that the full matrix G is never stored. 186

Algorithm 3 delineates the Cordell's method. Note that a single column $G[:, i_{max}]$ of the $D \times D$ matrix G187 (equation 3) is used per iteration, where i_{max} is the index of the maximum absolute value in r. As pointed out 188 by Cordell (1992), the method does not necessarily decrease monotonically along the iterations. Besides, 189 the method may not converge depending on how the vertical distances Δz_i , $i \in \{1:D\}$, controlling the 190 depths of the equivalent sources are set. According to Cordell (1992), the maximum absolute value $r_{\rm max}$ 191 in r decreases robustly at the beginning and oscillates within a narrowing envelope for the subsequent 192 iterations. 193

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

```
Initialization:
```

```
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 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_{\text{max}} in \mathbf{r};
 7 \ m = 1;
    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}}] + (a_{\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 r;
12
          m \leftarrow m + 1;
14 end
```

Row update 194 2.4

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Mendonça and Silva (1994) proposes an algebraic reconstruction technique (ART) (e.g., van der Sluis and van der Vorst, 1987, p. 58) to estimate a parameter vector $\tilde{\mathbf{p}}$ for a regular grid of P equivalent sources on a horizontal plane z_0 . Such methods iterate on the linear system rows to estimate corrections for the parameter vector, which may substantially save computer time and memory required to compute and store

199 the full linear system matrix along the iterations. The convergence of such *row-update methods* depends on

200 the linear system condition. The main advantage of such methods is not computing and storing the full

201 linear system matrix, but iteratively using its rows. The particular ART method proposed by Mendonça and

202 Silva (1994) considers that

$$\mathbf{d} = \begin{bmatrix} \mathbf{d}_e \\ \mathbf{d}_r \end{bmatrix} , \quad \mathbf{G} = \begin{bmatrix} \mathbf{G}_e \\ \mathbf{R}_r \end{bmatrix} , \tag{27}$$

203 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,

204 respectively. Mendonça and Silva (1994) designate d_e and d_r as, respectively, equivalent and redundant

205 data. With the exception of a normalization strategy, Mendonça and Silva (1994) calculate a $P \times 1$ estimated

206 parameter vector $\tilde{\mathbf{p}}$ by solving an underdetermined problem (equation 23) involving only the equivalent

207 data d_e (equation 27) for the particular case in which $H = W_p = I_P$ (equations 9 and 13), $W_d = I_{D_e}$

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

$$(\mathbf{F} + \mu \mathbf{I}_{D_e}) \mathbf{u} = \mathbf{d}_e$$

$$\tilde{\mathbf{p}} = \mathbf{G}_e^{\top} \mathbf{u} , \qquad (28)$$

where F is a $P \times P$ matrix that replaces $G_e G_e^{\top}$. Mendonça and Silva (1994) presume that the estimated

210 parameter vector $\tilde{\mathbf{p}}$ obtained from equation 28 leads to a $D_r \times 1$ residuals vector

$$\mathbf{r} = \mathbf{d}_r - \mathbf{G}_r \tilde{\mathbf{p}} \tag{29}$$

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

212 The overall method of Mendonça and Silva (1994) is defined by Algorithm 4. It is important noting

213 that the number D_e of equivalent data in \mathbf{d}_e increases by one per iteration, which means that the order

214 of the linear system in equation 28 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

216 efficiently updating $(\mathbf{F} + \mu \mathbf{I}_{D_e})$ at a given iteration (line 16 in Algorithm 4) by computing only its new

217 elements with respect to those computed in the previous iteration.

218 2.5 Reparameterization

219 Another approach for improving the computational performance of equivalent-layer technique consists

220 in setting a $P \times Q$ reparameterization matrix H (equation 9) with $Q \ll P$. This strategy has been used

in applied geophysics for decades (e.g., Skilling and Bryan, 1984; Kennett et al., 1988; Oldenburg et al.,

222 1993; Barbosa et al., 1997) and is known as subspace method. The main idea relies in reducing the linear

223 system dimension from the original P-space to a lower-dimensional subspace (the Q-space). An estimate

224 \tilde{q} for the reparameterized parameter vector q is obtained in the Q-space and subsequently used to obtain

