

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

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# 1 FUNDAMENTALS

2  $d_i$

3  $(x_i, y_i, z_i)$

4  $i \in \{1 : D\}$

5 approximate  $d_i$  by a harmonic function

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

6 where,

7  $p_j$

8  $(x_j, y_j, z_j)$

9  $j \in \{1 : P\}$

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

10 where  $\min\{z_j\}$  denotes the minimum  $z_j$  (or the vertical coordinate of the shallowest equivalent source).

$$\mathbf{f} = \mathbf{G}\mathbf{p}, \quad (3)$$

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

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

$$\mathbf{t} = \mathbf{A}\tilde{\mathbf{p}}, \quad (4)$$

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

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

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

## 23 1.1 Spatial distribution and total number of equivalent sources

24 There is no well-established criteria to define the optimum number  $P$  or the spatial distribution of the  
25 equivalent sources. We know that setting an equivalent layer with more (less) sources than potential-field

data usually leads to an underdetermined (overdetermined) inverse problem (e.g., Menke, 2018, p. 52–53). Concerning the spatial distribution of the equivalent sources, the only condition is that they must rely on a surface that is located below and does not cross that containing the potential field data. Soler and Uieda (2021) present a practical discussion about this topic.

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

CRITÉRIOS PARA DEFINIR A PROFUNDIDADE DA CAMADA: DAMPNEY (ESPAÇAMENTO DO GRID) E REIS (ESPAÇAMENTO DAS LINHAS)

## 1.2 Matrix G

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

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

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

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

and

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

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

A common assumption for most of the equivalent-layer methods is that the harmonic function  $g_{ij}$  (equation 2) is independent on the actual physical relationship between the observed potential field and their true sources (e.g., Cordell, 1992; Guspí and Novara, 2009; Li et al., 2014). Hence,  $g_{ij}$  can be defined according to the problem. The only condition imposed to this function is that it decays to zero as the observation point  $(x_i, y_i, z_i)$  goes away from the position  $(x_j, y_j, z_j)$  of the  $j$ -th equivalent source.

However, several methods use a function  $g_{ij}$  that preserves the physical relationship between the observed potential field and their true sources. For the case in which the observed potential field is gravity data,  $g_{ij}$  is commonly defined as a component of the gravitational field produced at  $(x_i, y_i, z_i)$  by a point mass or prism located at  $(x_j, y_j, z_j)$ , with unit density. On the other hand,  $g_{ij}$  is commonly defined as a component of the magnetic induction field produced at  $(x_i, y_i, z_i)$  by a dipole or prism located at  $(x_j, y_j, z_j)$ , with unit magnetization intensity, when the observed potential field is magnetic data.

For all harmonic functions discussed above, the sensitivity matrix  $\mathbf{G}$  (equation 3) is always dense. For scattered potential-field data,  $\mathbf{G}$  does not have a well-defined structure, regardless of whether the spatial 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 planar and regularly spaced grids, Takahashi et al. (2020, 2022) show that  $\mathbf{G}$  assumes a block-Toeplitz Toeplitz-block (BTTB) structure. In this case, the product of  $\mathbf{G}$  and an arbitrary vector can be efficiently computed via 2D fast Fourier transform as a discrete convolution.

### 1.3 General formulation

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

$$\mathbf{p} = \mathbf{H} \mathbf{q}, \quad (9)$$

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

$$\mathbf{f} = \mathbf{G} \mathbf{H} \mathbf{q}. \quad (10)$$

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

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

which is a combination of particular measures of length given by

$$\Phi(\mathbf{q}) = \|\mathbf{W}_d (\mathbf{d} - \mathbf{G} \mathbf{H} \mathbf{q})\|_2^2, \quad (12)$$

and

$$\Theta(\mathbf{q}) = \|\mathbf{W}_q (\mathbf{q} - \bar{\mathbf{q}})\|_2^2, \quad (13)$$

where  $\mu$  is a positive scalar controlling the trade-off between  $\Phi(\mathbf{q})$  and  $\Theta(\mathbf{q})$ ;  $\|\cdot\|_2$  is the 2-norm (or Euclidean norm);  $\mathbf{W}_q$  is a matrix imposing prior information on  $\mathbf{q}$  given by

$$\mathbf{W}_q = \mathbf{W}_p \mathbf{H}, \quad (14)$$

with  $\mathbf{W}_p$  being a matrix imposing prior information on  $\mathbf{p}$ ;  $\bar{\mathbf{q}}$  is a  $Q \times 1$  vector of reference values for  $\mathbf{q}$  satisfying

