Aplikace matematiky

Jaromír Jakeš

A numerical method of fitting a multiparameter nonlinear function to experimental data in the L_1 norm

Aplikace matematiky, Vol. 33 (1988), No. 3, 161–170

Persistent URL: http://dml.cz/dmlcz/104299

33 (1988) APLIKACE MATEMATIKY No. 3, 161—170

A NUMERICAL METHOD OF FITTING A MULTIPARAMETER NON-LINEAR FUNCTION TO EXPERIMENTAL DATA IN THE L_1 NORM

JAROMÍR JAKEŠ

(Received June 25, 1986)

Summary. A numerical method of fitting a multiparameter function, non-linear in the parameters which are to be estimated, to the experimental data in the L_1 norm (i.e., by minimizing the sum of absolute values of errors of the experimental data) has been developed. This method starts with the least squares solution for the function and then minimizes the expression $\sum_i (x_i^2 + a^2)^{1/2}$, where x_i is the error of the i-th experimental datum, starting with an a comparable with the root-mean-square error of the least squares solution and then decreasing it gradually to a negligibly small value, which yields the desired solution. The solution for each fixed a is searched by using the Hessian matrix. If necessary, a suitable damping of corrections is initially used. Examples are given of an application of the method to the analysis of some data from the field of photon correlation spectroscopy.

Keywords: Nonlinear function, adjustment of parameters by L_1 norm, photon correlation spectroscopy, analysis of experimental data.

INTRODUCTION

For many decades, the least squares method was the only numerical approach used for fitting experimental data. Recently, in connection with the difficulties met in adjusting the relaxation time distributions $G(\tau)$ to the experimental correlation functions measured in the photon correlation spectroscopy, use of the sum of absolute values of errors as a measure of goodness of fit instead of the sum of their squares has been suggested as an alternative to the least squares method [1]. For a linear function of parameters adjusted, this problem may be solved by the simplex method [1, 2]. This is the case of the analysis of the heterodyne autocorrelation data yielding the field autocorrelation function $g(t)$ sought as a superposition of several fixed relaxation times (the so-called comb) with the amplitudes as parameters. However, already in analyzing the homodyne autocorrelation data, where $g^2(t)$ with a sometimes unknown base is measured, the problem becomes non-linear. An iterative method bringing this problem back to the simplex method was developed [3], and several

tens of data sets were analyzed with it. Another way of analyzing the homodyne autocorrelation data used in Institute of Macromolecular Chemistry was to represent the function $g(t)$ as a superposition of several relaxation times with both the amplitudes and the relaxation times adjusted by the least squares method [4]. It turned out that for comparing the results of the two methods and for understanding their differences, the results of the adjustment of both the amplitudes and the relaxation times by minimizing the sum of the absolute values of errors of experimental values would be highly desirable. Here, the experimentally obtained correlation functions (both heterodyne and homodyne) are strongly non-linear in the relaxation times adjusted and we met with a serious difficulty since no numerical method of performing such a non-linear adjustment in the L_1 norm was available. Due to this fact, I developed a method for solving the problem, which is described in this paper.

MATHEMATICAL METHOD

A general method of minimization of a non-linear function F of parameters to be adjusted is based on the calculation of the vector $\boldsymbol{g}_i$ of the first derivatives of the function to be minimized with respect to the adjustable parameters, and of the matrix $\boldsymbol{H}_i$ of the second derivatives for a trial vector $\boldsymbol{x}_i$ of adjustable parameters. Then, an improved trial vector is calculated as

