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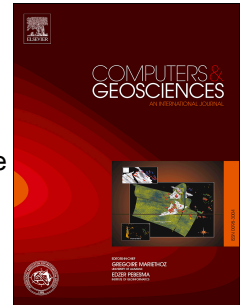
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GRAVPSO2D: A Matlab package for 2D gravity inversion in sedimentary basins using the Particle Swarm Optimization algorithm

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Abstract

In this paper GRAVPSO2D, a Matlab tool for two-dimensional gravity inversion in sedimentary basins using the Particle Swarm Optimization (PSO) algorithm, is presented. The package consists of a collection of functions and scripts that cover the main three parts of the process: (1) the model definition based on the observations, (2) the inversion itself, where the PSO is employed, and (3) the results processing, including best model estimation, uncertainty analysis and plots generation. GRAVPSO2D is freely available, and represents an effort for providing

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Author contributions: J.L.G.P., J.L.F.M., and Z.F.M. designed the methodology, developed the software, processed the data, and wrote the paper. G.G., and T.N. acquired the gravity data. S.B., G.G., and T.N. analyzed, discussed the inversion results corresponding to the real example, and wrote the related part of the paper.

the scientific community with the first tool based on the PSO algorithm in order to perform the inversion and the uncertainty assessment of the sedimentary basin gravity inversion problem, taking into account the gravity regional trend estimation, and vertically and horizontally density contrast variations. Synthetic and real examples are provided in order to show the software capabilities.

Keywords: Nonlinear gravity inversion, Particle Swarm Optimization, Uncertainty assessment, Sedimentary basin

1. Introduction

The interface separation between two media having different densities can be estimated in Geophysics using gravity measurements and by posing a nonlinear inverse problem. Gravity inversion in this kind of environments is a tool frequently used in Geophysics in tasks such as prospecting of oil and gas, or in hydrogeology and glaciology studies (Blakely, 1995; Dobrin, 1960; Hinze et al., 2013; Nettleton, 1976; Parker, 1994; Telford et al., 1976). The gravity inverse problem has a non-unique solution, leading to an infinity number of solutions (Al-Chalabi, 1971; Skeels, 1947; Zhdanov, 2015). It is therefore mandatory to introduce some kind of regularization and/or constraint(s) incorporating other geophysical information such as borehole and seismic profile data, contrasted prior models, etc. This will allow to restrict the set of possible solutions and stabilize the inversion.

The problem of the estimation of the basement relief in sedimentary basins using gravity observations is a nonlinear inverse problem, and the most used techniques for its solution are based on local optimization methods, either by the linearization of the problem plus regularization (see Silva et al. (2009) for example), or by the sequential application of the direct formulation (see Bott (1960) or Chen

and Zhang (2015) for example). GRAVPSO2D uses Particle Swarm Optimization (PSO), which is a global search method with excellent capabilities to perform the inverse problem uncertainty analysis and avoiding the weak points of the local optimization procedures, such as the dependency on the prior model and the lack of a proper uncertainty analysis (Fernández-Martínez et al., 2013, 2014b).

GRAVPSO2D works in two-dimensional environments. This approximation can be used when the dimension of an anomalous body is much larger than the other two dimensions (at least a $4\times$ or $6\times$ factor according to Nettleton (1976)). This situation is common in sedimentary basins, where their horizontal extensions are generally much larger than their depth, so profiles perpendicular to the principal dimensions can be used for the analysis in a 2D formulation (Pick et al., 1973; Telford et al., 1976).

2. Observations and basin modelization

GRAVPSO2D works with user-provided complete Bouguer gravity anomalies, Δg , along a profile. The software can also estimate a polynomial regional trend during the inversion, so if this effect exists in Δg it is not necessary to be previously suppressed by the user.

The 2D basin modeling used in GRAVPSO2D consists in the juxtaposition of rectangles along the profile as it was commonly employed by other authors (see for example Silva et al. (2009) or Ekinici et al. (2020)). As it can be seen in Fig. B.1, the rectangles' upper sides are located at the surface level (considered plane in the figure, although that is not mandatory, so they can be adapted to the terrain topography). It is common to set the horizontal dimensions to be equal for all rectangles, but GRAVPSO2D can also work with unequal widths. Then, the

bottom sides depict the sediments-basement interface.

FIGURE B.1 HERE (ONE COLUMN WIDTH)

Let N be the number of observed gravity points, $P_i(l_i, z_i)$, with $i = 1 \dots N$, and where l_i is the point position along the profile length, and z_i the point height. The gravity residual anomaly generated over each point by a model composed of M rectangles follows the equation

$$\Delta g_{P_i}^r = \sum_{j=1}^M F(\Delta \rho(z_j), z_j, \mathbf{r}_{ij}), \quad (1)$$

where F is the forward operator (see Appendix A), $\Delta \rho(z_j)$ is the particular rectangle density contrast, constant or variable with depth, z_j is the particular rectangle bottom side height (the problem unknowns), and \mathbf{r}_{ij} is the position vector of each rectangle related to each observation point. If a polynomial regional trend is added, which contributes with the anomaly Δg^t , the gravity anomaly over each observation point is:

$$\begin{aligned} \Delta g_{P_i} &= \Delta g_{P_i}^r + \Delta g_{P_i}^t \\ &= \sum_{j=1}^M \left[F(\Delta \rho(z_j), z_j, \mathbf{r}_{ij}) + \sum_{k=D}^0 A_k (l_i - l_r)^k \right], \end{aligned} \quad (2)$$

where D is the polynomial degree, A_k are the polynomial coefficients, and l_r is a reference position.

In real environments sediments' density typically increases with depth, so the density contrast sediments-basement, $\Delta \rho$, decreases. GRAVPSO2D can work with both, constant or variable density contrast. In the latter case, this variation can be vertical (with depth), and also horizontal.

Many models of density contrast variation with depth have been used in the literature. Constant values are frequently used (Barbosa et al., 1997, 1999), but vari-

able density contrast is also very common: Rao (1990) used a quadratic equation, Chakravarthi and Sundararajan (2007) a parabolic law, Litinsky (1989); Silva et al. (2006) a hyperbolic law, and Parker (1972); Granser (1987); Pham et al. (2018) an exponential law. All these models produce complicated equations hard to manage that do not match well the density variation with depth in some real environments (see for example density logs in Brocher (2005) or Silva et al. (2006)).

In order to manage the vertical density contrast variation, GRAVPSO2D can use a piecewise model, having the advantages of (1) any density variation can be used, and (2) only the formulation corresponding to the constant density model (Eq. (A.1)) is needed. An example can be seen in Fig. B.2, where a constant value of $\Delta\rho = -600 \text{ kg m}^{-3}$ is used between depths from 0 m to 100 m; then, a linear variation from $\Delta\rho = -570 \text{ kg m}^{-3}$ to $\Delta\rho = -520 \text{ kg m}^{-3}$ is used between depths 100 m to 150 m, and finally a constant value of $\Delta\rho = -520 \text{ kg m}^{-3}$ is employed for depths greater than 150 m. GRAVPSO2D divides each subsoil model's rectangle based on the density profile for computing the whole attraction, and uses constant density sub-rectangles of user-defined size to approximate the zones with density variation.

