

Gradient-boosted equivalent sources

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Abstract

The equivalent source technique is a powerful and widely used method for processing gravity and magnetic data. Nevertheless, its major drawback is the large computational cost in terms of processing time and computer memory. We present two techniques for reducing the computational cost of equivalent source processing: block-averaging source locations and the gradient-boosted equivalent source algorithm. Through block-averaging, we reduce the number of source coefficients that must be estimated while retaining the minimum desired resolution in the final processed data. With the gradient boosting method, we estimate the sources coefficients in small batches along overlapping windows, allowing us to reduce the computer memory requirements arbitrarily to conform to the constraints of the available hardware. We show that the combination of block-averaging and gradient-boosted equivalent sources is capable of producing accurate interpolations through tests against synthetic data. Moreover, we demonstrate the feasibility of our method by gridding a gravity dataset covering Australia with over 1.7 million observations using a modest personal computer.

1 Introduction

Measurements of anomalies in potential fields, like gravity disturbances and total-field magnetic anomalies, are widely used in geophysical exploration for their relatively low cost of acquisition. These data can be surveyed using ground, airborne, shipborne, or satellite systems. In ground surveys, the data are often gathered following irregular paths or networks along the surface of the terrain, leading to highly variable elevations in mountainous regions. On airborne surveys, the data are gathered along flight lines, producing a large number of measurements concentrated along almost straight lines. Measurement height can also change because of the vertical movement of the aircraft. Processing of the data often involves interpolation onto a regular grid at constant height, both to improve visualization for interpretation purposes as well as to prepare the data for further processing and modelling (e.g., reduction-to-the-pole, derivative calculations, upward continuation, Euler deconvolution).

Several methods exist in the literature for interpolation in two dimensions, for example continuous curvature splines in tension (Smith and Wessel, 1990), bi-harmonic (thin-plate) splines (Sandwell, 1987), and kriging (Hansen, 1993). These general-purpose methods have limitations when it comes to interpolating potential field data: (i) they are not able to take into account the variable height of the observation points and (ii) the interpolating functions

are not necessarily harmonic, which is the underlying assumption behind many processing techniques (e.g., upward continuation and vertical derivatives).

A widely used method for interpolating gravity and magnetic data is the equivalent sources technique (also known as equivalent layer, radial basis functions, or Green’s functions interpolation), first introduced by Dampney (1969). It consists in fitting a model of finite elementary sources to the data and using this model to predict new data values. Besides interpolation, equivalent sources have been used for reduction-to-the-pole of magnetic data (Guspí and Novara, 2009; Nakatsuka and Okuma, 2006; Silva, 1986), upward continuation (Emilia, 1973; Li and Oldenburg, 2010), joint processing of gravity gradient data (Barnes and Lumley, 2011), modelling the lithospheric magnetic field (Kother et al., 2015), recovering the magnetic induction vector from total-field magnetic anomalies (Li et al., 2020), and more.

Many variants of the equivalent sources technique have been proposed, often attempting to obtain faster or more accurate solutions. The key factors that vary between them are: (i) the type of source, (ii) the location of the sources, and (iii) the solution strategy. The type of source is most commonly a point mass for gravity or dipole for magnetics (e.g., Mendonça and Silva, 1994; Silva, 1986; Siqueira et al., 2017; von Frese et al., 1981). However, right-rectangular prisms (e.g., Barnes and Lumley, 2011; Jirigalatu and Ebbing, 2019; Li et al., 2020) and tesseroids (Bouman et al., 2016) have also been used successfully. In fact, even point sources with a simple inverse distance function, instead of actual gravity or magnetic fields, can be used as equivalent sources (Cordell, 1992). The sources are often distributed on a regular grid at a constant depth (e.g., Barnes and Lumley, 2011; Leão and Silva, 1989; Oliveira et al., 2013) or placed beneath each data point (e.g., Cordell, 1992; Siqueira et al., 2017). The model is usually estimated through damped least-squares, which imposes a heavy computational load when the number of data points is large (e.g., airborne and satellite surveys). To reduce the computational load, Mendonça and Silva (1994) built the solution iteratively by incorporating one data point at a time using the “equivalent data concept”. Leão and Silva (1989) processed the

input data using a moving window, only fitting the data inside the window and predicting observations at its center. Li and Oldenburg (2010) and Barnes and Lumley (2011) apply different operations to generate a sparse representation of the sensitive matrix (respectively, wavelet compression and quadtree discretization), which significantly improves the speed of the least-squares solution. Oliveira et al. (2013) parametrized the equivalent layer as a piecewise bivariate polynomial function, reducing the number of parameters in the solution. Siqueira et al. (2017) developed an iterative solution in which the sensitivity matrix is transformed into a diagonal matrix with constant terms through the “excess mass criterion”. Jirigalatu and Ebbing (2019) applied the Gauss-FFT method to speed up the forward modelling operations and solved the least-squares problem using steepest descent to avoid calculating the Hessian matrix and solving linear systems.

Many of the existing methods solve under-determined problems, requiring a much larger number of equivalent sources than the number of data points. Some achieve greater efficiency by restricting their applications to specific data types (Siqueira et al., 2017), interpolating only on regular grids (Leão and Silva, 1989), or requiring already gridded data (Takahashi et al., 2020), to name a few. Furthermore, many of the optimizations proposed are also complex to implement in a computer program, limiting their wider adoption.

In the present study, we propose a two strategies for reducing the computational load of the equivalent sources technique:

1. Reduce the number of equivalent sources for oversampled surveys through a *block-averaging* strategy while maintaining the quality of the solution.
2. Fit the equivalent source model iteratively along overlapping windows using a *gradient boosting* algorithm (Friedman, 2001).

The first strategy consists in dividing the survey area into horizontal blocks and assign one source to each block, located at the median horizontal location of the data points. For airborne, shipborne, and

satellite surveys, which are oversampled along tracks, this can greatly reduce the size of the inverse problem while retaining the same quality of interpolation.

The gradient boosting algorithm allows us to fit the equivalent source model iteratively by operating on individual overlapping windows. Thus, our method solves several much smaller least-squares problems instead of a large one. This has some similarities with the strategy used by [Leão and Silva \(1989\)](#) but without the requirement for sources and predictions to be on regular grids.

Through tests on synthetic data, we show that: (i) the *block-averaged* sources are able to achieve the same accuracy as other traditional equivalent source layouts while using a fraction of the number of sources, and (ii) the *gradient boosting* algorithm greatly reduces the computational memory required to fit very large datasets without sacrificing prediction accuracy. Finally, a combination of both strategies is used to process a collection of around 1.7 million ground gravity data measurements from Australia.

2 Methodology

2.1 The equivalent sources technique

Here, we will follow the “generalized equivalent sources” of [Cordell \(1992\)](#) and assume that any harmonic function $d(\mathbf{p})$ can be approximated by a sum of M discrete point source effects

$$d(\mathbf{p}) = \sum_{j=1}^M \frac{c_j}{\|\mathbf{p} - \mathbf{q}_j\|}, \quad (1)$$

in which \mathbf{p} and \mathbf{q}_j are position vectors in a 3D Cartesian space, c_j is a scalar coefficient related to the point source located at \mathbf{q}_j , and $\|\cdot\|$ represents the L_2 norm. The horizontal and vertical distribution of sources is discussed in section [2.4](#).

In case we have measured the value of the harmonic field on N points $\{\mathbf{p}_1 \mathbf{p}_2 \dots \mathbf{p}_N\}$, we can write a set of N equations of the form

$$d_i = \sum_{j=1}^M \frac{c_j}{\|\mathbf{p}_i - \mathbf{q}_j\|} \quad \forall i = 1, 2, \dots, N, \quad (2)$$

where d_i is the value of the potential field at the observation point \mathbf{p}_i . These equations can also be expressed as

$$\mathbf{d} = \mathbf{A} \mathbf{c}, \quad (3)$$

where \mathbf{d} is a column vector containing the N predicted values of the observed field at the observation points, \mathbf{c} is a column vector containing the M coefficients c_j , and \mathbf{A} is the $N \times M$ Jacobian matrix, whose elements are

$$a_{ij} = \frac{1}{\|\mathbf{p}_i - \mathbf{q}_j\|} \quad (4)$$

For a given set of N observed field values \mathbf{d}^o , we can find a least-squares solution to Eq. [3](#) and obtain the values of \mathbf{c} that best fit the observations. These values can, in turn, be used to predict the value of the harmonic field at any other point outside of the sources by evaluating Eq. [1](#). Gridding and upward continuation can thus be achieved by predicting values on points that fall on a regular grid or at different heights.

