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МЕТРИЧЕСКИЙ АНАЛИЗ И ПРИЛОЖЕНИЯ

А. В. Крянев¹, Г. В. Лукин¹, Д. К. Удумян¹

Предлагаются новый подход и основанные на нем схемы и алгоритмы интерполяции функций одной и многих переменных и экстраполяции (прогнозирования) временных рядов, названный авторами этого подхода метрическим анализом [1]. Показано, что метрический анализ с высокой степенью точности интерполирует функции многих переменных даже при сравнительно небольшом числе точек, в которых значение функции известны. Выявлено, что метрический анализ позволяет экстраполировать и прогнозировать значения функций более широкого класса, чем известный сингулярно-спектральный анализ [2]. Статья рекомендована к печати программным комитетом международной научной конференции “Математическое моделирование и вычислительная физика 2009” (ММСП2009, <http://mmcp2009.jinr.ru>).

Ключевые слова: метрический анализ, функции многих переменных, интерполяция, экстраполяция, прогнозирование временных рядов.

1. Introduction. The problems of interpolation and extrapolation of function values and the problems of forecasting the values of time processes are among the basic mathematical problems important for practice. From the time of Newton and Lagrange, the problems of interpolation were formulated and solved for functions of one variable; by now, quite complete results were obtained to develop various methods for interpolation and revealing the properties of interpolated values, including the analysis of interpolation errors and the problems of convergence of interpolated values to the exact ones [3, 4]. Recall that the classical scheme of interpolation is based on representing a function $y(x)$ in the form of the following linear combination:

$$y(x) \approx L_n(x) = \sum_{j=0}^m c_j \varphi_j(x). \quad (1.1)$$

Here $\varphi_j(x)$, $j = 0, \dots, m$, is a system of prescribed basis functions and c_j are the sought parameters.

We need to determine c_j in such a way that $y(x)$ be equal to known values Y_i at given points x_i , $i = 1, \dots, n$. For example, the Lagrange interpolation scheme uses the monomials $\varphi_j(x) = x^j$ as a basis system in (1.1). However, it was found that the Lagrange interpolation gives a uniform convergence of interpolation polynomials to the function under consideration for a certain class of smooth functions only (e.g., the class of integer functions). The reason for divergence is the presence of angular points at which the first derivative of the function exhibits discontinuity. The example of Bernstein shows that even one angular point may cause the divergence of interpolation polynomials on the entire interval under consideration. In the 1960–70s, as an alternative to the Lagrange interpolation scheme, the spline interpolation scheme was proposed. This scheme allows one to localize the effect of angular points and to ensure the uniform convergence of interpolating spline approximations for any continuous function [5–8].

The scheme of representing the functions as linear combinations of basis functions, including polynomials and spline approximations, in principle, can be generalized for the functions of several variables, but in practice such schemes are suitable only for the functions of two or three variables. So far, no efficient general schemes of interpolation and forecasting exist for the functions of many variables. There exist only some rough approximate schemes of interpolation, such as piecewise-linear schemes that require a large amount of data to enable their usage and often fail to provide a required accuracy even in the case when such an amount of data is available. Another example of rough schemes are neural nets used to interpolate the functions of several variables [9].

In this paper we propose a universal computer-based approach to efficiently interpolate and extrapolate the functions of several variables and to forecast time series without prior fixing a functional dependence on the arguments of the function under consideration, but only with the use of computed function values Y_1, \dots, Y_n at given points $\mathbf{X}_1, \dots, \mathbf{X}_n$, including in the case of chaotic errors in Y_1, \dots, Y_n .

¹ National Research Nuclear University МЕРНИ, Kashirskoe Shosse, 31, 115409, Moscow; А. В. Крянев, профессор, e-mail: avkryaney@mephi.ru; Г. В. Лукин, доцент, e-mail: gleb_lukin@letograf.ru; Д. К. Удумян, аспирант, e-mail: sinner5@mail.ru

2. Matrices of metric uncertainty and their properties. Below we consider the problems related to the functional dependence $Y = F(X_1, \dots, X_m) = F(\mathbf{X})$, where $F(\mathbf{X})$ is an unknown function to be reconstructed at a point \mathbf{X}^* or at a set of given points on the basis of the function values $Y_k, k = 1, \dots, n$, known at fixed points $\mathbf{X}_k = (X_{k1}, \dots, X_{km})^T$.

