

# 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  $i \in \{1:D\}$ . 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  $\mathbf{p}$  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.
- 57 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 the  $P \times 1$  parameter vector  $\mathbf{p}$  (equation 3) can be reparameterized into a  $Q \times 1$  vector  $\mathbf{q}$  according to:

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

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

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

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

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

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

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

78 and

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

- 79 where  $\mu$  is a positive scalar controlling the trade-off between  $\Phi(\mathbf{q})$  and  $\Theta(\mathbf{q})$ ;  $\mathbf{W}_q$  is a  $Q \times Q$  symmetric
- 80 matrix imposing prior information on q given by

$$\mathbf{W}_q = \mathbf{H}^\top \mathbf{W}_p \, \mathbf{H} \,, \tag{14}$$

81 with  $W_p$  being a  $P \times P$  symmetric matrix imposing prior information on p;  $\bar{q}$  is a  $Q \times 1$  vector of reference

82 values for q satisfying

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

- 83 with  $\bar{\bf p}$  being a  $P \times 1$  vector containing reference values for the original parameter vector  ${\bf p}$ ; and  ${\bf W}_d$  is a
- 84  $D \times D$  symmetric matrix defining the relative importance of each observed datum  $d_i$ . After obtaining an
- estimate  $\tilde{\mathbf{q}}$  for the reparameterized parameter vector  $\mathbf{q}$  (equation 9) minimizing  $\Gamma(\mathbf{q})$  (equation 11), the
- 86 estimate  $\tilde{p}$  for the original parameter vector (equation 3) is computed by

$$\tilde{\mathbf{p}} = \mathbf{H}\,\tilde{\mathbf{q}}\,. \tag{16}$$

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

$$\nabla \Gamma(\mathbf{q}) = -2 \mathbf{H}^{\top} \mathbf{G}^{\top} \mathbf{W}_d (\mathbf{d} - \mathbf{f}) + 2 \mu \mathbf{W}_q (\mathbf{q} - \bar{\mathbf{q}}) . \tag{17}$$

Then, by considering that  $\nabla\Gamma(\tilde{\mathbf{q}}) = \mathbf{0}$  (equation 17), 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

$$\tilde{\boldsymbol{\delta}}_q = \mathbf{B}\,\tilde{\boldsymbol{\delta}}_d\,,\tag{18}$$

90 where

$$\tilde{\boldsymbol{\delta}}_q = \tilde{\mathbf{q}} - \bar{\mathbf{q}} \,, \tag{19}$$

91

$$\tilde{\boldsymbol{\delta}}_d = \mathbf{d} - \mathbf{G} \,\mathbf{H} \,\bar{\mathbf{q}} \,, \tag{20}$$

92

$$\mathbf{B} = \left(\mathbf{H}^{\top} \mathbf{G}^{\top} \mathbf{W}_{d} \mathbf{G} \mathbf{H} + \mu \mathbf{W}_{q}\right)^{-1} \mathbf{H}^{\top} \mathbf{G}^{\top} \mathbf{W}_{d},$$
(21)

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

$$\mathbf{B} = \mathbf{W}_q^{-1} \mathbf{H}^{\top} \mathbf{G}^{\top} \left( \mathbf{G} \mathbf{H} \mathbf{W}_q^{-1} \mathbf{H}^{\top} \mathbf{G}^{\top} + \mu \mathbf{W}_d^{-1} \right)^{-1}.$$
 (22)

94 Evidently, we have considered that all inverses exist in equations 21 and 22.

Matrix B defined by equation 21 is commonly used for the cases in which D > P, i.e., when there are

96 more data than parameters (overdetermined problems). In this case, we consider that the estimate  $\tilde{q}$  is

obtained by solving the following linear system for  $\tilde{\delta}_q$  (equation 19):

$$\left(\mathbf{H}^{\top}\mathbf{G}^{\top}\mathbf{W}_{d}\mathbf{G}\mathbf{H} + \mu \mathbf{W}_{q}\right)\tilde{\boldsymbol{\delta}}_{q} = \mathbf{H}^{\top}\mathbf{G}^{\top}\mathbf{W}_{d}\tilde{\boldsymbol{\delta}}_{d}.$$
(23)

98 On the other hand, for the cases in which D < P (underdetermined problems), matrix B is usually defined

99 according to equation 22. In this case, we consider that the the estimate  $\tilde{q}$  is obtained in two steps, which

100 consists in first solving a linear system for a dummy vector u and then computing a matrix-vector product

101 as follows:

$$\left(\mathbf{G}\,\mathbf{H}\,\mathbf{W}_{q}^{-1}\,\mathbf{H}^{\top}\mathbf{G}^{\top} + \mu\,\mathbf{W}_{d}^{-1}\right)\,\mathbf{u} = \tilde{\boldsymbol{\delta}}_{d} \tilde{\boldsymbol{\delta}}_{q} = \mathbf{W}_{q}^{-1}\mathbf{H}^{\top}\mathbf{G}^{\top}\mathbf{u}$$
(24)

102 After obtaining  $\tilde{\delta}_q$  (equations 23 and 24), the estimate  $\tilde{\mathbf{q}}$  is computed with equation 19.

#### 2 COMPUTATIONAL STRATEGIES

- 103 Two important factors affecting the efficiency of a given matrix algorithm are the storage and amount of
- 104 required arithmetic. Here, we quantify this last factor by counting flops. A flop is a floating point addition,
- 105 subtraction, multiplication or division (Golub and Van Loan, 2013, p. 12–14).
- NÃO SEI SE TÁ BOM AQUI: To investigate the efficiency of equivalent-layer methods, we consider
- 107 how they (i) set up and (ii) solve the linear inverse problem to estimate the physical property distribution
- on the equivalent layer, as well as (iii) perform potential field transformations (equation 4).