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i - \boldsymbol{H}_i^{-1}\boldsymbol{g}_i , \tag{1}$$

and the whole procedure is repeated with this new trial vector. The matrix $\boldsymbol{H}$ is called the Hessian matrix. This general scheme applied to the least squares problem leads to the Newton-Raphson method [5]. For a quadratic function of the parameters adjusted, the Hessian matrix does not depend on the vector $\boldsymbol{x}$ and the convergence of Eq. (1) is attained within a single refinement cycle. If, for a general function, we make an initial guess $\boldsymbol{x}_i$ of the parameter vector close enough to the final solution $\boldsymbol{x}_{\min}$, so that the matrix $\boldsymbol{H}_i$ differs little from the matrix $\boldsymbol{H}_{\min}$, the iteration of Eq. (1) proceeds by the very fast quadratic convergence. The performance of various methods developed to treat the cases where such a close initial guess is not available was compared by Box [6]. Later, an alternative method was given by Murtagh and Sargent [7]. Perhaps the simplest way of solving the problem may be to scale (i.e. to multiply by factors less than unity) the corrections $\boldsymbol{x}_{i+1} - \boldsymbol{x}_i$ in Eq. (1), which may better be attained by adding some non-negative constants (damping factors) to the diagonal elements of the matrix $\boldsymbol{H}$ in early stages of the iteration [8, 9]. As I felt that using some general scheme for selecting the damping factors (e.g. proportional to the diagonal elements of $\boldsymbol{H}$ with the proportionality constant sought by a trial and error method as in [9]) may result in a nonnecessarily large number of iterations, I decided to control the damping factors from a terminal in an interactive calculation.

An obvious necessary condition for using the iterative scheme (1) is that the derivatives appearing in $\boldsymbol{g}_i$ and $\boldsymbol{H}_i$ do exist. This is not the case for the absolute value function which has neither the first nor the second derivative at the zero value of the argument. So, the general method mentioned above is inapplicable for fitting the experimental data in the L_1 norm. To avoid this difficulty, I replaced the function $|x|$ in the norm by the function $(x^2 + a^2)^{1/2}$, which for $a = 0$ is identical with $|x|$ and for $a > 0$ has the desired derivatives. Further, $(x^2 + a^2)^{1/2} = a + x^2/(a + (x^2 + a^2)^{1/2})$, which is close to $a + x^2/(2a)$, i.e. to a linear function of x^2 appearing in the L_2 norm, for large a. Thus, minimizing the expression

$$F = \sum_i ((f_i - \bar{f}_i)^2 + a^2)^{1/2} \tag{2}$$

with f_i and $\bar{f}_i$ being respectively the calculated and the experimental values at the i-th experimental point of the function f to be adjusted, leads in the limit $a \to \infty$ to the same solution as the least squares method.

Now, on the basis of the preceding paragraph, the following scheme of adjusting the parameters of a non-linear function f by minimizing the L_1 norm of $f - \bar{f}$ may be outlined: First, we adjust the parameters using the L_2 norm, i.e., solve the problem by the least squares method. Then we minimize expression (2) starting from the least squares solution, and use a value of a large enough to obtain a reasonable convergence. A value comparable with the root mean square error of least squares (its half or third) turned out to be suitable for this purpose. Then we use the solution obtained as the starting approximation for minimizing (2) with a smaller a and repeat the whole procedure until the solution for an a small enough to represent the solution of (2) for $a = 0$ is obtained. Decreasing a by a factor of about three in each step turned out to be appropriate, as it gives a reasonable convergence in the next minimization of expression (2). Whether an a is already small enough to represent the solution for $a = 0$, may be judged from a comparison of the solutions from two subsequent minimizations with various a's. Still much faster convergence may be obtained by using the linear extrapolation of the last and the last-but-one solutions already obtained as the starting approximation for calculation with the next smaller a, especially when a is already small enough compared with the mean square error of the least squares solution.