Without loss of generality, we may assume that the values of the arguments $X_i, i = 1, \dots, m$, are nondimensionalized and are brought into a common scale, for example, in such a way that the inequality $0 \leq X_i \leq 1$ is fulfilled for all X_i (i.e., the points \mathbf{X} belong to an m -dimensional unit cube $K \in E^m$ of space E^m).

In the space E^m , we choose a metric induced by the norm

$$\|\mathbf{X}\| = \sum_{j=1}^m w_j X_j^2, \tag{2.1}$$

where $w_j \geq 0, \sum_{j=1}^m w_j = m$, are some metric weights.

Remark. An essential part of our metric analysis is the choice of the weights $w_j, j = 1, \dots, m$, on the basis of the experimental data Y_k and $X_k, k = 1, \dots, n$ (see below), rather than the prior specification of weights, i.e., the specification of norm (2.1). For a while we assume that the weights w_j are given.

Let \mathbf{X}^* be a point at which the value of a function Y^* should be reconstructed. According to the metric analysis scheme, we compose the following $(n \times n)$ matrix W of metric uncertainty for the point \mathbf{X}^* with respect to the points $\mathbf{X}_1, \dots, \mathbf{X}_n$:

$$W = \begin{pmatrix} \rho^2(\mathbf{X}_1, \mathbf{X}^*)_{\mathbf{w}} & (\mathbf{X}_1, \mathbf{X}_2)_{\mathbf{w}} & \dots & (\mathbf{X}_1, \mathbf{X}_n)_{\mathbf{w}} \\ (\mathbf{X}_2, \mathbf{X}_1)_{\mathbf{w}} & \rho^2(\mathbf{X}_2, \mathbf{X}^*)_{\mathbf{w}} & \dots & (\mathbf{X}_2, \mathbf{X}_n)_{\mathbf{w}} \\ \dots & \dots & \dots & \dots \\ (\mathbf{X}_n, \mathbf{X}_1)_{\mathbf{w}} & (\mathbf{X}_n, \mathbf{X}_2)_{\mathbf{w}} & \dots & \rho^2(\mathbf{X}_n, \mathbf{X}^*)_{\mathbf{w}} \end{pmatrix}.$$

Here $\rho^2(\mathbf{X}_i, \mathbf{X}^*)_{\mathbf{w}} = \sum_{k=1}^m w_k (X_{ik} - X_k^*)^2, (\mathbf{X}_i, \mathbf{X}_j)_{\mathbf{w}} = \sum_{k=1}^m w_k (X_{ik} - X_k^*)(X_{jk} - X_k^*), i, j = 1, \dots, n$.

From the definition of the matrix W , it follows that this matrix is specified only by the location of the points $\mathbf{X}_1, \dots, \mathbf{X}^*$ and by the weights w_1, \dots, w_m only.

3. Metric interpolation of functions of several variables. Let us assume that the interpolation formula for the value Y^* of a function $Y = f(\mathbf{X})$ at a point \mathbf{X}^* is given by $Y^* = \sum_{i=1}^n z_i Y_i$, where the weights z_i

satisfy the normalization condition $\sum_{i=1}^n z_i = 1$, like for any interpolation formula.

Note that the weights z_i can be negative.

Let W be a nonsingular matrix. Let us define the following numerical characteristic $\sigma_{ND}^2(Y^*)$ of metric uncertainty for the reconstructed value Y^* at the point \mathbf{X}^* obtained on the basis of the known values of the function at the points $\mathbf{X}_1, \dots, \mathbf{X}_n$ with given weights $z_i, i = 1, \dots, n$:

$$\sigma_{ND}^2(Y^*; z) = (W(\mathbf{X}^*; \mathbf{X}_1; \dots; \mathbf{X}_n)\mathbf{z}, \mathbf{z}). \tag{3.1}$$

Here $\mathbf{z} = (z_1, \dots, z_n)^T$.