We focus on the overall strategies used by the selected methods

#### 110 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 **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 **i** of indices may be sorted or not and it may also have repeated indices. We may also define regular lists of indices by using the colon notation. For example,

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

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

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

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

The notation above can also be used to define submatrices. 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 **i** and **j** "pick out", respectively, the rows and columns of **G** that form the submatrix G[i, j]. The *i*-th row and the *j*-th column of **G** can be defined respectively by G[i, j] and G[i, j]. Finally, we may use the colon notation to define the following submatrix of G:

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

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

#### 113 **2.2 Moving windows**

- 114 The initial approach to enhance the computational efficiency of the equivalent-layer technique is
- 115 commonly denoted moving window and involves first splitting the observed data  $d_i$ ,  $i \in \{1 : D\}$ , into
- 116 M overlapping subsets (or data windows) formed by  $D^m$  data each,  $m \in \{1: M\}$ . The data inside the
- 117 m-th window are usually adjacent to each other and have indices defined by an integer list  $i^m$  having
- 118  $D^m$  elements. The number of data  $D^m$  forming the data windows are not necessarily equal to each other.
- 119 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
- 120 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
- 122 m-th window have indices defined by an integer list  $j^m$  having  $P^m$  elements. Each source window has a
- 123  $P^m \times 1$  parameter vector  $\mathbf{p}^m$  and is located right below the corresponding m-th data window. Then, each
- 124  $\mathbf{d}^m \equiv \mathbf{d}[\mathbf{i}^m]$  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 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  $\tilde{p}^m$  estimated for each window to obtain (i) an estimate  $\tilde{p}$  of the parameter vector for the entire equivalent layer or (ii) a given potential-field transformation t (equation 4). The main advantage of this approach is that the estimated parameter vector  $\tilde{p}$  or transformed potential field are not obtained by solving the full, but smaller linear systems.

Leão and Silva (1989) presented a pioneer work using the moving-window approach. Their method 131 requires a regularly-spaced grid of observed data on a horizontal plane  $z_0$ . The data windows are defined by 132 square local grids of  $\sqrt{D'} \times \sqrt{D'}$  adjacent points, all of them having the same number of points D'. The 133 equivalent sources in the m-th data window are located below the observation plane, at a constant vertical 134 distance  $\Delta z_0$ . They are arranged on a regular grid of  $\sqrt{P'} \times \sqrt{P'}$  adjacent points following the same 135 grid pattern of the observed data. The local grid of sources for all data windows have the same number 136 of elements P'. Besides, they are vertically aligned, but expands the limits of their corresponding data 137 windows, so that D' < P'. Because of this spatial configuration of observed data and equivalent sources, 138 we have that  $G^m = G'$  (equation 25) for all data windows (i.e.,  $\forall m \in \{1 : M\}$ ), where G' is a  $D' \times P'$ 139 constant matrix. 140

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

$$t_c^m = \left(\mathbf{G}'\mathbf{a}'\right)^{\top} \left[\mathbf{G}' \left(\mathbf{G}'\right)^{\top} + \mu \mathbf{I}_{D'}\right]^{-1} \mathbf{d}^m, \quad m \in \{1:M\},$$
(26)

where  $I_{D'}$  is the identity matrix of order D' and a' is a  $P' \times 1$  vector with elements computed by equation 5 by using all equivalent sources in the m-th subset and only the coordinate of the central point in the m-th data window. Due to the presumed spatial configuration of the observed data and equivalent sources, a' is the same for all data windows. Note that equation 26 combines the potential-field transformation (equation 4) with the solution of the undetermined problem (equation 24) for the particular case in which  $H = W_p = I_{P'}$  (equations 9 and 14),  $W_d = I_{D'}$  (equation 12),  $\bar{p} = 0$  (equation 15), where  $I_{P'}$  and  $I_{D'}$ are identity matrices of order P' and D', respectively, and 0 is a vector of zeros.

The method proposed by Leão and Silva (1989) can be outlined by the Algorithm 1. Note that Leão and Silva (1989) directly compute the transformed potential  $t_c^m$  at the central point of each data window without explicitly computing and storing an estimated for  $\mathbf{p}^m$  (equation 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 156 data on an undulating surface. A direct consequence of this generalization is that a different submatrix 157  $\mathbf{G}^m \equiv \mathbf{G}[\mathbf{i}^m, \mathbf{j}^m]$  (equation 25) must be computed for each window. Differently from Leão and Silva 158 (1989), Soler and Uieda (2021) store the computed  $\tilde{\mathbf{p}}^m$  for all windows and subsequently use them to obtain 159 a desired potential-field transformation (equation 4) as the superposed effect of all windows. The estimated 160  $\tilde{\mathbf{p}}^m$  for all windows are combined to form a single  $P \times 1$  vector  $\tilde{\mathbf{p}}$ , which is an estimate for original 161 parameter vector p (equation 3). For each data window, Soler and Uieda (2021) solve an overdetermined 162 problem (equation 23) for  $\tilde{\mathbf{p}}^m$  by using  $\mathbf{H} = \mathbf{W}_p = \mathbf{I}_{P^m}$  (equations 9 and 14),  $\mathbf{W}_d^m$  (equation 12) equal to 163 a diagonal matrix of weights for the data inside the m-th window and  $\bar{p} = 0$  (equation 15), so that

$$\left[ \left( \mathbf{G}^{m} \right)^{\top} \mathbf{W}_{d}^{m} \mathbf{G}^{m} + \mu \mathbf{I}_{P'} \right] \tilde{\mathbf{p}}^{m} = \left( \mathbf{G}^{m} \right)^{\top} \mathbf{W}_{d}^{m} \mathbf{d}^{m}.$$
 (27)

