

# Numerical Analysis

Edited by J. P. Hennart

# Lecture Notes in Mathematics

Edited by A. Dold and B. Eckmann

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## Numerical Analysis

Proceedings of the Fourth IIMAS Workshop  
held at Guanajuato, Mexico, July 23–27, 1984

Edited by J. P. Hennart



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## FOREWORD

During the five days 23rd-27th July 1984 in Guanajuato, Guanajuato, México, the Institute for Research in Applied Mathematics and Systems (IIMAS) of the National University of Mexico (UNAM) held its Fourth Workshop on Numerical Analysis. As in the first three versions in 1978, 1979 and 1981, the program of this research workshop concentrated on the numerical aspects of three main areas, namely optimization, linear algebra and differential equations, both ordinary and partial. J.H. Bramble, J.R. Cash, T.F. Chan, J.E. Dennis, Jr., J. Douglas, Jr., H.C. Elman, R. England, R.S. Falk, D. Goldfarb, A. Griewank, S.P. Han, J.P. Hennart, A.V. Levy, R.D. Skeel, M.F. Wheeler and M.H. Wright were invited to present lectures. In total 29 papers were delivered, of which 18 are offered in these Proceedings.

Like the Third Workshop, this one was supported by a generous grant from the Mexican National Council for Science and Technology (CONACyT) and the U.S. National Science Foundation, and was part of the Joint Scientific and Technical Cooperation Program existing between these two countries. In relation to this essential funding aspect, it is a pleasure to express again my thanks to R. Tapia, of the Mathematical Sciences Department at Rice, for his continual advice and help prior to the workshop. This time in particular, as the confirmation of the funding was very close to the beginning of the workshop, his role was fundamental in providing us with the above excellent list of invited speakers from the U.S.

My thanks also go to S. Gómez of IIMAS for the enthusiasm and energy she displayed at the local arrangements level, to my colleagues of the Numerical Analysis Department for their friendly cooperation and to IIMAS for its continuous support. Finally, I would like to acknowledge the invaluable help of Ms. A. Figueroa in the typing and retyping needed to transform a set of manuscripts into book form.

Mexico City, November 1985

J.P. HENNART

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## A GLOBAL ZERO RESIDUAL LEAST SQUARES METHOD

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### INTRODUCTION

In this work we want to find the least squares solution of a system of nonlinear equations

$$f_i(x) = 0 \quad i=1, \dots, m$$

where  $x \in \mathbb{R}^n$ ,  $f_i: \mathbb{R}^n \rightarrow \mathbb{R}$  and  $m \geq n$ . To solve this problem we seek for a minimum of the function  $F(x)$ , that is

$$\min_x F(x) = f^T(x) f(x)$$

In general there will exist local minima  $x^*$  of this function with small residuals ( $F(x^*) \neq 0$ ), but in this paper we shall assume that the zero residual solution ( $F(x^*) = 0$ ) also exists. It is this global solution the one that is of interest in the present work and will be referred as the global least squares solution. In order to avoid all local minima of  $F(x)$  we shall use a deflation technique called the tunneling function which preserves the global solution of  $F(x)$ . In order to find this solution the Gauss-Newton Method will be used.

The present method is not only able to avoid local solutions but also has the nice property of handling rank one deficiencies of the Jacobian  $J(x)$  of  $f(x)$ , which is a typical difficulty for the Gauss-Newton Method.

### 1. STATEMENT OF THE PROBLEM

We want to minimize a sum of squares

$$\min_x F(x) = f^T(x) f(x) \quad (1.1)$$

If  $J(x)$  is the Jacobian of  $f(x)$ , then the gradient of  $F(x)$  will be

$$g(x) = 2J^T(x) f(x) \quad (1.2)$$

Problem (1.1) has a local solution at  $x^*$  if

$$J^T(x^*) f(x^*) = 0 \quad (1.3)$$

and it is the global zero residual solution if

$$F(x_G^*) = f^T(x_G^*) f(x_G^*) = 0 \quad (1.4)$$

If  $G_i(x)$  is the Hessian of  $f_i(x)$ , then the Hessian of  $F(x)$  will be

$$G(x) = 2J^T(x) J(x) + 2 \sum_{i=1}^m f_i(x) G_i(x) \quad (1.5)$$

In practice, for small residual and for zero residual problems

$$G(x) \approx 2J^T(x) J(x) \quad (1.6)$$

It is this approximation the one we shall use in the present work.