FIGURE B.2 HERE (ONE COLUMN WIDTH)

GRAVPSO2D can also manage horizontal density contrast distributions. In this case the gravity profile is divided into horizontal sectors, and different vertical density contrast models are assigned to each one. All these configurations are provided via text files.

3. Particle Swarm Optimization

The PSO (Particle Swarm Optimization) algorithm (Kennedy and Eberhart, 1995) is a global optimizer based on the the behavior of swarms of animals (birds, fish schools) in the nature searching for food. A set of particles (models) explores the parameters' space with the goal of the optimization of a given cost function related to the inverse problem that is considered. As general overview, the algorithm works as follows: (1) in the first step, a set of particles (models) is created with random positions (the problem parameters) and velocities, and the objective function is employed to determine the fitness of each model in the set, (2) as time passes, the particles' position and velocity are updated based on their fitness and the corresponding values of their neighbors, i. e., the behavior of an individual is influenced by its own experience and that of its neighbors (Fernández-Martínez et al., 2008).

The algorithm depends internally of a set of parameters, where the more important are the so-called *inertia weight*, and *local* and *global accelerations*. Modifying how the velocities and accelerations of the particles are described a family of PSO variants are describable, and among them GRAVPSO2D can use the so-called GPSO, CC-PSO, CP-PSO, PC-PSO, PP-PSO, PR-PSO, RC-PSO, RP-PSO and RR-PSO family members (Fernández-Martínez and García-Gonzalo, 2009, 2012; García-Gonzalo et al., 2014). The cloud versions of these algorithms are used, i. e., no parameter tuning of inertia nor accelerations must be configured by the user, given that each the particle has its own PSO parameters, automatically chosen (García-Gonzalo and Fernández-Martínez, 2009).

Pioneer applications of PSO in the field of applied geophysics can be seen in Fernández-Álvarez et al. (2006); Fernández-Martínez et al. (2010a,b); Shaw and

107 [Srivastava \(2007\)](#). In [Fernández-Martínez et al. \(2010a\)](#), for example, an applica-
 108 tion of PSO to a 1D-DC resistivity inverse problem is presented. More recently,
 109 in [Luu et al. \(2018\)](#) an application to the seismic traveltime tomography problem
 110 can be seen, and in [Li et al. \(2019\)](#) PSO is applied to microseismic location. Nev-
 111 ertheless, in gravity and other potential field inversion methods the PSO algorithm
 112 has been barely used ([Essa and Elhussein \(2018\)](#), for example, apply PSO in the
 113 inversion of magnetic anomalies generated by simple structures).

114 In [Sanyi et al. \(2009\)](#) several simple gravity synthetic examples based on
 115 buried cylinders are solved using PSO, comparing the obtained results with other
 116 global search methods (genetic algorithms, simulated annealing, and ant colony
 117 optimization), and also with a classical Levenberg-Marquardt approach. In [Tou-
 118 shmalani \(2013a,b\)](#) PSO was employed to estimate the parameters of a fault based
 119 on gravity anomaly observations. The conclusion of the study is that PSO provides
 120 better agreement between the estimated and the synthetic model anomaly than the
 121 classical approach using linearization and the Levenberg-Marquardt method. In
 122 [Roshan and Singh \(2017\)](#) PSO is employed in the gravity inversion of a spher-
 123 ical and a vertical cylindrical models, as well as its application to a real exam-
 124 ple (modeled as a vertical cylinder). In all these papers PSO is employed as a
 125 global optimizer, and performance tests are performed in most cases against local
 126 optimization techniques. But the most important feature of global optimization
 127 algorithms is missed: their capability to perform an approximate nonlinear uncer-
 128 tainty analysis of the inverse solution by the sampling of the nonlinear uncertainty
 129 region(s). Few papers were found ([Singh and Biswas, 2016](#); [Ladino and Bassrei,
 130 2016](#)) where the inversion uncertainty is analyzed using the frequency distribution
 131 of the model parameters and/or cross-plots of parameters. In [Fernández-Muñiz](#)

et al. (2020) an application of PSO to gravity inversion of isolated anomalous bodies plus uncertainty assessment using PSO can also be seen.

In Pallero et al. (2015, 2017), a first attempts to apply the PSO algorithm to the gravity inverse problem in sedimentary basins were presented for 2D and 3D environments, respectively. In Ladino and Bassrei (2016) a mixed model of PSO plus regularized Gauss-Newton method is employed for 3D gravity inverse problem in sedimentary basins, where PSO provides the initial model for a final Gauss-Newton inversion and cross-plots are employed for uncertainty analysis. In Singh and Singh (2017) PSO is applied to a 2.5D gravity inversion in sedimentary basins, although in this case only comparisons with results obtained via the Marquardt method are performed. Finally, Ekinici et al. (2020) have recently used a different global optimization method, called *differential evolution algorithm* (DEA), to a 2D approximation of this kind of problem applied to the Aegean Graben System (Turkey), performing also uncertainty analysis.

4. The 2D basement relief gravity inverse problem and PSO

In this section a general overview about the 2D basement relief gravity inverse problem in the frame of the PSO algorithm is presented. The main configuration parameters and other details are enumerated and explained.

The first important parameters to impose for the PSO execution are the search space limits, which are established based on a first approximation model estimated using the Bouguer's plate formulation. It is important to stress that this first approximation model does not act as the initial model in the local optimization methods, but it is only a guidance for the PSO search bounds determination, therefore not much accuracy is needed (this topic is explained in detail in the

GRAVPSO2D reference manual). Then, other important parameters to select are the swarm size and the number of iterations. At each iteration, a number of models equal to the swarm size are generated, i. e., the search space is sampled during the PSO execution. After each iteration the cost function value for each model is computed, which is a value that has influence in the posterior swarm evolution. This cost function is defined as

$$c = \frac{\|\mathbf{v}\|_p}{\|\mathbf{o}\|_p} \cdot 100, \quad (3)$$

where p is a user-selected vector norm. In the last step of the algorithm all generated models are analyzed according to their cost function values.

The vector \mathbf{o} is defined as

$$\mathbf{o} = \Delta\mathbf{g}^o - \Delta\mathbf{g}^t, \quad (4)$$

i. e., the vector of observed gravity anomaly minus the regional trend values (if they are estimated during the inversion or imposed). The vector \mathbf{v} is defined as

$$\mathbf{v} = \Delta\mathbf{g}^o - \Delta\mathbf{g}^t - \Delta\mathbf{g}^r, \quad (5)$$

i. e., the vector of observed gravity anomaly minus the regional trend values (if they are estimated during the inversion or imposed) minus the residual gravity generated by the corresponding subsoil model in the swarm. If the observations have an associated standard deviation information, it can be used in GRAVPSO2D for weighting the cost function computation.