Now we choose weights $z_i, i = 1, \dots, n$, such that they satisfy the normalization condition $\sum_{i=1}^n z_i = 1$ and the numerical value of the uncertainty characteristic (3.1) is minimal:

$$\begin{cases} (W\mathbf{z}, \mathbf{z}) - \min_{\mathbf{z}} \\ (\mathbf{z}, \mathbf{1}) = 1, \quad \mathbf{1} = (1, \dots, 1)^T. \end{cases} \tag{3.2}$$

The sought interpolation value Y^* of the function $F(\mathbf{X})$ at the point \mathbf{X}^* obtained with the data $\mathbf{X}_i, Y_i, i = 1, \dots, n$, and with the minimum value of metric uncertainty as a solution to problem (3.2) is defined by the formula $Y^* = \frac{(W^{-1}\mathbf{Y}, \mathbf{1})}{(W^{-1}\mathbf{1}, \mathbf{1})}$, where $\mathbf{Y} = (Y_1, \dots, Y_n)^T$.

If the matrix W of metric uncertainty is singular, then the sought vector \mathbf{z}^* and the sought interpolation value Y^* (except for some special cases) are specified by the equalities (see [1])

$$\mathbf{z}^* = \frac{W^+ \mathbf{1}}{(W^+ \mathbf{1}, \mathbf{1})}, \quad Y^* = \frac{(W^+ \mathbf{Y}, \mathbf{1})}{(W^+ \mathbf{1}, \mathbf{1})}, \quad (3.4)$$

where W^+ is the pseudoinverse matrix or the inverse matrix after regularization of W [10–12].

Remark. When using (3.4), we assume that $(W^+ \mathbf{1}, \mathbf{1}) > 0$.

Let us define the metric uncertainty of the value Y^* given in (3.4). We have

$$\sigma_{ND}^2(Y^*) = (W\mathbf{z}^*, \mathbf{z}^*) = \frac{(WW^+ \mathbf{1}, W^+ \mathbf{1})}{(W^+ \mathbf{1}, \mathbf{1})^2} = \frac{(W^+ WW^+ \mathbf{1}, \mathbf{1})}{(W^+ \mathbf{1}, \mathbf{1})^2} = \frac{(W^+ \mathbf{1}, \mathbf{1})}{(W^+ \mathbf{1}, \mathbf{1})^2} = \frac{1}{(W^+ \mathbf{1}, \mathbf{1})}.$$

Here we take into account that the pseudoinverse matrix W^+ is symmetric and that $W^+ WW^+ = W^+$.

The value $\sigma_{ND}^2(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n) = \frac{1}{(W^+ \mathbf{1}, \mathbf{1})} > 0$ is called the measure of metric uncertainty in the reconstruction of the function at point \mathbf{X}^* on the basis of its known values at the points $\mathbf{X}_i, i = 1, \dots, n$.

The inverse value $I(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n) = (W^+ \mathbf{1}, \mathbf{1}) = \sum_{i=1}^n \sum_{j=1}^n W_{ij}^+$ is called the metric information of the point \mathbf{X}^* with respect to the set of the points $\mathbf{X}_1, \dots, \mathbf{X}_n$.

From the properties of pseudoinverse matrices it follows that, when a new point \mathbf{X}_{n+1} is added to the set of the points $\mathbf{X}_1, \dots, \mathbf{X}_n$, the metric information at any point \mathbf{X}^* with respect to the set of the points $\mathbf{X}_1, \dots, \mathbf{X}_n, \mathbf{X}_{n+1}$ is not less than the metric information at the point \mathbf{X}^* with respect to the set of the points $\mathbf{X}_1, \dots, \mathbf{X}_n$:

$$I(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n, \mathbf{X}_{n+1}) \geq I(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n).$$

The following equality is fulfilled for the measure of metric uncertainty:

$$\sigma_{ND}^2(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n, \mathbf{X}_{n+1}) \leq \sigma_{ND}^2(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n).$$

Now we consider the choice of the weights \mathbf{w} in norm (2.1) that defines the norm in space E^m [1]. Such a choice should take into account the nature of variation of the function under consideration when the independent arguments are varied; therefore, the “weight” matrix takes into account not only the geometric arrangement of the points in the original geometric space but also the different levels of the function’s variations with respect to different arguments of the function.

If the prior information on the degree of variation for the function in relation to the variations of the arguments (the values of partial derivatives) is known in the domain of the phase space E^m under consideration, then the normalized weights (the sum of the weights should be equal to m) are chosen in proportion to the absolute values of the corresponding partial derivatives.