## 2. THE TUNNELING FUNCTION CONCEPT

In order to avoid the local solutions of problem (1.1), we will now solve

$$\min_x \phi(x) = T^T(x)T(x) \quad (2.1)$$

where  $T(x)$  is the tunneling function defined as

$$T(x) = \frac{f(x)}{[(x-x^P)^T(x-x^P)]^k} = \frac{f(x)}{(\|x-x^P\|_2^2)^k} \quad (2.2)$$

and its Jacobian

$$T_x(x) = \frac{1}{(\|x-x^P\|_2^2)^k} \left[ J(x) - \frac{2k}{(\|x-x^P\|_2^2)} f(x)(x-x^P)^T \right] \quad (2.3)$$

Obviously if the parameter  $k$  is zero then  $T(x) \equiv f(x)$  and  $T_x(x) \equiv J(x)$ . Also it is clear that,  $T_x(x)$  is the Jacobian of the original function  $J(x)$  plus a rank one matrix. From the definition (2.2) it is very easy to show that the global solution for  $\phi(x)$ ,  $\phi(x_G^*)=0$  is the global solution for the original problem  $F(x_G^*)=0$ .

## 3. FEATURES OF THE ALGORITHM

### 3.1 The Gauss-Newton Step

The Gauss-Newton step for solving problem (1.1) will be

$$J(x)^T J(x) p = -J(x)^T f(x) \quad , \quad (3.1)$$

and in order to avoid ill conditioning of  $J(x)^T J(x)$ , a better definition of  $p$  is obtained by finding the least squares solution of

$$J(x)p = -f(x) \quad (3.2)$$

where  $p$  minimizes  $\|Jp + f\|_2$ .

The same consideration applies for solving problem (2.1), getting the Gauss-Newton step for the tunneling function

$$T_x(x)p = -T(x). \quad (3.3)$$

In order to obtain the solution of the systems (3.2) and (3.3) we can use the singular value decomposition of  $J$  and  $T$ :

$$J = U \begin{bmatrix} S \\ 0 \end{bmatrix} V^T, \quad \text{if } k=0$$

or

$$T = U \begin{bmatrix} S \\ 0 \end{bmatrix} V^T, \quad \text{if } k \neq 0$$

where  $S = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n)$  is the matrix of singular values with  $\sigma_i \geq 0$ ,  $U$  is an  $m \times m$  orthogonal matrix and  $V$  is an  $n \times n$  orthogonal matrix. Then the least squares solution for systems (3.2) and (3.3) are given by

$$p = -VS^{-1}V^T f, \quad \text{if } k = 0$$

or

$$p = -VS^{-1}V^T T, \quad \text{if } k \neq 0$$

where

$$S^{-1} = \begin{cases} \frac{1}{\sigma_j} & \text{if } \sigma_j \neq 0 \\ 0 & \text{if } \sigma_j = 0. \end{cases}$$

### 3.2 Parameter Computation

We start the algorithm using the step for the original system defined in Eq. (3.2), until we reach a point say  $x^P$ , at which one detects either a rank deficiency of the Jacobian  $J(x^P)$  (singular point) or a local solution  $J^T(x^P)f(x^P) = 0$  (critical point). At this point  $x^P$ , we deflate the original system using the tunneling function Eq. (2.2) (in practice this means that  $k$  will take a value different from zero, creating a pole at  $x^P$  with strength  $k$ ). We then proceed using the step defined in Eq. (3.3).