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

```
Initialization:

1 Set the indices \mathbf{i}^m for each data window, m \in \{1:M\};

2 Set the indices \mathbf{j}^m for each source window, m \in \{1:M\};

3 Set the constant depth z_0 + \Delta z_0 for all equivalent sources;

4 Compute the vector \mathbf{a}' associated with the desired potential-field transformation;

5 Compute the matrix \mathbf{G}';

6 Compute (\mathbf{G}'\mathbf{a}')^{\top} \left[\mathbf{G}' (\mathbf{G}')^{\top} + \mu \mathbf{I}_{D'}\right]^{-1};

7 m = 1;

8 while m < M do

9 | Compute t_c^m (equation 26);

10 | m \leftarrow m + 1;

11 end
```

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

```
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;
 4 Set a D \times 1 residuals vector \mathbf{r} = \mathbf{d};
 5 Set a P \times 1 vector \tilde{\mathbf{p}} = \mathbf{0};
 6 m = 1;
    while m < M do
          Set the matrix \mathbf{W}_d^m;
 8
          Compute the matrix G^m:
          Compute \tilde{\mathbf{p}}^m (equation 27);
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 \; ;
13
         m \leftarrow m + 1:
14 end
```

168 PAREI AQUI - APARENTEMENTE, A COLON NOTATION VAI SER UMA MÃO NA RODA

#### 169 2.3 Column update

- 170 Cordell (1992)
- 171 Guspí and Novara (2009)

### 172 **2.4 Row update**

- 173 Algebraic reconstruction techniques (ART) van der Sluis and van der Vorst (2004)
- Mendonça and Silva (1994)

# 175 2.5 Reparameterization

- 176 Barnes and Lumley (2011)
- 177 Oliveira Jr. et al. (2013)
- 178 Mendonça (2020)

#### 179 2.6 Wavelet compression

180 Li and Oldenburg (2010)

# 181 2.7 Iterative methods using the original ${f G}$

- 182 Xia and Sprowl (1991)
- 183 Xia et al. (1993)
- 184 Siqueira et al. (2017)
- 185 Jirigalatu and Ebbing (2019)

### 186 2.8 Discrete convolution

- 187 Takahashi et al. (2020)
- 188 Takahashi et al. (2022)

#### 3 TEXTO ANTIGO

- 189 Leão and Silva (1989) reduced the total processing time and memory usage of equivalent-layer technique
- 190 by means of a moving data-window scheme. A small moving data window with  $N_w$  observations and
- 191 a small equivalent layer with  $M_w$  equivalent sources  $(M_w > N_w)$  located below the observations are
- 192 established. For each position of a moving-data window, Leão and Silva (1989) estimate a stable solution
- 193  $p_{\mathbf{w}}^*$  by using a data-space approach with the zeroth-order Tikhonov regularization (?), i.e.,

$$\left(\mathbf{A}_{\mathbf{w}}\mathbf{A}_{\mathbf{w}}^{\top} + \mu \mathbf{I}\right)\mathbf{w} = \mathbf{d}_{\mathbf{w}}^{o}, \qquad (28a)$$

$$\mathbf{A_w}^{\top} \mathbf{w} = \mathbf{p_w}^*, \tag{28b}$$

- 194 where w is a dummy vector,  $\mu$  is a regularizing parameter,  $\mathbf{d_w}^o$  is an  $N_w$ -dimensional vector containing
- 195 the observed potential-field data,  $A_w$  is an  $N_w \times M_w$  sensitivity matrix related to a moving-data window, I
- 196 is an identity matrix of order  $N_w$  and the superscript  $\top$  stands for a transpose. After estimating an  $M_w \times 1$
- 197 parameter vector  $\mathbf{p_w}^*$  (equation 28b) the desired transformation of the data is only calculated at the central
- 198 point of each moving-data window, i.e.:

$$\hat{t}_k = \mathbf{t}_k^{\top} \ \mathbf{p_w}^* \,, \tag{29}$$

- 199 where  $\hat{t}_k$  is the transformed data calculated at the central point k of the data window and  $\mathbf{t}_k$  is an  $M_w \times 1$
- 200 vector whose elements form the kth row of the  $N_w \times N_w$  matrix of Green's functions T (equation ??) of
- 201 the desired linear transformation of the data.
- By shifting the moving-data window with a shift size of one data spacing, a new position of a data
- 203 window is set up. Next, the aforementioned process (equations 28b and 29) is repeated for each position of

a moving-data window, until the entire data have been processed. Hence, instead of solving a large inverse 204 problem, Leão and Silva (1989) solve several much smaller ones. 205

To reduce the size of the linear system to be solved, Soler and Uieda (2021) adopted the same strategy 206 proposed, originally, by Leão and Silva (1989) of using a small moving-data window sweeping the whole 207 data. In Leão and Silva (1989), a moving-data window slides to the next adjacent data window following a 208 sequential movement, the predicted data is calculated inside the data window and the desired transformation 209 are only calculated at the center of the moving-data window. Unlike Leão and Silva (1989), Soler and 210 Uieda (2021) do not adopt a sequential order of the data windows; rather, they adopt a randomized order of 211 windows in the iterations of the gradient-boosting algorithm (?, ? and ?). The gradient-boosting algorithm 212 in Soler and Uieda (2021) estimates a stable solution using the data and the equivalent sources that fall 213 within a moving-data window; however, it calculates the predicted data and the residual data in the whole 214 survey data. Next, the residual data that fall within a new position of the data window is used as input 215 data to estimate a new stable solution within the data window which in turn is used to calculated a new 216 predicted data and a new residual data in the whole survey data. Finally, unlike Leão and Silva (1989), 217 in Soler and Uieda (2021) neither the data nor the equivalent sources need to be distributed in regular 218 grids. Indeed, Leão and Silva (1989) built their method using regular grids, but in fact regular grids are not 219 necessary. Regarding the equivalent-source layout, Soler and Uieda (2021) proposed the block-averaged 220 sources locations in which the survey area is divided into horizontal blocks and one single equivalent 221 source is assigned to each block. Each single source per block is placed over the layer with its horizontal 222 coordinates given by the average horizontal positions of observation points. According to Soler and Uieda 223 (2021), the block-averaged sources layout reduces the number of equivalent sources significantly and the 224 gradient-boosting algorithm provides even greater efficiency in terms of data fitting. 225