2.2 Damped least-squares solution

We can obtain the values of the source coefficients \mathbf{c} that best fit the observed field values \mathbf{d}^o by minimizing the goal function

$$\phi(\mathbf{c}) = [\mathbf{d}^o - \mathbf{A} \mathbf{c}]^T \mathbf{W} [\mathbf{d}^o - \mathbf{A} \mathbf{c}] + \lambda_d \mathbf{c}^T \mathbf{c}, \quad (5)$$

where \mathbf{W} is a $N \times N$ diagonal matrix of data weights and λ_d is a positive *damping* parameter with the same units as the Jacobian matrix elements. The second term on the right-hand side of the equation is a zeroth-order Tikhonov regularization ([Tikhonov, 1977](#)) (also known as a damping regularization or ridge regression) that is used to stabilize the solution.

The range of acceptable values for the damping parameter λ_d will depend on the values of the Jacobian matrix \mathbf{A} and the coefficients. Consequently, this range will vary (often dramatically) between datasets, making it difficult to choose an appropriate value for λ_d in practice.

To solve this issue, we first scale the Jacobian matrix so that its elements are unitless and each column has unit variance. We define a diagonal matrix \mathbf{S}

$$\mathbf{S} = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_M \end{bmatrix}_{M \times M}, \quad (6)$$

in which σ_j is the standard deviation of the j -th column of \mathbf{A} . We then write the forward problem in Eq. 3 as

$$\mathbf{d} = \mathbf{A}\mathbf{S}^{-1}\mathbf{S}\mathbf{c} = [\mathbf{A}\mathbf{S}^{-1}][\mathbf{S}\mathbf{c}] = \mathbf{B}\mathbf{m} \quad (7)$$

where \mathbf{B} is the scaled and unitless Jacobian matrix and \mathbf{m} is a vector containing scaled coefficients with the same units as the data.

The goal function defined in Eq. 5 can be rewritten as

$$\phi(\mathbf{m}) = [\mathbf{d}^o - \mathbf{B}\mathbf{m}]^T \mathbf{W} [\mathbf{d}^o - \mathbf{B}\mathbf{m}] + \lambda \mathbf{m}^T \mathbf{m}, \quad (8)$$

where λ is a *dimensionless* damping parameter and regularization is applied on the scaled coefficients \mathbf{m} instead of \mathbf{c} . From experience, we recommend searching for suitable λ values between 10^{-8} and 10^2 varying by order-of-magnitude, irrespective of the dataset.

The vector of scaled coefficients $\hat{\mathbf{m}}$ that minimizes the goal function can be found by solving the *normal equation system* (Menke, 1989)

$$[\mathbf{B}^T \mathbf{W} \mathbf{B} + \lambda \mathbf{I}] \hat{\mathbf{m}} = \mathbf{B}^T \mathbf{W} \mathbf{d}^o. \quad (9)$$

Once the scaled coefficients are obtained, the estimated unscaled coefficients $\hat{\mathbf{c}}$ can be calculated by removing the scaling factor

$$\hat{\mathbf{c}} = \mathbf{S}^{-1} \hat{\mathbf{m}}. \quad (10)$$

The forward modeling operations used to perform predictions (e.g., for interpolation and upward continuation) are left unchanged by using vector $\hat{\mathbf{c}}$ instead of $\hat{\mathbf{m}}$.

2.3 Gradient boosting

Gradient boosting was first introduced by Friedman (2001, 2002) as a method for fitting additive parametric models of the form

$$d = \sum_{k=1}^K \alpha_k f(\mathbf{c}_k), \quad (11)$$

where α_k is a scalar coefficient called the *step-size* and f is a function of the parameter vector \mathbf{c}_k . For linear regression problems, these additive models can be written as the matrix equation

$$\mathbf{d} = \sum_{k=1}^K \alpha_k \mathbf{A}_k \mathbf{c}_k. \quad (12)$$

We can transform our equivalent source problem in Eq. 3 into an additive model by following these steps:

1. Define a set of M equivalent sources distributed throughout the survey area (see section 2.4 for details).
2. Define a set of K overlapping windows of equal size that cover the survey area.
3. Create K separate sets of equivalent sources, one for each window. Each set will be formed by the portion of the original M sources that fall inside the respective window. Since the windows overlap, the total number of sources from all sets will be greater than M .
4. Define the vector \mathbf{c}_k as the coefficients of the equivalent sources of the k -th window and matrix \mathbf{A}_k as the Jacobian matrix between those sources and every data point of the survey.
5. Model the predicted data as a superposition of the effects of the K separate sets of equivalent sources.

The gradient boosting algorithm works by fitting each component of the additive model, one at a time, to the residuals of the previous component. [Friedman \(2001\)](#) demonstrates that this corresponds to a steepest-descent optimization in the so-called “function space”, with α_k corresponding to step sizes in steepest descent. The adaptation of the gradient boosting method to find the damped least-squares solutions for the K parameters vectors \mathbf{c}_k and step sizes α_k in Eq. 12 is presented in Algorithm 1.

Algorithm 1: Gradient boosting solution for damped least-squares regression.

```

1 define the residual vector:  $\mathbf{r}_0 = \mathbf{d}^o$ 
2 for  $k = 1$  to  $K$  do
3   calculate  $N \times M_k$  Jacobian matrix  $\mathbf{A}_k$ 
4    $\mathbf{B}_k = \mathbf{A}_k \mathbf{S}_k^{-1}$ 
5    $\hat{\mathbf{m}}_k = [\mathbf{B}_k^T \mathbf{W}_k \mathbf{B}_k + \lambda \mathbf{I}]^{-1} \mathbf{B}_k^T \mathbf{W}_k \mathbf{r}_{k-1}$ 
6    $\hat{\mathbf{c}}_k = \mathbf{S}_k^{-1} \hat{\mathbf{m}}_k$ 
7    $\mathbf{d}_k = \mathbf{A}_k \hat{\mathbf{c}}_k$ 
8    $\alpha_k = \underset{\alpha}{\operatorname{argmin}} \left( \|\mathbf{r}_{k-1} - \alpha \mathbf{d}_k\|^2 \right) = \frac{\mathbf{r}_{k-1}^T \mathbf{d}_k}{\mathbf{d}_k^T \mathbf{d}_k}$ 
9    $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_k \mathbf{d}_k$ 
10 end for

```

After all α_k step sizes and \mathbf{c}_k coefficients vectors are estimated, we can predict the effect of the additive equivalent source model on any point through the summation

$$d(\mathbf{p}) = \sum_{k=1}^K \sum_{j=1}^{M_k} \alpha_k \frac{c_{kj}}{\|\mathbf{p} - \mathbf{q}_j\|}, \quad (13)$$

where c_{kj} is the j -th element of the \mathbf{c}_k vector.

To improve the convergence of the algorithm, [Friedman \(2002\)](#) suggests introducing randomness into the fitting process. We achieve this by randomizing the order in which the K windows are used in the gradient boosting algorithm.

The \mathbf{A}_k matrices have only $N \times M_k$ elements (where M_k is the number sources on the k -th window), which can be considerably smaller than the $N \times M$ elements of \mathbf{A} . Therefore, the gradient boosting method allows us to fit equivalent source models that would produce Jacobian matrices that are larger than the available computer memory. Furthermore, we can increase or decrease the size of the overlapping windows as needed depending on the number of sources in the model and the available computer memory.

We can improve the efficiency of the algorithm further by using only the N_k data points that fall within the k -th window for fitting the sources (steps 4 and 5 of algorithm 1), while using all available data when calculating the step size and residuals (steps 7, 8, and 9 of algorithm 1). By doing so, we can reduce the size of the Jacobian matrix further to $N_k \times M_k$ elements. The forward modeling operation performed in step 7 can be done by a summation (Eq. 2) instead of a matrix-vector product, which allows us to avoid computing and storing the larger $N \times M_k$ Jacobian at any point. Algorithm 2 incorporates these changes and is the final *gradient-boosted equivalent source algorithm*. Figure 1 shows a sketch of the gradient-boosted equivalent source algorithm with a set of observation points that simulate a ground survey and locating one source below each data point.

The influence of distance sources on the solution is maintained by using the entire set of data points when calculating the step size α_k and updating the residuals vector. In this case, the step size prevents the algorithm from worsening the fit on data points that fall outside of the current window. As such, it improves the convergence of the solution and ensures that the overall misfit decreases with iteration.