Starting with  $k=0.1$  and increasing  $k$  with  $\Delta k=0.1$ , the algorithm computes the appropriate non zero value of  $k$  to get a descent Gauss-Newton step for  $T(x)$ . To avoid division by zero when using Eq. (2.2) and (2.3), the above Gauss-Newton step is computed at the point

$$x = x^P + \epsilon r \quad (3.4)$$

where  $\epsilon$  is a very small parameter so that  $x$  is in a neighborhood of  $x^P$ , and  $r$  is a random vector  $r_i \in [-1,1]$ . Good results are obtained if  $\epsilon=0.1$ . See Ref. [1] for detailed description of the parameters.

Once  $k$  is non zero, according to Eq. (2.2) if  $\|x-x^P\|$  becomes larger than one, the shape of  $T(x)$  becomes very flat, slowing convergence. Therefore, if at some iterand  $x$ , the distance  $\|x-x^P\|_2 \geq 1$ , we move the position of the pole  $x^P$  along the vector  $(x-x^P)$  so that  $\|x-x^P\| = \epsilon$ . In this fashion we shall always have

$$\|x - x^P\|_2 \leq 1 \quad (3.5)$$

In the other hand, having  $\|x-x^P\|_2 \leq 1$  and  $k \neq 0$  leads to a situation where  $\|T(x)\|_2^2 > \|f(x)\|_2^2 = F(x)$ . Therefore, in order to improve convergence, by reducing  $T(x)$  it is desirable to reset  $k$  to zero as soon as possible and then proceed on the original system using the step defined in Eq. (3.2). This can be done whenever the norm of the residuals  $F = \|f(x)\|_2^2$  drops below the level of the norm at the point where  $k$  was increased from zero.

### 3.3 Main Features of the Algorithm

We want to point out here the main features of the algorithm which are:

- a) It can handle rank-one deficiency of the Jacobian (singular points).
- b) It does not stop at local solutions, and proceeds until it gets the global solution.

Briefly let us see how the tunneling idea achieves these features:

- a). At singular points where the Jacobian has a rank-one deficiency, the solution  $J(x)p = -f(x)$  is not unique ( $p$  is arbitrarily large), but if we choose  $x$ , so that  $(x-x^P)$  is not orthogonal to the null space of  $J(x)$ , then  $T_x(x)$  has full rank and  $T_x(x)p = -T(x)$  can be solved.

- b) At critical points  $J^T(x)f(x)=0$ , the Gauss Newton step of Eq. (3.1) is not defined. However, as stated in section 3.2 when this occurs  $k$  takes a value different from zero; then the expression

$$T_x^T(x)T(x) = \frac{1}{(\|x-x^D\|_2)^{2k}} \left[ J^T(x)f(x) - \frac{2k}{\|x-x^D\|_2^2} (x-x^D)f^T(x)f(x) \right] \quad (3.6)$$

shows that  $T_x^T(x)T(x) \neq 0$  unless  $x$  is the global solution, that is  $f^T(x)f(x)=0$ ; and therefore the Gauss-Newton step Eq. (3.3) is well defined, and since it is a descent direction for problem (2.1), the algorithm proceeds to the global solution.

There is another feature of the algorithm which is worth mentioning: when  $k$  is different from zero (because of a detection of a singular or a critical point somewhere before), the algorithm does not necessarily detect at  $x$  if  $J^T(x)f(x)=0$ , because  $T_x^T(x)T(x) \neq 0$ . This fact is important because the method approaches the global solution without the need to locate local solutions as was the case in our previous work in global optimization, Ref. [2], [3] and [4].

The value of  $k$  is calculated to get a descent Gauss-Newton step for system (2.2), but if  $k$  is not sufficiently large, one could also reach a critical point of the system  $T(x)$ , that is

$$T_x^T(x)T(x) = 0$$

which is not a critical point of system  $f(x)$ , that is  $J(x)^T f(x) \neq 0$ .

