Inversion of a model sedimentary basin using Simulated Annealing

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Overview

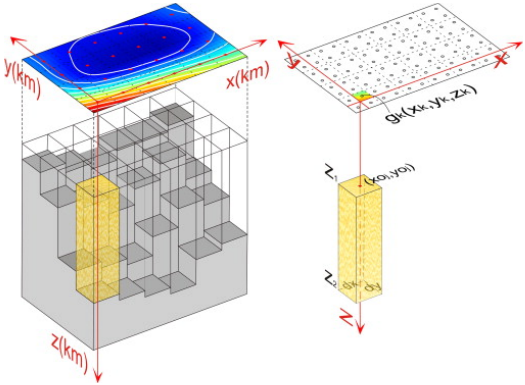
Introduction

According to Nagy, it is possible to **describe an arbitrary geological configuration in subsurface considering blocks composed of prisms with different dimensions**.

The distribution of vertical components associated with the gravitational attraction of a right rectangular prism with density varying with depth following a third order polynomial can be used to find this geological configuration through through the use of a global optimization algorithms.

Direct Model - Problem

A sedimentary basin is constituted by a sedimentary and an homogeneous basement. This sedimentary package is discretized by prisms contained in a finite region of space with a mesh in which the top coincides to the Earth's surface The arbitrary interface separating the sedimentary is described as points by the thickness of each of the prisms.



Direct Model

- In direct modeling we predict the field generated by a mathematical model and estimate the error with respect to the information obtained in the field.

The gravitational attraction of an elementary mass with respect to a unit mass located at a distance r is given by:

$$F_z = \int\int\int \frac{G\rho\cos\gamma}{r^2} dx' dy' dz' \quad (1)$$

Considering a coordinate system with the z-axis schematized according to the figure [citation] where the angle formed between the distance vector $r = \sqrt{(x' - x_0)^2 + (y' - y_0)^2 + (z' - z_0)^2}$ and the z-axis is given by γ. Applying the equation in the differential gravitational attraction component$dF_z = dF\cos\gamma$, we obtain the following expression:

Direct Model

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$$F_z = \int\int\int \frac{G\rho\cos\gamma}{r^2} dx' dy' dz' \tag{2}$$

and considering $\cos\gamma = (z' - z_0)/r$:

$$\begin{aligned} g_z &= G\int_{x_1'}^{x_2'}\int_{y_1'}^{y_2'}\int_{z_1'}^{z_2'} \frac{\rho(z')\cos\gamma}{r^3} dx' dy' dz' \\ &= G\int_{x_1'}^{x_2'}\int_{y_1'}^{y_2'}\int_{z_1'}^{z_2'} \frac{\rho(z')(z'-z_0)}{[(x'-x_0)^2+(y'-y_0)^2+(z'-z_0)^2]^{3/2}} dx' dy' dz' \end{aligned} \tag{3}$$

Direct Model

Applying the following transformation of coordinates:

$$x_n = x'_n - x_0 \tag{4}$$
$$x_n = y'_n - y_0 \tag{5}$$
$$z_n = z'_n - z_0 \tag{6}$$

with n=1,2 in which the prisms are limited by the planes $x' = x'_1, x'_2$, $y' = y'_1 . y'_2$ and $z' = z'_1, z'_2$; dx'=dx, dy'=dy e dz'=dz, we obtain:

$$g_z = G \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \int_{z_1}^{z_2} \frac{\rho(z')(z' - z_0)dz}{(x^2 + y^2 + z^2)^{3/2}} \tag{7}$$

Direct Model

Considering the following density as a function of the depth as:

$$\rho(z') = p + qz' + rz'^2 + sz'^3 \tag{8}$$

$$\begin{aligned}\rho(z) &= p + q(z+z_0) + r(z+z_0)^2 + s(z+z_0)^3 = (p + qz_0 + rz_0^2 + sz_0^3) \\ &+ (q + 2rz_0 + 3sz_0^2)z + (r + 3sz_0)z^2 + sz^3\end{aligned} \tag{9}$$