$$\bar{\mathbf{p}} = \mathbf{H} \bar{\mathbf{q}}, \quad (15)$$

with  $\bar{\mathbf{p}}$  being a  $P \times 1$  vector containing reference values for the original parameter vector  $\mathbf{p}$ ; and  $\mathbf{W}_d$  is a  $D \times D$  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 estimate  $\tilde{\mathbf{p}}$  for the original parameter vector (equation 3) is computed by

$$\tilde{\mathbf{p}} = \mathbf{H} \tilde{\mathbf{q}}. \quad (16)$$

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

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

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  $(\mathbf{H}^\top \mathbf{G}^\top \mathbf{W}_d^\top \mathbf{W}_d \mathbf{G} \mathbf{H}) \bar{\mathbf{q}}$ , we obtain

$$\tilde{\boldsymbol{\delta}}_q = \mathbf{B} \tilde{\boldsymbol{\delta}}_d, \quad (18)$$

where

$$\tilde{\boldsymbol{\delta}}_q = \tilde{\mathbf{q}} - \bar{\mathbf{q}}, \quad (19)$$

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

$$\mathbf{B} = \left( \mathbf{H}^\top \mathbf{G}^\top \mathbf{W}_d^\top \mathbf{W}_d \mathbf{G} \mathbf{H} + \mu \mathbf{H}^\top \mathbf{W}_p^\top \mathbf{W}_p \mathbf{H} \right)^{-1} \mathbf{H}^\top \mathbf{G}^\top \mathbf{W}_d^\top \mathbf{W}_d, \quad (21)$$

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

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

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

Matrix  $\mathbf{B}$  defined by equation 21 is commonly used for the cases in which  $D > P$ , i.e., when there are more data than parameters (overdetermined problems). In this case, we consider that the estimate  $\tilde{\mathbf{q}}$  is obtained by solving the following linear system for  $\tilde{\boldsymbol{\delta}}_q$  (equation 19):

$$\left( \mathbf{H}^\top \mathbf{G}^\top \mathbf{W}_d^\top \mathbf{W}_d \mathbf{G} \mathbf{H} + \mu \mathbf{H}^\top \mathbf{W}_p^\top \mathbf{W}_p \mathbf{H} \right) \tilde{\boldsymbol{\delta}}_q = \mathbf{H}^\top \mathbf{G}^\top \mathbf{W}_d^\top \mathbf{W}_d \tilde{\boldsymbol{\delta}}_d. \quad (23)$$

On the other hand, for the cases in which  $D < P$  (underdetermined problems), matrix  $\mathbf{B}$  is usually defined according to equation 22. In this case, we consider that the the estimate  $\tilde{\mathbf{q}}$  is obtained in two steps, which consists in first solving a linear system for a dummy vector  $\mathbf{u}$  and then computing a matrix-vector product as follows:

$$\begin{aligned} \left[ \mathbf{G} \mathbf{H} \left( \mathbf{H}^\top \mathbf{W}_p^\top \mathbf{W}_p \mathbf{H} \right)^{-1} \mathbf{H}^\top \mathbf{G}^\top + \mu \left( \mathbf{W}_d^\top \mathbf{W}_d \right)^{-1} \right] \mathbf{u} &= \tilde{\boldsymbol{\delta}}_d \\ \tilde{\boldsymbol{\delta}}_q &= \left( \mathbf{H}^\top \mathbf{W}_p^\top \mathbf{W}_p \mathbf{H} \right)^{-1} \mathbf{H}^\top \mathbf{G}^\top \mathbf{u} \end{aligned} \quad (24)$$

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

## 2 COMPUTATIONAL STRATEGIES

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

NÃO SEI SE TÁ BOM AQUI: To investigate the efficiency of equivalent-layer methods, we consider 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

### 2.1 Moving-data windows

Split the observed data  $d_i, i \in \{1, \dots, D\}$ , into  $M$  overlapping subsets (or data windows) formed by  $D^m$  data each,  $m \in \{1, \dots, M\}$ .

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

The data forming a given window are usually adjacent to each other.

Each window has an  $D^m \times 1$  observed data vector  $\mathbf{d}^m$ .

Let each data window be approximated by a local equivalent layer composed of  $P^m$  sources, so that its predicted data vector is given by

$$\mathbf{f}^m = \mathbf{G}^m \mathbf{p}^m, \quad (25)$$

where  $\mathbf{p}^m$  is a  $P^m \times 1$  vector containing the scalar physical properties of the equivalent sources in the  $m$ -th subset and  $\mathbf{G}^m$  is an  $D^m \times P^m$  matrix whose elements are computed with equation 2 by using only the coordinates of the observed data and equivalent sources in the  $m$ -th subset.