Below we propose one of the possible schemes to estimate the weights on the basis of the degree of influence of each argument (factor) on the variation of the function by eliminating this factor and by reconstructing the values of the function at the point \mathbf{X}^* of interest when this factor is included or not to the truncated point $\mathbf{X}^{(j)*} = (X_1^*, \dots, X_{j-1}^*, X_{j+1}^*, \dots, X_m^*)^T$ of dimension $m - 1$ by the formulas $Y^{(l)*} = \frac{(\widetilde{W}^{(l)+} \mathbf{1}, \mathbf{Y})}{(\widetilde{W}^{(l)+} \mathbf{1}, \mathbf{1})}, l =$

$1, \dots, m$, where $\widetilde{W}^{(l)}$ is the matrix of metric uncertainty whose elements are $\widetilde{W}_{ij}^{(l)} = \sum_{\substack{k=1 \\ k \neq l}}^m (X_{ik} - X_k^*)(X_{jk} - X_k^*),$
 $i, j = 1, \dots, n$.

The sought weights \mathbf{w} are calculated as

$$w_k = \frac{m \widetilde{w}_k}{\sum_{k=1}^m \widetilde{w}_k}, \quad k = 1, \dots, m, \quad (3.5)$$

where $\widetilde{w}_k = (Y^{(k)*} - \tilde{Y}^*)^2$ and $\tilde{Y}^* = \frac{(\widetilde{W}^+ \mathbf{1}, \mathbf{Y})}{(\widetilde{W}^+ \mathbf{1}, \mathbf{1})}$. The elements \widetilde{W}_{ij} of the matrix \widetilde{W} of metric uncertainty are

obtained by the formulas $\widetilde{W}_{ij} = \sum_{k=1}^m (X_{ik} - X_k^*)(X_{jk} - X_k^*), i, j = 1, \dots, n$.

Remark. From (3.5) it follows that $\sum_{k=1}^m w_k = m$. Therefore, if $w_k > 1$ ($w_k < 1$), then the level of variations of the function becomes higher (lower) when the k -th argument is varied under the condition that the sensitivity degree of the function is the same with respect to the variations of its arguments.

Thus, the above weight metric choice scheme allows one to specify the degree of influence of each argument and to take into account the distinction in this degree by passing to a new metric with the corresponding unequal weights.

Let us consider the degenerate case when the function under consideration has an argument (factor) that the function does not depend on. Then, when we implement the scheme of finding the new metric's weights, we get an unambiguous result: the metric weight for this factor is equal to zero and this factor is automatically eliminated from further consideration. Therefore, the above scheme of transition to the metric with weights allows one to take into account the influence of arguments on the variations of a function and to eliminate the inessential arguments, thus decreasing the dimension of the factor space, as is done in factor analysis.

The following theorems are true [1].

Theorem 1 (an inequality for the measure of metric uncertainty). *The measure of metric uncertainty for any interpolation value of a function Y at a point \mathbf{X}^* with respect to the known values of this function at points $\mathbf{X}_1, \dots, \mathbf{X}_n$ satisfies the following inequality of metric uncertainty:*

$$\sigma_Y^2(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n) \geq \left(I_Y(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n) \right)^{-1}. \tag{3.6}$$

Here $I_Y(\mathbf{X}^*/\mathbf{X}_1, \dots, \mathbf{X}_n)$ is the metric information on the function Y at the point \mathbf{X}^* with respect to the points $\mathbf{X}_1, \dots, \mathbf{X}_n$.

Definition. The interpolation value of a function Y^* at a point \mathbf{X}^* is said to be effective if (3.6) becomes the equality for its measure of metric uncertainty.

Theorem 2 (on the effectiveness of the interpolation value of a function). *The interpolation value of a function Y^* at a point \mathbf{X}^* is effective.*