#### 3.0.1 The equivalent-data concept 226

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To reduced the total processing time and memory usage of equivalent-layer technique, Mendonça and 227 Silva (1994) proposed a strategy called 'equivalent data concept'. The equivalent data concept is grounded 228 on the principle that there is a subset of redundant data that does not contribute to the final solution and 229 thus can be dispensed. Conversely, there is a subset of observations, called equivalent data, that contributes 230 effectively to the final solution and fits the remaining observations (redundant data). Iteractively, Mendonça 231 and Silva (1994) selected the subset of equivalent data that is substantially smaller than the original dataset. 232 This selection is carried out by incorporating one data point at a time.

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According to Mendonça and Silva (1994), the number of equivalent data is about one-tenth of the total number of observations. These authors used the equivalent data concept to carry out an interpolation of gravity data. They showed a reduction of the total processing time and memory usage by, at least, two orders of magnitude as opposed to using all observations in the interpolation process via the classical equivalent-layer technique.

#### The wavelet compression and lower-dimensional subspace 3.0.2

For large data sets, the sensitivity matrix A (equation 3) is a drawback in applying the equivalent-layer 240 technique because it is a large and dense matrix. 241

? transformed a large and full sensitivity matrix into a sparse one by using fast wavelet transforms. In the wavelet domain, ? applyied a 2D wavelet transform to each row and column of the original sensitivity matrix A to expand it in the wavelet bases. This operation can be done by premultiplying the original sensitivity matrix A by a matrix representing the 2D wavelet transform W<sub>2</sub> and then the resulting is

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

$$\tilde{\mathbf{A}} = \mathbf{W_2} \, \mathbf{A} \, \mathbf{W_2}^{\top} \,, \tag{30}$$

where  $\tilde{\mathbf{A}}$  is the expanded original sensitivity matrix in the wavelet bases with many elements zero or close 247 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 248 is obtained by retaining only the large elements of the A. Thus, the elements of A whose amplitudes 249 fall below a relative threshold are discarded. In ?, the original sensitivity matrix A is high compressed 250 resulting in a sparce matrix A<sub>s</sub> with a few percent of nonzero elements and the the inverse problem is 251 solved in the wavelet domain by using  $A_s$  and a incomplete conjugate gradient least squares, without an 252 253 explicit regularization parameter and a limited number of iterations. The solution is obtained by solving the 254 following linear system

$$\tilde{\mathbf{A}}_{\mathbf{L}}^{\top} \tilde{\mathbf{A}}_{\mathbf{L}} \tilde{\mathbf{p}}_{\mathbf{L}}^{*} = \tilde{\mathbf{A}}_{\mathbf{L}}^{\top} \tilde{\mathbf{d}}^{o}, \tag{31}$$

where  $\tilde{\mathbf{p}}_{\mathbf{L}}^*$  is obtained by solving the linear system given by equation 31,

$$\tilde{\mathbf{A}}_{\mathbf{L}} = \tilde{\mathbf{A}}_{\mathbf{s}} \tilde{\mathbf{L}}^{-1}, \tag{32a}$$

$$\tilde{\mathbf{p}}_{\mathbf{L}} = \tilde{\mathbf{L}}\tilde{\mathbf{p}}, \tag{32b}$$

$$\tilde{\mathbf{d}}^o = \mathbf{W}_{\mathbf{2}} \mathbf{d}^o, \tag{32c}$$

$$\tilde{\mathbf{d}}^o = \mathbf{W_2} \, \mathbf{d}^o, \tag{32c}$$

where  $\tilde{\mathbf{L}}$  is a diagonal and invertible weighting matrix representing the finite-difference approximation in 256 the wavelet domain. Finally, the distribution over the equivalent layer in the space domain p is obtained by 257 applying an inverse wavelet transform in two steps, i.e.: 258

$$\tilde{\mathbf{p}} = \tilde{\mathbf{L}}^{-1} \, \tilde{\mathbf{p}}_{\mathbf{L}}^* \,, \tag{33}$$

259 and

$$\mathbf{p} = \mathbf{W_2} \, \tilde{\mathbf{p}} \,. \tag{34}$$

260 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 261 calculated via equation ?? which uses a full matrix of Green's functions T. 262

? used the equivalent-layer technique with a wavelet compression to perform an upward continuation 263 of total-field anomaly between uneven surfaces. For regularly spaced grid of data, ? reported that high 264 compression ratios are achived with insignificant loss of accuracy. As compared to the upward-continued 265 total-field anomaly by equivalent layer using the dense matrix, ?'s (?) approach, using the Daubechies 266 wavelet, decreased CPU (central processing unit) time by up to two orders of magnitude. 267

? overcame the solution of intractable large-scale equivalent-layer problem by using the subspace method 268 (e.g., ?, ?; ?, ?; ?, ?; ?, ?). The subspace method reduces the dimension of the linear system of equations to 269 be solved. Given a higher-dimensional space (e.g., M-dimensional model space,  $\mathbb{R}^M$ ), there exists many 270 lower-dimensional subspaces (e.g., Q-dimensional subspace) of  $\mathbb{R}^M$ . The linear inverse problem related 271 to the equivalent-layer technique consists in finding an M-dimension parameter vector  $\mathbf{p} \in \mathbb{R}^M$  which 272 adequately fits the potential-field data. The subspace method looks for a parameter vector who lies in a 273 Q-dimensional subspace of  $\mathbb{R}^M$  which, in turn, is spanned by a set of Q vectors  $\mathbf{v}_i = 1, ..., Q$ , where 274