Substituting equation (9) into (7) :

$$g_z = G\int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \int_{z_1}^{z_2} \frac{(\rho_1 z + \rho_2 z^2 + \rho_3 z^3 + \rho_4 z^4)dz}{(x^2+y^2+z^2)^{3/2}} \tag{10}$$

$$\rho_1 = p + qz_0 + rz_0^2 + sz_0^3 \tag{11}$$

$$\rho_2 = q + 2rz_0 + 3sz_0^2 \tag{12}$$

$$\rho_3 = r + 3sz_0 \tag{13}$$

$$\rho_4 = s \tag{14}$$

Direct Model

Equation (10) can be simplified:

$$g_z = G \sum_{n=1}^{n=4} \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \int_{z_1}^{z_2} \frac{(\rho_k z^k) dz}{(x^2 + y^2 + z^2)^{3/2}} = G \sum_{n=1}^{n=4} I_k \tag{15}$$

for k=1:

$$\begin{aligned} I_1 = -\rho_1 \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} \frac{1}{(x^2 + y^2 + z^2)^{1/2}} dy \Big|_{z_1}^{z_2} = \\ -\rho_1 \int_{x_1}^{x_2} \ln\left(y + \sqrt{x^2 + y^2 + z^2}\right) dx \Big|_{y_1}^{y_2} \Big|_{z_1}^{z_2} \end{aligned} \tag{16}$$

Direct Model

Integration $\int fdg = fg - \int gdf$ in the equation (16) as dg=dx :

$$
\begin{aligned}
I_1 &= -\rho_1[x\ln\left(y+\sqrt{x^2+y^2+z^2}\right)|_{x_1}^{x_2} \\
&- \int_{x_1}^{x_2} \frac{x^2(\sqrt{x^2+y^2+z^2}-y)}{(x^2+z^2)\sqrt{x^2+y^2+z^2}}dx]|_{y_1}^{y_2}|_{z_1}^{z_2} \\
&= -\rho_1[x\ln\left(y+\sqrt{x^2+y^2+z^2}\right)|_{x_1}^{x_2} - \int_{x_1}^{x_2} \frac{x^2}{x^2+z^2}dx \\
&+ y\int_{x_1}^{x_2} \frac{x^2}{(x^2+z^2)\sqrt{x^2+y^2+z^2}}]|_{y_1}^{y_2}|_{z_1}^{z_2}
\end{aligned}
\tag{17}
$$

Direct Model

But the second term of the previous equation is 0, which means:

$$
\begin{aligned}
I_1 &= -\rho_1[x\ln\left(y+\sqrt{x^2+y^2+z^2}\right) \\
&+y[\int_{x_1}^{x_2}\frac{x^2+z^2-z^2}{(x^2+z^2)\sqrt{x^2+y^2+z^2}}]]|_{y_1}^{y_2}|_{z_1}^{z_2} \\
&= -\rho_1\left[x\ln\left(y+\sqrt{x^2+y^2+z^2}\right)|_{x_1}^{x_2}+I\right]|_{y_1}^{y_2}|_{z_1}^{z_2}
\end{aligned}
\tag{18}
$$

$$
\begin{aligned}
I &= y\int_{x_1}^{x_2}\frac{dx}{\sqrt{x^2+y^2+z^2}}-yz^2\int_{x_1}^{x_2}\frac{dx}{(x^2+z^2)\sqrt{x^2+y^2+z^2}} \\
&= y\left[\ln\left(x+\sqrt{x^2+y^2+z^2}\right)|_{x_1}^{x_2}-z^2\int_{x_1}^{x_2}\frac{dx}{(x^2+z^2)\sqrt{x^2+y^2+z^2}}\right] \\
&= y[\ln\left(x+\sqrt{x^2+y^2+z^2}\right)-\frac{z}{y}\arctan\left(\frac{xy}{z\sqrt{x^2+y^2+z^2}}\right)]|_{x_1}^{x_2}
\end{aligned}
\tag{19}
$$