225 an estimate \tilde{p} for the parameter vector p (equation 3) in the P-space by using equation 9. Hence, the key

aspect of this reparameterization approach is solving an appreciably smaller linear inverse problem for \tilde{q}

227 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

229 equivalent layer in terms of piecewise bivariate polynomials. Specifically, their method consists in splitting

230 a regular grid of equivalent sources into source windows inside which the physical-property distribution

231 is described by bivariate polynomial functions. The key aspect of their method relies on the fact that the

232 total number of coefficients required to define the bivariate polynomials is considerably smaller than the

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_{max} in r;
   Define the index i_{max} of r_{max};
Define the list of indices i_r of the remaining data in r;
   Define \mathbf{d}_e = \mathbf{d}[i_{\text{max}}];
    Compute (\mathbf{F} + \mu \mathbf{I}_{D_e}) and \mathbf{G}_e;
    Compute \tilde{\mathbf{p}} (equation 28);
10 Compute \mathbf{r} = \mathbf{d}[\mathbf{i}_r] - \mathbf{G}[\mathbf{i}_r, :] \tilde{\mathbf{p}};
11 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};
13
          Define the list of indices i_r of the remaining elements in r;
14
15
          Update (\mathbf{F} + \bar{\mu} \mathbf{I}_{D_e}) and \mathbf{G}_e;
16
          Update \tilde{\mathbf{p}} (equation 28);
17
          Update \mathbf{r} = \mathbf{d}[\mathbf{i}_r] - \mathbf{G}[\mathbf{i}_r,:] \tilde{\mathbf{p}};
18
          Define the maximum absolute value r_{max} in r;
19
20 end
```

- 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 $\tilde{\bf q}$ with ${\bf W}_d={\bf I}_D$ (equation 12) and $\bar q={\bf 0}$ (equation 14), so that

$$\left(\mathbf{H}^{\top}\mathbf{G}^{\top}\mathbf{G}\,\mathbf{H} + \mu\,\mathbf{W}_{q}\right)\tilde{\mathbf{q}} = \mathbf{H}^{\top}\mathbf{G}^{\top}\,\mathbf{d}\,,\tag{30}$$

- 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 ${\bf H}$ 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 ${\bf W}_q = {\bf I}_Q$ (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 H (equation 9) with $Q \ll P$. Instead, they used a matrix H with $Q \approx 1.7 P$. Their central idea is setting a

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- 253 reparameterization scheme that groups distant equivalent sources into blocks by using a bisection process.
- 254 This scheme leads to a quadtree representation of the physical-property distribution on the equivalent layer,
- 255 so that matrix GH (equation 10) is notably sparse. Barnes and Lumley (2011) explore this sparsity in
- 256 solving the overdetermined problem for $\tilde{\mathbf{q}}$ (equation 30) via conjugate-gradient method. Here, we consider
- 257 the conjugate gradient normal equation residual (CGNR) Golub and Van Loan (2013, sec. 11.3) as a
- 258 reference, which is also known as *conjugate gradient least squares* (CGLS) (Aster et al., 2019, p. 165).

259 2.6 Wavelet compression

- 260 Previously to Barnes and Lumley (2011), the idea of transforming the dense matrix G (equation 3) into a
- sparse one has already been used in the context of equivalent-layer technique. Li and Oldenburg (2010)
- 262 proposed a method that applies the wavelet transform to the original dense matrix G and sets to zero the
- small coefficients that are below a given threshold, which results in an approximating sparse representation
- 264 of G in the wavelet domain. Their method requires
- 265 PAREI AQUI

266

2.7 Iterative methods using the original G

- 267 Ideia: descrever o conjugate gradient e depois as diferenças dos outros métodos iterativos esta ideia é
- 268 ruim porque vai ser necessario reescrever os sistemas com matrizes CCT e CTC. Isso necessita definir as
- 269 matrizes Wq e Wd como WqTWq ou WqWqT, a depender do problema.
- 270 Xia and Sprowl (1991)
- 271 Xia et al. (1993)
- 272 Siqueira et al. (2017)
- 273 Jirigalatu and Ebbing (2019)

274 2.8 Discrete convolution

- 275 Takahashi et al. (2020)
- 276 Takahashi et al. (2022)

3 TEXTO ANTIGO

- 277 3.0.1 The wavelet compression and lower-dimensional subspace
- For large data sets, the sensitivity matrix A (equation 3) is a drawback in applying the equivalent-layer