275  $\mathbf{v}_i \in \mathbb{R}^M$  In matrix notation, the parameter vector in the subspace method can be written as

$$p = V \alpha, (35)$$

- where V is an  $M \times Q$  matrix whose columns  $\mathbf{v}_i = 1, ..., Q$  form a basis vectors for a subspace Q of  $\mathbb{R}^M$ .
- 277 In equation 35, the parameter vector  $\mathbf{p}$  is defined as a linear combination in the space spanned by Q basis
- 278 vectors  $\mathbf{v}_i = 1, ..., Q$  and  $\boldsymbol{\alpha}$  is a Q-dimensional unknown vector to be determined. The main advantage of
- 279 the subspace method is that the linear system of M equations in M unknowns to be originally solved is
- 280 reduced to a new linear system of Q equations in Q unknowns which requires much less computational
- 281 effort since  $Q \ll M$ , i.e.:

$$\mathbf{V}^{\top} \mathbf{A}^{\top} \mathbf{A} \mathbf{V} \alpha^* = \mathbf{V}^{\top} \mathbf{d}^o. \tag{36}$$

- 282 To avoid the storage of matrices A and V, ? evaluates an element of the matrix AV by calculating the dot
- product between the row of matrix A and the column of the matrix B. After estimating  $\alpha^*$  (equation 36)
- 284 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 35. The choice of the Q basis vectors  $\mathbf{v}_i = 1, ..., Q$  (equation 35) in the
- 286 subspace method is not strict. ?, for example, chose the eigenvectors yielded by applying the singular value
- 287 decomposition of the matrix containing the gridded data set. The number of eigenvectors used to form
- 288 basis vectors will depend on the singular values.
- The proposed subspace method for solving large-scale equivalent-layer problem by ? was applied to
- 290 estimate the mass excess or deficiency caused by causative gravity sources.

# 291 3.0.3 The quadtree discretization

- To make the equivalent-layer technique tractable, ? also transformed the dense sensitivity matrix A (equation 3) into a sparse matrix. In ?, a sparce version of the sensitivity matrix is achived by grouping
- 294 equivalent sources (e.g., they used prisms) distant from an observation point together to form a larger prism
- 295 or larger block. Each larger block has averaged physical properties and averaged top- and bottom-surfaces
- 296 of the grouped smaller prisms (equivalent sources) that are encompassed by the larger block. The authors
- 297 called it the 'larger averaged block' and the essence of their method is the reduction in the number of
- 298 equivalent sources, which means a reduction in the number of parameters to be estimated implying in
- 299 model dimension reduction.
- 300 The key of the ?'s (?) method is the algorithm for deciding how to group the smaller prisms. In
- 301 practice, these authors used a recursive bisection process that results in a quadtree discretization of the
- 302 equivalent-layer model.
- By using the quadtree discretization, ? were able to jointly process multiple components of airborne
- 304 gravity-gradient data using a single layer of equivalent sources. To our knowledge, ? are the pioneers on
- processing full-tensor gravity-gradient data jointly. In addition to computational feasibility, ?'s (?) method
- 306 reduces low-frequency noise and can also remove the drift in time-domain from the survey data. Those
- 307 authors stressed that the  $G_{zz}$ -component calculated through the single estimated equivalent-layer model
- 308 projected on a grid at a constant elevation by inverting full gravity-gradient data has the low-frequency error
- 309 reduced by a factor of 2.4 as compared to the inversion of an individual component of the gravity-gradient
- 310 data.

#### The reparametrization of the equivalent layer 311

Oliveira Jr. et al. (2013) reparametrized the whole equivalent-layer model by a piecewise bivariate-312 polynomial function defined on a set of Q equivalent-source windows. In Oliveira Jr. et al.'s (2013) 313 approach, named polynomial equivalent layer (PEL), the parameter vector within the kth equivalent-source 314 window  $p^k$  can be written in matrix notation as 315

$$\mathbf{p}^k = \mathbf{B}^k \, \mathbf{c}^k \,, \qquad k = 1 \dots Q \,, \tag{37}$$

where  $\mathbf{p}^k$  is an  $M_w$ -dimensional vector containing the physical-property distribution within the kth equivalent-source window,  $c^k$  is a P-dimensional vector whose lth element is the lth coefficient of the 317  $\alpha$ th-order polynomial function and  $\mathbf{B}^k$  is an  $M_w \times P$  matrix containing the first-order derivative of the 318  $\alpha$ th-order polynomial function with respect to one of the P coefficients. 319

By using a regularized potential-field inversion, Oliveira Jr. et al. (2013) estimates the polynomial 320 coefficients for each equivalent-source window by solving the following linear system 321

$$\left(\mathbf{B}^{\top} \mathbf{A}^{\top} \mathbf{A} \mathbf{B} + \mu \mathbf{I}\right) \mathbf{c}^{*} = \mathbf{B}^{\top} \mathbf{A}^{\top} \mathbf{d}^{o}, \tag{38}$$

where  $\mu$  is a regularizing parameter,  $\mathbf{c}^*$  is an estimated H-dimensional vector containing all coefficients 322 describing all polynomial functions within all equivalent-source windows which compose the entire 323 equivalent layer, I is an identity matrix of order H(H = PQ) and B is an  $M \times H$  block diagonal matrix 324 such that the main-diagonal blocks are  $\mathbf{B}^k$  matrices (equation 37) and all off-diagonal blocks are zero 325 matrices. For ease of the explanation of equation 38, we keep only the zeroth-order Tikhonov regularization 326 and omitting the first-order Tikhonov regularization (?) which was also used by Oliveira Jr. et al. (2013). 327

The main advantage of the PEL is solve H-dimensional system of equations (equation 38), where H328 totalizes the number of polynomial coefficients composing all equivalent-source windows, requiring a 329 lower computational effort since  $H \ll N$ . To avoid the storage of matrices A and B, Oliveira Jr. et al. 330 (2013) evaluate an element of the matrix AB by calculating the dot product between the row of matrix A 331 and the column of the matrix B. After estimating all polynomial coefficients of all windows, the estimated 332 coefficients (c\* in equation 38) are transformed into a single physical-property distribution encompassing 333 the entire equivalent layer. 334