It is worth noting that two sets of equivalent sources obtained through two adjacent overlapping windows have some portion of the sources on the same locations, specifically the ones that fall on the intersection between the two windows. We can interpret this as the gradient-boosting algorithm fitting the source coefficients multiple times: one time for every window that covers each source. This fact can be exploited in order to save some computational memory. Instead of storing all of the multiple \mathbf{c}_k vec-

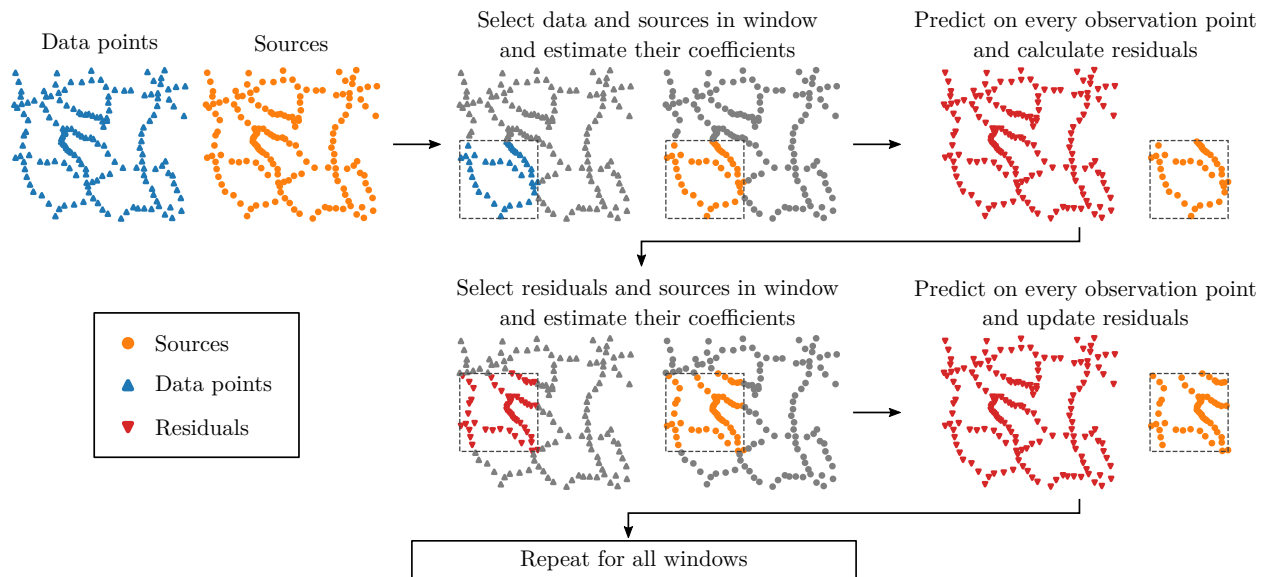


Figure 1: Sketch of the gradient-boosted equivalent source algorithm. Data points are represented by blue upwards-facing triangles, equivalent sources by orange dots, data residuals by red downwards-facing triangles, and the current window by black dashed lines. The algorithm starts by selecting the data and sources inside the first window and estimating the source coefficients using the selected data points. Then, the effect of the estimated sources is predicted on all data points and used to calculate the residuals. Another window is used to select residuals and sources and estimate the coefficients using the selected residuals instead of the original data. Again, the effect of the estimated sources is predicted on all data points and the residuals are updated. These steps are repeated for every window in a randomized order.

Algorithm 2: Gradient-boosted equivalent source algorithm.

```

1 define the residual vector:  $\mathbf{r}_0 = \mathbf{d}^o$ 
2 for  $k = 1$  to  $K$  do
3   select weights  $\tilde{\mathbf{W}}_k$  and residuals  $\tilde{\mathbf{r}}_{k-1}$  for
   data points inside the  $k$ -th window only
4   calculate  $N_k \times M_k$  Jacobian matrix  $\tilde{\mathbf{A}}_k$ 
   with data points and sources inside the
    $k$ -th window only
5    $\mathbf{B}_k = \tilde{\mathbf{A}}_k \mathbf{S}_k^{-1}$ 
6    $\hat{\mathbf{m}}_k = \left[ \mathbf{B}_k^T \tilde{\mathbf{W}}_k \mathbf{B}_k + \lambda \mathbf{I} \right]^{-1} \mathbf{B}_k^T \tilde{\mathbf{W}}_k \tilde{\mathbf{r}}_{k-1}$ 
7    $\hat{\mathbf{c}}_k = \mathbf{S}_k^{-1} \hat{\mathbf{m}}_k$ 
8   calculate  $\mathbf{d}_k$ , where
   
$$d_{ki} = \sum_{j=1}^{M_k} \frac{c_{kj}}{\|\mathbf{p}_i - \mathbf{q}_{kj}\|} \quad \forall i = 1 \text{ to } N$$

9    $\alpha_k = \underset{\alpha}{\operatorname{argmin}} \left( \|\mathbf{r}_{k-1} - \alpha \mathbf{d}_k\|^2 \right) = \frac{\mathbf{r}_{k-1}^T \mathbf{d}_k}{\mathbf{d}_k^T \mathbf{d}_k}$ 
10   $\mathbf{r}_k = \mathbf{r}_{k-1} - \alpha_k \mathbf{d}_k$ 
11 end for
```

tors (Eq. 12), we can initialize a single \mathbf{c} vector with zeros, where each element represents the coefficient of each one of the original M sources. After each iteration of the gradient-boosting algorithm, we add the multiplication of the estimated coefficients $\hat{\mathbf{c}}_k$ and the step-size α_k to the corresponding elements of vector \mathbf{c} . Because the relation between the source coefficients and the effect they generate is linear, we can safely compute the resulting field through Equation 1. This way, the memory needed to store the entire set of estimated coefficients is limited to a single vector of M elements.

Our gradient boosting algorithm for overlapping windows is similar to the “bootstrap inversion” used in von Frese et al. (1988), which also iteratively fits portions of an equivalent source model to the data

residuals. The key differences are that in our method: (i) the sources in the overlapping portions of the windows are fitted more than once, allowing the algorithm to self-correct for poor solutions to any given window; (ii) we use only data points within the window when fitting, what enables the use of larger datasets; (iii) experience shows that the step size parameter improves the convergence of the solution, particularly when using only the data inside the windows for fitting.

2.4 Location of sources

The ideal number of sources and their locations, both horizontally and vertically, has been debated since the inception of the equivalent sources technique with Dampney (1969). The choices made regarding these parameters can play an important role on the accuracy of the predictions and the computational resources needed to estimate the source coefficients. An ideal distribution of sources should simultaneously be able to reproduce the measured data on the survey points, make accurate predictions on non-surveyed locations, and minimize the required computational resources.

A large number of evenly distributed sources along the survey region are capable of reproducing the observed data. Nevertheless, the computational load can be prohibitive and such underdetermined problems are prone to overfitting the data, leading to poor predictive power when interpolating and extrapolating. On the other hand, using few sources will reduce the computational requirements but the model may be incapable of reproducing the full spectral content of the measured data.

Particular survey characteristics also play a role in the choice of equivalent source distribution. In a ground survey, observations are usually located along irregular paths and scattered points. The coverage of the survey region is often uneven, leaving large areas without any observation. On the other hand, observations from airborne surveys are located along almost straight and closely spaced flight lines. Measurements are usually taken at a high temporal frequency, leading to observation points along the flight lines that are several times closer to each other than

the flight line spacing. This creates a bias in the sampling, which can cause aliasing artifacts in gridded products.

2.4.1 Horizontal source layouts

The most widely used layouts for distributing equivalent sources horizontally are:

1. *Sources below data points*: one equivalent source is placed at the horizontal location of each data point (Fig. 2b). Therefore, the number of sources is be equal to the number of observations ($N = M$).
2. *Regular grid*: a homogeneous distribution of point sources below the survey region (Fig. 2c). A padding region is often added to help reduce edge effects. In practice, it often leads to underdetermined problems since a large number of sources is required ($N < M$).

For ground surveys, the *regular grid* layout needs a sufficiently small grid spacing to be able to fit the observed data. This creates an unnecessarily large number of sources in areas where no observations exist. In contrast, the *sources below data* layout is more likely to accurately fit the observed data with many fewer sources, reducing the computational load. But when applied to airborne surveys, the *sources below data* layout may place an undesirably large number of sources along the flight paths. This could lead to aliasing effects on the predicted values, such as the stripes parallel to flight lines that are often observed when gridding airborne magnetic data. The *regular grid* layout can avoid this effect by evenly distributing sources and using a continuous source layer (e.g., right-rectangular prisms or tesseroids).

We propose a new way of distributing equivalent sources horizontally that could simultaneously reduce the computational load and mitigate some of the drawbacks of existing layouts. In the *block-averaged sources* layout, point sources are placed in the average position of data points that fall within specified spatial blocks (Fig. 2d). This is done by:

1. Dividing the survey region into rectangular blocks of equal size.

2. Computing the median horizontal position of the observation points that fall inside each block. Blocks without any observation point are omitted.
3. Assign one point source to the median horizontal position calculated in step 2.

The number of sources created by this new layout will be less than the number of observations if the block size is chosen appropriately (i.e., making sure that blocks are large enough to contain more than a single data point). The overdetermined problem that arises from this layout has a lower computational load and is less prone to overfitting the data since the model complexity is lower. Moreover, the block averaging process can balance the spacing between sources along a flight line and between adjacent lines, helping to reduce aliasing effects in generated grids. We will demonstrate through tests on synthetic data that the block-averaged sources layout is able to interpolate with comparable accuracy to other layouts while using a fraction of the equivalent sources.