- 279 technique because it is a large and dense matrix.
- 280 ? transformed a large and full sensitivity matrix into a sparse one by using fast wavelet transforms. In
- 281 the wavelet domain, ? applyied a 2D wavelet transform to each row and column of the original sensitivity
- 282 matrix A to expand it in the wavelet bases. This operation can be done by premultiplying the original
- 283 sensitivity matrix A by a matrix representing the 2D wavelet transform W_2 and then the resulting is

postmultiplied by the transpose of $\mathbf{W_2}$ (i.e., $\mathbf{W_2}^{\top}$). 284

$$\tilde{\mathbf{A}} = \mathbf{W_2} \, \mathbf{A} \, \mathbf{W_2}^{\top} \,, \tag{31}$$

where $\tilde{\mathbf{A}}$ is the expanded original sensitivity matrix in the wavelet bases with many elements zero or close 285 to zero. Next, the matrix $\hat{\bf A}$ is replaced by its sparse version $\hat{\bf A}_{\rm s}$ in the wavelet domain which in turn 286 is obtained by retaining only the large elements of the A. Thus, the elements of A whose amplitudes 287 fall below a relative threshold are discarded. In ?, the original sensitivity matrix A is high compressed 288 resulting in a sparce matrix A_s with a few percent of nonzero elements and the the inverse problem is 289 solved in the wavelet domain by using A_s and a incomplete conjugate gradient least squares, without an 290 explicit regularization parameter and a limited number of iterations. The solution is obtained by solving the 291 292 following linear system

$$\tilde{\mathbf{A}}_{\mathbf{L}}^{\top} \tilde{\mathbf{A}}_{\mathbf{L}} \tilde{\mathbf{p}}_{\mathbf{L}}^{*} = \tilde{\mathbf{A}}_{\mathbf{L}}^{\top} \tilde{\mathbf{d}}^{o}, \tag{32}$$

where $\tilde{\mathbf{p}}_{\mathbf{L}}^*$ is obtained by solving the linear system given by equation 32,

$$\tilde{\mathbf{A}}_{\mathbf{L}} = \tilde{\mathbf{A}}_{\mathbf{s}} \tilde{\mathbf{L}}^{-1}, \tag{33a}$$

$$\tilde{\mathbf{p}}_{\mathbf{L}} = \tilde{\mathbf{L}}\tilde{\mathbf{p}},$$
 (33b)

$$\tilde{\mathbf{p}}_{\mathbf{L}} = \tilde{\mathbf{L}}\tilde{\mathbf{p}}, \tag{33b}$$

$$\tilde{\mathbf{d}}^{o} = \mathbf{W}_{\mathbf{2}} \mathbf{d}^{o}, \tag{33c}$$

where $\tilde{\mathbf{L}}$ is a diagonal and invertible weighting matrix representing the finite-difference approximation in 294 the wavelet domain. Finally, the distribution over the equivalent layer in the space domain p is obtained by 295 applying an inverse wavelet transform in two steps, i.e.: 296

$$\tilde{\mathbf{p}} = \tilde{\mathbf{L}}^{-1} \, \tilde{\mathbf{p}}_{\mathbf{L}}^* \,, \tag{34}$$

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$$\mathbf{p} = \mathbf{W_2} \, \tilde{\mathbf{p}} \,. \tag{35}$$

298 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 299 calculated via equation ?? which uses a full matrix of Green's functions T. 300

? used the equivalent-layer technique with a wavelet compression to perform an upward continuation 301 of total-field anomaly between uneven surfaces. For regularly spaced grid of data, ? reported that high 302 compression ratios are achived with insignificant loss of accuracy. As compared to the upward-continued 303 total-field anomaly by equivalent layer using the dense matrix, ?'s (?) approach, using the Daubechies 304 305 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 higherdimensional 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

314 parameter vector in the subspace method can be written as

$$p = V \alpha, (36)$$

- where 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 .
- 316 In equation 36, the parameter vector \mathbf{p} is defined as a linear combination in the space spanned by Q basis
- 317 vectors $\mathbf{v}_i = 1, ..., Q$ and $\boldsymbol{\alpha}$ is a Q-dimensional unknown vector to be determined. The main advantage of
- 318 the subspace method is that the linear system of M equations in M unknowns to be originally solved is
- 319 reduced to a new linear system of Q equations in Q unknowns which requires much less computational
- 320 effort since $Q \ll M$, i.e.:

$$\mathbf{V}^{\top} \mathbf{A}^{\top} \mathbf{A} \mathbf{V} \alpha^* = \mathbf{V}^{\top} \mathbf{d}^o. \tag{37}$$

- 321 To avoid the storage of matrices A and V, ? evaluates an element of the matrix AV by calculating the dot