335 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 336 within the equivalent layer is generally much smaller than the number of equivalent sources. Consequently, 337 this leads to a considerably smaller linear system that needs to be solved. Hence, the main strategy of 338 polynomial equivalent layer is the model dimension reduction. 339

The polynomial equivalent layer was applied to perform upward continuations of gravity and magnetic 340 data and reduction to the pole of magnetic data. 341

#### 3.0.5 The iterative scheme without solving a linear system 342

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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) 344 and later expanded upon by Guspí and Novara (2009) updates the physical property of sources, located 345 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

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

$$\tilde{\tilde{\mathbf{A}}} = 2 \,\pi \,\gamma \,\Delta \mathbf{S}^{-1} \,, \tag{39}$$

- 356 where  $\gamma$  is Newton's gravitational constant and  $\Delta S^{-1}$  is a diagonal matrix of order N whose diagonal
- 357 elements  $\Delta s_i$ , i = 1, ..., N are the element of area centered at the ith horizontal coordinates of the ith
- 358 observation point. The physical foundations of Siqueira et al.'s (2017) method rely on two constraints: i) the
- 359 excess of mass; and ii) the positive correlation between the gravity observations and the mass distribution
- 360 over the equivalent layer.
- 361 Although Siqueira et al.'s (2017) method does not solve any linear system of equations, it can be
- 362 theoretically explained by solving the following linear system at the kth iteration:

$$\tilde{\tilde{\mathbf{A}}}^{\top} \tilde{\tilde{\mathbf{A}}} \Delta \hat{\mathbf{p}}^k = \tilde{\tilde{\mathbf{A}}}^{\top} \mathbf{r}^k, \tag{40}$$

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

$$r_i^k = d_i^o - d_i^k . (41)$$

- and  $\Delta \hat{\mathbf{p}}^k$  is an estimated N-dimensional vector of parameter correction.
- Because  $\tilde{\tilde{A}}$ , in equation 40, is a diagonal matrix (equation 39), the parameter correction estimate is
- directly calculated without solving system of linear equations, and thus, an ith element of  $\Delta \hat{\mathbf{p}}^k$  is directly
- 368 calculated by

$$\Delta \hat{p}^k_{\ i} = \frac{\Delta s_i \, r_i^k}{2 \, \pi \, \gamma} \,. \tag{42}$$

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

$$\hat{p}_i^{k+1} = \hat{p}_i^k + \Delta \hat{p}_i^k. \tag{43}$$

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

$$p_i^o = \frac{\Delta s_i \, d_i^o}{2 \, \pi \, \gamma} \,. \tag{44}$$

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

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374 For jointly process two gravity gradient components, Jirigalatu and Ebbing (2019) used the Gauss-FFT 375 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 376 mask matrix M is defined in the following way: if the corresponding pixel does not contain the original 377 data, the element of M is set to zero; otherwise, it is set to one. The kth Landweber iteration is given by 378

$$\mathbf{p}_{k+1} = \mathbf{p}_k + \omega \left[ \mathbf{A_1}^{\top} (\mathbf{d_1} - \mathbf{M} \mathbf{A_1} \mathbf{p}_k) + \mathbf{A_2}^{\top} (\mathbf{d_2} - \mathbf{M} \mathbf{A_2} \mathbf{p}_k) \right], \tag{45}$$

where  $\omega$  is a relaxation factor,  $d_1$  and  $d_2$  are the two gravity gradient components and  $A_1$  and  $A_2$  are the 379 corresponding gravity gradient kernels. Jirigalatu and Ebbing (2019) applied their method for processing 380 two horizontal curvature components of Falcon airborne gravity gradient. 381

#### 382 The convolutional equivalent layer with BTTB matrices

383 ? (?, ?) introduced the convolutional equivalent layer for gravimetric and magnetic data processing, 384 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 386 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 392 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 398 processing, ? developed the convolutional equivalent layer for magnetic data processing. By assuming 399 a regularly spaced grid of magnetic data at a constant height and a planar equivalent layer of dipoles,? 400 proved that the sensitivity matrix linked with this layer possess a BTTB structure in the specific scenario 401 where each dipole is exactly beneath each observed magnetic data point. ? used a conjugate gradient 402 least-squares (CGLS) algorithm which does not require an inverse matrix or matrix-matrix multiplication. 403 Rather, it only requires matrix-vector multiplications per iteration, which can be effectively computed using 404 405 the 2D FFT as a discrete convolution. The matrix-vector product only uses the elements that constitute the first column of the associated BTTB matrix, resulting in computational time and memory savings. ? (?) 406 showed the robustness of the convolutional equivalent layer in processing magnetic survey that violates the 407 requirement of regular grids in the horizontal directions and flat observation surfaces. 408

409 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 410

$$\mathbf{w} = \mathbf{C}\mathbf{v} \,, \tag{46}$$

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

$$\mathbf{C} = (\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P})^* \mathbf{\Lambda} (\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}) , \qquad (47)$$

- 416 where the symbol " $\otimes$ " denotes the Kronecker product (?),  $\mathbf{F}_{2Q}$  and  $\mathbf{F}_{2P}$  are the  $2Q \times 2Q$  and  $2P \times 2P$
- 417 unitary DFT matrices (?, p. 31), respectively, the superscritpt "\*" denotes the complex conjugate and  $\Lambda$  is
- 418 a  $4QP \times 4QP$  diagonal matrix containing the eigenvalues of C. Due to the diagonalization of the matrix
- 419 C, the auxiliary system (equation 46) can be rewritten by using equation 47 and premultiplying both sides
- 420 of the result by  $(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P})$ , i.e.,

$$\Lambda \left( \mathbf{F}_{2O} \otimes \mathbf{F}_{2P} \right) \mathbf{v} = \left( \mathbf{F}_{2O} \otimes \mathbf{F}_{2P} \right) \mathbf{w} . \tag{48}$$