2.4.2 Depth of sources

It is widely known from potential theory that the depth of a point source influences the wavelength of the observed field at the surface. This makes the source depth a key parameter affecting the outcome of interpolation and other operations done with equivalent sources. Several different strategies for assigning the depths of equivalent sources have been proposed in the literature. Here, we will highlight the following (Fig. 3):

1. *Constant depth*: The simplest option is to locate all sources at the same depth (Fig. 3a). If the measurements were taken at significantly different altitudes, some measurements will be more distant to the sources than others, which may create problems for reproducing short wavelengths in high altitude points.
2. *Relative depth*: The depths of sources are determined by shifting the vertical coordinate of data points downward by a fixed amount (Fig. 3b).

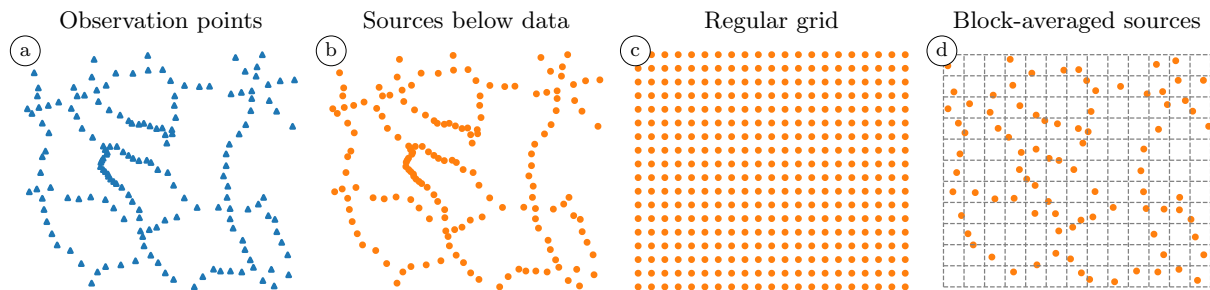


Figure 2: Sketch of different horizontal layouts for equivalent source models. Blue points represent the locations of observations and orange points represent the locations of equivalent sources according to different layout strategies. (a) Set of 166 observation points that simulate a ground survey. (b) Location of the 166 sources obtained through the *sources below data* layout. (c) Location of the 378 sources obtained through the *regular grid* layout. (d) Location of the 87 sources obtained through the *block-averaged sources* layout. Grey dashed lines represent the spatial blocks within which the median observation location is calculated.

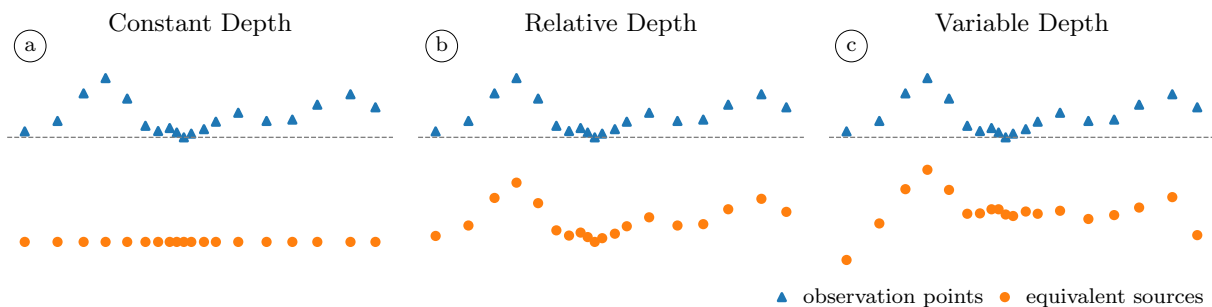


Figure 3: Examples of different strategies for assigning depths to equivalent sources. Here we assign one source for each observation point, located at the same horizontal coordinates as the data points. Source depths are (a) a *constant depth* at a chosen vertical coordinate, (b) a *relative depth* determined by uniformly downward shifting the vertical coordinate of data points, and (c) a *variable depth* determined by shifting the vertical coordinates of the observation points by an amount proportional to the average distance to neighbouring sources. The distance between data points and their respective sources (a) depends on observation height, (b) is constant, and (c) is proportional to the horizontal distribution of sources. Notice how the closely spaced sources in the middle of the profile (c) are shallower than their counterparts in (b).

The sources will not all be at the same vertical coordinate, but they will all be at the same vertical distance from the observation points.

3. *Variable depth*: The depths of sources are proportional to the horizontal distance to the nearest neighbouring data points or sources (Fig. 3c). Different variations of this strategy have been proposed before, for example Cordell (1992), Guspí et al. (2004), and Guspí and Novara (2009). The rationale for this strategy is that if a survey has data points clustered in some areas, we may want the sources below those areas to be shallower in order to preserve the shorter wavelengths that can be measured.

Our approach to the *variable depth* strategy will be:

$$z = z_{obs} + \Delta z + \alpha h, \quad (14)$$

in which z is the depth of an equivalent source, Δz is a relative depth shift that is the same for all sources, α is an adimensional depth factor, h is the median horizontal distance to the k nearest neighbouring sources, and z_{obs} is a vertical observation coordinate that will depend on the horizontal layout strategy. For *sources below data*, it is the vertical coordinate of the data point corresponding to the given source. For *regular grid*, it can be interpolated from the vertical coordinates of all data points. Finally, for *block-averaged sources* it will be the average vertical coordinate of data within the corresponding block.

In the following sections, we will test the effectiveness and trade-offs of each of these strategies on synthetic data.

3 Tests on synthetic data

We have used synthetic gravity datasets to test the interpolation accuracy of the difference horizontal and vertical source distribution strategies as well as the gradient-boosted equivalent source method. To generate the data, we created a model that is made out of 64 right-rectangular prisms, distributed on a region of 111319 m \times 111319 m with depths varying between

10000 m and zero. The density contrast of prisms ranges from -900 kg m^{-3} to 500 kg m^{-3} . The model includes prisms of different shapes, sizes, and depths to create gravity disturbances with a variety of wavelengths.

We created two synthetic datasets from the model, one simulating a ground survey and another an airborne acquisition (Fig. 4). To create the synthetic ground survey, we selected measurement positions from a portion of a public domain dataset for Southern Africa, available through the NOAA National Centers for Environmental Information (NCEI). For the synthetic airborne survey, we used a portion of the Great Britain Aeromagnetic Survey acquired by Hunting Geology and Geophysics Ltd and Canadian Aeroservices Ltd between 1955 and 1965 and made publicly available by the British Geological Survey (BGS). In both cases, we rescaled the horizontal coordinates of each survey portion to span an area of 111319 m \times 110576 m, matching the model dimensions. The ground survey contains 963 observations distributed at heights between 0 m and 2052.2 m (Fig. 4a). The airborne survey has 5673 observations at heights between 359 m and 1255 m (Fig. 4c).

The vertical component of the gravitational acceleration generated by the model was computed using the method of Nagy et al. (2000, 2002) with recent modifications by Fukushima (2020), as implemented in the open-source software Harmonica (Uieda et al., 2020b). We generated a *target grid* of 57 \times 56 points with a spacing of 2 km and located 2000 m above the zero height plane (Fig. 5) to serve as a reference when calculating the interpolation error. We then generated synthetic ground (Fig. 4b) and airborne (Fig. 4d) data to which we added pseudo-random Gaussian noise with zero mean and 1 mGal standard deviation.

3.1 Source distribution strategies

We investigated the effect of different strategies for distributing the equivalent sources horizontally and vertically on interpolation accuracy. To do this, we used the damped least-squares solution described in Section 2.2 (without gradient boosting) to interpolate the synthetic datasets (Fig. 4) and compared the

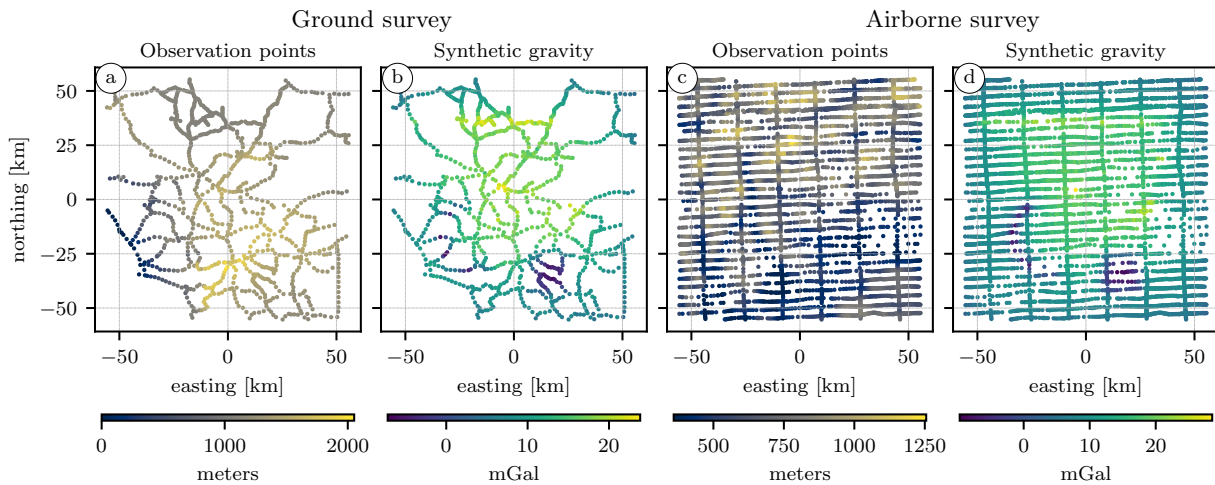


Figure 4: Maps of the observation locations and gravity values for the synthetic ground and airborne surveys. (a) Horizontal position and height of the ground survey points. (b) Synthetic gravity data calculated on the ground survey points with added pseudo-random Gaussian noise. (c) Horizontal position and height of the airborne survey points. (d) Synthetic gravity data calculated on the airborne survey points with added pseudo-random Gaussian noise. Heights are given in meters above the zero height plane.

results against the target grid (Fig. 5). This process was repeated for each combination of horizontal layout (*sources below data* and *block-averaged sources*) and depth type (*constant*, *relative*, and *variable*) and for regular grid sources with a constant depth, totalling 7 different combinations.