Other important aspect in GRAVPSO2D is model filtering. The direct application of global search algorithms to the sedimentary basin gravity inverse problem produces unrealistic models characterized by a sawtooth profile (Boschetti et al.,

175 1997; Parker, 1999; Pallero et al., 2015). This can be mitigated via a moving av-
 176 erage filtering applied to the generated PSO models, and prior to the computation
 177 of the pertinent cost function value. Filtering is in this case the way to introduce
 178 relative constraints (Barbosa et al., 1997) in the problem, and the use of aver-
 179 age filtering technique permits a flexible configuration of the method behavior for
 180 different values in the filtering window.

181 Finally, using absolute constraints (Barbosa et al., 1997) is also possible. Ab-
 182 solute constraints are values of sediments-basement interface depths (or minimum
 183 depths) that can come from boreholes, seismic profiles or other sources. These
 184 data can be used to fix (or permit a small variation around a value) the depth value
 185 of parts of the subsoil model and its surroundings.

186 5. The GRAVPSO2D package

187 The GRAVPSO2D package is a Matlab software, so it is possible to work with
 188 it in any operating system where Matlab¹ is present.

189 5.1. Package organization and installation

190 Once the user has downloaded and uncompressed the package, a folder called
 191 grav-pso-2d/ will be obtained. This folder contains the following elements:

- 192 • A folder called pso_programs_v3/ containing the Particle Swarm Opti-
 193 mization code.

¹Matlab 9.2.0.538062 (R2017a) Linux version (under Debian GNU Linux) was employed in the writing of the software, but, as no special packages nor extensions are used, any version should be capable to execute GRAVPSO2D.

- 194 • A folder called `doc/` that stores a complete and self-contained 61-page ref-
195 erence manual.
- 196 • A folder called `examples/` containing the example data.
- 197 • A collection of 14 files whose names follow the template `grav2d_*.m`.

198 5.2. *Main scripts*

199 On the user side, `GRAVPSO2D` is composed by three main scripts, which are:

- 200 • `grav2d_ModelDefinition.m`. This script helps to prepare the data prior
201 to the inversion. Based on the observations data file and several user con-
202 figuration variables, this script performs the subsoil partition.
- 203 • `grav2d_Inversion.m`. This script performs the inversion using the PSO
204 algorithm. The user can select several parameters, such as the PSO fam-
205 ily member, the swarm size and the number of iterations, the activation of
206 weights, the vector norm for the cost function evaluation, and others. As
207 a result, the script generates a file containing, among other internal infor-
208 mation, all the sampled models, which will be the data to use in the post
209 processing stage.
- 210 • `grav2d_Plot.m`. This script analyzes the results obtained by `grav2d_Inversion.m`,
211 providing the inversion results in text and graphical modes, which can be
212 configured by the user through some variables.

213 5.3. *Input data files*

214 In this section, the different input data files will be enumerated (a detailed
215 description of the different formats is stated in the user's manual). All input data

216 files used by GRAVPSO2D are ASCII files, so it can be opened and edited by any
 217 text editor.

- 218 • **Observations data file.** The observations data file contains a gravity profile
 219 in rectangular coordinates, and is the fundamental file in GRAVPSO2D.
- 220 • **Subsoil data file.** This file describes the subsoil partition in rectangles,
 221 which is the model used by the software, as it was described in section 2.
- 222 • **Regional trend data file.** If the user wants to use a regional trend in inver-
 223 sion (estimation or only using a predefined one), a first approximation must
 224 be introduced via a configuration file. This first approximation does not act
 225 as initial approximation as in local optimization algorithms, but only as a
 226 reference to compute the search space for the polynomial coefficients in the
 227 PSO algorithm.
- 228 • **Density contrast definition data files.** Two files can be configured related
 229 to this topic, one for the vertical, and one for the horizontal density contrast
 230 variations. In the former case, the vertical variation is configured piecewise
 231 providing information about depths and the corresponding density contrast.
 232 Multiple configurations can be defined, each one marked by an identifier. In
 233 the case of the horizontal density distribution the corresponding file stores a
 234 set of segments, and a vertical contrast density configuration is assigned to
 235 each of them via the identifier.
- 236 • **Filtering data file.** For the filtering step the user must provide the window
 237 filter coefficients, which are stored in a file and can be freely selected.

- **Boreholes data file.** In this file borehole information is stored. The user can configure a fixed value or an influence area for a prescribed basement depth.

5.4. Output files

The `grav2d_Inversion.m` script generates after its execution a unique file, stored as Matlab `*.mat` format (version 7), containing the inversion's results. It contains a structure comprising all the generated models during the PSO execution, as well as all the inversion details (an in-depth description of the structure is presented in the GRAVPSO2D reference manual). This file is loaded by the `grav2d_Plot.m` in order to generate its results.

6. Synthetic example

In this section a synthetic example is presented in order to illustrate the behavior of the GRAVPSO2D software. A synthetic subsoil composed by 126 rectangles of 200 m horizontal width with upper sides from height 976 m to 1439 m, and depths are comprised between 10 m and 513 m has been created. The density contrast $\Delta\rho$ is variable with depth and also horizontally: two sectors dividing the profile at the middle, the first one with $\Delta\rho = -580 \text{ kg m}^{-3}$ between depths from 0 m to 100 m, and $\Delta\rho = -540 \text{ kg m}^{-3}$ for depths greater than 150 m ($\Delta\rho$ varies linearly between 100 m, and 150 m), and the second one with $\Delta\rho = -600 \text{ kg m}^{-3}$ between depths from 0 m to 110 m, and $\Delta\rho = -570 \text{ kg m}^{-3}$ for depths greater than 150 m ($\Delta\rho$ varies linearly between 110 m, and 150 m). Then a set of 99 points near uniformly distributed, and whose heights coincide with the rectangles top sides were generated. For this points the gravity anomaly corresponding to the subsoil model was generated, and then contaminated with white noise distributed

as $N(0, 0.25)$ mGal. Finally, a linear regional anomaly was added to each point following the trend

$$\Delta g^t = A_1 (l - l_r) + A_0, \quad (6)$$

where $A_1 = 1.2 \cdot 10^{-3}$ mGal m⁻¹, $A_0 = -99.042$ mGal, $l_r = 10\,798.699$ m, and l is the position in the profile of each point.

The previous configuration was employed, as it was explained, for the gravity signal generation. But for the inversion a reduced model was used in order to mimic a real situation, i. e., in a real application the subsoil model is always an idealized and simplified version of a real environment. First of all, the subsoil model in the reduced version is composed by 51 rectangles of 500 m horizontal width, while the vertical and horizontal density contrast variations are the same as in the original model. The number of observation points used in the inversion is in this case 39, which were randomly selected from the original set of 99 points. Finally, the linear regional trend model will be estimated during the inversion.

For the inversion, the CP-PSO family member was selected, and three repetitions of the algorithm were combined using in each one a swarm of 200 models, and performing in each case 100 iterations, i. e., a total of 60 000 models were generated. The user is strongly encouraged to read the GRaVPSO2D reference manual in order to obtain an extended discussion about the behavior of the different PSO family members and about the different approaches to perform an inversion.