In the least squares method, the expressions for the elements g_j and H_{jk} of the vector $\boldsymbol{g}/2$ and the matrix $\boldsymbol{H}/2$ (halves are usually calculated here to remove the common factor of two) are as follows:

$$g_j = \sum_i (f_i - \bar{f}_i)\, \partial f_i/\partial x_j\,, \tag{3}$$

$$H_{jk} = \sum_i ((\partial f_i/\partial x_j)\, \partial f_i/\partial x_k + (f_i - \bar{f}_i)\, \partial^2 f_i/\partial x_j\, \partial x_k)\,, \tag{4}$$

where x_j, x_k are the parameters adjusted. These are the formulae for the Newton-Raphson method. The respective formulae for minimizing expression (2) differ from

them only by two multiplicative factors common for all parameters adjusted, but varying from one experimental point to another. They read as follows:

$$g_j = \sum_i F_1(f_i - \bar{f}_i)\,\partial f_i/\partial x_j\,, \tag{5}$$

$$H_{jk} = \sum_i (F_2(\partial f_i/\partial x_j)\,\partial f_i/\partial x_k + F_1(f_i - \bar{f}_i)\,\partial^2 f_i/\partial x_j\,\partial x_k)\,, \tag{6}$$

where $F_1 = ((f_i - \bar{f}_i)^2 + a^2)^{-1/2}/2$ and $F_2 = a^2((f_i - \bar{f}_i)^2 + a^2)^{-3/2}/2$. Thus, once the Newton-Raphson method of least squares for some problem has been programmed, one can proceed straightforward to modify the program for minimizing expression (2).

CONVERGENCE CONSIDERATIONS

Let us start the discussion of convergence of minimizing (2) by investigating the convergence properties of the function $(x^2 + a^2)^{1/2}$. Its first and second derivatives, $x/(x^2 + a^2)^{1/2}$ and $a^2/(x^2 + a^2)^{3/2}$, respectively, give the correction $-x(x^2 + a^2)/a^2$. We see that the desired correction $-x$ is overestimated by the factor of $1 + x^2/a^2$. Convergence is obtained if this factor is less than two, i.e. if $|x| < |a|$. In the opposite case, the iteration process (1) oscillates. The best value of the damping factor to be added to the second derivative to improve convergence is $x^2/(x^2 + a^2)^{3/2}$, leading immediately to the correct value. For a given ratio of x/a, this value is inversely proportional to a.

It is known that if the function of the adjusted parameters is linear, the solution minimizing the L_1 norm fits exactly as many experimental points as is the number of the adjusted parameters [2]. The deviations $f_i - \bar{f}_i$ at these points are independent linear functions of the original parameters and may be regarded as a new parameter set. The left and right derivatives of the L_1 norm with respect to the new parameters at zero value differ by sign as the absolute value function, but generally they also differ in their absolute value unlike the absolute value function. Due to this, minimization of (2) with a non-zero a leads to some offset of experimental and calculated values even at these points. For small a this offset is expected to be proportional to the value of a. It may be inferred that, if in the adjusting scheme a is decreased by the same factor in each step and a strategy for minimizing (2) is found, then the same strategy but with the damping factors increased by the same ratio by which a is being decreased is expected to work about as well in the next step. In the non-linear case, the number of points fitted exactly may be smaller than that of the adjusted parameters and the situation becomes more complicated. Experience shows that in this case some damping factors should be increased with decreasing a while others should not. Furthermore, experience shows the following strategy as appropriate: we fix some parameters (those weakly affecting the function f) at their trial values by giving them very large damping factors, and try to adjust the remaining ones.

If expression (2) increases, a return to the previous cycle is made and some other parameters are fixed. If (2) increases even with a single parameter adjusted, then the latter is given a non-zero finite value of the damping factor found by trial and error and decreased to zero in the course of adjustment. Once a group of parameters has been adjusted to a reasonable extent (not to full precision), one or several parameters so far fixed are given zero damping factors and the adjustment is re-tried. If adding a single parameter to the adjustment increases (2), this parameter is again given a non-zero finite damping factor, and this factor is later decreased to zero. This process is repeated until all parameters have been given zero damping factors, at which stage it already rapidly yields the final solution. In accordance with what has been said above about the convergence properties of the function $(x^2 + a^2)^{1/2}$, the necessity of using finite non-zero damping factors in this strategy frequently appeared in minimizing (2). The damping factors should be controlled from a terminal in an interactive mode with a program allowing interference after a prescribed number of iterations to decrease the damping factors, and also if the computer finds unreasonable (e.g. negative) values of parameters obtained by (1) or an increase in expression (2), or if the damped $\boldsymbol{H}$ matrix is found not to be positively definite.