Each source distribution strategy requires certain hyper-parameters to be chosen in order to build the set of point sources. For example, using a constant depth needs the definition of the depth and using block-averaged sources requires the definition of the block size. The predictive capabilities of the equivalent sources depend on the choice of these hyper-parameters. To ensure that our comparisons are fair, we perform an exhaustive search over combinations of hyper-parameter values (including the damping parameter from Eq. 8) to obtain the best prediction that can be achieved by each source distribution strategy. Here, the best prediction is defined as the one that minimizes the root mean-square error (RMS) between interpolated values and the target grid (Fig. 5). The parameter values used in these searches and the

one producing the smallest RMS error are outlined in Tables 1 and 2.

Fig 6 and 7 show the differences between the target grid and the best prediction achieved by each source distribution strategy for the ground and airborne synthetic surveys, respectively. For the synthetic ground survey, the horizontal layouts produced similar RMS values of approximately 0.8 mGal regardless of the depth type, with the exception of the regular grid layout which produced a larger RMS of 0.97 mGal. The differences between the target grid and the interpolated values are larger in regions of poor data coverage. Edge effects are present for all strategies but are noticeably smaller for the combination of block-averaged sources with a variable depth based on the nearest neighbour distance. For the synthetic airborne survey, all strategies (including the regular grid) produced similar RMS errors of approximately 0.3 mGal. The maps of the differences between the target grid and interpolation results are visually indistinguishable from each other.

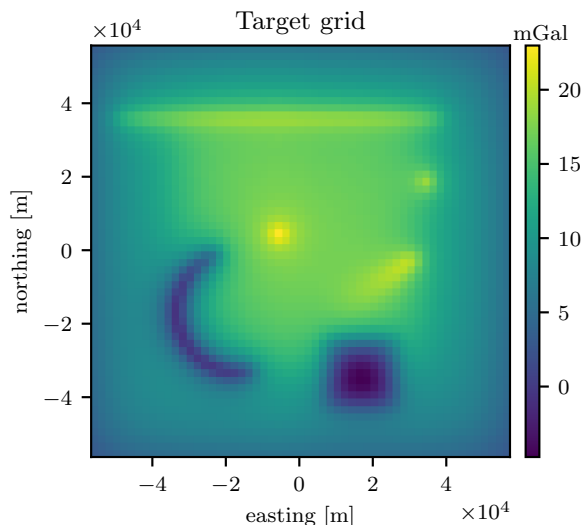


Figure 5: Pseudo-color map of the target grid of synthetic gravity data. The grid is composed of 57×56 points with a spacing of 2 km. The grid height is 2000 m above the zero height plane.

3.2 Window size and overlap in gradient boosting

We assessed the trade-offs in interpolation accuracy and computation time of the gradient-boosted equivalent sources algorithm as a function of the two key controlling factors: the window size and the amount of overlap between adjacent windows. The comparisons were performed against a regular least-squares solution (Eq. 9) using the synthetic airborne data (Fig. 4c-d). To avoid biasing the results, we used the same locations of equivalent sources for both the regular and gradient-boosted interpolations, namely block-averaged sources with a block size of 2000 m and a relative depth of 9000 m.

3.2.1 Window size

The size of the windows controls the size of the Jacobian matrices $\tilde{\mathbf{A}}_k$ by limiting the number of data points and equivalent sources used in each step of the gradient-boosting algorithm (Alg. 2). Thus, using

smaller windows will reduce the total amount of computer memory required to estimate the source coefficients. Nevertheless, smaller windows may produce less accurate interpolations by failing to achieve the global minimum of the goal function in Eq. 8. The window size might also impact the computation time in non-intuitive ways since smaller windows generate smaller least-squares problems but also require more gradient-boosting iterations.

We calculated the interpolation RMS error and computation time for a fixed window overlap of 50% and several window sizes. To avoid any biases introduced by the shuffling of windows, the calculations were repeated using different seeds for the pseudo-random number generator used in the shuffling. Figs. 8a and 8c show the RMS error and computation time required for estimating the source coefficients, respectively, as a function of the window size.

The results show that the interpolation error for gradient-boosting is generally larger than the error for regular equivalent sources. The error decreases asymptotically to within $\sim 40\%$ of the regular equivalent sources for windows with an area greater than $\sim 10\%$ of the survey area. The computation time similarly decreases with window size, with the gradient-boosting being generally faster than the regular equivalent sources for windows with an area greater than $\sim 5\%$ of the survey area. As the window size increases, both RMS error and computation time appear to stabilize to nearly constant levels.

3.2.2 Window overlap

The amount of overlap between adjacent windows plays an important role in the performance of the gradient-boosted equivalent sources. It controls the number of iterations and how often a particular source is used in the least-squares fitting process. While the experiments in the previous section showed that 50% overlap was sufficient to achieve acceptable interpolation accuracy, we separately studied the impacts of the amount of window overlap on both accuracy and computation time.

We performed a similar experiment to one in section 3.2.1 but this time kept the window size fixed to