However, from Eq. (3.6) it can be seen that increasing  $k$  will be enough to get

$$T_x^T(x)T(x) \neq 0.$$

Geometrically it means that for  $k$  sufficiently large the error function  $\phi(x)=T_x^T(x)T(x)$  stretches out.

#### 4. Numerical Examples

Several numerical examples were solved, in order to test the method, which are reported in Ref. [1]. In this paper we illustrate only one of those examples.

Consider the problem (Cragg-Levy)

$$\begin{aligned}
 f_1 &= (e^{x_1} - x_2)^2 \\
 f_2 &= 10(x_2 - x_3)^3 \\
 f_3 &= [\sin(x_3 - x_4) / \cos(x_3 - x_4)]^2 \\
 f_4 &= x_1^4 \\
 f_5 &= x_4 - 1
 \end{aligned} \tag{4.1}$$

for which we have found the following local minima

$$\begin{aligned}
 x &= (0, 1, 0, 0) & \text{with } f^T(x)f(x) &= 1.01 \times 10^2 \\
 x &= (0, 1, 1, 0) & &= 6.8 \times 10^0 \\
 x &= (-0.631, 0, 0, 0) & &= 1.1 \times 10^0 \\
 x &= (0.552, 2, 2, 2) & &= 1.01 \times 10^0 \\
 x &= (-1.110, -2, -2, -2) & &= 4.07 \times 10^1
 \end{aligned} \tag{4.2}$$

and the global minimum

$$f^T(x)f(x) = 0 \quad \text{at} \quad x = (0, 1, 1, 1) \tag{4.3}$$

The above local minima were found using a Levenberg-Marquard algorithm (Moré's version) when the following initial points were used

$$\begin{aligned}
 x_i &= (0, 0, 0, 0), (0, 1, 0, 0), (0, 1, 1, 0) \\
 & (1, 2, 2, 2), (-1, -2, -2, -2)
 \end{aligned} \tag{4.4}$$

Obviously at the local minima the Levenberg-Marquard algorithm terminated since it is a local method.

The tunneling algorithm starting from the same initial points (4.4) arrived at the global solution requiring the computing effort given in the following table:

Initial Point	Iter	fn	Jac
(0, 0, 0, 0)	6	9	8
(0, 1, 0, 0)	8	11	10
(0, 1, 1, 0)	7	10	9
(1, 2, 2, 2)	8	13	10
(-1, -2, -2, -2)	8	12	10

Final error  $10^{-6}$

TABLE I. Numerical results for example (4.1), showing the required number of iterations, function evaluations and Jacobian evaluations for the present method to reach the global zero residual solution.

On its way to the global minimum the present method detected the following points as "singular": where there is a rank deficiency of the Jacobian

$$\begin{aligned} x &= (0, 0, 0, 0) & \text{with } f^T(x)f(x) &= 2 \times 10^0 \\ x &= (1, 2, 2, 2) & &= 2.26 \times 10^0 \quad (4.5) \\ x &= (-1, -2, -2, -2) & &= 4.1 \times 10^1 \end{aligned}$$

however, by automatically increasing the value of the parameter  $k$  at these points, the method was able to get the global solution.

## 5. CONCLUSIONS

In this paper another application of the tunneling concept to least square problems is presented. To arrive to the global zero residuals least squares solution of the problem, the Gauss-Newton method is used as the basis of the algorithm, and the tunneling mapping is employed to deal with singular or critical points for which the Gauss-Newton step Eq. (3.1) would not be defined. The numerical results clearly illustrate one of the basic properties of this method: if the pole strength  $k$  is sufficiently large the local solutions of the original problem are smoothed out and the Gauss-Newton displacements move towards the global solution.

We only outline here the basic ideas, a full description of the algorithm and the behaviour and sensitivity of the parameters can be found in Ref. [1].

## 6. AN IDEA IN PROGRESS

In section 3 we pointed out as one feature of the algorithm, the local stretching of the function, cancelling the critical points.