For the filtering step, a window of width 5 elements was selected, being all the coefficients of value 1. Two passes of the filter were employed, because it was observed that in order to obtain smooth results (and in this synthetic example this is the kind of the sediments-basement interface) it is more convenient to use a narrow window combined with two passes instead of a single pass with a

286 wider filtering window. Also borehole information as absolute constraints were
 287 used, considering semi fixed (with a 10 m freedom) the depths of three rectangles
 288 (numbers 12, 13, and 31). About the cost function computation, the L_2 norm is
 289 employed considering weights based on the inverse of the observations variances.

FIGURE B.3 HERE (TWO COLUMN WIDTH)

290 Fig. B.3 (left) shows the general results of the inversion corresponding to the
 291 best model (the one among all the generated models which produces the mini-
 292 mum cost function value, which corresponds to a 2.91 % relative misfit). This
 293 plot is generated by the `grav2d_Plot.m` script, and it is composed mainly by two
 294 parts. The upper one shows the inversion residuals corresponding to each obser-
 295 vation point, while the lower part presents a general overview of the estimated
 296 sediments-basement interface. This interface is composed, in turn, by the depths
 297 corresponding to the best model, and a range of depths comprising all generated
 298 models inside the equivalent region with relative misfit lower than a selected value
 299 by the user, 4.5 %, in this case. **At this point there is a limitation related to the fil-**
 300 **tering step that must be taken into account. Due to border effects in filtering the**
 301 **rectangles close to the profile ends must be analyzed carefully, and sometimes**
 302 **ignored. In such rectangles, where in general the sediments depth is shallow, the**
 303 **border effects of the filtering step produce in many cases unrealistic results that**
 304 **could not match the actual basement-sediments interface.**

305 Fig. B.4 presents an important plot also generated by the `grav2d_Plot.m`
 306 script. For each rectangle, this plot contains in its upper part the cumulative dis-
 307 tribution function computed using all the models inside the working equivalent
 308 region (4.5 % in this example), and in its lower part the corresponding histogram.
 309 These plots are important because the user can inspect the probability distribution

of each parameter in detail. In this case, the distribution for the rectangle number 22 is clearly unimodal with depth 491.3 m, and quasi-symmetrical. This is a more convenient way to describe the uncertainty in nonlinear inverse problems than its classical expression through the most probable value plus a standard deviation, specially when the probability is far from the normal distribution (Pallero et al., 2018). But in B.4 it can also be seen that the most probable depth according to the histogram for rectangle number 22 (491.3 m) does not match the depth deduced from the best model (497.5 m), i. e., the global best model (the one with the lowest relative misfit) is not necessary composed by the set of the most probable depths of each individual rectangle. In this particular case, the relative difference in depths with respect to the depth from the best model is 1.25 %.

FIGURE B.4 HERE (ONE COLUMN WIDTH)

In addition to the best model, a model composed by the individual most probable depths of each rectangle is generated by `grav2d_Plot.m` and called median model. In this example, the median model has a relative misfit of 3.33 % (see Fig. B.3, right), and together with the best model and the individual histograms provides a powerful information to perform the inverse problem uncertainty assessment.

FIGURE B.5 HERE (TWO COLUMN WIDTH)

Fig. B.5 shows the CDFs and histograms corresponding to the rectangle number 15 after the inversion using absolute constraints (left) and without using absolute constraints² (right). The rectangle number 15 is situated in the neighborhood of one of the absolute constraints, but not strictly contiguous, so it is a good can-

²All the other parameters in this inversion are the same as in the case of the previous experiment.

331 didate to check the influence of this kind of constraints not only in the affected
 332 rectangles itself, but also in a small area around it. As it can be seen, in both
 333 cases the histogram presents only one maximum and a near symmetrical shape,
 334 but in the inversion with absolute constraints the estimated depth is closer to the
 335 true one that in the case of inversion without absolute constraints. So the use of
 336 absolute constraints has influence not only in the affected rectangles, but also in
 337 their neighborhood. Finally, the estimated regional trend has parameters of value
 338 $A_0 = -98.675 \text{ mGal}$, and $A_1 = 1.2117 \cdot 10^{-3} \text{ mGal m}^{-1}$, presenting their corre-
 339 sponding histograms (not shown here) only one mode.

340 Figs. B.3, B.4, and B.5 show, together with the estimated model, the true
 341 model (green line). As it can be shown, there are differences between it and the
 342 best and median models. All these differences are a consequence of the well
 343 known characteristics of inverse problems, i. e., their inherent non-uniqueness in
 344 the case of potential field based methods, the presence of noise in observations
 345 (Fernández-Martínez et al., 2014a,b), the always finite number of observations,
 346 the idealization of the model, which is in all cases a simplification of the reality,
 347 etc. All these sources of uncertainty make the task of the inverse problems not
 348 only to find the *best* model, considered as the one that adjusts the observations
 349 with minimum misfit, but a task of determination of a collection of models that are
 350 compatible at a certain level of error with all the prior information (observations,
 351 previous models, particular information of a specific parameter, etc.) at a disposal
 352 (Scales and Snieder, 2000; Tarantola, 2006).

7. Real example

An application of GravPSO2D package for the inversion of observed gravity data is provided in this section. For more reliability with our previous works describing the theoretical aspects of the inversion scheme (Pallero et al., 2015; Fernández-Martínez et al., 2017) we provide here the original data corresponding to the gravity profile already discussed in these papers. In addition, with the aim at giving more replicable examples for users we have also extended this dataset with 3 other available gravity profiles also acquired during the same survey.

This dataset, acquired from a gravity survey carried out in the Atacama Desert (north Chile) by Gabalda et al. (2005), with the purpose of the basement relief of a sedimentary basin estimation, where irregular sediment thickness was suspected (presence of paleo-valleys). This region of central Andes (see Fig. B.6 for a general overview) is characterized by these continental sediments, known as the Atacama Gravels formation, derived from the Andes mountains' erosion, and deposited in a central depression formed during the built up of the Andean system in response to the subduction of the oceanic Nazca plate beneath the South American continent (Mortimer, 1973; Riquelme, 2003). These sediments deposited on the western flank of the Andean system in El Salado valley are composed of low density materials (fluvial gravels, sand and clays intercalated with ignimbrite layers (Cornejo et al., 1993)). As described in Nalpas et al. (2008), the Atacama Gravels preserved along of the Río Salado catchment represent the infill of a drainage system of paleo-valleys converging to a canyon outlet open towards the Pacific Ocean (see Fig. B.7, dash line with arrow), indicating exoreic conditions just before sedimentation. The preservation of the Atacama Gravels was related to a fall of fluvial transport capacity (limiting the mass transfer to the ocean and initiat-

ing the sedimentation) consecutive to a progressive climatic shift towards aridity during the Miocene. Field observations suggest that the thickness of the Atacama Gravels may reach around 150 m to 200 m in the Central Depression, and up to 500 m in the “Pampa del Inca” paleovalley north of Potrerillos in the Domeyko Cordillera (Nalpas et al., 2008).