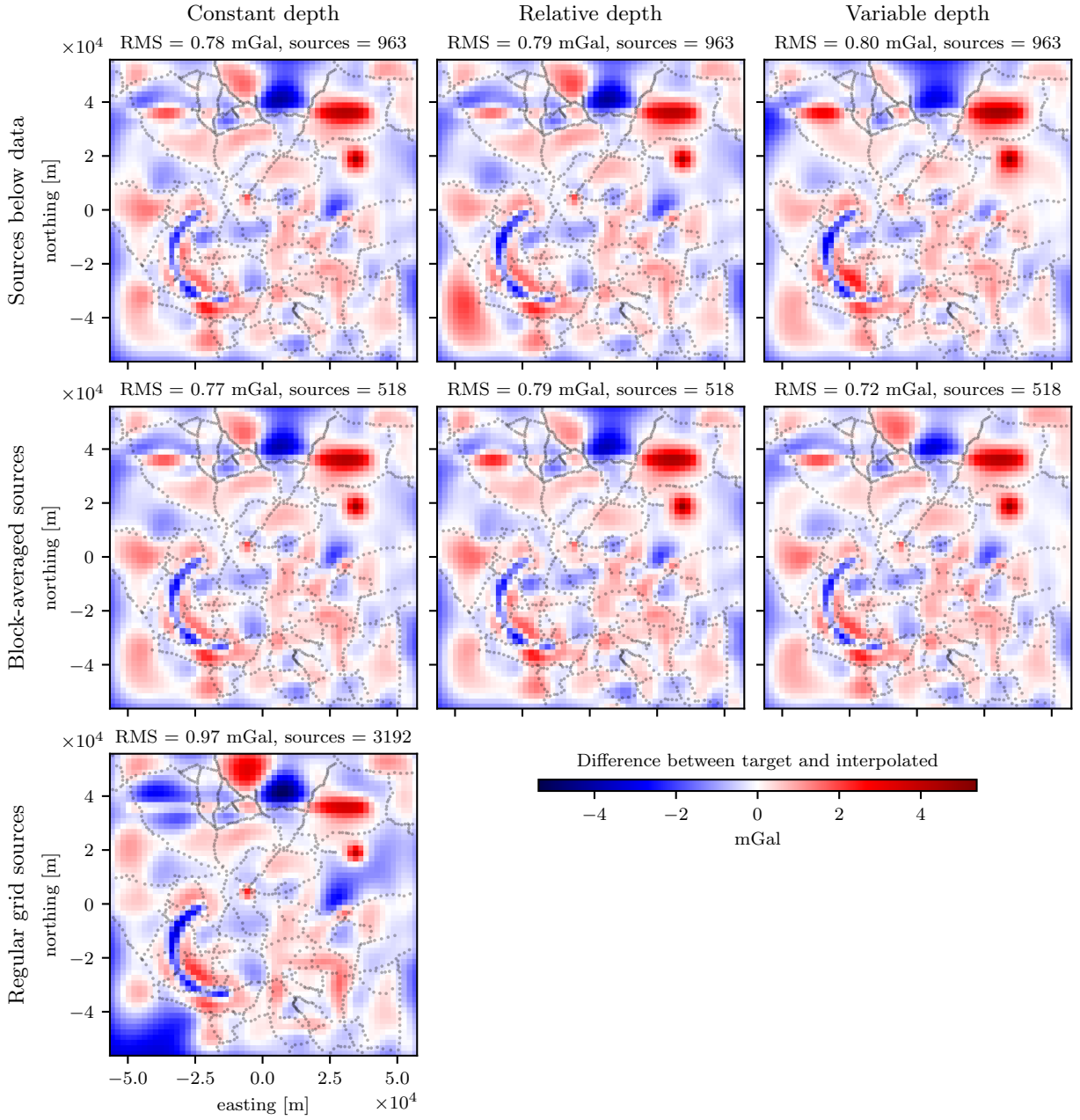


Figure 6: Pseudo-color maps of the differences between the target grid and the interpolated synthetic ground survey data produced by each source distribution strategy. The black dots represent the horizontal location of the synthetic data points. The RMS error and total number of equivalent sources is reported for each strategy at the top of the respective maps.

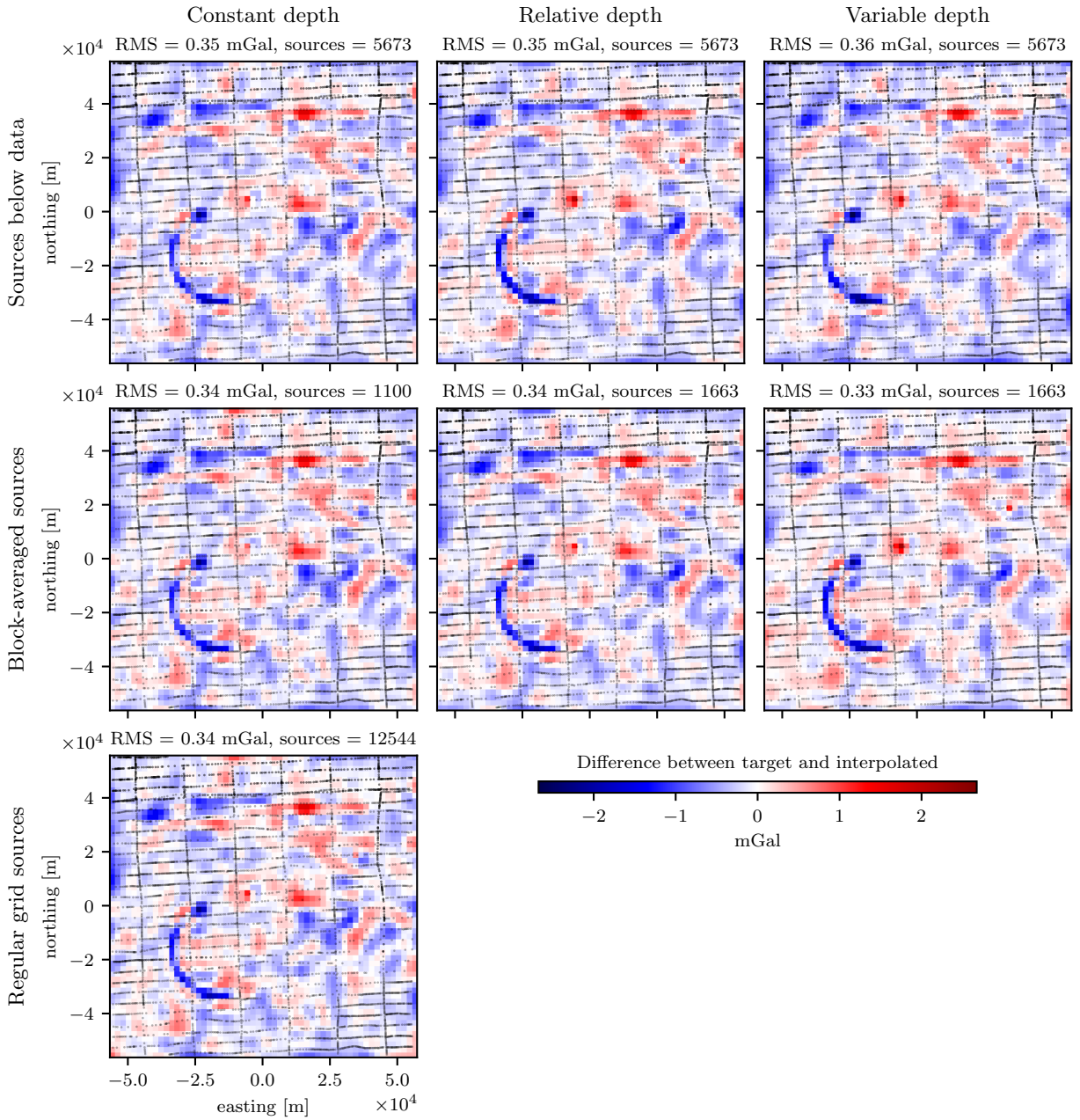


Figure 7: Pseudo-color maps of the differences between the target grid and the interpolated synthetic airborne survey data produced by each source distribution strategy. The black dots represent the horizontal location of the synthetic data points. The RMS error and total number of equivalent sources is reported for each strategy at the top of the respective maps.

30000 m and varied the amount of overlap from 0% to 95% with a step size of 5%. All other experimental procedures remained unchanged. Figs. 8b and 8d show the RMS error and computation time required for estimating the source coefficients, respectively, as a function of the window overlap.

Our results show that the interpolation RMS error decreases with the amount of overlap, reaching the same accuracy as the regular equivalent sources at approximately 90% overlap. On the other hand, the computation time increases with the amount of overlap, becoming larger than that of the regular equivalent sources for overlaps greater than 70%. This is expected since increasing the overlap adds iterations to the gradient boosting algorithm without decreasing the individual least-squares problem sizes to compensate.

4 Gridding gravity data from Australia

This section will demonstrate how gradient-boosted equivalent sources can be used to interpolate large datasets of gravity data onto a regular grid at uniform height. For this purpose, we selected an open-access compilation of ground gravity surveys over Australia made by Wynne (2018) and filtered and referenced to the WGS84 ellipsoid by Uieda (2021). It contains over 1.7 million data points and covers most of the Australian territory at variable point spacings. Our goal is to create a 1 arc-minute resolution grid of gravity disturbances at a constant geometric height of 2127.58 m (the largest height of observations).

We computed the gravity disturbance by removing the normal gravity of the WGS84 ellipsoid from the observed gravity data (Fig. 9). Here, normal gravity was computed at each observation point through the closed-form formula of Li and Götze (2001) using the Boule software (Uieda and Soler, 2020). Finally, we converted the observations to planar Cartesian coordinates by applying a Mercator projection.

We start the interpolation process by defining a set of block-averaged sources at a relative depth of 4000 m and a block size of 1.8 km, resulting in a total

of 796744 point sources. The block size was chosen to match the desired resolution of the final grid (1 arc-minute is approximately 1.8 km at the equator). The coefficients of the gradient-boosted equivalent sources are estimated using a damping equal to 100 and a window size of 225 km, which was chosen in order to limit the amount of computer memory needed to store the Jacobian matrix to under 10 Gigabytes. Finally, we used the estimated source coefficients to predict the values of the gravity disturbance on a regular grid of 2442×2085 points at 2127.58 m above the ellipsoid. Fig. 9 shows the original data distribution and the interpolated regular grid. Grid points that are further than 50 km from the nearest data point are masked to avoid unrealistic extrapolations.

The resulting grid preserves the high resolution of the original data while avoiding aliasing artifacts due to the block averaging. Some parts of the grid are smoother and with reduced amplitude (e.g., some southwestern parts), which is expected from the upward continuation that was performed to have the grid at a constant height. On a modest workstation with 16 cores and 16 Gigabytes of RAM, estimating the 796744 coefficients with gradient-boosting took ~ 1.3 hours and the forward modelling step took ~ 18 minutes.

5 Discussion

5.1 Location of sources

The results of our tests on synthetic data (Figs 6 and 7) show that there are no significant differences between source distribution strategies, both in terms of the interpolation RMS errors and from visual inspection of the difference maps. Therefore, we argue that all source distribution strategies are able to produce comparably accurate interpolations. Nevertheless, the *block-averaged sources* strategy make use of fewer sources when compared with other strategies, which reduces the computational load of estimating the sources coefficients and forward modelling. To ensure that the interpolation is able to reproduce the high frequencies in the data, the block size used in the averaging should be chosen to match the desired

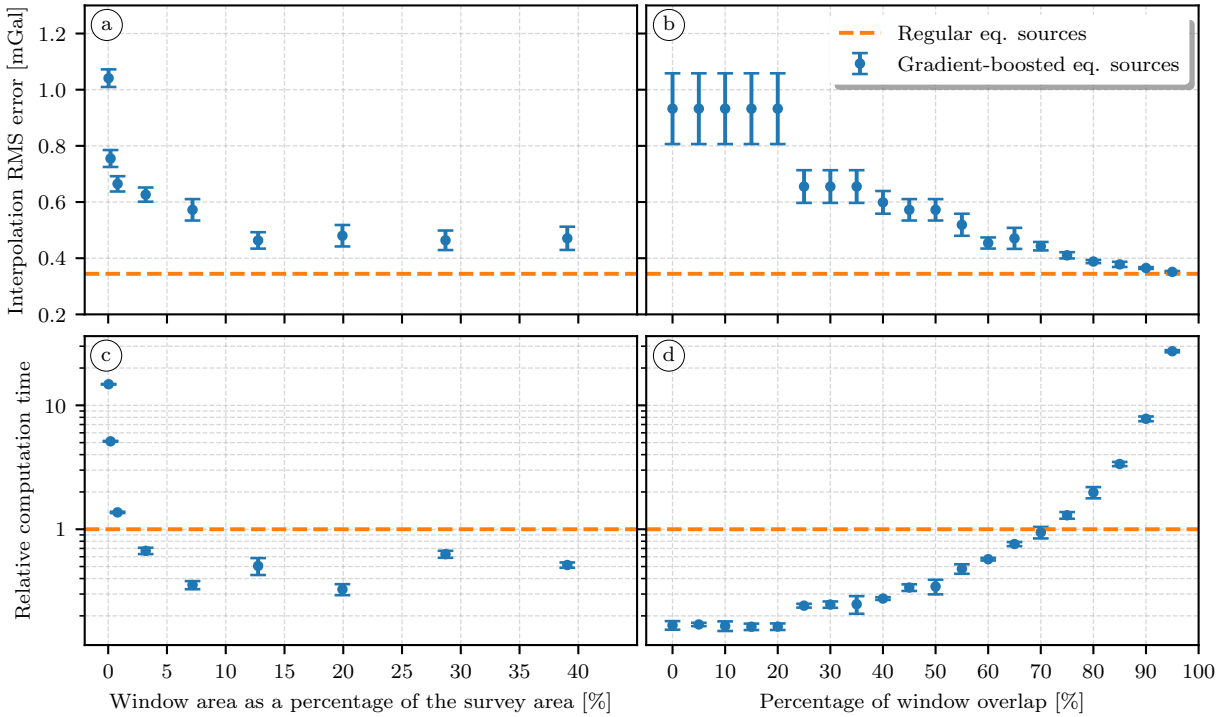


Figure 8: Comparison of the interpolation RMS error and computation time for regular least-squares equivalent sources (orange dashed lines) and gradient-boosted equivalent sources (blue dots and error bars). Both methods used the same source positions (block-averaged sources with a relative depth). Window sizes are given as a percentage of the survey area (e.g., 100% represents a window with the same area as the survey) and window overlap is given as a percentage of the window size (an overlap of 50% means that two adjacent windows share an area half of the size of the entire window). Computation time refers to the time required to estimate the source coefficients and is reported as a ratio between the gradient-boosted and the regular equivalent sources. For gradient-boosting, the RMS errors and computation times are the means (error bars represent 1 standard deviation) of results using different seeds for the pseudo-random number generator. (a) RMS error between the target grid and interpolation results and (b) RMS error between the target grid and interpolation results and (c) computation time as a function of window size. (d) computation time as a function of window overlap.

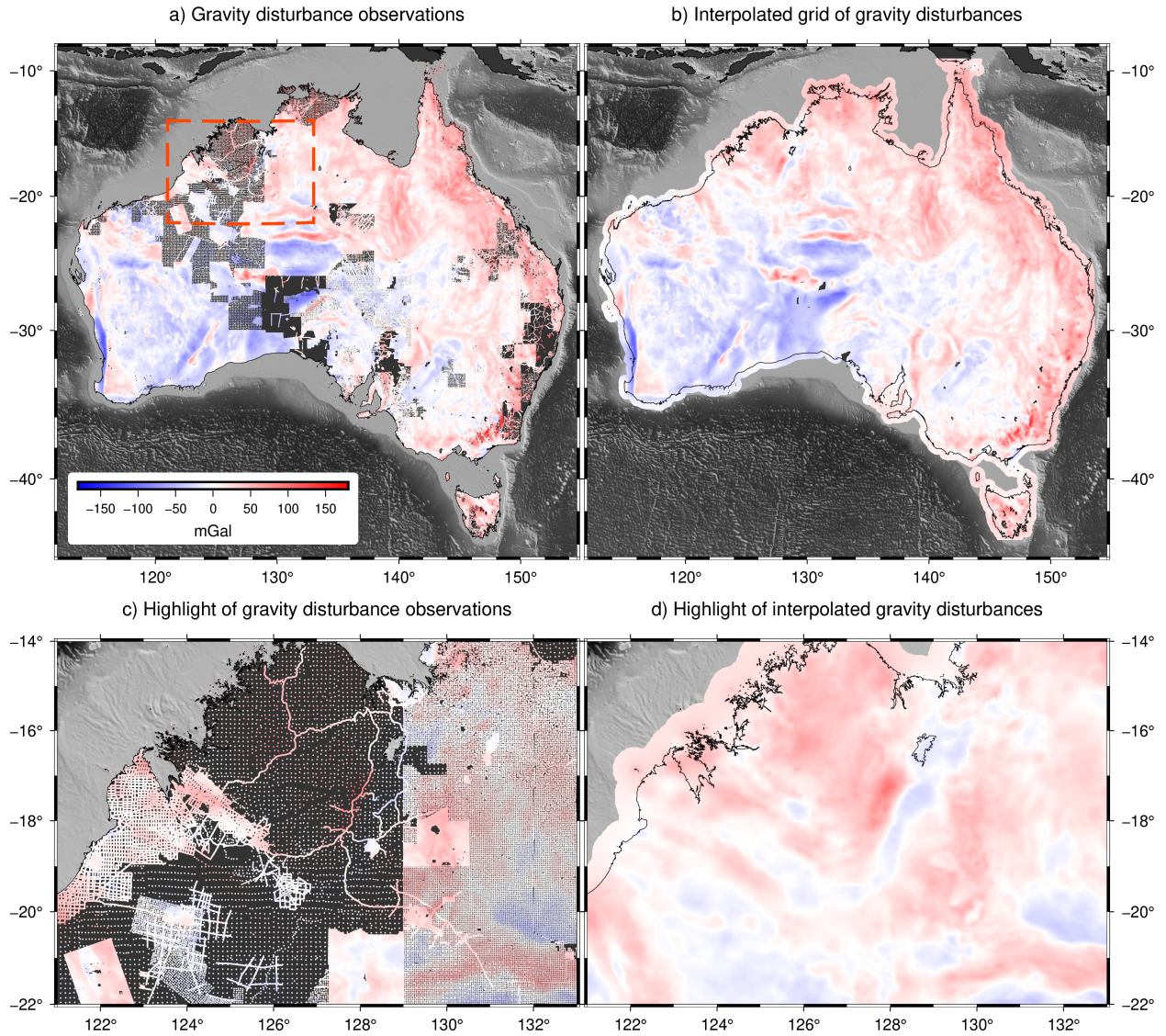


Figure 9: Pseudo-color maps of observed (a and c) and interpolated (b and d) gravity disturbance of Australia. The observed values in a and c are plotted as colored circles. The red rectangle marks the boundaries of the highlight maps in c and d. Observations are part of a compilation by [Wynne \(2018\)](#) of over 1.7 million ground gravity measurements. Interpolated values were obtained through gradient-boosted equivalent sources and calculated on a regular grid at 2127.58 m over the WGS84 ellipsoid.

grid resolution.

The choice of source depth strategy does not appear to significantly impact the interpolation RMS error. In the particular case of a sparse ground survey with block-averaged sources, the use of a variable depth visibly reduced edge effects and artifacts in areas of poor data coverage. At a first glance, the choice of a depth strategy would not seem to impact the computation time. However, when searching for the set of hyper-parameters that produce the most accurate interpolation (e.g., through cross-validation), one must solve the inverse problem once for every possible combination of parameters. A depth strategy like the *variable depth* requires a higher number of hyper-parameters (depth shift Δz , depth factor α , and the number of nearest neighbours k from Eq. 14) than other strategies which only require a single parameter. Having more parameters means increasing the dimensions of the parameter space and thus increasing the number of possible combinations. Thus, we recommend using a *constant depth* or a *relative depth* when processing large datasets in order to minimize computation time.

