Numerical Filtration as Method of Précising of Computing Results and Error Estimation

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Abstract[1]

In the paper numerical filtration is applied for more precise definition of results, its error estimation and reliability increase. The criterions of reliability estimates are developed. The offered filtration methods are demonstrated by the concrete examples.

1. Introduction

If the analytical methods are absent the most reliable error estimate is the difference between approximate and accurate results. But it is possible only for test examples having an analytical solution. Application of such estimate for other examples is not reliable. In this case an approximate value (but more accurate in comparison with a tested one) can be used. This value may be only three times as more precise as the tested value. But two questions arise: how the more accurate value can be obtained and how to verify that its precision is really greater than precision of the tested value.

If more accurate value is computed by the same method as the tested one, unreal additional recourses can be required. The other way is the using of more rough results (with less nodes number and computing time). If the method error changes according to known (for example as the power or exponential dependence) low, it is possible to make identification and extrapolation of results and to predict approximately the value corresponding to infinite number of nodes [1].

The answer on the second question is given with the help of the second extrapolation (extrapolation of the extrapolated results obtained for different sets of initial data [2]). In this case we have an error estimate of the extrapolated results (or fuzziness of the error estimate). This estimate must satisfy the requirement to be three and more times as less as the error of initial data (the relative fuzziness is less than 1/3), otherwise the given method of estimation in concrete case is unreliable.

Moreover the extrapolation results can be used instead of computed data as more accurate ones for good estimates. Then additional extrapolation is required to check reliability of the obtained results. In some cases the repeated extrapolation allows obtaining more accurate (high order) results than the results obtained by using of a numerical method directly. It is impossible to realize by computing because of great time expense.

2. Problem Statement

2.1. Numerical Filtration

For extrapolation a priori knowledge of dependence of calculations result on the nodes number (or error mathematical model) is required, for example as following

$$z_n = z + c_1 n^{-k_1} + c_2 n^{-k_2} + \ldots + c_L n^{-k_L} + \delta(n) \quad (1)$$

where L is the typical size independent on time, z is the accurate value; z_n is the approximate result obtained for n nodes; c_j are coefficients independent on n; $\delta(n)$ is a

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small quantity in comparison with $c_j n^{-k_j}$ for given n, $k_1,\ldots, k_L$ are arbitrary real numbers ($k_1 > k_2 > \ldots > k_L$).

In mathematical analysis only the first term is usually estimated as far as the other terms are asymptotically (for $n \to \infty$) infinite-small quantities of higher order. But for finite n the other terms must be under consideration.

If a solution is nonsingular it can be expended by the Taylor formula, then k_j is a part of the positive integers.

The solving of the numerical filtration problem is sequential removing of power terms of the sum (1) by means of computing of linear combinations of results obtained for different n.

Let $q = n_{j-1} / n_j < 1$, $m>L$. According to (1) the system of linear algebraic equations is written as

$$z_{n_1} = z + c_1 + c_2 + \ldots + c_L + v_1 ,$$

$$z_{n_2} = z + c_1 q^{k_1} + c_2 q^{k_2} + \ldots + c_L q^{k_L} + v_2 ,$$

....

$$z_{n_m} = z + c_1 q^{(m-1)k_1} + c_2 q^{(m-1)k_2} + \ldots + c_L q^{(m-1)k_L} + v_m$$

or in the matrix form

$$A = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & q^{k_1} & \cdots & q^{k_L} \\ . & . & . & . \\ 1 & q^{(m-1)k_1} & \cdots & q^{(m-1)k_L} \end{pmatrix}, \quad v = \begin{pmatrix} \delta(n_1) \\ \vdots \\ \delta(n_m) \end{pmatrix}$$

$$y = Ax + v , \ x = \begin{pmatrix} z \\ c_1 \\ \vdots \\ c_L \end{pmatrix}, \quad y = \begin{pmatrix} z_{n_1} \\ \vdots \\ z_{n_m} \end{pmatrix}, \tag{2}$$

2.2. Minimization Method of Dispersion of Expected Error

The problem statement is the following. Let's consider a system of m linear algebraic equations (2) with $n=L+1$ unknowns, supposing error existence in the every equation.

Error values are unknown and the system (2) is always underdetermined independently on ratio of m and n and on rank of the matrix A. The error vector v is characterized either by the norm (maximum value $|v_i|$) or by the dispersions σ^2_i or by the covariance matrix. Mathematical expectation $M(v_j)$ is assumed to be equal to zero as a rule.

It is necessary to find the estimate of the system solution and the error estimate of result.

Let the matrix A be constant and accurately known for the equations system (2). Indeterminacy domains of expected variation of the error vector v and the required vector x are preassigned. Square sizes of the domains are determined by the covariance matrixes K_v and K_x

$$K_v = \begin{pmatrix} \sigma_1^2 & r_{12}\sigma_1\sigma_2 & \ldots & r_{1m}\sigma_1\sigma_m \\ r_{12}\sigma_1\sigma_2 & \sigma_2^2 & \ldots & r_{2m}\sigma_2\sigma_m \\ \ldots & \ldots & \ldots & \ldots \\ r_{1m}\sigma_1\sigma_m & r_{2m}\sigma_2\sigma_m & \ldots & \sigma_m^2 \end{pmatrix}$$

where σ_j^2 are the dispersions of the random quantities v_j, r_{ij} are the correlation coefficients of v_i and v_j, (the matrix K_x is defined analogously).