As $(x^2 + a^2)^{1/2} - a \leqq |x| < (x^2 + a^2)^{1/2}$ (a positive), the desired minimum value of the L_1 norm of the errors is bounded by F-na and F (cf. Eq. (2)), where n is the number of experimental points. Thus, by selecting a small enough, we can obtain the minimum of the L_1 norm with any desired accuracy. When high accuracy is required, difficulties due to the loss of significant digits may appear in the case when the number of the experimental points fitted exactly is smaller than that of the adjusted parameters; switching to a higher (quadruple) precision solves this problem.

After decreasing a some two or three orders of magnitude below the root mean square error of least squares, a comparison of errors of the individual experimental points from two subsequent minimizations with different a allows us to find points fitted exactly by the solution sought: errors of these points decrease approximately by the ratio of the a values, whereas the errors of the other points remain approximately constant. Then, in cases when the number of points fitted exactly is equal to that of the adjusted parameters, the minimal L_1 norm solution can be found by solving the system of nonlinear equations originating from the conditions of exact fit much faster than by a further decrease of a: using the approximate solution already found as the starting iteration for the Newton method should yield fast convergence. In the cases when the number of points fitted exactly is smaller than that of the adjusted parameters, the conditions of exact fit should be added as constraints to the minimization problem. After removing the absolute values by using the signs of errors from the approximate solution, this problem can be solved by the method of Lagrange multipliers, again using the approximate solution as the first iteration. In both cases, a post-check should be made whether, if the parameters are varied so that the exact fit is violated at a single point, the L_1 norm increases in both +

and − directions. A linear transformation of differentials of parameters is sufficient for this purpose.

APPLICATION OF THE METHOD TO THE ANALYSIS OF CORRELATION SPECTROSCOPY DATA

The above method was applied to the analysis of the homodyne autocorrelation data, where the value of $g^2(t) + b$, i.e., the square of the field autocorrelation function $g(t)$ plus an unknown additive constant b, was measured. The function $g(t)$ is the Laplace transform of the relaxation spectrum $G(\tau)$, and the latter is sought for as a superposition of N discrete relaxation times τ_j with both times τ_j and their amplitudes x_j adjusted. All τ_j's and x_j's are requested to be positive. Including the unknown base, the total number of adjusted parameters is $2N + 1$. Sometimes, one of the τ_j's converges to infinity and, if $1/\tau_j$ is adjusted, to a negative value of $1/\tau_j$. In this case, the respective τ_j is fixed to 10^{30} and the number of parameters decreases to $2N$. If for the shortest experimental time $f - \bar{f}$ is negative, addition of a new very short τ_j decreases the norm, compensating for the error of this point and essentially unaffecting the other experimental points. This is equivalent to removing this point from the data set. Hence, we have

$$f(t) = g^2(t) + b\,, \tag{7}$$

$$g(t) = \sum_{j=1}^{N} x_j \exp\left(-t/\tau_j\right), \quad x_j > 0\,, \quad \tau_j > 0\,, \tag{8}$$

and a set of pairs $(t_i, \bar{f}_i)$ of experimental data for which

$$\sum_i |f(t_i) - \bar{f}_i| \tag{9}$$

should be minimized by adjusting x_j, τ_j, and b. Having a minimal solution for a given N, we may try to find a new τ_{N+1} which, if added to the $g(t)$ with a very small positive amplitude x_{N+1}, decreases the norm. This can be achieved by calculating the derivative of the norm with respect to x_{N+1} at $x_{N+1} = 0$. Where this derivative is negative, the respective τ_{N+1} meets the above condition. If such a τ_{N+1} exists, adjustment may be continued to a better minimum, usually corresponding to $N + 1$, but it may also happen that N decreases during the adjustment if some x_j vanishes. If no such τ_{N+1} exists, adjustment cannot be continued by increasing N. All solutions presented below are of this last type unless otherwise stated.