FIGURE B.6 HERE (TWO COLUMN WIDTH)

The density contrast sediments-basement has been estimated at around $\Delta\rho = -800 \text{ kg m}^{-3}$ (Gabalda et al., 2005). This high density contrast and the well preserved nature of these basins, due to the arid climatic conditions in this region, make the Atacama Gravels formation a suitable candidate for basement relief estimation via the gravity inverse problem. Moreover, two observable contacts along the El Salado valley between the dense substratum and the low density sedimentary filling (Figs. B.6 and B.7, red stars) provide valuable information for the gravity data inversion interpretation. Details on the gravity and GPS data acquisition and processing performed according to the state-of-the-art for precise gravity surveys can be found in Gabalda et al. (2003, 2005).

FIGURE B.7 HERE (TWO COLUMN WIDTH)

The dataset is composed of four gravity profiles acquired in uneven topography area with elevations ranges between 800 m to 2400 m (see location of the 4 profiles on Figs. B.6, and B.7). Three of them (P1, P2, and P3) have an orientation W-E and an average altitude between 1200 m and 1500 m, while the fourth one (P4) shows an orientation mainly NW-SE and an average altitude of about 2100 m (in any case, all profiles present an ascending topography eastward). The number of observed gravity measurements and the lengths for each profile are respectively 52 points and 25 km for P1, 53 points and 31 km for P2, 51 points

401 and 18 km for P3, and 32 points and 14 km for P4. The uncertainties of grav-
 402 ity and height data are estimated to be better than 20 μGal and 5 cm respectively.
 403 The interpreted final gravity values (complete Bouguer anomalies) include terrain
 404 corrections computed using a 90 m resolution topographic model.

405 In order to apply GRAVPSO2D to the observed profiles, we have used in all
 406 cases the CP-PSO family member, a swarm of 200 models with 200 iterations,
 407 and 3 repetitions were combined, which means that a total of 120 000 generated
 408 models for each profile inversion. The L_2 norm was used for the cost function
 409 evaluation, and two passes of a 3-element filter window with coefficients equal
 410 to 1 was applied. In all cases, a fixed density contrast sediments-basement of
 411 $\Delta\rho = -800 \text{ kg m}^{-3}$ was employed accordingly to previous estimations (Gabalda
 412 et al., 2005). The subsoil for each profile has been discretized into vertical rect-
 413 angles of width corresponding to the mean separation of the observed gravity
 414 measurements. We thus obtain, 52 rectangles of width equal to 490 m for P1, 53
 415 rectangles of width equal to 550 m for P2, 52 rectangles of width 360 m for P3
 416 and 33 rectangles of width 420 m for P4. A first regional trend approximation is
 417 automatically subtracted from the observed Bouguer anomaly profile with the ob-
 418 jective of isolate the residual gravity anomaly. The final regional trend (first order
 419 polynomial was chosen) is automatically estimated during the inversion process
 420 for removing the long wavelength gravity signal produced by the regional grav-
 421 ity (here mostly related with the deep crustal root of the Andes). In our case,
 422 the residual signal is thus supposed to be generated by the sedimentary filling of
 423 the Atacama Gravels formation in a local pre-existing morphological basin. The
 424 results of the inversion process are discussed hereafter.

FIGURE B.8 HERE (TWO COLUMN WIDTH)

Fig. B.8 shows the median estimated models for P1 (left), and P2 (right), together with the 5% relative error equivalent region. In the case of P1, the profile shows two sub-basins, separated at approximately a length of 15 km along the profile by an outcropped basement observable in the field. The westwards sub-basin presents a maximum depth of 100 m with limits for the 5% equivalent region between 92 m, and 108 m. The eastwards sub-basin shows a maximum depth of 93 m with limits for the 5% equivalent region between 86 m, and 100 m. Fig. B.11 (left and center) shows the cumulative distribution functions and the corresponding histograms for the two described rectangles corresponding to the maximum thickness. In P2 a deeper filling is observed in the first half of the profile, where the maximum depth reaches 227 m, with limits for the 5% equivalent region between 196 m and 256 m. Fig. B.11 (right) shows the cumulative distribution function and the corresponding histogram for this deepest point. As it can be seen, although the depth amplitude for the 5% equivalent region in this case is apparently wide (around 60 m), the histogram shows there is a clear maximum between depths 220 m and 230 m, so this region contains the maximum probability for the rectangle's depth.

FIGURE B.9 HERE (TWO COLUMN WIDTH)

Fig. B.9 shows the median estimated models for P3 (left), and P4 (right), together with the 5% relative error equivalent region. In the case of P3, the profile shows an irregular basin bottom topography, with a shallow region around a distance of 7 km from the initial point that divides the profile in two sub-basins. The westwards sub-basin presents a maximum depth of about 109 m with limits for the 5% equivalent region between 96 m, and 122 m. The eastwards sub-basin shows a maximum depth of 110 m with limits for the 5% equivalent region between

100 m, and 121 m. Fig. B.12 (left and center) shows the cumulative distribution functions and the corresponding histograms for the two described rectangles. In P4 the deepest region corresponds roughly to the center of the profile, where the maximum depth reaches around 322 m, being the deepest point in the four profiles. The limits for the 5% equivalent region are between 300 m, and 344 m. Fig. B.12 (right) shows the cumulative distribution function and the corresponding histogram for the rectangle. About the estimated regional trend, all profiles present a slope of value $\sim -3.26 \text{ mGal km}^{-1}$ (the adjusted values corresponding to the median models are $-3.35 \text{ mGal km}^{-1}$, $-3.23 \text{ mGal km}^{-1}$, $-3.26 \text{ mGal km}^{-1}$, and $-3.23 \text{ mGal km}^{-1}$ for profiles P1, P2, P3, and P4 respectively). Fig. B.13 shows the original and residual anomaly, as well as the adjusted trend for the P1 (left), and P2 (right) profiles, while Fig. B.14 represents the same data for the P3 (left), and P4 (right) profiles.

In addition to the geological constraints given on the termination of the sedimentary filling (outcropping basement) along the surveyed gravity profiles, we also have direct field observations of the actual thickness of the Atacama Gravels near the profiles P2 and P4 revealed by the erosion of the Río Salado, which allows to see locally the altitude of the base of the gravels (see Figs. B.6, and B.7, red stars). These deposits correspond to a sedimentary layer with a variable thickness, moderate in the central depression (100 m to 200 m) and more important upstream for the paleovalleys, which reach the Cordillera of Domeyco (going up to 500 m), like the “Pampa del Inca” paleovalley, north of Potrerillos (Nalpas et al., 2008).

For the P4 profile the “Quebrada El Salado” completely intersects the Atacama Gravels NE of the profile, a little upstream of the paleovalley of the “Pampa del Inca”, where the maximum thickness of the Graves of Atacama is about 360 m

(base at 1820 m, top at 2180 m). This value in the field is entirely in agreement with the thickness deduced from the inversion of the P4 profile which is 322 m (see Figs. B.9, right, and B.12, right), about 40 m less which corresponds to the gradual decrease in the thickness of the Atacama Gravels on along the paleovalley towards the central depression.