- 322 product between the row of matrix A and the column of the matrix B. After estimating α^* (equation 37)
- 323 belonging to a Q-dimensional subspace of \mathbb{R}^M , the distribution over the equivalent layer p in the \mathbb{R}^M is
- obtained by applying equation 36. The choice of the Q basis vectors $\mathbf{v}_i = 1, ..., Q$ (equation 36) in the
- 325 subspace method is not strict. ?, for example, chose the eigenvectors yielded by applying the singular value
- 326 decomposition of the matrix containing the gridded data set. The number of eigenvectors used to form
- 327 basis vectors will depend on the singular values.
- The proposed subspace method for solving large-scale equivalent-layer problem by ? was applied to
- 329 estimate the mass excess or deficiency caused by causative gravity sources.

330 3.0.2 The quadtree discretization

- To make the equivalent-layer technique tractable, ? also transformed the dense sensitivity matrix A 331 (equation 3) into a sparse matrix. In ?, a sparce version of the sensitivity matrix is achived by grouping 332 333 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 334 of the grouped smaller prisms (equivalent sources) that are encompassed by the larger block. The authors 335 336 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 337 model dimension reduction. 338
- 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 342 gravity-gradient data using a single layer of equivalent sources. To our knowledge, ? are the pioneers on 343 processing full-tensor gravity-gradient data jointly. In addition to computational feasibility, ?'s (?) method 344 reduces low-frequency noise and can also remove the drift in time-domain from the survey data. Those 345 authors stressed that the G_{zz} -component calculated through the single estimated equivalent-layer model 346 projected on a grid at a constant elevation by inverting full gravity-gradient data has the low-frequency error 347 reduced by a factor of 2.4 as compared to the inversion of an individual component of the gravity-gradient 348 349 data.

350 3.0.3 The reparametrization of the equivalent layer

Oliveira Jr. et al. (2013) reparametrized the whole equivalent-layer model by a piecewise bivariatepolynomial 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

$$\mathbf{p}^k = \mathbf{B}^k \, \mathbf{c}^k \,, \qquad k = 1 \dots Q \,, \tag{38}$$

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 α th-order polynomial function and \mathbf{B}^k is an $M_w \times P$ matrix containing the first-order derivative of the α th-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

$$\left(\mathbf{B}^{\top} \mathbf{A}^{\top} \mathbf{A} \mathbf{B} + \mu \mathbf{I}\right) \mathbf{c}^{*} = \mathbf{B}^{\top} \mathbf{A}^{\top} \mathbf{d}^{o}, \tag{39}$$

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 38) and all off-diagonal blocks are zero matrices. For ease of the explanation of equation 39, 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 39), 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 A and B, Oliveira Jr. et al. (2013) evaluate an element of the matrix AB by calculating the dot product between the row of matrix AB and the column of the matrix BB. After estimating all polynomial coefficients of all windows, the estimated coefficients (C^* in equation 39) 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.

381 3.0.4 The iterative scheme without solving a linear system

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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

- 387 updating the distribution of physical properties within the equivalent layer in the wavenumber and space
- 388 domains, respectively. Specifically, in Xia and Sprowl's (1991) method the physical-property distribution is
- 389 updated by using the ratio between the squared depth to the equivalent source and the gravitational constant
- 390 multiplied by the residual between the observed and predicted observation at the measurement station.
- 391 Neither of these methods solve linear systems.
- Following this class of methods of iterative equivalent-layer technique that does not solve linear systems,
- 393 Siqueira et al. (2017) developed a fast iterative equivalent-layer technique for processing gravity data in