Direct Model

Considering $x = \tan\theta\sqrt{y^2+z^2}$ and $y\sin\theta = \rho$ we can compute I_1 through 24 terms after substituting the intergration limits:

$$I_1 = \rho_1(-x\ln\left(y+\sqrt{x^2+y^2+z^2}\right) - y\ln\left(x+\sqrt{x^2+y^2+z^2}\right)$$
$$+z\arctan\left(\frac{xy}{z\sqrt{x^2+y^2+z^2}}\right))\Big|_{x_1}^{x_2}\Big|_{y_1}^{y_2}\Big|_{z_1}^{z_2} \tag{20}$$

This solution is applied to problems whose prisms exhibits a constant density ($\rho_1 = cte, \rho_2 = rho_3 = \rho_4 = 0$). **Our model is based on the density as a cubic polynomial equation**, which guides us towards the recurrence formulas for I_2, I_3 e I_4.

Direct Model

For k=2:

$$
\begin{aligned}
I_2 &= \rho_2 \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \int_{z_1}^{z_2} \frac{z^2 dz}{(x^2+y^2+z^2)^{3/2}} \\
&= \rho_2 \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \left[\ln(z+r) - \frac{z}{r}\right] \Big|_{z_1}^{z_2} \\
&= \rho_2 \int_{x_1}^{x_2} dx \left[y \ln(z+r) - x \arctan\left(\frac{zy}{xr}\right)\right] \Big|_{y_1}^{y_2} \Big|_{z_1}^{z_2} \\
&= \rho_2 [yx \ln(z+r) - \frac{y^2}{2} \arctan\left(\frac{zx}{yr}\right) - \frac{x^2}{2} \arctan\left(\frac{zy}{xr}\right) \\
&+ \frac{z^2}{2} \arctan\left(\frac{xy}{zr}\right)] \Big|_{x_1}^{x_2} \Big|_{y_1}^{y_2} \Big|_{z_1}^{z_2}
\end{aligned}
\tag{21}
$$

Direct Model

For k=3:

$$
\begin{aligned}
I_3 &= \rho_3 \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \int_{z_1}^{z_2} \frac{z^3 dz}{(x^2+y^2+z^2)^{3/2}} \\
&= \rho_3 \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \left[r + \frac{(x^2+y^2)}{r} \right] \Big|_{z_1}^{z_2} \\
&= \rho_3 \int_{x_1}^{x_2} dx \left[x^2 \ln(y+r) + yr \right] \Big|_{y_1}^{y_2} \Big|_{z_1}^{z_2} \\
&= \rho_3 \left[\frac{y^3}{3} \ln(x+r) + \frac{x^3}{3} \ln(y+r) + \frac{z^3}{3} \arctan\left(\frac{xy}{zr}\right) - \frac{2}{3} xyr \right] \Big|_{x_1}^{x_2} \Big|_{y_1}^{y_2} \Big|_{z_1}^{z_2}
\end{aligned} \tag{22}
$$

Direct Model

For k=4:

$$
\begin{aligned}
I_4 &= \rho_4 \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \int_{z_1}^{z_2} \frac{z^4 dz}{(x^2+y^2+z^2)^{3/2}} \\
&= \rho_4 \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \left[\frac{1}{2} zr + \frac{(x^2+y^2)}{r} z - \frac{3}{2}(x^2+y^2)\ln(z+r) \right] \Big|_{z_1}^{z_2} \\
&= \rho_4 \int_{x_1}^{x_2} dx [\frac{1}{2} yzr + x^3 \arctan\left(\frac{yz}{xr}\right) - \frac{1}{2} y^3 \ln(z+r) - \frac{3}{2} x^2 y \ln(z+r)] \Big|_{y_1}^{y_2} \\
&= \rho_4 [\frac{z^4}{4} \arctan\left(\frac{xy}{zr}\right) + \frac{x^4}{4} \arctan\left(\frac{yz}{xr}\right) + \frac{y^4}{4} \arctan\left(\frac{zx}{yr}\right) \\
&\quad - \frac{xy}{2}(x^2+y^2)\ln(z+r) - \frac{xyzr}{4}] \Big|_{x_1}^{x_2} \Big|_{y_1}^{y_2} \Big|_{z_1}^{z_2}
\end{aligned}
$$