It is necessary to find an optimal method of determination of the estimate $\hat{x}$ of the required parameters vector x by the results of measurements or calculations $y_1, \ldots ,y_n$.

Minimum of mathematical expectation of error square of the unknown x_1 is assumed as optimality criterion

$$F_1 = M|\hat{x}_1 - x_1|^2 \to \min \tag{3}$$

The estimate $\hat{x}$ is found in the form $\hat{x} = By$, where B is a matrix $n \times m$ (only linear operators B are under consideration).

The analogous problem is solved in [3].

$$B = \left(A^T K_v^{-1} A + K_x^{-1}\right)^{-1} A^T K_v^{-1} ,$$

or if $K_x^{-1} = 0$

$$B = \left(A^T K_v^{-1} A\right)^{-1} A^T K_v^{-1} . \tag{4}$$

So the problem of the unknown z determination is solved by the least squares method.

Notes, for $L=1$, $m=2$ the filtration formula coincides with the Richardson extrapolation formula

$$z^*_{n_2} = z_{n_2} + \frac{z_{n_2} - z_{n_1}}{Q^{k_j} - 1} . \tag{5}$$

Extrapolation fulfils for all pairs of neighboring values. Then the filtered dependence without the term n^{-k_j} is

$$z^*_n = z + c^*_1 n^{-k_1} + \ldots + c^*_{j-1} n^{-k_{j-1}} + c^*_{j+1} n^{-k_{j+1}} +$$

$$+ c^*_L n^{-k_L} + \delta^*(n) , \tag{6}$$

Where

$$c^*_l = c_l \frac{Q^{k_j} - Q^{k_l}}{Q^{k_j} - 1} . \tag{7}$$

The filtered sequence $z^*_{n_j}$ has by one term less than the initial one. If it contains more than one term then it can be filtered removing of the power component n^{-k_l}. The filtration is repeated consequently for $n^{-k_1},\ldots,n^{-k_L}$ if the initial sequence contains sufficient number of terms. It is convenient to present the extrapolation results in the form of triangle matrix

$$\begin{array}{lllll} n & z_n & z_n^* & z_n^{**} & z_n^{***} & \ldots \\ 10 & z_{10} & - & - & - \\ 20 & z_{20} & z_{20}^* & - & - \\ 40 & z_{40} & z_{40}^* & z_{40}^{**} & - \\ 80 & z_{80} & z_{80}^* & z_{80}^{**} & z_{80}^{***} \\ \ldots \end{array} \qquad (8)$$

The using of the second extrapolation is known as the Romberg's method. But its application leads to restrictions that don't allow to use automatically the obtained by extrapolation values. It requires the development of methods of certainty increase of defined estimates.

3. Certainty Increase

3.1. Estimate Fuzziness Criterion

The error estimate in the Runge rule is reduced to comparison of the value z_n with the extrapolated value z_n^*. As far as this estimate is correct for the assumption that the quantity z_n^* is more accurate than z_n, it is necessary to verify validity of this assumption. For this we repeat the extrapolation and find the value z_n^{**}. The difference $\Delta_n = z_n - z_n^*$ is the error estimate of the approximate value z_n. The difference $\Delta_{\Delta n} = z_n^* - z_n^{**}$ represents error estimate of the extrapolated value z_n^* or error estimate of the error estimate (fig. 1). The relation $\delta_n = |\Delta_{\Delta n}/\Delta_n|$ means relative fuzziness of the error estimate.

If $\delta_n << 1$ then the relative fuzziness of the estimate Δ_n is small and this estimate is to be trusted.

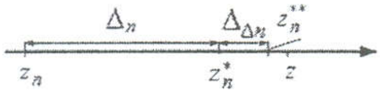

Figure 1. Fuzziness of Error Estimate

Let's assume that the error estimate is presented as the interval $z = z_n^* \pm \Delta_n$. For definition of the limited value δn (for acceptation or rejection of obtained estimate) it needs on the base of available information to determine the possibility of falling of the values outside the interval between $z_n = z_n^* - \Delta_n$ and $z_n^* + \Delta_n$. Let's suppose for this purpose that with following hypothetical extrapolation the value δ_n (as a coefficient of distance decrease between neighbors extrapolated values) remains as $\delta_n = \delta$. Then maximal difference between the limited value and z_n^* is determined as the sum of the geometrical progression $\Delta_{\max} = \Delta_n^* / (1-\delta)$. Then

$$K\frac{\Delta_n^*}{1-\delta} \le \Delta_n ,$$

where $K \ge 1$ is a coefficient of error estimate reserve. It is introduced to obtain rather reliable estimates in indeterminacy conditions because of influence of irregular components of error. Then the criterion of estimate acceptation is written as

$$\delta \le \frac{1}{K+1} . \qquad (9)$$

Let's assume K=2. Then the limited value $\delta = 1/3$, for $\delta \le 1/3$ the estimate is accepted and for $\delta > 1/3$ it is rejected. The practice shows [3] that this criterion really operates.