- 394 which the sensitivity matrix A (equation 3) is replaced by a diagonal matrix $N \times N$, i.e.:

$$\tilde{\tilde{\mathbf{A}}} = 2 \,\pi \,\gamma \,\Delta \mathbf{S}^{-1} \,, \tag{40}$$

- 395 where γ is Newton's gravitational constant and ΔS^{-1} is a diagonal matrix of order N whose diagonal
- 396 elements Δs_i , i=1,...,N are the element of area centered at the ith horizontal coordinates of the ith
- 397 observation point. The physical foundations of Siqueira et al.'s (2017) method rely on two constraints: i) the
- 398 excess of mass; and ii) the positive correlation between the gravity observations and the mass distribution
- 399 over the equivalent layer.
- 400 Although Siqueira et al.'s (2017) method does not solve any linear system of equations, it can be
- 401 theoretically explained by solving the following linear system at the kth iteration:

$$\tilde{\tilde{\mathbf{A}}}^{\top} \tilde{\tilde{\mathbf{A}}} \Delta \hat{\mathbf{p}}^k = \tilde{\tilde{\mathbf{A}}}^{\top} \mathbf{r}^k, \tag{41}$$

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

$$r_i^k = d_i^o - d_i^k . (42)$$

- 404 and $\Delta \hat{\mathbf{p}}^k$ is an estimated N-dimensional vector of parameter correction.
- Because $\tilde{\tilde{A}}$, in equation 41, is a diagonal matrix (equation 40), the parameter correction estimate is
- 406 directly calculated without solving system of linear equations, and thus, an ith element of $\Delta \hat{\mathbf{p}}^k$ is directly
- 407 calculated by

$$\Delta \hat{p}^k_{\ i} = \frac{\Delta s_i \, r_i^k}{2 \, \pi \, \gamma} \,. \tag{43}$$

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

$$\hat{p}_i^{k+1} = \hat{p}_i^k + \Delta \hat{p}_i^k. \tag{44}$$

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

$$p_i^o = \frac{\Delta s_i \, d_i^o}{2 \, \pi \, \gamma} \,. \tag{45}$$

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

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

$$\mathbf{p}_{k+1} = \mathbf{p}_k + \omega \left[\mathbf{A_1}^{\top} (\mathbf{d_1} - \mathbf{M} \mathbf{A_1} \mathbf{p}_k) + \mathbf{A_2}^{\top} (\mathbf{d_2} - \mathbf{M} \mathbf{A_2} \mathbf{p}_k) \right], \tag{46}$$

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

421 3.0.5 The convolutional equivalent layer with BTTB matrices

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

? demonstrated that the sensitivity matrix **A** (equation 3) associated with a planar equivalent layer formed by a set of point masses, each one directly beneath each observation point and considering a regular grid of observation points at a constant height has a symmetric block-Toeplitz Toeplitz-block (BTTB) structure. A symmetric BTTB matrix has, at least, two attractive properties. The first one is that it can be defined by using only the elements forming its first column (or row). The second attractive property is that any BTTB matrix can be embedded into a symmetric Block-Circulat Circulant-Block (BCCB) matrix. This means that the full sensitivity matrix **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 437 processing, ? developed the convolutional equivalent layer for magnetic data processing. By assuming 438 a regularly spaced grid of magnetic data at a constant height and a planar equivalent layer of dipoles,? 439 proved that the sensitivity matrix linked with this layer possess a BTTB structure in the specific scenario 440 where each dipole is exactly beneath each observed magnetic data point. ? used a conjugate gradient 441 least-squares (CGLS) algorithm which does not require an inverse matrix or matrix-matrix multiplication. 442 Rather, it only requires matrix-vector multiplications per iteration, which can be effectively computed using 443 the 2D FFT as a discrete convolution. The matrix-vector product only uses the elements that constitute the 444 first column of the associated BTTB matrix, resulting in computational time and memory savings. ? (?) 445 showed the robustness of the convolutional equivalent layer in processing magnetic survey that violates the 446 requirement of regular grids in the horizontal directions and flat observation surfaces. 447

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

$$\mathbf{w} = \mathbf{C}\mathbf{v} \,, \tag{47}$$