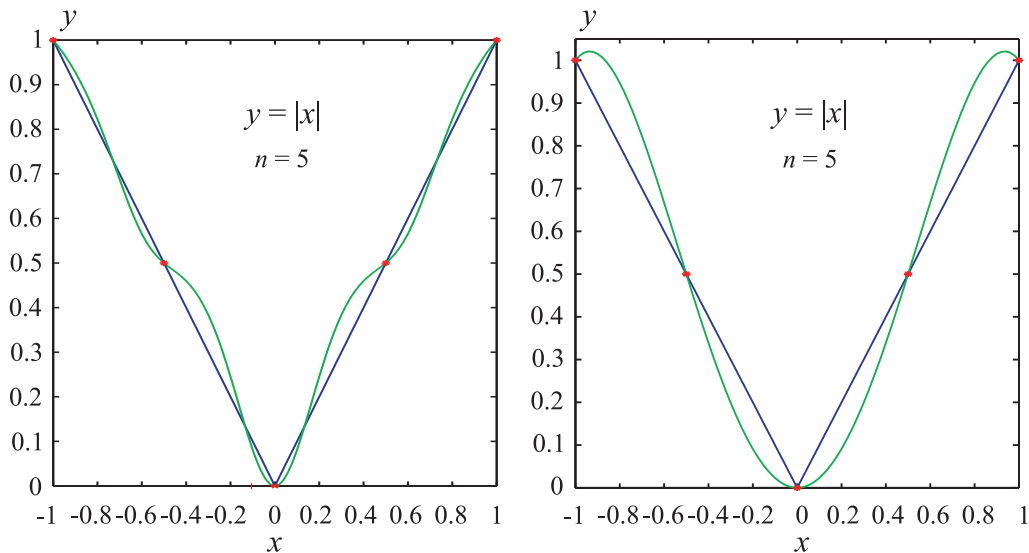


Fig. 1. The results of interpolation with 5 nodes

Example 1. Let us consider the interpolation of the function $y(x) = |x|$ on the interval $[a, b]$, where $a = -1$ and $b = 1$. For $n \in \mathbb{N}$ we have $h = \frac{b-a}{n}$; $x_k = a + kh$, $k = 0, \dots, n$, are the nodes of interpolation, i.e., we know the values of the function $y(x)$ at the points x_k . As mentioned above, the existence of one angular point may cause divergence of interpolation polynomials in the Lagrange method. The results of interpolation by the metric analysis method and by the Lagrange method with different grid steps are shown in Figs. 1 and 2.

From these figures it follows that, when the grid steps are decreased, the Lagrange interpolation diverges, whereas the accuracy of interpolation values obtained by the metric analysis method increases.

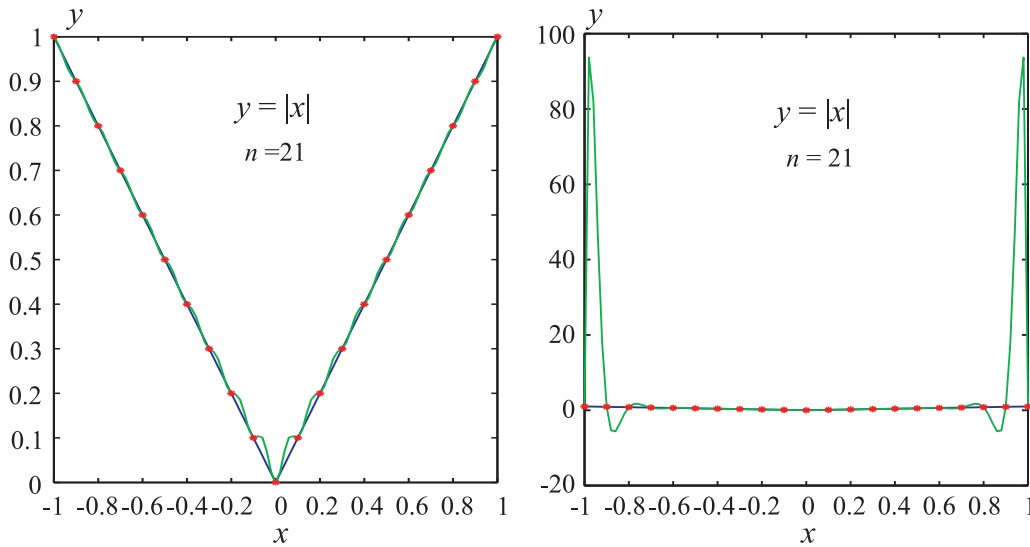


Fig. 2. The results of interpolation with 21 nodes

Example 2. Let us consider the function $Y = f(\mathbf{x}) = (V\mathbf{x}, \mathbf{x}) + (\mathbf{c}, \mathbf{x})$, $\mathbf{x} = (x_1, \dots, x_m)^T$, $0 \leq x_i \leq 1$, $i = 1, \dots, m$, where V is an $(m \times m)$ constant matrix, $\mathbf{c} = (c_1, \dots, c_m)^T$ is a constant vector and $m = 12$ is the space dimension. Let $Y(\mathbf{X}_k) = Y_k$, $k = 1, \dots, 25$, where \mathbf{X}_k are the nodes of interpolation and Y_k are the values of the function at the nodal points. Let $N = 20$ be the number of points at which the function should be reconstructed. Both the nodal points and the points at which the function is reconstructed are chosen using a random number generator in E^m .