The main advantage of this approach is that the estimated parameter vector  $\tilde{\mathbf{p}}$  is not obtained by solving the full linear system, but several smaller ones.

Leão and Silva (1989) presented a pioneer work using this approach.

Their method requires a regularly-spaced grid of observed data on a horizontal plane  $z_0$ .

The data windows are defined by square local grids of  $\sqrt{D'} \times \sqrt{D'}$  adjacent points, all of them having the same number of points  $D'$ .

The equivalent sources in the  $m$ -th data window are located below the observation plane, at a constant vertical distance  $\Delta z_0$ . They are arranged on a regular grid of  $\sqrt{P'} \times \sqrt{P'}$  adjacent points following the same grid pattern of the observed data. The local grid of sources for all data windows have the same number of elements  $P'$ . Besides, they are vertically aligned, but expands the limits of their corresponding data windows, so that  $D' < P'$ .

Because of this spatial configuration of observed data and equivalent sources, we have that  $\mathbf{G}^m = \mathbf{G}'$  (equation 25) for all data windows (i.e.,  $\forall m \in \{1, \dots, M\}$ ), where  $\mathbf{G}'$  is a  $D' \times P'$  constant matrix.

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

as follows:

$$t_c^m = (\mathbf{G}' \mathbf{a}')^\top \left[ \mathbf{G}' (\mathbf{G}')^\top \right]^{-1} \mathbf{d}^m, \quad m \in \{1, \dots, M\}, \quad (26)$$

where  $\mathbf{a}'$  is a  $P' \times 1$  vector with elements computed by equation 5 by using all equivalent sources in the  $m$ -th subset and only the coordinate of the central point in the  $m$ -th data window. Due to the presumed spatial configuration of the observed data and equivalent sources,  $\mathbf{a}'$  is the same for all data windows. Note that equation 26 combines the potential-field transformation (equation 4) with the solution of the undetermined problem (equation 24) for the particular case in which  $\mathbf{H} = \mathbf{W}_p = \mathbf{I}_{P'}$  (equations 9 and 14),  $\mathbf{W}_d = \mathbf{I}_{D'}$ ,  $\bar{\mathbf{p}} = \mathbf{0}$  (equations 15, 19 and 20) where  $\mathbf{I}_{P'}$  and  $\mathbf{I}_{D'}$  are identity matrices of order  $P'$  and  $D'$ , respectively, and  $\mathbf{0}$  is a vector of zeros.

The method proposed by Leão and Silva (1989) can be outlined by the following pseudo-code:

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

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**Initialization :**

```

1 Set the  $\mathbf{d}^m$  for each data window,  $m \in \{1, \dots, M\}$  ;
2 Set the constant depth  $z_0 + \Delta z_0$  for all equivalent sources ;
3 Compute the vector  $\mathbf{b}'$  associated with the desired potential-field transformation ;
4 Compute the matrix  $\mathbf{A}'$  ;
5 Compute  $(\mathbf{A}' \mathbf{b}')^\top \left[ \mathbf{A}' (\mathbf{A}')^\top \right]^{-1}$  ;
6  $\ell = 1$  ;
7 while  $\ell < M$  do
8   | Compute  $t_c^m$  (equation 26) ;
9   |  $\ell \leftarrow \ell + 1$  ;
10 end
```

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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  $\mathbf{p}^m$  (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 data on an undulating surface.

PAREI AQUI

The overall steps of their method are defined by the following pseudo-code:

## 2.2 Column update

Cordell (1992)

Guspí and Novara (2009)

## 2.3 Row update

Algebraic reconstruction techniques (ART) van der Sluis and van der Vorst (2004)

Mendonça and Silva (1994)

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

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**Initialization :**

```

1 Set the  $\mathbf{d}^m$  for each data window,  $m \in \{1, \dots, M\}$  ;
2 Set the depth scheme for all equivalent sources ;
3 Compute the vector  $\mathbf{b}'$  associated with the desired potential-field transformation ;
4 Compute the matrix  $\mathbf{A}'$  ;
5 Compute  $(\mathbf{A}'\mathbf{b}')^\top [\mathbf{A}' (\mathbf{A}')^\top]^{-1}$  ;
6  $\ell = 1$  ;
7 while  $\ell < M$  do
8   | Compute  $t_c^m$  (equation 26) ;
9   |  $\ell \leftarrow \ell + 1$  ;
10 end
```

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160 **2.4 Reparameterization**