- 450 where w and v are, respectively, vectors of data and parameters completed by zeros and C is a BCCB
- 451 matrix formed by $2Q \times 2Q$ blocks, where each block C_q , $q = 0, \dots, Q 1$, is a $2P \times 2P$ circulant matrix.
- 452 The first column of C is obtained by rearranging the first column of the sensitivity matrix A (equation 3).
- 453 Because a BCCB matrix is diagonalized by the 2D unitary discrete Fourier transform (DFT), C can be
- 454 written as

$$\mathbf{C} = (\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P})^* \mathbf{\Lambda} (\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}) , \qquad (48)$$

- 455 where the symbol " \otimes " denotes the Kronecker product (?), \mathbf{F}_{2Q} and \mathbf{F}_{2P} are the $2Q \times 2Q$ and $2P \times 2P$
- 456 unitary DFT matrices (?, p. 31), respectively, the superscritpt "*" denotes the complex conjugate and Λ is
- 457 a $4QP \times 4QP$ diagonal matrix containing the eigenvalues of C. Due to the diagonalization of the matrix
- 458 C, the auxiliary system (equation 47) can be rewritten by using equation 48 and premultiplying both sides
- 459 of the result by $(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P})$, i.e.,

$$\Lambda \left(\mathbf{F}_{2O} \otimes \mathbf{F}_{2P} \right) \mathbf{v} = \left(\mathbf{F}_{2O} \otimes \mathbf{F}_{2P} \right) \mathbf{w} . \tag{49}$$

- 460 By applying the vec-operator (?) to both sides of equation 49, by premultiplying both sides of the result by
- 461 \mathbf{F}_{2O}^* and then postmultiplying both sides of the result by \mathbf{F}_{2P}^*

$$\mathbf{F}_{2Q}^* \left[\mathbf{L} \circ \left(\mathbf{F}_{2Q} \mathbf{V} \mathbf{F}_{2P} \right) \right] \mathbf{F}_{2P}^* = \mathbf{W} , \qquad (50)$$

- 462 where " \circ " denotes the Hadamard product (?, p. 298) and L, V and W are $2Q \times 2P$ matrices obtained
- 463 by rearranging, along their rows, the elements forming the diagonal of matrix Λ , vector v and vector w,
- 464 respectively. The left side of equation 50 contains the 2D Inverse Discrete Fourier Transform (IDFT) of the
- 465 term in brackets, which in turn represents the Hadamard product of matrix L and the 2D DFT of matrix V.
- 466 Matrix L contains the eigenvalues of Λ (equation 48) and can be efficiently computed by using only the
- 467 first column of the BCCB matrix C (equation 47).
- Actually, in ? (?, ?) a fast 2D discrete circular convolution (Van Loan, 1992) is used to process very
- 469 large gravity and magnetic datasets efficiently. The convolutional equivalent layer was applied to perform
- 470 upward continuation of large magnetic datasets. Compared to the classical Fourier approach, ?'s (?) method
- 471 produces smaller border effects without using any padding scheme.
- Without taking advantage of the symmetric BTTB structure of the sensitivity matrix (?, ?) that arises
- 473 when gravimetric observations are measured on a horizontally regular grid, on a flat surface and considering
- 474 a regular grid of equivalent sources whithin a horizontal layer, ? explored the symmetry of the gravity
- 475 kernel to reduce the number of forward model evaluations. By exploting the symmetries of the gravity
- 476 kernels and redundancies in the forward model evaluations on a regular grid and combining the subspace
- 477 solution based on eigenvectors of the gridded dataset, ? estimated the mass excess or deficiency produced
- 478 by anomalous sources with positive or negative density contrast.

479 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.
- 481 Equation 50 shows that estimate the matrix V, containing the elements of parameter vector p, is a
- 482 inverse problem that could be solved by deconvolution. From equation 50, the matrix V can be obtain by
- 483 deconvolution, i.e.

$$\mathbf{V} = \mathbf{F}_{2Q}^* \left[\frac{\left(\mathbf{F}_{2Q} \mathbf{W} \, \mathbf{F}_{2P} \right)}{\mathbf{L}} \right] \mathbf{F}_{2P}^* \,. \tag{51}$$

- 484 Equation 51 shows that the parameter vector (in matrix V) can be theoretically obtain by dividing each
- 485 potential-field observations (in matrix W) by each eigenvalues (in matrix L). Hence, the parameter vector
- 486 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
- 488 to an enormous change in the estimated parameter. Hence, equation 51 requires regularization to be useful.
