Some mathematical and numerical developments for improvements in computational efficiency applied to geophysics

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Abstract

Computational efficiency can be greatly improved from preliminary mathematical developments capable of, for example, saving the processing time required in performing numerical calculations present in geophysical studies. Here, we present some well-known numerical methodologies (others not so much) applied in different areas of geophysics, such as: seismic, gravimetry and geothermal. A more in-depth mathematical study of a geophysical problem allows the construction and intelligent use of numerical methods capable of exploring shortcuts that capable of exploring shortcuts that are invisible to the computational use of brute force type. This allows the potentially optimized application of the computational resources available to approach the considered geophysical problem. In many sciences, including geophysics, to solve a problem consist in analysis, model proposing, and then solve the problem based on such model. This last part, generally the whole process involve some complicated relations, things that would be kind of hard to solve with a calculator and a pencil, and it is where numerical methods come in. They are algorithms that, step by step, solve problems like: find zeros of functions of several types, solve linear systems of big size, integrate and take derivatives of a huge number of functions, and they are widely applicable in a great part of geophysics.

1 Introduction

A great matter that is often left aside in the courses of geophysics and mathematics is how the computer solve numerical problems, because as far the calculus class teaches, it's made analytically. Many scientists, in turn the geophysicist, must know how to analyze problems, create models, and then solve them, however this last part, in most of the problems of the science, is just solvable numerically.

The computer is a powerful tool, but in essence only accept orders in a quite directed way, step by step, called algorithm. So, the numerical methods create algorithms in order to solve problems. Since, this article got as objective expose some of that methods with examples of application in the geophysical situations.

2 Theory

The following topics in this section are three numerical methods: Gauss-Newton, Gauss elimination, and Monte Carlo; giving emphasis to the intuitive idea and applications examples instead of the algorithm itself.

2.1 Gauss-Newton's method to find zero of functions

Find zeros of functions is, in general, one of the first subjects to be study in numerical analysis, given the simplicity of the methods, besides the solving impossibility of analytical problems involving high degree polynomial equations. This was proved by the great young mathematician Évariste Galois, that determined the necessary and sufficient conditions to find the roots analytically, and started a study of numerical resolution of equations. There are some methods to find the zeros of functions, like the bisection, secant, Muller, but Gauss-Newton is without doubts the fastest among all; with order of convergence $\rho = 2$, while the secant method got $\rho = 1.618$ and the bisection only has $\rho = 0.5$ (Atkinson, 1988). In practice this means that it is possible to calculate with a desirable precision, the root of a function only with paper, pen and a pocket calculator (and sometimes not even that).

What the Gauss-Newton's method proposes is that would be given a certain value that counts as an initial solution, then find the tangent line of the function at that value, and find the root of it, repeating that process until the difference between two consecutive values is less than the error proposed, or until reach a maximum number of repetitions. This process is illustrated at the Figure 1.

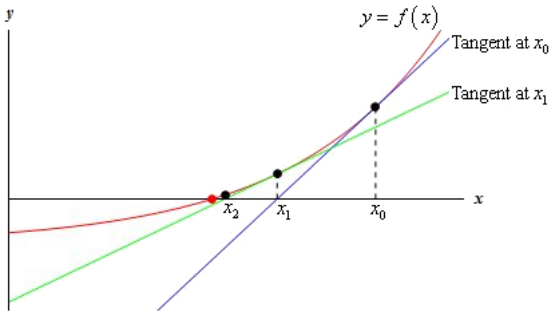

Figure 1: Illustration of the Gauss-Newton's Method (Dawkins)

The equation of the tangent line is an linear approximation of the function, which is nothing more than a first order Taylor polynomial. That can be written as follows:

$$T(x) = f(x_0) + f'(x_0)(x - x_0). \tag{1}$$

Being x_0 the point which the tangent line refers to. So the root of that line look like this:

$$x = x_0 - \frac{f(x_0)}{f'(x_0)}. \tag{2}$$

Well, as will this procedure is repeated a lot of times, the formula for each iteration looks as follow:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}. \tag{3}$$

Despite the fast convergence, to ensure it some conditions must be taken into account, such as: the initial value is supposed to be close to the desirable solution, so it is good to have an interval that is certain to contain a solution. This can be assured in a interval $I =]a, b[$ if the following statement is true:

$$f(a) \cdot f(b) < 0. \tag{4}$$

Also, it is necessary to have an analytic equation of the derivative of the function.