- By applying the vec-operator (?) to both sides of equation 48, by premultiplying both sides of the result by
- 422  $\mathbf{F}_{2O}^*$  and then postmultiplying both sides of the result by  $\mathbf{F}_{2P}^*$

$$\mathbf{F}_{2D}^* \left[ \mathbf{L} \circ \left( \mathbf{F}_{2Q} \mathbf{V} \mathbf{F}_{2P} \right) \right] \mathbf{F}_{2P}^* = \mathbf{W} , \qquad (49)$$

- 423 where " $\circ$ " denotes the Hadamard product (?, p. 298) and L, V and W are  $2Q \times 2P$  matrices obtained
- 424 by rearranging, along their rows, the elements forming the diagonal of matrix  $\Lambda$ , vector v and vector w,
- 425 respectively. The left side of equation 49 contains the 2D Inverse Discrete Fourier Transform (IDFT) of the
- 426 term in brackets, which in turn represents the Hadamard product of matrix L and the 2D DFT of matrix V.
- 427 Matrix L contains the eigenvalues of  $\Lambda$  (equation 47) and can be efficiently computed by using only the
- 428 first column of the BCCB matrix C (equation 46).
- 429 Actually, in ? (?, ?) a fast 2D discrete circular convolution (Van Loan, 1992) is used to process very
- 430 large gravity and magnetic datasets efficiently. The convolutional equivalent layer was applied to perform
- 431 upward continuation of large magnetic datasets. Compared to the classical Fourier approach, ?'s (?) method
- 432 produces smaller border effects without using any padding scheme.
- Without taking advantage of the symmetric BTTB structure of the sensitivity matrix (?, ?) that arises
- 434 when gravimetric observations are measured on a horizontally regular grid, on a flat surface and considering
- 435 a regular grid of equivalent sources whithin a horizontal layer, ? explored the symmetry of the gravity
- 436 kernel to reduce the number of forward model evaluations. By exploting the symmetries of the gravity
- 437 kernels and redundancies in the forward model evaluations on a regular grid and combining the subspace
- 438 solution based on eigenvectors of the gridded dataset, ? estimated the mass excess or deficiency produced
- 439 by anomalous sources with positive or negative density contrast.

#### 440 3.0.7 The deconvolutional equivalent layer with BTTB matrices

- To avoid the iterations of the conjugate gradient method in ?, we can employ the deconvolution process.
- 442 Equation 49 shows that estimate the matrix V, containing the elements of parameter vector p, is a
- 443 inverse problem that could be solved by deconvolution. From equation 49, the matrix V can be obtain by
- 444 deconvolution, i.e.

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

- 445 Equation 50 shows that the parameter vector (in matrix V) can be theoretically obtain by dividing each
- 446 potential-field observations (in matrix W) by each eigenvalues (in matrix L). Hence, the parameter vector
- 447 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
- 449 to an enormous change in the estimated parameter. Hence, equation 50 requires regularization to be useful.
- 450 We used ewiener deconvolution to obtain a stable solution, i.e.,

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

- 451 where the matrix L\* contains the complex conjugate eigenvalues and  $\mu$  is a parameter that controls the
- 452 degree of stabilization.

## 453 3.1 Solution stability

- The solution stability of the equivalent-layer methods is rarely addressed. Here, we follow the numerical
- 455 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
- 457 solution) within the equivalent layer. Then, the noise-free data d are contaminated with additive D different
- 458 sequences of pseudorandom Gaussian noise, creating different noise-corrupted potential-field data  $d_{\ell}^{o}$ ,
- 459  $\ell = 1, ..., D$ . From each  $\mathbf{d}_{\ell}^{\mathbf{o}}$ , we estimate a physical-property distribution  $\hat{\mathbf{p}}_{\ell}$  within the equivalent layer.
- Next, for each noise-corrupted data  $\mathbf{d}_{\ell}^{\mathbf{o}}$  and estimated solution  $\hat{\mathbf{p}}_{\ell}$ , the  $\ell$ th model perturbation  $\delta p_{\ell}$  and the
- 461  $\ell$ th data perturbation  $\delta d_{\ell}$  are, respectively, evaluated by

$$\delta p_{\ell} = \frac{\parallel \hat{\mathbf{p}}_{\ell} - \mathbf{p} \parallel_2}{\parallel \mathbf{p} \parallel_2}, \quad \ell = 1, ..., D,$$
 (52)

462 and

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

$$(53)$$

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

$$\delta p_{\ell} < \kappa \, \delta d_{\ell}, \quad \ell = 1, ..., D,$$
 (54)

- 464 where  $\kappa$  is the constant of proportionality between the model perturbation  $\delta p_{\ell}$  (equation 52) and the data
- 465 perturbation  $\delta d_{\ell}$  (equation 53). The constant  $\kappa$  acts as the condition number of an invertible matrix in a
- 466 given inversion, and thus measures the instability of the solution. The larger (smaller) the value of  $\kappa$  the
- 467 more unstable (stable) is the estimated solution.
- Equation 54 shows a linear relationship between the model perturbation and the data perturbation. By
- 469 plotting  $\delta p_{\ell}$  (equation 52) against  $\delta d_{\ell}$  (equation 53) produced by a set of D estimated solution obtained by
- 470 applying a given equivalent-layer method, we obtain a straight line behaviour described by equation 54.
- 471 By applying a linear regression, we obtain a fitted straight line whose estimated slope ( $\kappa$  in equation 54)
- 472 quantifies the solution stability.
- 473 Here, the analysis of solution stability is numerically conducted by applying the classical equivalent-
- 474 layer technique with zeroth-order Tikhonov regularization, the convolutional method for gravimetric and

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475 magnetic data, the deconvolutional method (equation 50) and the deconvolutional method with different 476 values for the Wiener stabilization (equation 51).