- 489 We used ewiener deconvolution to obtain a stable solution, i.e.,

$$\mathbf{V} = \mathbf{F}_{2Q}^* \left[\left(\mathbf{F}_{2Q} \mathbf{W} \, \mathbf{F}_{2P} \right) \frac{\mathbf{L}^*}{\left(\mathbf{L} \, \mathbf{L}^* + \mu \right)} \right] \mathbf{F}_{2P}^* \,, \tag{52}$$

490 where the matrix L^* contains the complex conjugate eigenvalues and μ is a parameter that controls the

491 degree of stabilization.

492 3.1 Solution stability

- The solution stability of the equivalent-layer methods is rarely addressed. Here, we follow the numerical stability analysis presented in Signaira et al. (2017).
- 494 stability analysis presented in Siqueira et al. (2017).
- Let us assume noise-free potential-field data d, we estimate a physical-property distribution p (estimated
- 496 solution) within the equivalent layer. Then, the noise-free data d are contaminated with additive D different
- 497 sequences of pseudorandom Gaussian noise, creating different noise-corrupted potential-field data d_{ℓ}^{o} ,
- 498 $\ell = 1, ..., D$. From each $\mathbf{d}_{\ell}^{\mathbf{o}}$, we estimate a physical-property distribution $\hat{\mathbf{p}}_{\ell}$ within the equivalent layer.
- Next, for each noise-corrupted data $\mathbf{d}^{\mathbf{o}}_{\ell}$ and estimated solution $\hat{\mathbf{p}}_{\ell}$, the ℓ th model perturbation δp_{ℓ} and the
- 500 ℓ th data perturbation δd_{ℓ} are, respectively, evaluated by

$$\delta p_{\ell} = \frac{\parallel \hat{\mathbf{p}}_{\ell} - \mathbf{p} \parallel_2}{\parallel \mathbf{p} \parallel_2}, \quad \ell = 1, ..., D,$$
 (53)

501 and

$$\delta d_{\ell} = \frac{\parallel \mathbf{d}_{\ell}^{\mathbf{o}} - \mathbf{d} \parallel_2}{\parallel \mathbf{d} \parallel_2}, \quad \ell = 1, ..., D.$$
 (54)

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

$$\delta p_{\ell} \le \kappa \, \delta d_{\ell}, \quad \ell = 1, ..., D,$$
 (55)

- 503 where κ is the constant of proportionality between the model perturbation δp_{ℓ} (equation 53) and the data
- 504 perturbation δd_{ℓ} (equation 54). The constant κ acts as the condition number of an invertible matrix in a
- 505 given inversion, and thus measures the instability of the solution. The larger (smaller) the value of κ the
- 506 more unstable (stable) is the estimated solution.
- 507 Equation 55 shows a linear relationship between the model perturbation and the data perturbation. By
- 508 plotting δp_{ℓ} (equation 53) against δd_{ℓ} (equation 54) produced by a set of D estimated solution obtained by
- 509 applying a given equivalent-layer method, we obtain a straight line behaviour described by equation 55.
- 510 By applying a linear regression, we obtain a fitted straight line whose estimated slope (κ in equation 55)
- 511 quantifies the solution stability.
- Here, the analysis of solution stability is numerically conducted by applying the classical equivalent-
- 513 layer technique with zeroth-order Tikhonov regularization, the convolutional method for gravimetric and

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magnetic data, the deconvolutional method (equation 51) and the deconvolutional method with different values for the Wiener stabilization (equation 52).

522

4 NUMERICAL SIMULATIONS

- 516 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
- 518 data we measure of the computational effort by counting the number of floating-point operations (*flops*),
- 519 such as additions, subtractions, multiplications, and divisions (Golub and Van Loan, 2013) for different
- 520 number of observation points, ranging from 10,000 up to 1,000,000. The results generated when using
- 521 iterative methods are set to it = 50 for the number of iterations.

4.1 Floating-point operations calculation

- To measure the computational effort of the different algorithms to solve the equivalent layer linear system,
- 524 a non-hardware dependent method can be useful because allow us to do direct comparison between them.
- 525 Counting the floating-point operations (flops), i.e., additions, subtractions, multiplications and divisions
- 526 is a good way to quantify the amount of work of a given algorithm (Golub and Van Loan, 2013). For
- 527 example, the number of flops necessary to multiply two vectors \mathbb{R}^N is 2N. A common matrix-vector