For the P2 profile the “Quebrada El Salado” cuts the Atacama Gravels near the western end of the El Salvador runway, where the maximum observed thickness of the Graves of Atacama is about 70 m (base at 1425 m, and top at 1495 m). As the point is located on the southern edge of the paleovalley coming from El Salvador, it is expected to have a slightly smaller thickness compared to the value of the profile, around 80 m, which is more in the axis of this paleovalley.

8. Conclusions

In this paper GRAVPSO2D, a Matlab software for 2D gravity inversion in sedimentary basins using the Particle Swarm Optimization algorithm has been presented. This software represents the first effort to provide the scientific community with a tool based on the PSO for this particular problem. GRAVPSO2D is freely available and includes an exhaustive reference manual where all the details related to the input data, file formats, and output results are exposed and analyzed.

It is of particular importance for results interpretation the analysis of the posterior probability distributions of the parameters, an important task that can be accomplished with the help of the powerful and smart ability of the PSO algorithm for sampling the parameters space. We showed its application to sedimentary basin relief estimation in synthetic and real cases.

The real test case presented in this paper contains a dataset of various profiles

corresponding to different basin geometries and depths. This dataset acquired in a context of uneven topography and of significant regional gravity anomaly also represent a standard gravity dataset that will enable the user to better handle the inversion and the parameterization taking into account the actual terrain topography and the regional trend. It can be concluded that GRAVPSO2D is a powerful software to invert and assess the uncertainty of the solution in this kind of problems via a whole family of PSO optimizers.

9. Computer code availability

The source code of GRAVPSO2D will be available free of charge in the BGI's webpage (<http://bgi.obs-mip.fr/>), and in <https://github.com/jgpallero/grav-pso-2d>.

10. Declaration of competing interest

The authors declare that they have no known competing financial interests nor personal relationships that could have appeared to influence the work reported in this paper.

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520 **Appendix A. Gravity attraction due to a constant density rectangle over an**
 521 **exterior point**

522 Let a rectangle of density ρ , defined by the coordinates (see Fig. B.10) x mini-
 523 mum x_m , x maximum x_M , z of top side z_t , and z of bottom side z_b . The gravitational
 524 attraction generated by this polygon at an arbitrary point $P(x, y)$ is (Barbosa and
 525 Silva, 1994; Telford et al., 1976)

$$\begin{aligned}
 F &= F(x, z, x_m, x_M, z_t, z_b, \rho) \\
 &= G\rho \left[A \ln \frac{A^2 + D^2}{A^2 + C^2} - B \ln \frac{B^2 + D^2}{B^2 + C^2} \right. \\
 &\quad \left. - 2C \left(\arctan \frac{A}{C} - \arctan \frac{B}{C} \right) \right. \\
 &\quad \left. + 2D \left(\arctan \frac{A}{D} - \arctan \frac{B}{D} \right) \right], \tag{A.1}
 \end{aligned}$$

526 where $A = x - x_m$, $B = x - x_M$, $C = z - z_t$, $D = z - z_b$, and G is the Newton's
 527 constant.

FIGURE B.10 HERE (ONE COLUMN WIDTH)

528 **Appendix B. Additional figures**

529 In this appendix some auxiliary figures referred in section 7 are shown.

FIGURE B.11 HERE (TWO COLUMN WIDTH)

FIGURE B.12 HERE (TWO COLUMN WIDTH)

FIGURE B.13 HERE (TWO COLUMN WIDTH)

FIGURE B.14 HERE (TWO COLUMN WIDTH)

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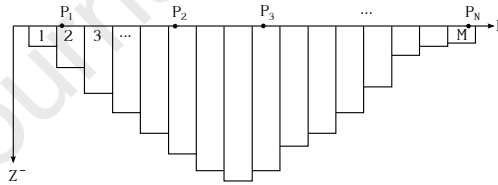


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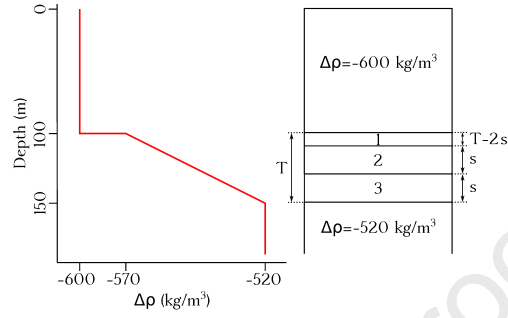


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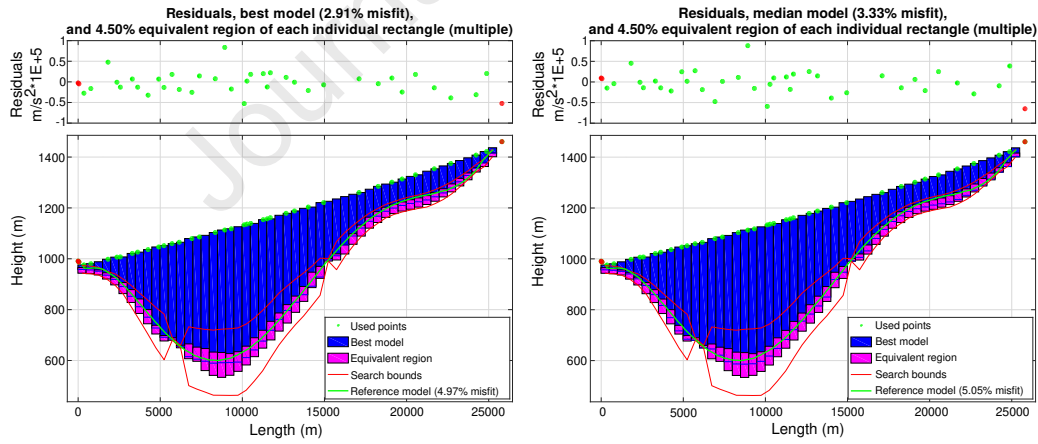


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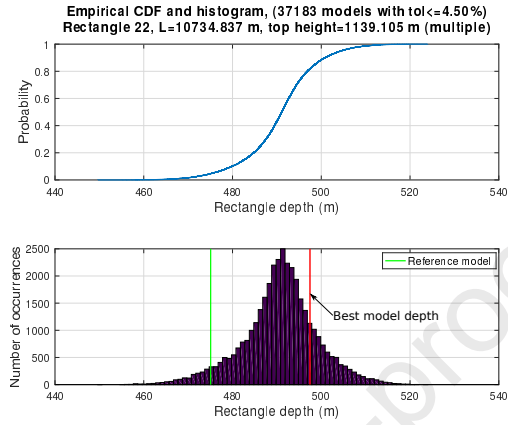