483

#### 4 NUMERICAL SIMULATIONS

- 477 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
- 479 data we measure of the computational effort by counting the number of floating-point operations (*flops*),
- 480 such as additions, subtractions, multiplications, and divisions (Golub and Van Loan, 2013) for different
- 481 number of observation points, ranging from 10,000 up to 1,000,000. The results generated when using
- 482 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,
- a non-hardware dependent method can be useful because allow us to do direct comparison between them.
- 486 Counting the floating-point operations (*flops*), i.e., additions, subtractions, multiplications and divisions
- 487 is a good way to quantify the amount of work of a given algorithm (Golub and Van Loan, 2013). For
- 488 example, the number of flops necessary to multiply two vectors  $\mathbb{R}^N$  is 2N. A common matrix-vector
- 489 multiplication with dimension  $\mathbb{R}^{N\times N}$  and  $\mathbb{R}^N$ , respectively, is  $2N^2$  and a multiplication of two matrices
- 490  $\mathbb{R}^{N \times N}$  is  $2N^3$ . Figure ?? shows the total flops count for the different methods presented in this review
- 491 with a crescent number of data, ranging from 10,000 to 1,000,000 for the gravity equivalent layer and
- 492 figure ?? for magnetic data.

## 493 4.1.1 Normal equations using Cholesky decomposition

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

$$f_{classical} = \frac{5}{6}N^3 + 4N^2 \tag{55}$$

## 498 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 sizes
- 500 (equation 28b). For our results we are considering a data-window of the same size of wich the authors
- presented in theirs work ( $N_w = 49$ ) and the same number of equivalent sources ( $M_w = 225$ ). We are doing
- 502 this process for all the other techniques to standardize the resolution of our problem. Using the Cholesky
- 503 decomposition with this method the *flops* are

$$f_{window} = N\frac{5}{6}M_w N_w^2 + 4N_w M_w (56)$$

#### 504 4.1.3 PEL method (Oliveira Jr. et al., 2013)

- 505 The polynomial equivalent layer uses a simliar approach od moving windows from Leão and Silva (1989).
- 506 For this operations calculation (equation 38) we used a first degree polynomial (two variables) and each
- 507 window contains  $N_s = 1,000$  observed data and  $M_s = 1,000$  equivalent sources. Following the steps
- 508 given in (Oliveira Jr. et al., 2013) the total flops becomes

$$f_{pel} = \frac{1}{3}H^3 + 2H^2 + 2NM_sH + H^2N + 2HN + 2NP$$
 (57)

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

## 511 4.1.4 Conjugate gradient least square (CGLS)

- The CGLS method is a very stable and fast algorithm for solving linear systems iteratively. Its
- 513 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) (?)

$$f_{cals} = 2N^2 + it(4N^2 + 12N) (58)$$

# 515 4.1.5 Wavelet compression method with CGLS (?)

- For the wavelet method (equation 31) we have calculated a coompression rate of 98% (  $C_r = 0.02$  )
- for the threshold as the authors used in ? and the wavelet transformation requiring  $\log_2(N)$  flops each
- 518 (equations 30 and 32c), with its inverse also using the same number of operations (equation 34). Combined
- 519 with the conjugate gradient least square necessary steps and iterations, the number of *flops* are

$$f_{wavelet} = 2NC_r + 4N\log_2(N) + it(4N\log_2(N) + 4NC_r + 12C_r)$$
(59)

## 520 4.1.6 Fast equivalent layer for gravity data (Sigueira et al., 2017)

- The fast equivalent layer from Siqueira et al. (2017) solves the linear system in it iterations. The main
- 522 cost of this method (equations 40,41, 42 and 43)is the matrix-vector multiplication to asses the predicted
- 523 data  $(2N^2)$  and three simply element by element vector sum, subtraction and division (3N total)

$$f_{siqueira} = it(3N + 2N^2) \tag{60}$$

#### 524 4.1.7 Convolutional equivalent layer for gravity data (?)

- This methods replaces the matrix-vector multiplication of the iterative fast-equivalent technique (Siqueira
- 526 et al., 2017) by three steps, involving a Fourier transform, an inverse Fourier transform, and a Hadamard
- 527 product of matrices (equation 49). Considering that the first column of our BCCB matrix has 4N elements,
- 528 the flops count of this method is

$$f_{convgrav} = \kappa 4N \log_2(4N) + it(27N + \kappa 8N \log_2(4N)) \tag{61}$$

- In the resultant count we considered a *radix-2* algorithm for the fast Fourier transform and its inverse,
- 530 which has a  $\kappa$  equals to 5 and requires  $\kappa 4N \log_2(4N)$  flops each. The Hadarmard product of two matrices
- 531 of 4N elements with complex numbers takes 24N flops. Note that equation 61 is different from the one
- 532 presented in ? because we also added the flops necessary to calculate the eigenvalues in this form. It does
- 533 not differentiate much in order of magnitude because the iterative part is the most costful.

#### 534 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 49), 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 58.

$$f_{convmag} = \kappa 16N \log_2(4N) + 24N + it(\kappa 16N \log_2(4N) + 60N)$$
(62)

#### 539 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 50 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 ( $\kappa 4N \log_2(4N)$ ).

$$f_{deconv} = \kappa 12N \log_2(4N) + 24N \tag{63}$$

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  $\mu$  as shown in equation 51

$$f_{deconvwiener} = \kappa 12N \log_2(4N) + 76N \tag{64}$$

## **CONFLICT OF INTEREST STATEMENT**

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

#### **AUTHOR CONTRIBUTIONS**

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

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#### DATA AVAILABILITY STATEMENT

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

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