The results of interpolation for Example 2 is given in the table. In the first column, we indicate the number of points at which the function is reconstructed; the second column contains the exact values of the function; the third column contains the reconstructed values; and the fourth column contains the relative errors in percentage.

Results of multidimensional interpolation

N	exact values	reconstructed values	relative errors (in %)	N	exact values	reconstructed values	relative errors (in %)
1	38.00	38.59	1.54	11	35.18	35.89	2.02
2	44.38	45.81	3.20	12	44.57	45.28	1.59
3	44.40	46.44	4.58	13	42.63	44.04	3.30
4	49.94	49.42	1.04	14	49.50	49.89	0.79
5	36.30	37.66	3.74	15	25.84	25.22	2.38
6	44.76	45.42	1.48	16	41.00	41.38	0.92
7	43.19	42.45	1.70	17	55.39	53.83	2.83
8	43.46	42.82	1.47	18	42.05	44.93	6.86
9	37.43	36.51	2.45	19	38.95	39.86	2.35
10	30.78	29.06	5.60	20	47.37	47.22	0.32

In spite of a small number of nodal points, we achieve a high accuracy in the reconstructed values.

4. Extrapolation of functions by the metric analysis method using nonlinear autoregression.

Let us consider a function $y = f(x)$ with its values $y_1 = f(x_1), \dots, y_n = f(x_n)$ at points $x_1, \dots, x_n \in E^1$. It is required to find a value y_{n+1} at x_{n+1} . The problem of finding the extrapolation value y_{n+1} can be reduced to the problem of interpolating a multidimensional function using nonlinear autoregression: $y_{m+1} = F(y_1, \dots, y_m)$, $y_{m+2} = F(y_2, \dots, y_{m+1}), \dots, y_n = F(y_{n-m}, \dots, y_{n-1})$. Then, the extrapolation of $y = f(x)$ is reduced to the interpolation of the function $Y = F(y_1, y_2, \dots, y_m)$ whose values are known at the $n - m$ points $\mathbf{X}_1 = (y_1, \dots, y_m), \dots, \mathbf{X}_{n-m} = (y_{n-m}, \dots, y_n)$.

The value y_{n+1} is determined as an interpolation value of the m -dimensional function F at the point \mathbf{X}^* : $y_{n+1} = F(\mathbf{X}^*)$, where $\mathbf{X}^* = (y_{n-m+1}, \dots, y_n)$.

The parameter m is very important in this scheme and is unknown in advance. Using the scheme of extrapolation with different m for forecasting the value y_n , we can determine m as follow: $m = \arg \min (\tilde{y}_n - y_n)$, where \tilde{y}_n is determined using the above scheme of extrapolation.

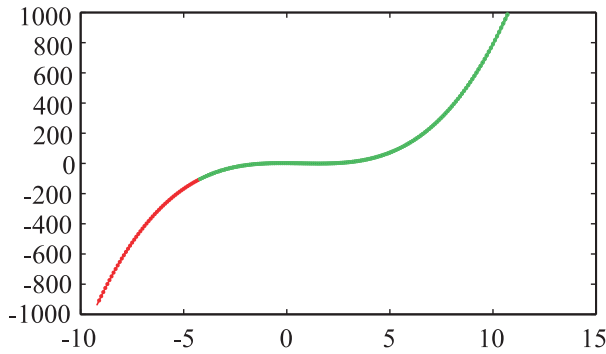


Fig. 3. The results of extrapolation

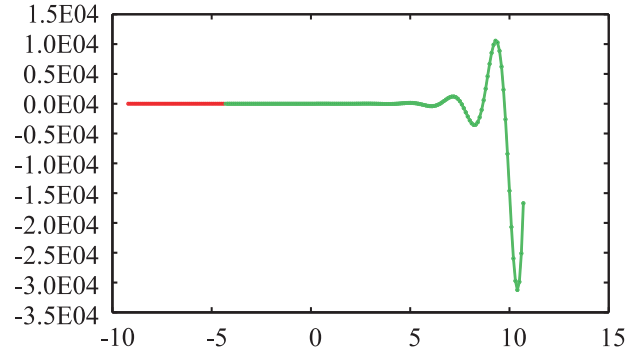


Fig. 4. The results of extrapolation

Example 3. Let us consider the function $y = (x + 1)(x - 1)(x - 2)$ on the interval (a, b) , $a = -9.2$, $b = -4.2$ with the step $h = 0.1$, so we have $N = 50$ points at which we know the values of this function. The results of extrapolation for $N_{\text{ext}} = 150$ points are illustrated in Fig. 3.