161 Barnes and Lumley (2011)

162 Oliveira Jr. et al. (2013)

163 Mendonça (2020)

164 **2.5 Wavelet compression**

165 Li and Oldenburg (2010)

166 **2.6 Iterative methods using the original A**

167 Xia and Sprowl (1991)

168 Xia et al. (1993)

169 Siqueira et al. (2017)

170 Jirigalatu and Ebbing (2019)

171 **2.7 Discrete convolution**

172 Takahashi et al. (2020)

173 Takahashi et al. (2022)

**3 TEXTO ANTIGO**

174 Leão and Silva (1989) reduced the total processing time and memory usage of equivalent-layer technique  
 175 by means of a moving data-window scheme. A small moving data window with  $N_w$  observations and  
 176 a small equivalent layer with  $M_w$  equivalent sources ( $M_w > N_w$ ) located below the observations are  
 177 established. For each position of a moving-data window, Leão and Silva (1989) estimate a stable solution



178  $\mathbf{p}_w^*$  by using a data-space approach with the zeroth-order Tikhonov regularization (?), i.e.,

$$\left(\mathbf{A}_w \mathbf{A}_w^\top + \mu \mathbf{I}\right) \mathbf{w} = \mathbf{d}_w^o, \quad (27a)$$

$$\mathbf{A}_w^\top \mathbf{w} = \mathbf{p}_w^*, \quad (27b)$$

179 where  $\mathbf{w}$  is a dummy vector,  $\mu$  is a regularizing parameter,  $\mathbf{d}_w^o$  is an  $N_w$ -dimensional vector containing  
 180 the observed potential-field data,  $\mathbf{A}_w$  is an  $N_w \times M_w$  sensitivity matrix related to a moving-data window,  $\mathbf{I}$   
 181 is an identity matrix of order  $N_w$  and the superscript  $\top$  stands for a transpose. After estimating an  $M_w \times 1$   
 182 parameter vector  $\mathbf{p}_w^*$  (equation 27b) the desired transformation of the data is only calculated at the central  
 183 point of each moving-data window, i.e.:

$$\hat{t}_k = \mathbf{t}_k^\top \mathbf{p}_w^*, \quad (28)$$

184 where  $\hat{t}_k$  is the transformed data calculated at the central point  $k$  of the data window and  $\mathbf{t}_k$  is an  $M_w \times 1$   
 185 vector whose elements form the  $k$ th row of the  $N_w \times N_w$  matrix of Green's functions  $\mathbf{T}$  (equation ??) of  
 186 the desired linear transformation of the data.

187 By shifting the moving-data window with a shift size of one data spacing, a new position of a data  
 188 window is set up. Next, the aforementioned process (equations 27b and 28) is repeated for each position of  
 189 a moving-data window, until the entire data have been processed. Hence, instead of solving a large inverse  
 190 problem, Leão and Silva (1989) solve several much smaller ones.

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

### 211 3.0.1 The equivalent-data concept

212 To reduced the total processing time and memory usage of equivalent-layer technique, Mendonça and  
 213 Silva (1994) proposed a strategy called 'equivalent data concept'. The equivalent data concept is grounded  
 214 on the principle that there is a subset of redundant data that does not contribute to the final solution and

thus can be dispensed. Conversely, there is a subset of observations, called equivalent data, that contributes effectively to the final solution and fits the remaining observations (redundant data). Iteratively, Mendonça and Silva (1994) selected the subset of equivalent data that is substantially smaller than the original dataset. This selection is carried out by incorporating one data point at a time.

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.

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

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

? transformed a large and full sensitivity matrix into a sparse one by using fast wavelet transforms. In the wavelet domain, ? applied a 2D wavelet transform to each row and column of the original sensitivity matrix  $\mathbf{A}$  to expand it in the wavelet bases. This operation can be done by premultiplying the original sensitivity matrix  $\mathbf{A}$  by a matrix representing the 2D wavelet transform  $\mathbf{W}_2$  and then the resulting is postmultiplied by the transpose of  $\mathbf{W}_2$  (i.e.,  $\mathbf{W}_2^\top$ ).