3.2. Visualization of Extrapolation Results

The results of extrapolation and error estimation are presented as dependence of $-\lg\Delta$ (common logarithm of relative error) on $-\lg n$. In fig. 2-4 the curves *0* corresponds to the error of computed data, the curves *1-3* are the results of the first, second and third extrapolation.

The visualization allows to filtrate at interactive mode and to find decision of estimate certainty on the base of general analysis of data obtained by extrapolation.

4. Examples of Filtration Application

Numerical filtration is applied to processing of results obtained by different numerical methods. As examples the results of a derivative computation by the symmetric difference formula of the second order are presented in fig.2 and the results of numerical integration by the right rectangles method are demonstrated in fig.3. The results analysis shows that the computed integral values have 1-5 precise decimal digits and the result of the first extrapolation has 3-10 digits for relative fuzziness less than 0.1.

A restriction on the level of 16 digits is explained by round-off error. Notes, the round-off error increase with growth of n. The growth is not so essential for the numerical integration.

The results of processing of numerical data obtained by solving of differential equations (ordinary and with partial derivative) look analogously.

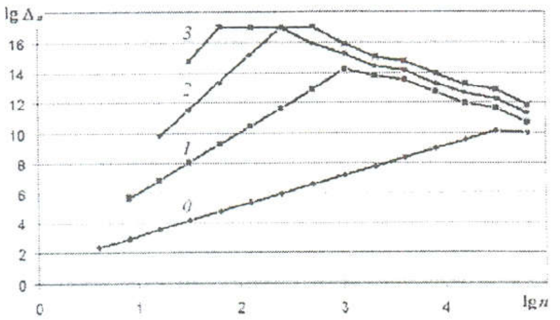

Figure 2. Extrapolation Results for Numerical Differentiation

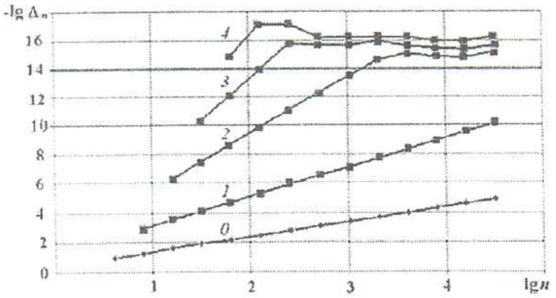

Figure 3. Extrapolation Results for Numerical Integration

In nonlinear problems [4] error components of higher order of smallness can exceed components of lower order. In this case the error can change the sign with growth of n (as in fig. 4). Thus, the results having the first order look as dependencies of the second order. The filtration allows determining existence of all components.

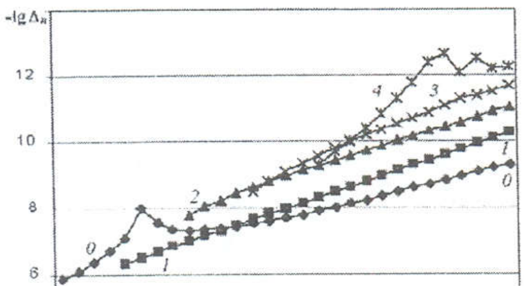

Figure 4. Extrapolation Results for Nonlinear Problem

The extrapolation is often complicated by definition of maximum values of distributed parameters. Different locations of the extreme value with respect to the nodes lead to irregular component of error. In this case the general filtration formula (4) improves the result with corresponding choice of analyzing values number. In fig.5 the solutions indexes related to logarithm of nodes number linearly are put on the abscissa axis.

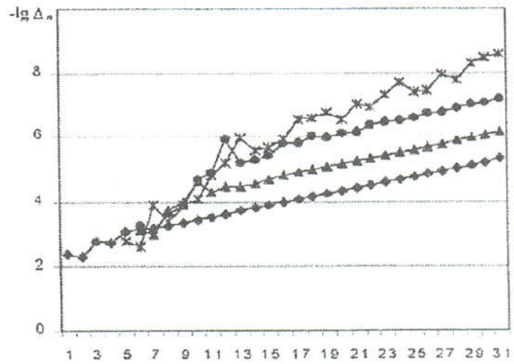

Figure 5. Extrapolation Results for Irregular Error Components

5. Conclusions

It is shown that application of numerical filtration on the base of extrapolation allows increasing essentially the precision of numerical results almost without time expense. Moreover, analysis of several components of error, using of the fuzziness criterion and visualization of results in the form of diagrams increase estimate certainty.

Multicomponent analysis also helps to determine the algorithm imperfection that is not obvious because of more essential components of error.

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