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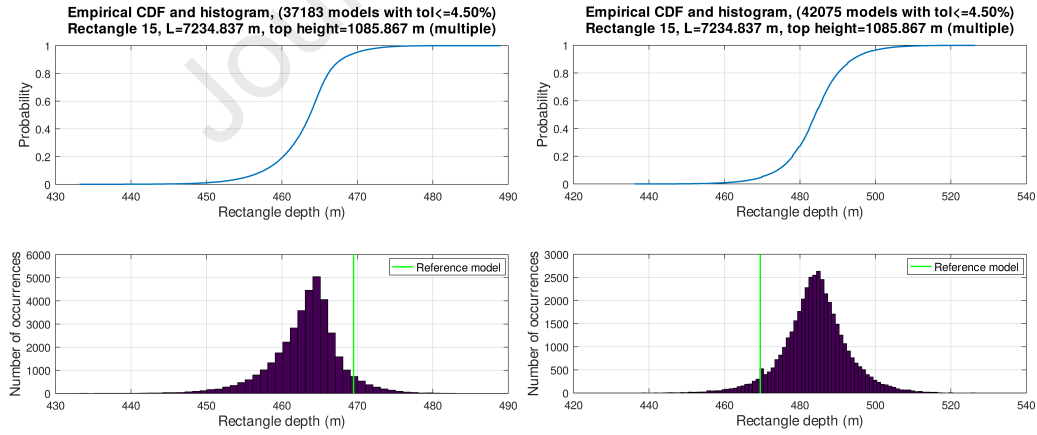


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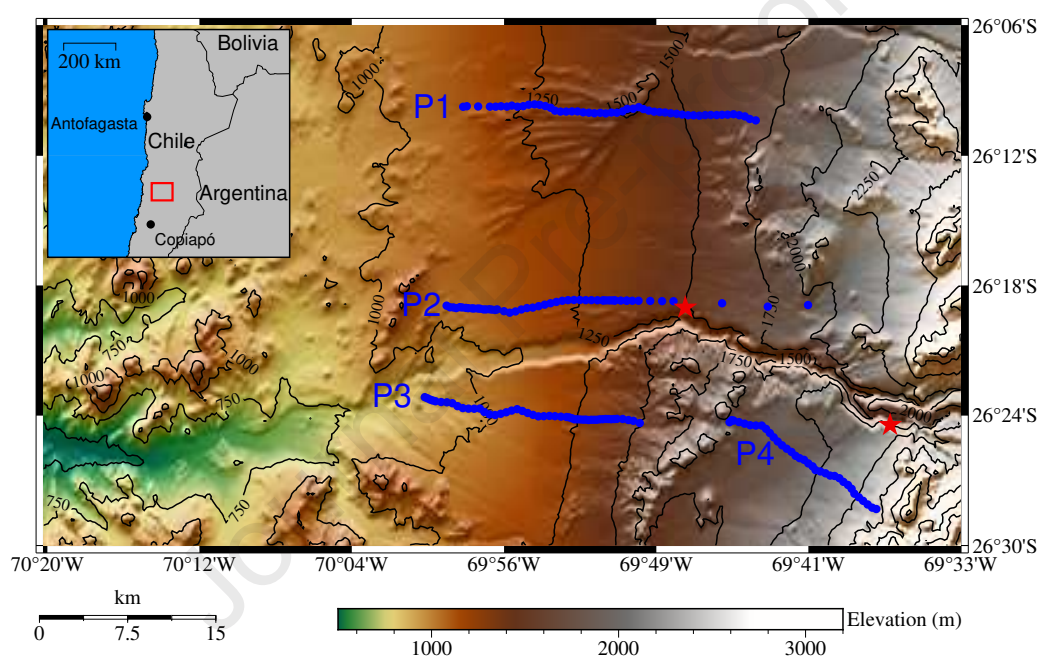


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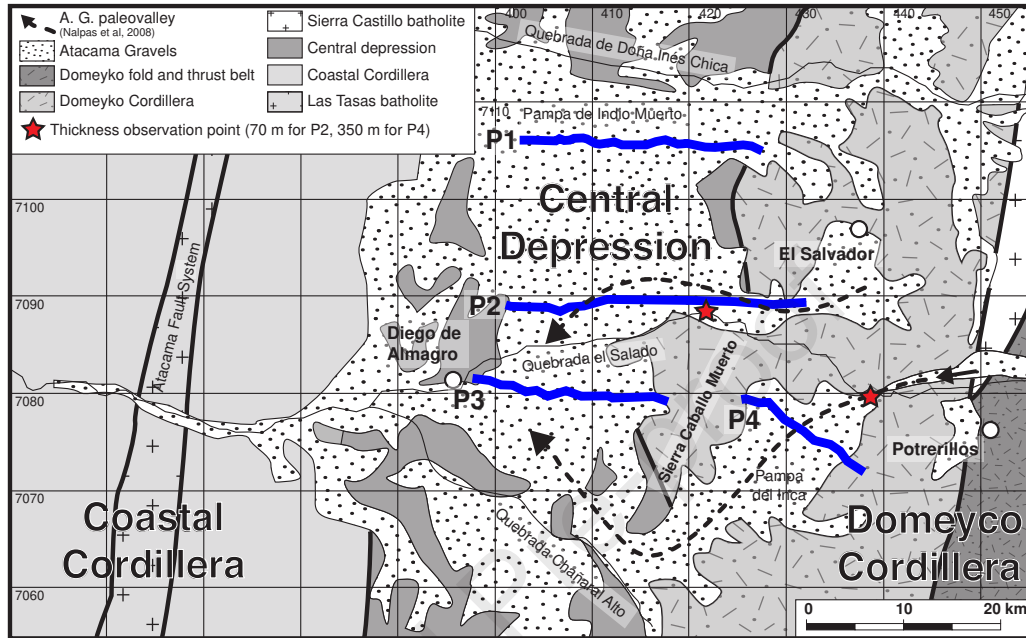


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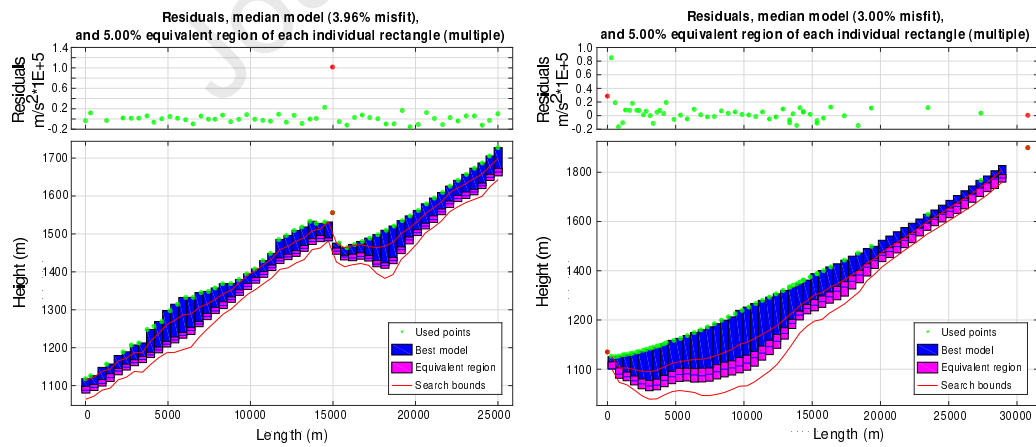