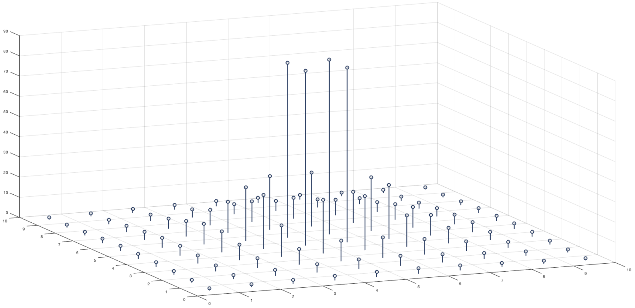


Figure: Rectangular Prism : $x_1 = 4, y_1 = 4, z_1 = 0, x_2 = 6, y_2 = 6, z_1 = 3$ $p_1 = 2560, q_1 = 0, r_1 = 0, s_1 = 0$, grid from 0 until 10 km.

Direct Model - Prism 40x40x60x60x3

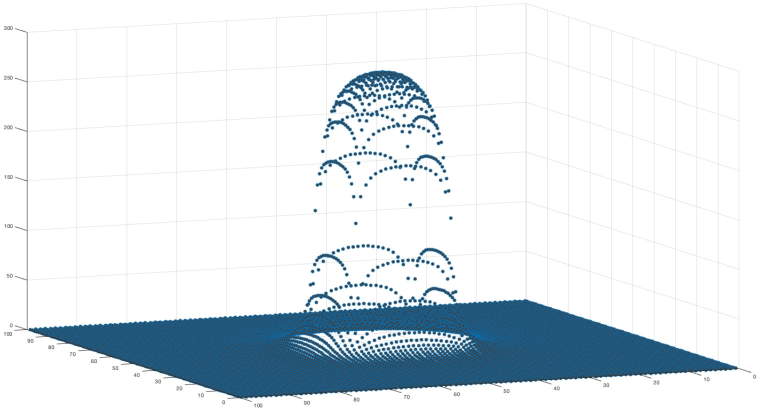


Figure: .

Inversion - SA Algorithm

- How to solve this problem using optimization algorithms?

Evolutionary Algorithms

The simulated annealing method simulates the process of slow cooling of molten metal to achieve the minimum function value in a minimization problem. The cooling phenomenon of the molten metal is simulated by introducing a temperature-like parameter and controlling it using the concept of Boltzmann's probability distribution.

Boltzmann's probability distribution implies that the energy (E) of a system in thermal equilibrium at temperature T is distributed probabilistically according to:

$$P(E) = exp(\frac{E}{k_b T}) \tag{24}$$

Inversion - SA Algorithm

- The convergence of the simulated annealing algorithm can be controlled by controlling the temperature T.
- Start with an initial design vector X1 (iteration number i = 1) and a high value of temperature T .
- Generate a new design point randomly in the vicinity of the current design point and find the difference in function values: $\Delta E = E_{i+1} - E_i = f_{X_{i+1}} - f_{X_i}$
- If $\Delta E \leq 0$ than $P[E_{i+1}] = 1$ and X_{i+1} is accepted
- If $\Delta E > 0$ then the probability of accepting the point X_{i+1}, in spite of its being worse than X_i in terms of the objective function value, is finite (although it may be small) according to the Metropolis criterion.

Inversion - SA Algorithm

Metropolis criterion

According to Metropolis criterion, the probability of the next design point (state) X_{i+1} depends on the difference in the energy state or function values at the two design points (states). $P[E_{i+1}] = [exp(\frac{\Delta E}{T})]$

- If the temperature T is large, the probability will be high for design points X_{i+1} with larger function values, even worse design can be accepted.
- if the temperature T is small, the probability of accepting worse design points X_{i+1}
- as the temperature values get smaller the process gets closer to the optimum solution.