The red points correspond to the exact values of the function, whereas the green points correspond to the extrapolated values. In all the examples below, they have the same meaning. The extrapolated values of the function almost coincide with the exact values; that is why it is impossible to distinguish them in the figures. The relative error of extrapolation is $\varepsilon = \frac{y_{\text{ext}} - y_{\text{exact}}}{y_{\text{exact}}} = 10^{-3}$, where y_{exact} is the exact value of the function at the end of the extrapolation interval, i.e., $y_{\text{exact}} = y(x_{N+N_{\text{ext}}})$. The optimal space dimension is $m_{\text{opt}} = 31$.

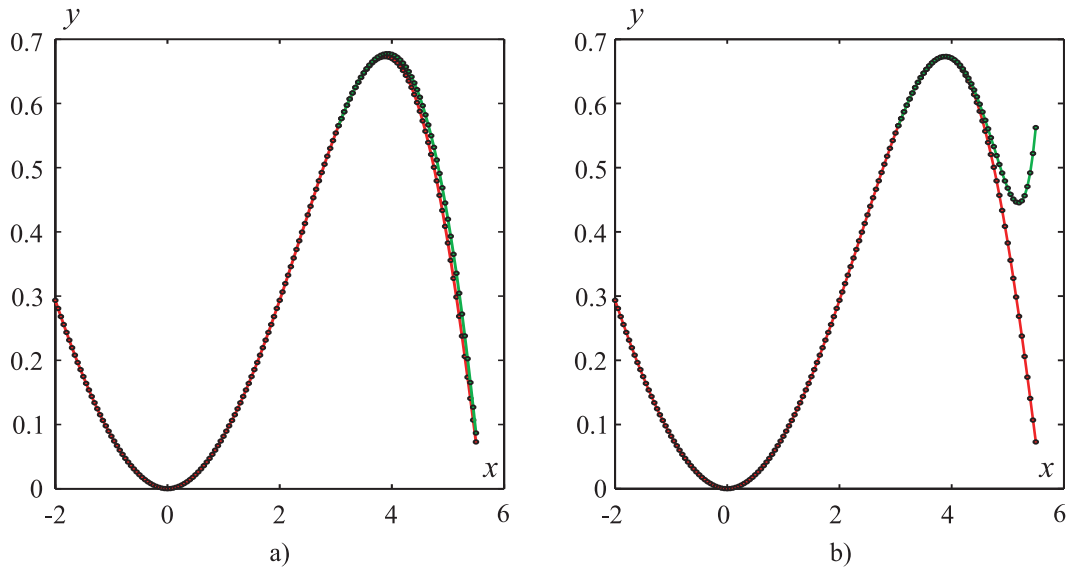


Fig. 5. The results of extrapolation

Example 4. Let $y = e^x \sin(\omega x)$, $\omega = 2.9$, $a = -9.2$, $b = -4.2$, $h = 0.1$, $N = 50$, and $N_{\text{ext}} = 150$. The results of extrapolation are illustrated in Fig. 4. Here $\varepsilon = 10^{-10}$ and $m_{\text{opt}} = 32$.

Note that the well-known SSA method [2] yields adequate results for the extrapolation of functions being superpositions of polynomials, exponentials, and sinusoids. For a wider class of functions, however, the SSA method fails, whereas the metric analysis method gives acceptable results.

Example 5. Let $y = e^{-0.2\sqrt{|x|}} \sin(\omega x^2)$, $a = -2$, $b = 3$, $h = 0.05$, $\omega = 0.1$, $N = 100$, and $N_{\text{ext}} = 50$. The comparison results are given in Fig. 5. Figure 5a illustrates the results obtained by the metric analysis method; the results obtained by the SSA method are represented in Fig. 5b. The optimal space dimension is $m_{\text{opt}} = 77$.

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