This problem can be solved using the secant method, but in this one is not treated in this paper.

2.2 Gaussian Elimination

Gaussian elimination is a method to solve well behaved linear system, whether it is homogeneous or not; but it is essential to solve a lot of problems involving matrices, like matrix inversion, find determinants, obtain dimension of the space spanned by the columns vectors, calculate eigenvalues and eigenvectors. In this subsection it is presented the algorithm of gaussian elimination with a little bit of theory behind, and ways to decrease the numerical error, as well how to find determinant using this method. The whole point of the Gaussian elimination is to obtain a row equivalent matrix, in other words the space spanned by the row vectors are the same by isomorphism. From the matrix point of view, it is intended to obtain an upper triangular matrix, but for it works there are only permited to operate rows multiplying, subtracting and permuting. Supposing an matrix $\boldsymbol{A} = (a_{ij})$ with dimension $n \times n$:

```
Do this process for 1 ⩽ k ⩽ n − 1
   If a_kk ≠ 0 then:
      Do the below process for every
      row index i > k
         m_ik = a_ik / a_kk
         L_i = L_i − m_ik L_k
      end do
    end if
end do
```

Where L_i is the i-th row of the matrix and a_{kk} are the pivots. The terms m_{ik} are the row multipliers, and there is a reason why they got row and column indexes attached to it. The next sub-section shows how the system is solved.

2.3 Linear systems

The described algorithm can be used to solve linear system of this shape:

$$\boldsymbol{Ax} = \boldsymbol{b}. \tag{5}$$

Being $\boldsymbol{A}$ the coefficient matrix of dimension $n \times n$, $\boldsymbol{b}$ the term independent vector of dimension n, and x the unknown vector. By doing the same operations of the Gaussian elimination on both $\boldsymbol{A}$ and $\boldsymbol{b}$, what is obtained is an equivalent linear system $\boldsymbol{Ux} = \boldsymbol{g}$ of the shape:

$$\begin{bmatrix} u_{11} & \cdots & u_{1n} \\ 0 & \ddots & \vdots \\ \vdots & & \\ 0 & \cdots & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} g_1 \\ \vdots \\ g_n \end{bmatrix} \tag{6}$$

As $\boldsymbol{U}$ is upper triangular, it is easy to find a solution vector, because it is only necessary to do back substitution as follows:

$$x_n = \frac{g_n}{u_{nn}} \tag{7}$$

and

$$x_k = \frac{1}{u_{kk}}[g_k - \sum_{j=k+1}^{n} u_{kj} x_j] \tag{8}$$

where $k = n-1, n-2, \cdots, 1$.

2.4 LU decomposition

A lot of modeling problems in geophysics have the same structure of linear systems, but in that case, the matrix $\boldsymbol{A}$, generally, is composed of geometric quantities, and the vector $\boldsymbol{b}$ the observed data (such as travel time of the seismic waves), and $\boldsymbol{x}$ the parameters of the subsurface model (such as P-wave velocity and layer thickness). However, in realistic life problems, the same matrix $\boldsymbol{A}$ is applied to various $\boldsymbol{b}_k$, so it is interesting to store the values of the row multipliers m_{ik} somewhere. Suppose you store them in an

lower triangular matrix of the following shape:

$$\boldsymbol{L} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ m_{21} & 1 & & \vdots \\ \vdots & & \ddots & 0 \\ m_{n1} & m_{n2} & \cdots & 1 \end{bmatrix}, \tag{9}$$

and with that, it is possible to do the same Gaussian elimination. calculations on the new vector, but with the same row multipliers, saving computer power. The best option though is to store those row multiplyers below the diagonal of the $\boldsymbol{A}$ matrix, because it will save RAM memory since there only got zeros and not going to be used. The $\boldsymbol{A}$ with $n \times n$ dimension should be as follows:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & & a_{1n} \\ m_{21} & a_{22} & & & \vdots \\ \vdots & & \ddots & & \\ & & & a_{(n-1)n} & a_{(n-1)n} \\ m_{n1} & m_{n2} & \cdots & m_{n(n-1)} & a_{nn} \end{bmatrix}, \tag{10}$$