$$\tilde{\mathbf{A}} = \mathbf{W}_2 \mathbf{A} \mathbf{W}_2^\top, \quad (29)$$

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

$$\tilde{\mathbf{A}}_L^\top \tilde{\mathbf{A}}_L \tilde{\mathbf{p}}_L^* = \tilde{\mathbf{A}}_L^\top \tilde{\mathbf{d}}^o, \quad (30)$$

where  $\tilde{\mathbf{p}}_L^*$  is obtained by solving the linear system given by equation 30,

$$\tilde{\mathbf{A}}_L = \tilde{\mathbf{A}}_s \tilde{\mathbf{L}}^{-1}, \quad (31a)$$

$$\tilde{\mathbf{p}}_L = \tilde{\mathbf{L}} \tilde{\mathbf{p}}, \quad (31b)$$

$$\tilde{\mathbf{d}}^o = \mathbf{W}_2 \mathbf{d}^o, \quad (31c)$$

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

$$\tilde{\mathbf{p}} = \tilde{\mathbf{L}}^{-1} \tilde{\mathbf{p}}_L^*, \quad (32)$$

and

$$\mathbf{p} = \mathbf{W}_2 \tilde{\mathbf{p}}. \quad (33)$$

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

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

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

$$\mathbf{p} = \mathbf{V} \boldsymbol{\alpha}, \quad (34)$$

where  $\mathbf{V}$  is an  $M \times Q$  matrix whose columns  $\mathbf{v}_i = 1, \dots, Q$  form a basis vectors for a subspace  $Q$  of  $\mathbb{R}^M$ . In equation 34, the parameter vector  $\mathbf{p}$  is defined as a linear combination in the space spanned by  $Q$  basis vectors  $\mathbf{v}_i = 1, \dots, Q$  and  $\boldsymbol{\alpha}$  is a  $Q$ -dimensional unknown vector to be determined. The main advantage of the subspace method is that the linear system of  $M$  equations in  $M$  unknowns to be originally solved is reduced to a new linear system of  $Q$  equations in  $Q$  unknowns which requires much less computational effort since  $Q \ll M$ , i.e.:

$$\mathbf{V}^T \mathbf{A}^T \mathbf{A} \mathbf{V} \boldsymbol{\alpha}^* = \mathbf{V}^T \mathbf{d}^o. \quad (35)$$

To avoid the storage of matrices  $\mathbf{A}$  and  $\mathbf{V}$ , ? evaluates an element of the matrix  $\mathbf{A}\mathbf{V}$  by calculating the dot product between the row of matrix  $\mathbf{A}$  and the column of the matrix  $\mathbf{B}$ . After estimating  $\boldsymbol{\alpha}^*$  (equation 35) belonging to a  $Q$ -dimensional subspace of  $\mathbb{R}^M$ , the distribution over the equivalent layer  $\mathbf{p}$  in the  $\mathbb{R}^M$  is obtained by applying equation 34. The choice of the  $Q$  basis vectors  $\mathbf{v}_i = 1, \dots, Q$  (equation 34) in the subspace method is not strict. ?, for example, chose the eigenvectors yielded by applying the singular value decomposition of the matrix containing the gridded data set. The number of eigenvectors used to form basis vectors will depend on the singular values.

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

### 3.0.3 The quadtree discretization

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

equivalent sources, which means a reduction in the number of parameters to be estimated implying in model dimension reduction.

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

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

### 3.0.4 The reparametrization of the equivalent layer

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

$$\mathbf{p}^k = \mathbf{B}^k \mathbf{c}^k, \quad k = 1 \dots Q, \quad (36)$$

where  $\mathbf{p}^k$  is an  $M_w$ -dimensional vector containing the physical-property distribution within the  $k$ th equivalent-source window,  $\mathbf{c}^k$  is a  $P$ -dimensional vector whose  $l$ th element is the  $l$ th coefficient of the  $\alpha$ th-order polynomial function and  $\mathbf{B}^k$  is an  $M_w \times P$  matrix containing the first-order derivative of the  $\alpha$ 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

$$\left( \mathbf{B}^\top \mathbf{A}^\top \mathbf{A} \mathbf{B} + \mu \mathbf{I} \right) \mathbf{c}^* = \mathbf{B}^\top \mathbf{A}^\top \mathbf{d}^o, \quad (37)$$

where  $\mu$  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  $H$  ( $H = PQ$ ) and  $\mathbf{B}$  is an  $M \times H$  block diagonal matrix such that the main-diagonal blocks are  $\mathbf{B}^k$  matrices (equation 36) and all off-diagonal blocks are zero matrices. For ease of the explanation of equation 37, 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 37), where  $H$  totalizes the number of polynomial coefficients composing all equivalent-source windows, requiring a lower computational effort since  $H \ll N$ . To avoid the storage of matrices  $\mathbf{A}$  and  $\mathbf{B}$ , Oliveira Jr. et al. (2013) evaluate an element of the matrix  $\mathbf{A}\mathbf{B}$  by calculating the dot product between the row of matrix  $\mathbf{A}$  and the column of the matrix  $\mathbf{B}$ . After estimating all polynomial coefficients of all windows, the estimated coefficients ( $\mathbf{c}^*$  in equation 37) are transformed into a single physical-property distribution encompassing the entire equivalent layer.

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

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

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

There exists a class of methods that iteratively estimate the distribution of physical properties within an equivalent layer without the need to solve linear systems. The method initially introduced by Cordell (1992) and later expanded upon by Guspí and Novara (2009) updates the physical property of sources, located beneath each potential-field data, by removing the maximum residual between the observed and fitted data. In addition, Xia and Sprowl (1991) and Xia et al. (1993) have developed efficient iterative algorithms for updating the distribution of physical properties within the equivalent layer in the wavenumber and space domains, respectively. Specifically, in Xia and Sprowl's (1991) method the physical-property distribution is updated by using the ratio between the squared depth to the equivalent source and the gravitational constant multiplied by the residual between the observed and predicted observation at the measurement station. Neither of these methods solve linear systems.

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

$$\tilde{\mathbf{A}} = 2 \pi \gamma \Delta \mathbf{S}^{-1}, \quad (38)$$

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

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

$$\tilde{\mathbf{A}}^\top \tilde{\mathbf{A}} \Delta \hat{\mathbf{p}}^k = \tilde{\mathbf{A}}^\top \mathbf{r}^k, \quad (39)$$

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

$$r_i^k = d_i^o - d_i^k. \quad (40)$$

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

Because  $\tilde{\mathbf{A}}$ , in equation 39, is a diagonal matrix (equation 38), the parameter correction estimate is directly calculated without solving system of linear equations, and thus, an  $i$ th element of  $\Delta \hat{\mathbf{p}}^k$  is directly

353 calculated by

$$\Delta \hat{p}_i^k = \frac{\Delta s_i r_i^k}{2 \pi \gamma} . \quad (41)$$

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

$$\hat{p}_i^{k+1} = \hat{p}_i^k + \Delta \hat{p}_i^k . \quad (42)$$

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

$$p_i^o = \frac{\Delta s_i d_i^o}{2 \pi \gamma} . \quad (43)$$

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

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

$$\mathbf{p}_{k+1} = \mathbf{p}_k + \omega \left[ \mathbf{A}_1^\top (\mathbf{d}_1 - \mathbf{M} \mathbf{A}_1 \mathbf{p}_k) + \mathbf{A}_2^\top (\mathbf{d}_2 - \mathbf{M} \mathbf{A}_2 \mathbf{p}_k) \right] , \quad (44)$$

364 where  $\omega$  is a relaxation factor,  $\mathbf{d}_1$  and  $\mathbf{d}_2$  are the two gravity gradient components and  $\mathbf{A}_1$  and  $\mathbf{A}_2$  are the  
365 corresponding gravity gradient kernels. Jirigalatu and Ebbing (2019) applied their method for processing  
366 two horizontal curvature components of Falcon airborne gravity gradient.

### 367 3.0.6 The convolutional equivalent layer with BTTB matrices

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

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

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

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

$$\mathbf{w} = \mathbf{C}\mathbf{v} , \quad (45)$$

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

$$\mathbf{C} = (\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P})^* \mathbf{\Lambda} (\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}) , \quad (46)$$

where the symbol “ $\otimes$ ” denotes the Kronecker product (?),  $\mathbf{F}_{2Q}$  and  $\mathbf{F}_{2P}$  are the  $2Q \times 2Q$  and  $2P \times 2P$  unitary DFT matrices (? , p. 31), respectively, the superscript “ $*$ ” denotes the complex conjugate and  $\mathbf{\Lambda}$  is a  $4QP \times 4QP$  diagonal matrix containing the eigenvalues of  $\mathbf{C}$ . Due to the diagonalization of the matrix  $\mathbf{C}$ , the auxiliary system (equation 45) can be rewritten by using equation 46 and premultiplying both sides of the result by  $(\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P})$ , i.e.,

$$\mathbf{\Lambda} (\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}) \mathbf{v} = (\mathbf{F}_{2Q} \otimes \mathbf{F}_{2P}) \mathbf{w} . \quad (47)$$

By applying the vec-operator (?) to both sides of equation 47, by premultiplying both sides of the result by  $\mathbf{F}_{2Q}^*$  and then postmultiplying both sides of the result by  $\mathbf{F}_{2P}^*$

$$\mathbf{F}_{2Q}^* [\mathbf{L} \circ (\mathbf{F}_{2Q} \mathbf{V} \mathbf{F}_{2P})] \mathbf{F}_{2P}^* = \mathbf{W} , \quad (48)$$

where “ $\circ$ ” denotes the Hadamard product (? , p. 298) and  $\mathbf{L}$ ,  $\mathbf{V}$  and  $\mathbf{W}$  are  $2Q \times 2P$  matrices obtained by rearranging, along their rows, the elements forming the diagonal of matrix  $\mathbf{\Lambda}$ , vector  $\mathbf{v}$  and vector  $\mathbf{w}$ , respectively. The left side of equation 48 contains the 2D Inverse Discrete Fourier Transform (IDFT) of the term in brackets, which in turn represents the Hadamard product of matrix  $\mathbf{L}$  and the 2D DFT of matrix  $\mathbf{V}$ . Matrix  $\mathbf{L}$  contains the eigenvalues of  $\mathbf{\Lambda}$  (equation 46) and can be efficiently computed by using only the first column of the BCCB matrix  $\mathbf{C}$  (equation 45).

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

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

### 3.0.7 The deconvolutional equivalent layer with BTTB matrices

To avoid the iterations of the conjugate gradient method in  $\mathbf{F}$ , we can employ the deconvolution process. Equation 48 shows that estimate the matrix  $\mathbf{V}$ , containing the elements of parameter vector  $\mathbf{p}$ , is a inverse problem that could be solved by deconvolution. From equation 48, the matrix  $\mathbf{V}$  can be obtain by deconvolution, i.e.

$$\mathbf{V} = \mathbf{F}_{2Q}^* \left[ \frac{(\mathbf{F}_{2Q} \mathbf{W} \mathbf{F}_{2P})}{\mathbf{L}} \right] \mathbf{F}_{2P}^* . \quad (49)$$

Equation 49 shows that the parameter vector (in matrix  $\mathbf{V}$ ) can be theoretically obtain by dividing each potential-field observations (in matrix  $\mathbf{W}$ ) by each eigenvalues (in matrix  $\mathbf{L}$ ). Hence, the parameter vector is constructed by element-by-element division of data by eigenvalues.

However, the deconvolution often is extremely unstable. This means that a small change in data can lead to an enormous change in the estimated parameter. Hence, equation 49 requires regularization to be useful. We used wiener deconvolution to obtain a stable solution, i.e.,

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

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

## 3.1 Solution stability

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

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

Next, for each noise-corrupted data  $\mathbf{d}_\ell^o$  and estimated solution  $\hat{\mathbf{p}}_\ell$ , the  $\ell$ th model perturbation  $\delta p_\ell$  and the  $\ell$ th data perturbation  $\delta d_\ell$  are, respectively, evaluated by

$$\delta p_\ell = \frac{\|\hat{\mathbf{p}}_\ell - \mathbf{p}\|_2}{\|\mathbf{p}\|_2}, \quad \ell = 1, \dots, D, \quad (51)$$

and

$$\delta d_\ell = \frac{\|\mathbf{d}_\ell^o - \mathbf{d}\|_2}{\|\mathbf{d}\|_2}, \quad \ell = 1, \dots, D. \quad (52)$$



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

$$\delta p_\ell \leq \kappa \delta d_\ell, \quad \ell = 1, \dots, D, \quad (53)$$

449 where  $\kappa$  is the constant of proportionality between the model perturbation  $\delta p_\ell$  (equation 51) and the data  
450 perturbation  $\delta d_\ell$  (equation 52). The constant  $\kappa$  acts as the condition number of an invertible matrix in a  
451 given inversion, and thus measures the instability of the solution. The larger (smaller) the value of  $\kappa$  the  
452 more unstable (stable) is the estimated solution.

453 Equation 53 shows a linear relationship between the model perturbation and the data perturbation. By  
454 plotting  $\delta p_\ell$  (equation 51) against  $\delta d_\ell$  (equation 52) produced by a set of  $D$  estimated solution obtained by  
455 applying a given equivalent-layer method, we obtain a straight line behaviour described by equation 53.  
456 By applying a linear regression, we obtain a fitted straight line whose estimated slope ( $\kappa$  in equation 53)  
457 quantifies the solution stability.

458 Here, the analysis of solution stability is numerically conducted by applying the classical equivalent-  
459 layer technique with zeroth-order Tikhonov regularization, the convolutional method for gravimetric and  
460 magnetic data, the deconvolutional method (equation 49) and the deconvolutional method with different  
461 values for the Wiener stabilization (equation 50).

## 4 NUMERICAL SIMULATIONS

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

### 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. Counting the floating-point operations (*flops*), i.e., additions, subtractions, multiplications and divisions is a good way to quantify the amount of work of a given algorithm (Golub and Loan, 2013). For example, the number of *flops* necessary to multiply two vectors  $\mathbb{R}^N$  is  $2N$ . A common matrix-vector multiplication with dimension  $\mathbb{R}^{N \times N}$  and  $\mathbb{R}^N$ , respectively, is  $2N^2$  and a multiplication of two matrices  $\mathbb{R}^{N \times N}$  is  $2N^3$ . Figure ?? shows the total *flops* count for the different methods presented in this review with a crescent number of data, ranging from 10, 000 to 1, 000, 000 for the gravity equivalent layer and figure ?? for magnetic data.

#### 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 will use the Cholesky decompositions method to calculate the necessary *flops*. In this method it is calculated the lower triangle of  $\mathbf{A}^T \mathbf{A}$  ( $1/2N^3$ ), the Cholesky factor ( $1/3N^3$ ), a matrix-vector multiplication ( $2N^2$ ) and finally solving the triangular system ( $2N^2$ ), totalizing

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

#### 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 (equation 27b). For our results we are considering a data-window of the same size of wich the authors presented in theirs work ( $N_w = 49$ ) and the same number of equivalent sources ( $M_w = 225$ ). We are doing this process for all the other techniques to standardize the resolution of our problem. Using the Cholesky decomposition with this method the *flops* are

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

#### 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). For this operations calculation (equation 37) we used a first degree polynomial (two variables) and each window contains  $N_s = 1, 000$  observed data and  $M_s = 1, 000$  equivalent sources. Following the steps given in (Oliveira Jr. et al., 2013) the total *flops* becomes

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

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

#### 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 involves a matrix-vector product outside the loop ( $2N^2$ ), two matrix-vector products inside the loop ( $4N^2$ ) and six vector products inside the loop ( $12N$ ) (?)

$$f_{cglS} = 2N^2 + it(4N^2 + 12N) \quad (57)$$

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

For the wavelet method (equation 30) we have calculated a coompression rate of 98% ( $C_r = 0.02$ ) for the threshold as the authors used in ? and the wavelet transformation requiring  $\log_2(N)$  flops each (equations 29 and 31c), with its inverse also using the same number of operations (equation 33). Combined with the conjugate gradient least square necessary steps and iterations, the number of flops are

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

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

The fast equivalent layer from Siqueira et al. (2017) solves the linear system in  $it$  iterations. The main cost of this method (equations 39,40, 41 and 42)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)

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

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

This methods replaces the matrix-vector multiplication of the iterative fast-equivalent technique (Siqueira et al., 2017) by three steps, involving a Fourier transform, an inverse Fourier transform, and a Hadamard product of matrices (equation 48). Considering that the first column of our BCCB matrix has  $4N$  elements, the flops count of this method is

$$f_{convgrav} = \kappa 4N \log_2(4N) + it(27N + \kappa 8N \log_2(4N)) \quad (60)$$

In the resultant count we considered a *radix-2* algorithm for the fast Fourier transform and its inverse, which has a  $\kappa$  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 60 is different from the one presented in ? because we also added the flops necessary to calculate the eigenvalues in this form. It does not differentiate much in order of magnitude because the iterative part is the most costful.

#### 518 4.1.8 Convolutional equivalent layer for magnetic data (?)

519 The convolutional equivalent layer for magnetic data uses the same flops count of the main operations as  
 520 in the gravimetric case (equation 48), the difference is the use of the conjugate gradient algorithm to solve  
 521 the inverse problem. It requires a Hadamard product outside of the iterative loop and the matrix-vector and  
 522 vector-vector multiplications inside the loop as seen in equation 57.

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

#### 523 4.1.9 Deconvolutional method

524 The deconvolution method does not require an iterative algorithm, rather it solves the estimative of the  
 525 physical properties in a single step using the  $4N$  eigenvalues of the BCCB matrix as in the convolutional  
 526 method. From equation 49 it is possible to deduce this method requires two fast Fourier transform  
 527 ( $\kappa 4N \log_2(4N)$ ), one for the eigenvalues and another for the data transformation, a element by element  
 528 division ( $24N$ ) and finally, a fast inverse Fourier transform for the final estimative ( $\kappa 4N \log_2(4N)$ ).

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

529 Using the deconvolutional method with a Wiener stabilization adds two multiplications of complex  
 530 elements of the conjugates eigenvalues ( $24N$  each) and the sum of  $4N$  elements with the stabilization  
 531 parameter  $\mu$  as shown in equation 50

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

## CONFLICT OF INTEREST STATEMENT

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

## AUTHOR CONTRIBUTIONS

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

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## DATA AVAILABILITY STATEMENT

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

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