For the analysis, four data sets supplied by R. Johnsen from Uppsala for an IUPAC project of comparing various methods of analysis of homodyne autocorrelation data were used. Data set 1 was simulated as a mixture of three relaxation times at 65, 91, and 205 μs with the ratio ·63: ·30: ·07, data sets 2 and 4 were doublets at 63 and 82 μs with the ratio ·82: ·18 and at 51 and 76 μs with the ratio ·89: ·11. To all these data sets a random normal noise with the standard deviation of 5×10^{-4} was added and the base constant b was zero. Data set 3 was a real measurement

of a mixture of two samples, each of which was expected to have a single relaxation time while the ratio of the relaxation times was expected to be about 1·7 : 1. The root mean square experimental error was about 5×10^{-4} here. So closely spaced doublets and triplet are hardly expected to be resolved even in the case when $g(t)$ instead of $g^2(t) + b$ is known, and the results presented below fully confirm this expectation. All data sets give the values of $g^2(t) + b$ for t running from 3 μs to 128 μs by the step of 1 μs. The results of the analysis by least squares ($a = \infty$) and for $a = 10^{-9}$ and $a = 3 \times 10^{-9}$ are summarized in Table 1. Examination of Table 1 shows that in most cases five or more digits (significant digits in τ_j, decimal digits in x_j and b) are obtained in the adjusted parameters with $a = 10^{-9}$. The only exception is the value τ_2 for data set 3. Here, a very large but not infinite τ was found. Further decrease in a to 3×10^{-11} and 10^{-11} led to some change in τ_2 (see Table 1), but already with $a = 10^{-9}$ and $a = 10^{-11}$ the calculated values of the function $f(t_i)$ differed only in the eighth or still less significant digit. Here the experimental values of $\bar{f}_i$ spanned the range from about zero to about 0·65. It is a general experience with all the methods mentioned in Introduction that if a τ_j beyond the region of t where $f(t)$ is measured is found, this τ_j is very ill-conditioned. In this connection, the behaviour of τ_2 in data set 3 is not surprising. In data set 1, $f - \bar{f}$ is negative for the first t_i (3 μs). The removal of this experimental datum from the data set leads to the same result as before in the L_1 norm calculation. This rather exceptional behaviour is caused by the fact that both solutions fit exactly the same experimental points (5, 12, 43, 92, and 117 μs) and the number of points fitted exactly equals the number of the adjusted parameters. In all other data sets the number of points fitted exactly is one less than the number of the adjusted parameters.

The method was also applied to some measured (not simulated) data sets. The largest value of $N = 7$ with one infinite τ_j has been found (14 parameters adjusted). Even in this case (as in all the others) no difficulty arose in calculations (with the 16 digit accuracy), although calculations appeared rather lengthy. In all the cases considered, only small differences between the results of adjustments by the L_2 and L_1 norms were found. Greater differences may be expected in cases when the noise distribution deviates considerably from normality, e.g. if far-off outliers caused by scarce rough errors appear in the experimental data.

CONCLUSIONS

A method of adjusting parameters of a function non-linear in the adjusted parameters by minimizing the L_1 norm of its deviations from the experimental data was developed. This method, although rather laborious, yielded results without difficulties in all the cases to which it was applied (about a dozen of data sets from the field of photon correlation spectroscopy). In all cases considered, only small differences between the solutions obtained by the L_1 and L_2 norms were found (cf. also Tab. 1).