One interesting property of this matrix $\boldsymbol{L}$ is that

$$\boldsymbol{A} = \boldsymbol{L} \times \boldsymbol{U}. \tag{11}$$

This property is due a certain theorem and the proof for it can be found at Atkinson (1988). Despite of that, it is pretty important, mostly when the determinant operator is applied to both sides of the equation:

$$\det \boldsymbol{A} = \det \boldsymbol{L} \times \det \boldsymbol{U}, \tag{12}$$

and as $\det \boldsymbol{L} = 1$, because it is an lower triangular matrix with all the terms in the diagonal equals to one:

$$\det \boldsymbol{A} = \det \boldsymbol{U}. \tag{13}$$

Therefore the determinant of $\boldsymbol{A}$ can be obtained by the product of the terms on the diagonal of $\boldsymbol{U}$.

2.5 Pivoting and Scaling

Although being useful, the pure Gaussian elimination algorithm have a lot of failures. First of all, if the pivot is equal to zero, the row multiplier is impossible to be found (division by zero). Besides that, applying this method on a big linear system, the number of arithmetic operations becomes an great source of numerical error. One of the reasons is because the computer works in binary base, the calculations are made in that base, so it is necessary to convert from decimal to binary, and then convert the result from binary to decimal; generating error (Lopes and Ruggiero, 1988).

To deal with that problem a lot of techniques had arisen, such as pivoting and scaling. Pivoting is nothing more than permuting rows and columns to select an specific pivot, and scaling is multiplying the terms of a row for a given value.

Partial pivoting just permute rows, to obtain a bigger pivot, preventing error. The criteria for that is to use a bigger number in the column (k) being operated, so the term that row multipliers becomes smaller. In an mathematical way:

$$c_k = \max |a_{ik}|, \tag{14}$$

being c_k the pivot to the column k, therefore the row of the pivot and the k row are swapped, and the for optimizing even more, it is good to store the index of the pivot row, so it becomes possible do the same permutations when applying the Gaussian elimination in the independent term vector $\boldsymbol{b}$.

Implicit scaling is an simple trick to make partial pivoting more efficient, only changing the criteria for swapping. To reach that criteria, first is necessary to define a vector with the biggest numbers of each row:

$$s_i = \max |a_{ij}| \; for \; j = 1, \cdots, n; \tag{15}$$

with $i = 1, \cdots, n$. Then the pivot will be the number in the column with the bigger relation between his value and the bigger term at his row. In an mathematical way:

$$c_k = \max \left| \frac{a_i k}{s_i} \right|. \tag{16}$$

2.6 Monte Carlo for integration

The Monte Carlo method is one of the many stochastic ones, on which are generated pseudo random number to obtain numerical results. It is useful to study the behavior of atomic particles, simulating their movement from the principle that they move in an random way. Also, it is useful to calculate the digits of the number π and compute areas, besides compose a relatively simple code.

To calculate the area of one quadrant of an circle of radius r, it is possible to apply the formula for the whole circle, and divide by four, so we have $area = \frac{\pi}{4} r^2$. However, if this quadrant is put inside an square of side length equals r, becomes possible to shot a lot of random numbers to x and y axis. An illustration is shown at Figure 2

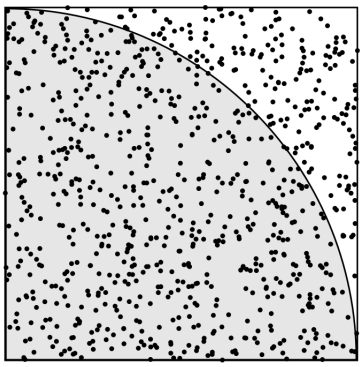

Figure 2: Computing area with Monte Carlo (Cedric, 2013)

Since random numbers generally have a continuous probability distribution on all square, the relation between the numbers of points inside the circle quadrant (n_c) and those that belongs to the whole square (n_q) is given by:

$$\frac{n_c}{n_q} = \frac{C}{Q}, \tag{17}$$

being C the circle quadrant area, and Q is the square area. So isolating the C we have.

$$C = r^2 \frac{n_c}{n_q}. \tag{18}$$

In that way, it is possible to calculate the area of the circle multiplying C by four. If the analytic expression for the area were applied would be possible to calculate π.