Another idea that presently is being explored, is that of a pole supported on a hypersphere.

In previous papers on global optimization, Ref. [2], [3], [4] the tunneling function has been used to deflate unwanted local minima of a function  $f(x)$  at  $x^*$  using the expression

$$T(x) = \frac{f(x) - f(x^*)}{[(x - x^*)^T(x - x^*)]^k} \quad (6.1)$$

and during the tunneling phase a zero of  $T(x)$  is sought, to get a starting point of the next minimization phase.

If the solution of  $T(x)=0$  is not found within a specified CPU time, the assumption is taken that probably the global minimum has been found at  $x^*$  and the global optimization algorithm terminates.

Obviously this is only a necessary but not a sufficient condition for global optimality.

In order to increase the confidence, that really a solution of  $T(x)=0$  does not exist, on the basis of a finite CPU time allocation, an idea that seems promising is to use a different mapping function instead of Eq. (6.1), defined by

$$\tau(x) = \frac{T(x)}{[R^2 - (x-x^*)^T(x-x^*)]^k} \quad (6.2)$$

We note that in Eq. (6.2) a smoothing effect on  $T(x)$  occurs not by the action of a single pole at  $x^*$  (as it was using Eq. (6.1)), but by a region of poles located at the boundary of the hypersphere of radius  $R$ .

This smoothing effect can easily be seen in Figs. 1 and 2, where the zero of the pulse like function is preserved by the mapping Eq. (6.2), and yet the function has been smoothed within the interior of the hypersphere increasing tremendously the zone of attraction of the zero.

Obviously, we are expressing here only the concept of an "idea in progress" and for conclusive numerical results, we shall have to wait for the next IIMAS workshop.

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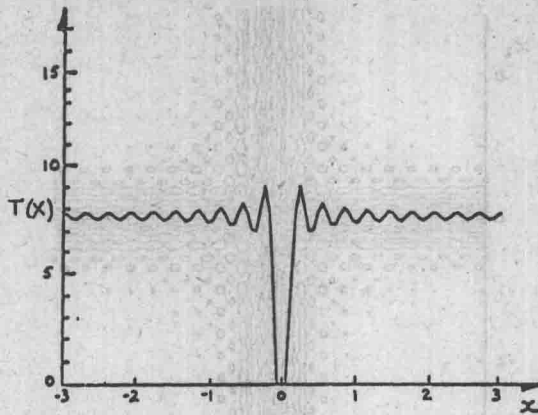


Figure 1a. Original pulse-like function, with zeroes near the origin and multiple singular points that cause a small region of attraction to the zeroes

$$T(x) = -10 \left[ \sum_{n=1}^{20} \left\{ \frac{2}{n\pi} \sin(n\pi/36) \cos(xn) \right\} + \frac{2}{\pi} \sin(\pi/36) \right] + 8$$

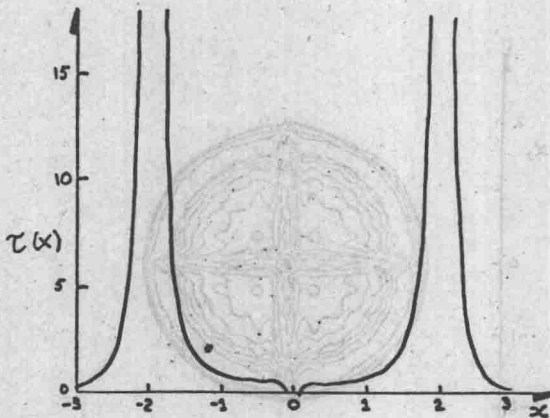


Figure 1b. Effect of the Mapping  $\tau(x)$  on  $T(x)$ , Eq. (6.2) with  $R=2$ ,  $k=2$ ,  $x^*=0$ . The zeroes near the origin are preserved, while the singular points are smoothed, causing the region of attraction of the zeroes to increase.