Code

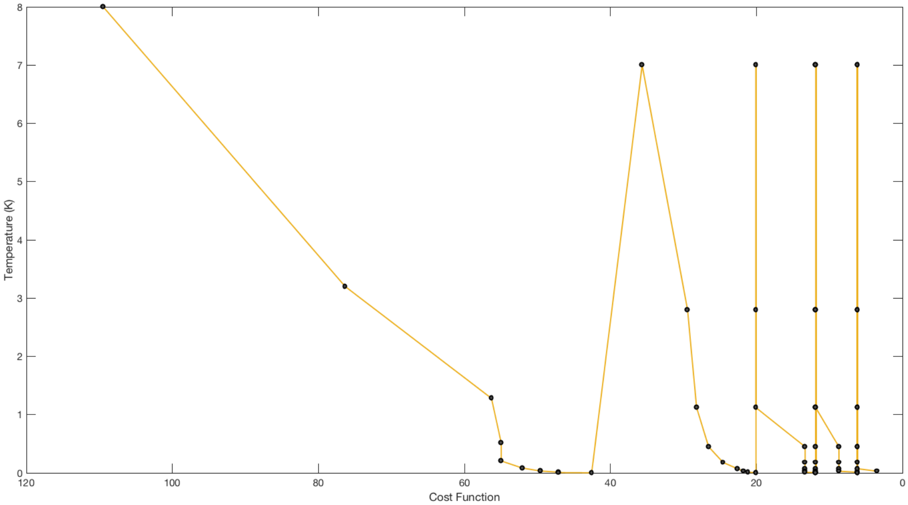
- Generate z and density:
  $z_n(i,j) = REAL(z(i,j) + 2 * e * z(i,j) * (ran3(idum) - 0.5))$
  $p_n = REAL(p1 + 2 * e * p1 * (ran3(idum) - 0.5))$
  $q_n = REAL(q1 + 2 * e * q1 * (ran3(idum) - 0.5))$
  $r_n = REAL(r1 + 2 * e * r1 * (ran3(idum) - 0.5))$
  $s_n = REAL(s1 + 2 * e * s1 * (ran3(idum) - 0.5))$
- Metropolis :
  $IF(fx_n < fx)$THEN - accept
  ELSE $IF((EXP(-(fx_n - fx)/temperatura) >$
  $ran3(idum)).and.(naccepted < a))$ THEN - accept
- Temperature decay:
  $temperatura = temperatura * tfactor$
- Heating process:
  $IF((temperatura < 0.001).and.(emin > 0.1))$ THEN
  $temperatura = 7.0$
  END IF

Parameters to start the optimization:

Parameters

$p_1 = 2000.0000000000000$; $q_1 = 100.00000000000000$
$r_1 = 100.00000000000000$; $s_1 = 1000.0000000000000$
$z_0 = 0.0000000000000000$; $z_1 = 0.0000000000000000$
$xmin = 0.0000000000000000$; xmax = 10.000000000000000
$ymin = 0.0000000000000000$; ymax = 10.000000000000000
temperature = 8.0000000000000000 ; tfactor = 0.40000000000000002
nsteps = 1000 ; idum = 10 ; istep = 1 ; jstep = 1
FINISH-start 880.25350200000003 seconds
Solution: $p_1 = 2562.0402832031250$; $q_1 = 5.3528009448200464E\text{-}004$
$r_1 = 1.8700489774346352E\text{-}002$; $s_1 = 8.7235484897973947E\text{-}006$
Cost function: 3.4913883283133424

Temperature x Cost function



Temperature x Cost function

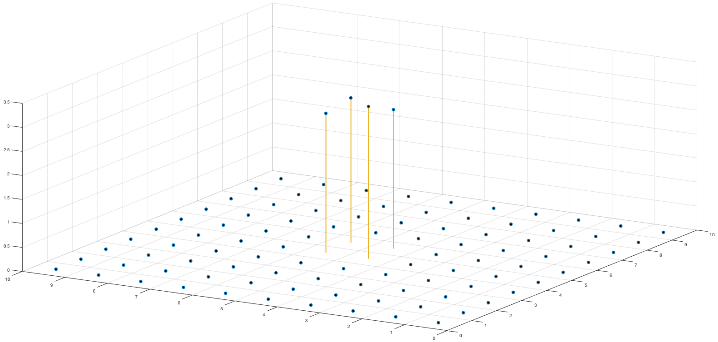


Figure: Prediction of the subsurface after 14 min with an error ¡ $10^{-}3$ due to the chosen cutoff of 3 for the cost function.

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