It is easy to make an relation between the definite integral and area calculations, because to a certain extent is the same thing. That said, it is possible to compute the integral by defining the $\max f(x)\ for\ a \leqslant x \leqslant b$, being a and b the limits of integration; and then apply the Monte Carlo in the plane, however there is an alternative approach to that problem. One of the implications of the Mean Value Theorem is that the definite integral $\int_a^b f(x)\mathrm{d}x$ is determined by the mean value of f(x) at the interval $a \leqslant x \leqslant b$ (Gould et al., 1996). That way is possible to calculate an approximation to the average picking n values of $f(x_i)$ with x_i being a sequence of random numbers inside the interval. Like this the integral can be defined as follows:

$$\int_a^b f(x)\mathrm{d}x \approx (b-a)\frac{1}{n}\sum_{i=1}^{n} f(x_i). \tag{19}$$

At lower dimensions, other methods like Simpson's Rule, rectangular and trapezoidal approximation are more precise; but at multidimensional integral Monte Carlo is the most efficient method, (Gould et al., 1996).

3 Examples of application at geophysics

This section shows three examples of applications of the numerical methods seen above in different fields of geophysics.

3.1 Geothermal gradient modeling

Suppose there is an model described at Figure 3.

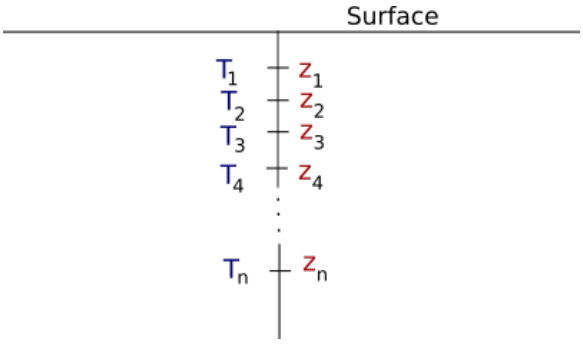

Figure 3: Geothermal prospecting model

In this model are placed temperature T_i at the depths z_i for $i = 1, \cdots, n$. Suppose that theoretically after studying the data, statistically the geothermal gradient at the region is given by the following expression:

$$T(z) = a + bz + cz^2 + dz^3 + ez^4 + fz^5 \tag{20}$$

Then, what remains for the model to be complete is to determine the coefficients a, b, c, e and f. To have this, is necessary to solve the following linear system:

$$\begin{aligned}
T_1 &= T(z_1) = a + bz_1 + cz_1^2 + dz_1^3 + ez_1^4 + fz_1^5 \\
T_2 &= T(z_2) = a + bz_2 + cz_2^2 + dz_2^3 + ez_2^4 + fz_2^5 \\
T_3 &= T(z_3) = a + bz_3 + cz_3^2 + dz_3^3 + ez_3^4 + fz_3^5 \\
&\vdots \\
T_n &= T(z) = a + bz_n + cz_n^2 + dz_n^3 + ez_n^4 + fz_n^5
\end{aligned} \tag{21}$$

The way is presented, the linear system have more equations than variables, and in that case there is two options: Apply the least square method to optimize (and approximate the linear system to one with six equations), or to curtail the excess of equations. Each one of then gives an linear system of the following matrix view point:

$$\begin{bmatrix} 1 & z_1 & z_1^2 & \cdots & z_1^5 \\ 1 & z_2 & z_2^2 & \cdots & z_2^5 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & z_n & z_n^2 & \cdots & z_n^5 \end{bmatrix} \begin{bmatrix} a \\ b \\ \vdots \\ f \end{bmatrix} = \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_n \end{bmatrix} \tag{22}$$

which is an linear system solvable by Gaussian elimination needing a minimum of six measurements.

3.2 Travel time in a curved reflecting interface

Suppose an model on which a layer of homogeneous seismic velocity V, that at the lower boundary has an reflecting curved interface, that is described by the function $h(x)$, as shown at Figure 4.