5.2 Gradient boosting

From Fig. 8a and 8c, we can see that the gradient-boosted equivalent sources produce slightly less accurate interpolation results but are able to achieve smaller computation times than regular equivalent sources. The reduction of the accuracy might be due to the gradient boosting algorithm failing to converge to the global minimum of the goal function. As the windows increase in size, interpolation error decreases because more data points are included into the least-squares fitting of the source coefficients. At the same time, the fitting process becomes faster because of a reduction in the number of iterations. Our results indicate that it is desirable to maximize the window size up to the point that the Jacobian matrices still fit within the available computer memory.

The results shown in Figs 8b and 8d indicate that using window overlap values between 40% and 70% strike a balance between accuracy and computation time. This corroborates our initial choice of 50% overlap, which is good enough for producing accu-

rate predictions in reasonable times.

6 Conclusions

The equivalent source technique has been proven to be well suited for interpolating gravity disturbances and magnetic anomalies. The two main reasons that make it to stand out from other 2D interpolation methods is the fact that the equivalent sources take into account the height of the observations and that the interpolated values will always be harmonic functions. The main challenge of using equivalent sources in practice is the high computational load of estimating the coefficients of the equivalent sources, specially on the computer memory needed to store the Jacobian matrix. In this work we present two strategies that could be simultaneously applied in order to interpolate very large datasets (millions of points) in reasonable computation times on modest hardware: block-averaging source locations, which reduce the number of equivalent sources needed for the interpolation, and the gradient-boosted equivalent source algorithm, which breaks down the inverse problem into smaller sets of equivalent sources defined by overlapping windows. Both methods were tested against synthetic datasets in order to compare their accuracy and how they perform in terms of computational resources.

Our results show that the block-averaged sources reduce the computational load needed to estimate source coefficients in comparison to the two traditional strategies of placing sources below data points or on regular grids. We also showed that this reduction of the number of sources does not affect the accuracy of the predictions. The use of block-averaged sources may also prevent aliasing of the interpolated values, specially when the observations are unevenly sampled (e.g., airborne and shipborne surveys). Special attention must be payed when choosing the size of the blocks for averaging: as a thumb rule, we recommend choosing a size approximately equal to the resolution of the regular grid where the values will be interpolated.

Tests that compared strategies for the vertical location of the sources showed that any one of the three

strategies tested (*constant depth*, *relative depth* and *variable depth*) produces comparable accuracy of interpolation. Nevertheless, we are more prone to recommending either the *constant depth* or the *relative depth* for most applications because they involve less hyper-parameters that would need to be configured before the actual interpolation.

Gradient-boosted equivalent sources were shown to heavily reduce the computer memory needed to estimate source coefficients, making it possible to interpolate large datasets with millions of points that would otherwise produce Jacobian matrices larger than the available memory. The interpolations obtained though this new method achieve close to the same accuracy than the regular equivalent sources, while reducing the computation time needed to estimate the source coefficients by approximately three times. We also show that an overlap of 50% between adjacent windows achieves a good compromise between accuracy and computation time. The size of the overlapping windows should be chosen as the maximum value possible that creates Jacobian matrices that still fit into computer memory.

The gradient-boosting method developed here can be used in conjunction with any horizontal source layout, depth strategy, or source type (e.g., point sources, prisms, tesseroids) because it does not rely on assumptions about the sources. Future research should investigate the application of gradient boosting to other equivalent source methods.

7 Data and code availability

The Python source code used to produce all results and figures presented here is available at <https://doi.org/10.6084/m9.figshare.13604360> and <https://github.com/compgeolab/eql-gradient-boosted> under the BSD 3-clause open-source license.

The gradient-boosted equivalent sources implementation is based on the equivalent source code in the Harmonica library (Uieda et al., 2020b). Other software used in this study includes: Pooch (Uieda et al., 2020a) for downloading and caching datasets, Verde (Uieda, 2018) for block reductions and coordinate manipulations, Boule (Uieda and Soler, 2020)

for normal gravity calculations, xarray (Hoyer and Hamman, 2017) and Numpy (Harris et al., 2020) for handling multidimensional arrays and numerical computations, Numba (Lam et al., 2015) for just-in-time compilation and parallelization, Matplotlib (Hunter, 2007) and PyGMT (Uieda et al., 2020c) for generating the figures and maps, and the Jupyter notebook programming environment (Kluyver et al., 2016). Harmonica, Boule, Pooch, and Verde are part of the Fatiando a Terra project (Uieda et al., 2013).

All datasets used are open-access and publicly available. The synthetic surveys were generated using a public domain gravity dataset for Southern Africa distributed by the NOAA NCEI (<https://www.ngdc.noaa.gov/mgg/gravity/gravity.html>) and the Great Britain Aeromagnetic Survey distributed by the British Geological Survey (BGS) under an Open Government License (<https://www.bgs.ac.uk/products/geophysics/aeromagneticRegional.html>). The shaded relief in Fig. 9 is the SRTM15+ dataset by Tozer et al. (2019). The Australian ground gravity data is based on a compilation distributed by Geoscience Australia under a Creative Commons Attribution 4.0 International Licence (Wynne, 2018) which was filtered and referenced to the WGS84 ellipsoid by Uieda (2021) and is distributed under the same license (<https://doi.org/10.6084/m9.figshare.13643837>).

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S.R. Soler and L. Uieda jointly developed the initial idea, analysed the results, and wrote the paper. S.R. Soler produced all results and developed the software implementation with minor revisions by L. Uieda.

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A Source position parameters used for the tests on synthetic data

Tables 1 and 2 show the parameter values tested and their optimal values for creating the equivalent source distributions tested in Section 3.1. The optimal values were used to produce the results in Figs 6 and 7.

Table 1: Parameters used to produce each source distribution for interpolating the synthetic ground survey data. Also contains the set of parameters that generates the smallest RMS error for each source distribution and their corresponding RMS.

Source layout	Depth type	Parameters	Values	Best	RMS
Source Below Data	Constant	Depth (m)	1000 to 17000, step size 2000	7000	0.78
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-1}	
	Relative	Depth (m)	1000 to 17000, step size 2000	9000	0.79
Damping		$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-1}		
Block Averaged Sources	Variable	Depth (m)	0 to 1400, step size 200	1000	0.80
		Depth factor	0.1, 0.5, 1, 2, 3, 4, 5 and 6	1	
		k neighbours	1, 5, 10 and 15	15	
	Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	1		
Constant	Constant	Depth (m)	1000 to 17000, step size 2000	7000	0.77
		Block size (m)	1000, 2000, 3000 and 4000	3000	
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-1}	
Relative	Relative	Depth (m)	1000 to 17000, step size 2000	7000	0.79
		Block size (m)	1000, 2000, 3000 and 4000	3000	
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-1}	
Variable	Variable	Depth (m)	0 to 1400, step size 200	600	0.72
		Depth factor	0.1, 0.5, 1, 2, 3, 4, 5 and 6	1	
		k neighbours	1, 5, 10 and 15	15	
		Block size (m)	1000, 2000, 3000 and 4000	3000	
Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-1}			
Grid Sources	Constant	Depth (m)	1000 to 9000, step size 2000	3000	0.97
		Grid spacing (m)	1000, 2000, 3000 and 4000	2000	
		Damping	$10^1, 10^2, 10^3$ and 10^4	10^2	

Table 2: Parameters used to produce each source distribution for interpolating the synthetic airborne survey data. Also contains the set of parameters that generates the smallest RMS error for each source distribution and their corresponding RMS.

Source layout	Depth type	Parameters	Values	Best	RMS
Source Below Data	Constant	Depth (m)	1000 to 17000, step size 2000	7000	0.35
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-2}	
	Relative	Depth (m)	1000 to 17000, step size 2000	9000	0.35
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-2}	
	Variable	Depth (m)	50 to 1450, step size 200	1450	0.36
		Depth factor	1 to 6, step size 1	1	
		k neighbours	1, 5, 10 and 15	15	
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	1	
Block Averaged Sources	Constant	Depth (m)	1000 to 17000, step size 2000	9000	0.34
		Block size (m)	1000, 2000, 3000 and 4000	3000	
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-4}	
	Relative	Depth (m)	1000 to 17000, step size 2000	9000	0.34
		Block size (m)	1000, 2000, 3000 and 4000	2000	
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-3}	
	Variable	Depth (m)	50 to 1450, step size 200	50	0.33
		Depth factor	1 to 6, step size 1	2	
		k neighbours	1, 5, 10 and 15	15	
		Block size (m)	1000, 2000, 3000 and 4000	2000	
		Damping	$10^{-4}, 10^{-3}, \dots, 10^2$	10^{-2}	
Grid Sources	Constant	Depth (m)	1000 to 9000, step size 2000	7000	0.34
		Grid spacing (m)	1000, 2000 and 3000	1000	
		Damping	$10^{-3}, 10^{-2}, \dots, 10^2$	10^{-1}	