- multiplication with dimension $\mathbb{R}^{N\times N}$ and \mathbb{R}^N , respectively, is $2N^2$ and a multiplication of two matrices
- 529 $\mathbb{R}^{N\times N}$ is $2N^3$. Figure ?? shows the total flops count for the different methods presented in this review
- 530 with a crescent number of data, ranging from 10,000 to 1,000,000 for the gravity equivalent layer and
- 531 figure ?? for magnetic data.

532 4.1.1 Normal equations using Cholesky decomposition

- 533 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
- 535 the lower triangule of A^TA (1/2N³), the Cholesky factor (1/3N³), a matrix-vector multiplication (2N²)
- 536 and finally solving the triangular system $(2N^2)$, totalizing

$$f_{classical} = \frac{5}{6}N^3 + 4N^2 \tag{56}$$

537 4.1.2 Window method (Leão and Silva, 1989)

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

$$f_{window} = N\frac{5}{6}M_w N_w^2 + 4N_w M_w (57)$$

543 4.1.3 PEL method (Oliveira Jr. et al., 2013)

- The polynomial equivalent layer uses a simliar approach od moving windows from Leão and Silva (1989).
- 545 For this operations calculation (equation 39) we used a first degree polynomial (two variables) and each
- 546 window contains $N_s = 1,000$ observed data and $M_s = 1,000$ equivalent sources. Following the steps
- 547 given in (Oliveira Jr. et al., 2013) the total flops becomes

$$f_{pel} = \frac{1}{3}H^3 + 2H^2 + 2NM_sH + H^2N + 2HN + 2NP$$
 (58)

- 548 where H is the number of constant coefficients for the first degree polynomial (P=3) times the number 549 of windows $(P \times N/N_s)$.
- 550 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) (?)

$$f_{cals} = 2N^2 + it(4N^2 + 12N) (59)$$

- 554 4.1.5 Wavelet compression method with CGLS (?)
- For the wavelet method (equation 32) we have calculated a coompression rate of 98% ($C_r = 0.02$)
- 556 for the threshold as the authors used in ? and the wavelet transformation requiring $\log_2(N)$ flops each
- 557 (equations 31 and 33c), with its inverse also using the same number of operations (equation 35). Combined
- 558 with the conjugate gradient least square necessary steps and iterations, the number of *flops* are

$$f_{wavelet} = 2NC_r + 4N\log_2(N) + it(4N\log_2(N) + 4NC_r + 12C_r)$$
(60)

- 559 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
- 561 cost of this method (equations 41,42, 43 and 44)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)

$$f_{siqueira} = it(3N + 2N^2) \tag{61}$$

- 563 4.1.7 Convolutional equivalent layer for gravity data (?)
- This methods replaces the matrix-vector multiplication of the iterative fast-equivalent technique (Siqueira
- 565 et al., 2017) by three steps, involving a Fourier transform, an inverse Fourier transform, and a Hadamard
- product of matrices (equation 50). Considering that the first column of our BCCB matrix has 4N elements,
- 567 the flops count of this method is

$$f_{convqrav} = \kappa 4N \log_2(4N) + it(27N + \kappa 8N \log_2(4N)) \tag{62}$$

- In the resultant count we considered a *radix-2* algorithm for the fast Fourier transform and its inverse,
- 569 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 62 is different from the one
- 571 presented in ? because we also added the flops necessary to calculate the eigenvalues in this form. It does
- 572 not differentiate much in order of magnitude because the iterative part is the most costful.

573 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 50), 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 59.

$$f_{convmag} = \kappa 16N \log_2(4N) + 24N + it(\kappa 16N \log_2(4N) + 60N)$$
(63)

578 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 51 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 ($\kappa 4N \log_2(4N)$).

$$f_{deconv} = \kappa 12N \log_2(4N) + 24N \tag{64}$$

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 52

$$f_{deconvwiener} = \kappa 12N \log_2(4N) + 76N \tag{65}$$

CONFLICT OF INTEREST STATEMENT

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

AUTHOR CONTRIBUTIONS

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

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DATA AVAILABILITY STATEMENT

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

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