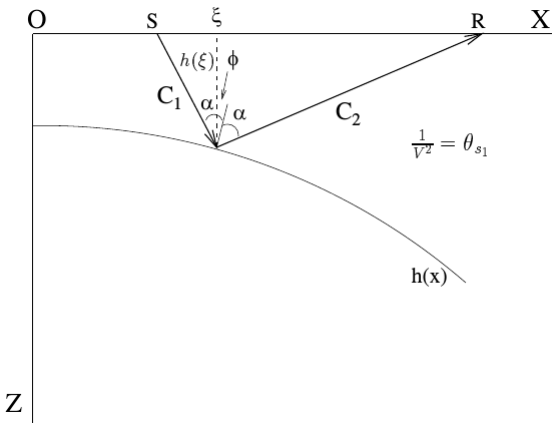

Figure 4: Isotropic layer model with an curved reflecting interface (Figueiró, 1994)

Being S the source position, and R the seismic receiver. The travel time is given by the following expression:

$$t(S,R) = \frac{h(\xi)}{V}\left[\frac{1}{cos(\alpha-\phi)} + \frac{1}{cos(\alpha+\phi)}\right], \quad (23)$$

where:

$$\alpha - \phi = \arctan\left(\frac{\xi - S}{h(\xi)}\right), \quad (24)$$

$$\alpha + \phi = \arctan\left(\frac{R - \xi}{h(\xi)}\right), \quad (25)$$

$$\phi = \arctan\left[\frac{\mathrm{d}h}{\mathrm{d}x}(\xi)\right], \quad (26)$$

Subtracting the Eq.(24) by the (25) and replacing ϕ with the Eq.(26), we have:

$$2\arctan\left[\frac{\mathrm{d}h}{\mathrm{d}x}(\xi)\right] - \arctan\left(\frac{R-\xi}{h(\xi)}\right) + \arctan\left(\frac{\xi - S}{h(\xi)}\right) = 0. \quad (27)$$

Then, it becomes a problem of finding the zero of Eq.(27), ($f(\xi) = 0$), so that way ξ is found, so ϕ and α are found by Eq.(26) and (24). That way the problem can be solved with the Gauss-Newton's method. The demonstration of the above equations can be found in Figueiró (1994).

3.3 Gravimetric model for multiple spheres

Suppose a model that have ten spheres, each one defined by: r_i, x_{ci}, z_{ci}, ρ_i; being respectively the sphere radius, horizontal coordinate of the center of sphere, the vertical one and the density. In field is measured the gravitational anomaly of the spheres (g_{obs}), caused by a buried heterogeneous body, that is supposed to be represented by the union of such ten sphere. Then, for direct modeling, the gravimetric anomaly caused by such body given by:

$$g_{calc}(x) = \frac{4}{3}G\pi\sum_{i=1}^{10}\frac{(\rho_i - \rho_o)z_{ci}\,r_i^3}{[z_{ci}^2 + (x - x_{ci})^2]^{\frac{3}{2}}}. \quad (28)$$

In the actual model there is 41 parameters, counting with the density ρ_o of the medium. The problem is how to find then. The demonstration for the equation above can be found at Átila Joaquim Costa (2012).

There are a lot of possible methods, but one interesting way to solve it is to use the Monte Carlo method to raffle the parameters, defining an plausible geological interval,

$$\Delta g = |g_{obs} - g_{calc}|. \quad (29)$$

When the Δg reach an acceptable level, it's time to stop the raffling and just add small disturbances at the values of the parameters to decrease even more Δg. Despite of that, the criteria for the algorithm to stop can be very well the time spent on calculations, or the number of iterations, but those alone are not good ones.

4 Conclusions

Even though the algorithms shown here are not the most efficient, the purpose were to show what they can do, and how to apply in realistic geophysical problems. In fact, there are situations that other algorithms do a best job, like the bisection method together with the Gauss-Newton's method, or iterative methods to solve linear equations, such as Gauss-Seidel, or Jacobi. Despite of that, is not just the numerical method, but also the code implementation that must seek efficient use of RAM memory and computer power, to become possible to have a fast and precise result.

Also, studies like that presented in this paper emphasize the importance to study numerical methods to improve the toolbox necessary to solve problems of different nature, including geophysical ones. There are universities that don't offer sufficient numerical analysis related course in compulsory disciplines for the geophysics degree. Therefore is important to, along the degree, the students to have access to models and numerical methods needed to solve the mentioned problems.

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