The present hand-operated method may of course be used in the linear case as

Table 1

Example of adjusting parameters of a nonlinear function by minimizing the L_1 norm.

j	τ_j	x_j	τ_j	x_j	τ_j	x_j
	Data set 1; 5, 12, 43, 92, and 117 μs fitted exactly at $a = 0$					
	$a = \infty$[a]		$a = 10^{-9}$		$a = 3 \times 10^{-9}$	
	$b = -\cdot0043908945$		$b = -\cdot0012934582$		$b = -\cdot0012933735$	
1	70·9318850	·724032234	68·9824695	·677667683	68·9823497	·677664468
2	∞	·047060425	218·705130	·091491892	218·696547	·091495056
	Data set 1, point 3 μs removed; 5, 12, 43, 92, and 117 μs fitted exactly at $a = 0$					
	$a = \infty$[a]		$a = 10^{-9}$		$a = 3 \times 10^{-9}$	
	$b = -\cdot0043210075$		$b = -\cdot0012935282$		$b = -\cdot0012935836$	
1	70·9687856	·724325458	68·9825974	·677671036	68·9827334	·677674528
2	∞	·046700110	218·713753	·091488580	218·722417	·091485120
	Data set 2; 3, 10, 41, 110, and 126 μs fitted exactly at $a = 0$					
	$a = \infty$[a]		$a = 10^{-9}$		$a = 3 \times 10^{-9}$	
	$b = -\cdot0004853826$		$b = -\cdot0001114527$		$b = -\cdot0001114923$	
1	65·0945173	·767522175	65·3149917	·769650163	65·3149625	·769649913
2	∞	·007090179	∞	·004701271	∞	·004701561
3	2·51050180	·000538746	1·64107405	·000236794	1·64107401	·000236740
	Data set 3; 3, 17, 39, 43, 101, and 126 μs fitted exactly at $a = 0$					
	$a = \infty$[a]		$a = 10^{-9}$		$a = 3 \times 10^{-9}$	
	$b = -\cdot0136693032$		$b = -\cdot0140965650$		$b = -\cdot0140957222$	
1	91·3964240	·715046762	91·1625488	·713410510	91·1622901	·713407309
2	∞	·096547201	228786·582	·098466243	217608·359	·098469014
3	2·80086484	·003087207	4·84871102	·001608514	4·84768792	·001608585
			$a = 10^{-11}$		$a = 3 \times 10^{-11}$	
			$b = -\cdot0140970246$		$b = -\cdot0140970150$	
1			91·1626885	·713412241	91·1626856	·713412205
2			235344·745	·098464748	235204·041	·098464779
3			4·84926652	·001608475	4·84925492	·001608476
	Data set 4; 5, 23, 38, and 100 μs fitted exactly at $a = 0$					
	$a = \infty$[a]		$a = 10^{-9}$		$a = 3 \times 10^{-9}$	
	$b = \cdot0003326506$		$b = \cdot0001641259$		$b = \cdot0001641287$	
1	53·3214945	·784017862	54·0185340	·762784884	54·0185254	·762785058
2	14·0554828	·002869849	31·8795824	·024058478	31·8796105	·024058297

[a] Least squares solution.

For the meaning of the parameter a see Eq. (2), for the other parameters see Eqs. (7) and (8).

well, but here the fully automated algorithms, e.g. those referred to in monographs [2], [10], and [11], should be preferred despite the fact that the present method may consume considerably less CPU time than the LP methods in those cases when there are many experimental points and few parameters to be adjusted.

Acknowledgements. I am very indebted to Dr. P. Štěpánek and Dr. K. Zimmermann for introducing me to problems of photon correlation spectroscopy, which stimulated the development of the method presented in this paper, to Prof. I. Marek, corresponding member of the Academy, from The Faculty of Mathematics and Physics, Charles University, Prague, and to Dr. P. Štěpánek for reading the manuscript and making valuable comments.

References

[1] *K. Zimmermann, M. Delaye, P. Licinio:* Analysis of multiexponential decay by a linear programming method: Application to light scattering spectroscopy. J. Chem. Phys. 82 (1985) 2228.
[2] *G. B. Dantzig:* Linear Programming and Extensions. Princeton University Press, Princeton, New Jersey 1963.
[3] *K. Zimmermann, J. Jakeš:* Unpublished results.
[4] *J. Jakeš, P. Štěpánek:* To be published.
[5] *A. J. Pope:* Two approaches to nonlinear least squares adjustments. Can. Surveyor 28 (1974) 663.
[6] *M. J. Box:* A comparison of several current optimization methods, and the use of transformations in constrained problems. Computer J. 9 (1966) 67.
[7] *B. A. Murtagh, R. W. H. Sargent:* Computational experience with quadratically convergent minimisation methods. Computer J. 13 (1970) 185.
[8] *K. Levenberg:* A method for the solution of certain non-linear problems in least squares. Quart. Appl. Mathematics 2 (1944) 164.
[9] *D. W. Marquardt:* An algorithm for least-squares estimation of nonlinear parameters. J. Soc. Indust. Appl. Math. 11 (1963) 431.
[10] *P. Bloomfield, W. L. Steiger*: Least Absolute Deviations. Theory, Applications, and Algorithms. Birkhäuser, Boston—Basel—Stuttgart 1983.
[11] *T. S. Arthanari, Y. Dodge:* Mathematical Programming in Statistics. Wiley, New York 1981.

Souhrn

NUMERICKÁ METODA ADJUSTACE MNOHOPARAMETROVÉ NELINEÁRNÍ FUNKCE K EXPERIMENTÁLNÍM DATŮM POMOCÍ L_1 NORMY

JAROMÍR JAKEŠ

Byla vypracována metoda adjustace mnohoparametrové funkce nelineární vzhledem k hledaným parametrům pomocí L_1 normy, tj. minimalisací součtu absolutních hodnot odchylek funkce od experimentálních dat. Metoda vychází z řešení získaného metodou nejmenších čtverců a potom

minimalisuje výraz $\sum_i (x_i^2 + a^2)^{1/2}$, kde x_i je odchylka i-tého experimentálního bodu, při čemž začíná s hodnotou a srovnatelnou se střední kvadratickou odchylkou řešení metodou nejmenších čtverců a potom postupně snižuje hodnotu a k zanedbatelně malé hodnotě, která poskytuje hledané řešení. Řešení pro každé fixované a se hledá pomocí Hessovy matice a na počátku se používá přiměřené tlumení oprav parametrů, je-li to nutné. Jsou uvedeny příklady použití této metody k analyse experimentálních dat z oblasti fotonové korelační spektroskopie.

Резюме

ЧИСЛЕННЫЙ МЕТОД АДЪЮСТАЦИИ НЕЛИНЕЙНОЙ ФУНКЦИИ С МНОГИМИ ПАРАМЕТРАМИ К ЭКСПЕРИМЕНТАЛЬНЫМ ДАННЫМ С ПОМОЩЬЮ НОРМЫ L_1

JAROMÍR JAKEŠ

Разработан метод адъюстации функции со многими параметрами, нелинейной по отношению к искомым параметрам, с помощью нормы L_1, т. е. путем минимизации суммы абсолютных значений отклонений функции от экспериментальных данных. Метод основан на решении, полученном с использованием метода наименьших квадратов, после чего минимуют выражение $\sum_i (x_i^2 + a^2)^{1/2}$, где x_i — отклонение i-той экспериментальной точки, причем начинают со значения a, сопоставимого со средним квадратным отклонением решения по методу наименьших квадратов, а затем постепенно уменьшают a до пренебрежимо малой величины, которая приводит к искомому решению. Решение для каждого фиксированного a ишут с помощью матрицы Гесса; в начале, если это необходимо, используют соответствующее демпфирование поправок к параметрам. Приводятся примеры использования данного метода в анализе экспериментальных данных из области фотонной корреляционной спектроскопии.

Author's address: RNDr. *Jaromír Jakeš*, CSc., Ústav makromolekulární chemie ČSAV, Heyrovského nám. 2, 162 06 Praha 6.