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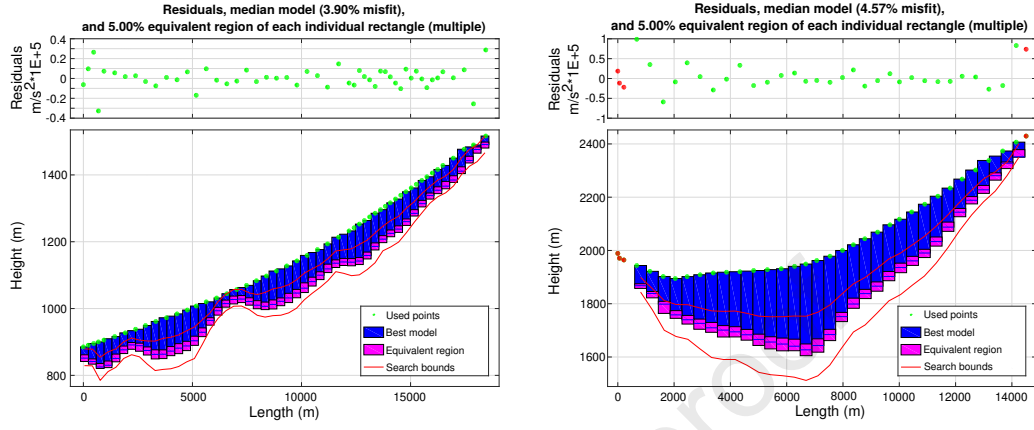


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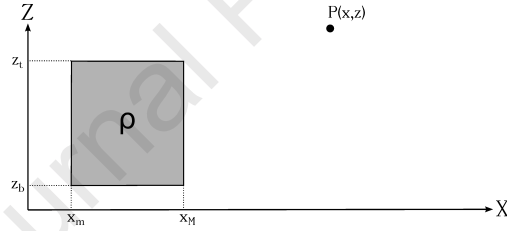


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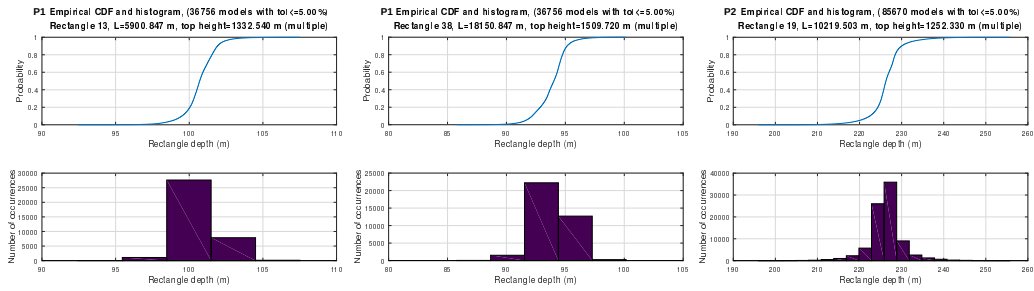


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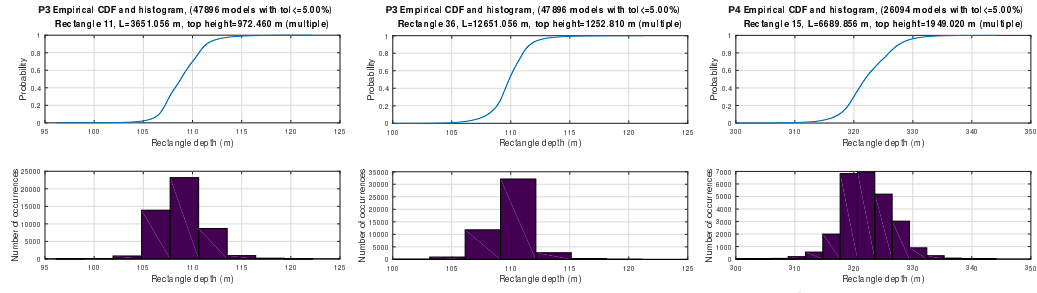


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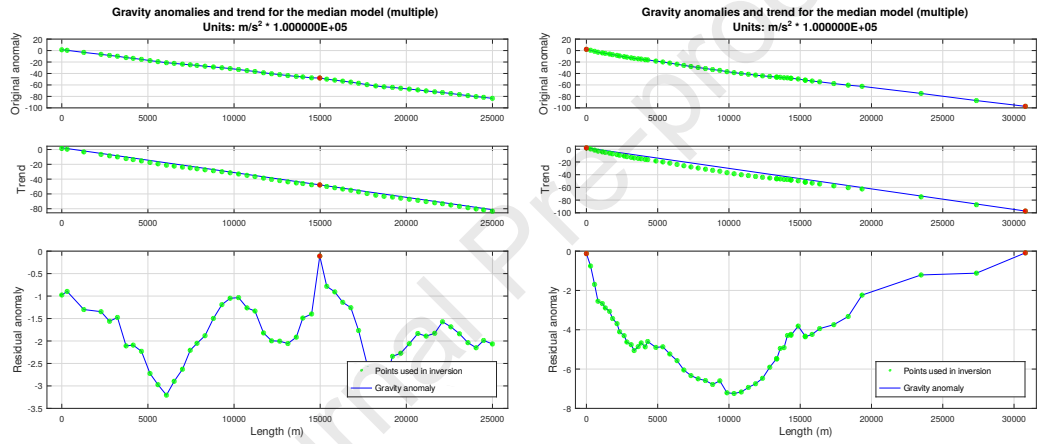


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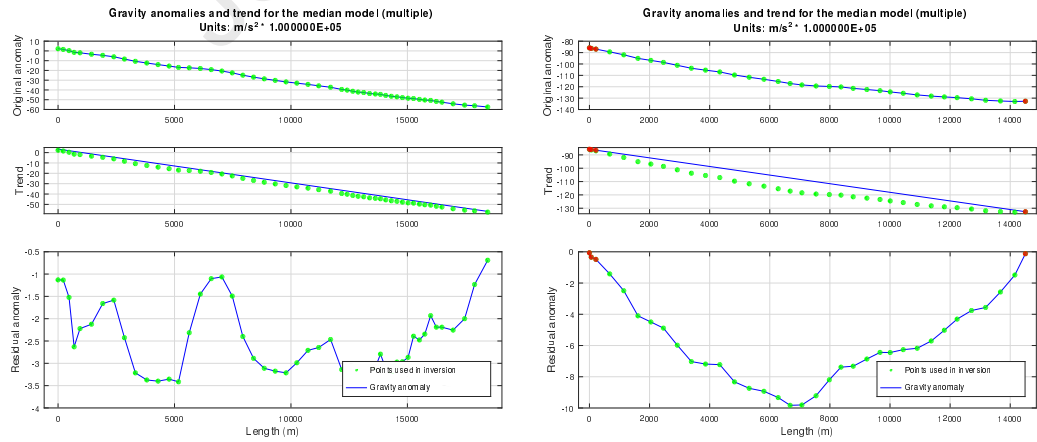


Figure B.14: