A novel method of interpolation and extrapolation of functions by a linear initial value problem

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Abstract

A novel method of function approximation using an initial value, linear, ordinary differential equation (ODE) is presented. The main advantage of this method is to obtain the approximation expressions in a closed form. This technique can be taught in the classroom to undergraduates that have completed a first course in ODE using DERIVE or some other computer algebra system (CAS), because of the computing power available today. It can also be included in an ODE course as an "application" of ODE using DERIVE or some other CAS.

1 Introduction

The main idea of the new method presented here is that we obtain an approximation of a function on a fixed interval by means of a Cauchy problem (an initial value problem (IVP)) for an ODE with unknown constant coefficients and unknown initial values. The goal function is formulated as a positive definite function with non-negative weight function. The unknown coefficients and initial conditions of the IVP are then defined by means of minimization of the goal function. Such an approach was first suggested in [1]. In that paper the identification of dynamical systems by means of the integration of each equation of the system (using quadrature rules and statistics) was used.

The classical approach to function approximation is based on a particular choice of functions, for example polynomial, rational, exponential functions or Fourier series. There are several disadvantages to the classical approach. For example, polynomial interpolation may seldom be used for the purposes of extrapolation due to the fast divergence of higher order polynomials outside of the interpolation interval. The main disadvantage of a Fourier series approximation is that it is not applicable to non-periodic functions and hence, could not be used for extrapolation purposes. The method we propose allows us to approximate functions by means of linear combination of polynomials, trigonometric and exponential functions, products of polynomials and exponents, polynomials and

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periodic functions, periodic functions and exponents, and polynomials, exponents and periodic functions. It is well suited for the purposes of interpolation and extrapolation of physical and chemical processes, which are usually described in terms of systems of linearised ODE. An example of this approximation technique is discussed below.

2 Formulation of classical regression problems

A conventional problem of regression is formulated as follows. Assume that the following table of data (either experimental or functional) is given in table 1.

Table 1

I	0	1	2	$\cdots$	N
X	$x_0 = 0$	x_1	x_2	$\cdots$	x_N
Y	y_0	y_1	y_2	$\cdots$	y_N

The following conventional methods might be applied to “fit” a function to the tabled data (see, for instance, [2]):

Problem A. A linear regression fit:

$$y = a \cdot x + b \tag{1}$$

where a, b are unknown coefficients.

Problem B. An exponential regression fit:

$$y = \beta \cdot e^{\alpha \cdot x} \quad \Rightarrow \quad \ln(y) = \alpha \cdot x + \ln(\beta), \tag{2}$$

which can be reduced to the previous problem by means of the logarithm where α, β are the unknown coefficients.

Problem C. For two given functions $f_{1,2}(x)$ that do not contain any unknown parameters, attempt a non-linear regression fit (which is linear with regards to coefficients):

$$y = a_1 f_1(x) + a_2 f_2(x), \tag{3}$$

where a_1, a_2 are unknown coefficients.

Problem D. A non-linear exponential regression fit:

$$y = a_1 e^{b_1 \cdot x} + a_2 e^{b_2 \cdot x}, \tag{4}$$

where all parameters a_1, a_2, b_1, b_2 are unknown.

Conventionally, a graphical method is used in an attempt to solve the non-linear exponential regression ***Problem D,*** which arises, for example, in chemical technology and bio-chemical kinetics. In this paper we consider an analytic method for solving ***Problem D.***

3 Non-linear regression as the solution to an IVP

Consider the non-linear exponential regression ***Problem D*** of equation (4).

Equation (4) is a general solution to the following initial value problem (IVP):

$$\frac{d^2y}{dx^2} + c_1 \frac{dy}{dx} + c_0 y = 0, \qquad x = x_0 = 0: \ \ y(0) = \tilde{y}_0, \ \ \left.\frac{dy}{dx}\right|_{x=0} = \tilde{y}_1 \tag{5}$$

where $c_0, c_1, \tilde{y}_0, \tilde{y}_1$ are unknowns.

Hence the original problem of the determination of four unknowns a_1, a_2, b_1, b_2 is equivalent to the determination of the following four unknowns $c_0, c_1, \tilde{y}_0, \tilde{y}_1$, where c_0, c_1 are unknown coefficients of the linear second order differential equation ($\frac{d^2y}{dx^2} + c_1 \frac{dy}{dx} + c_0 y = 0$) and $\tilde{y}_0, \tilde{y}_1$ are unknown initial conditions of this equation.

In this case the original unknowns (a_1, a_2, b_1, b_2) are functions of $(c_0, c_1, \tilde{y}_0, \tilde{y}_1)$:

$$\begin{cases} a_i = a_i\left(c_0, c_1, \tilde{y}_0, \tilde{y}_1\right) \\ b_i = b_i\left(c_0, c_1, \tilde{y}_0, \tilde{y}_1\right) \end{cases} \quad (i = 1, 2) \tag{6}$$

4 Solution to the problem of non-linear regression

Let us consider the ordinary differential equation of the IVP (5):

$$\frac{d^2y}{dx^2}+c_1\frac{dy}{dx}+c_0y=0 \tag{7}$$

and integrate it twice with regards to *x*. The resulting integral equation is as follows:

$$y+c_0I_2(x)+c_1I_1(x)+d_0+d_1x=0 \tag{8}$$

where $I_1(x)=\int_{x_0=0}^{x} y(\tau)d\tau$, $I_2(x)=\int_{x_0=0}^{x} I_1(\tau)d\tau$, and c_0, c_1, $d_0=-\tilde{y}_0$, $d_1=-(\tilde{y}_1+c_1\tilde{y}_0)$ are new unknowns.

To calculate the unknowns c_0, c_1, d_0, d_1 let us enlarge table 1 as follows:

Table 2

i	0	1	2	$\cdots$	*N*
x	$x_0=0$	x_1	x_2	$\cdots$	x_N
y	y_0	y_1	y_2	$\cdots$	y_N
$I_1(x)$	0	I_{11}	I_{12}	$\cdots$	I_{1N}
$I_2(x)$	0	I_{21}	I_{22}	$\cdots$	I_{2N}

where $I_{1j}=\int_{x_0=0}^{x_j} y(\tau)d\tau$, $I_{2j}=\int_{x_0=0}^{x_j} I_1(\tau)d\tau$. In this table the last two rows are obtained by means of numerical integration of the *y*–row using any quadrature scheme (trapezoidal rule, Simpson's rule, *et cetera*) or alternately by fitting a cubic spline to the x and y data to obtain a function y(x) that can be integrated by the CAS.

After that the problem is converted to ***Problem C*** (expression (3)) with $f_1(x)=-I_2(x)$, $f_2(x)=-I_0(x)$, $f_3(x)=-1$, $f_4(x)=-x$. Unknown coefficients c_0, c_1, d_0, d_1 are found by the well known least square method (LSM) with the goal function:

$$F_1(c_0,c_1,d_0,d_1)=\frac{1}{2}\sum_{j=0}^{N}\left[y_j+c_0I_{2j}+c_1I_{1j}+d_0+d_1x_j\right]^2 \rightarrow \min \tag{9}$$

Goal function minimization occurs when we set

$$\frac{\partial F_1}{\partial c_0}=\frac{\partial F_1}{\partial c_1}=\frac{\partial F_1}{\partial d_0}=\frac{\partial F_1}{\partial d_1}=0. \tag{10}$$

This yields a system of linear algebraic equations:

$$M \cdot [c_0, c_1, d_0, d_1]^T = N \tag{11}$$

where

$$M = \begin{bmatrix} \sum_{j=0}^{N} I_{2j}^2 & \sum_{j=0}^{N} I_{2j} I_{1j} & \sum_{j=0}^{N} I_{2j} & \sum_{j=0}^{N} I_{2j} x_j \\ & \sum_{j=0}^{N} I_{1j}^2 & \sum_{j=0}^{N} I_{1j} & \sum_{j=0}^{N} I_{1j} x_j \\ & & N+1 & \sum_{j=0}^{N} x_j \\ (Symm) & & & \sum_{j=0}^{N} x_j^2 \end{bmatrix}, \qquad N = (-1) \cdot \begin{bmatrix} \sum_{j=0}^{N} I_{2j} y_j \\ \sum_{j=0}^{N} I_{1j} y_j \\ \sum_{j=0}^{N} y_j \\ \sum_{j=0}^{N} x_j y_j \end{bmatrix}. \tag{12}$$

Hence, unknowns $c_0, c_1, d_0 = -\tilde{y}_0, d_1 = -(\tilde{y}_1 + c_1 \tilde{y}_0)$ are found from the system:

$$M \cdot [c_0, c_1, d_0, d_1]^T = N \,. \tag{13}$$

Consequently the coefficients (c_0, c_1) of the ODE as well as the initial conditions of the IVP can be determined. Indeed for the initial conditions we have:

$$\tilde{y}_0 = -d_0, \qquad \tilde{y}_1 = -d_1 + c_1 d_0 \tag{14}$$

To determine the coefficients, we note that the characteristic equation of the ODE is:

$$\lambda^2 + c_1 \lambda + c_0 = 0 \,. \tag{15}$$

Hence the eigenvalues of the ODE are:

$$\lambda_{1,2} = -\frac{c_1}{2} \pm \sqrt{\left(\frac{c_1}{2}\right)^2 - c_0} \,. \tag{16}$$

Let us denote $b_1 = \lambda_1$, $b_2 = \lambda_2$ and introduce new functions $f_1(x) = e^{b_1 x}$, $f_2(x) = e^{b_2 x}$. The non-linear exponential regression ***Problem D*** is converted to the non-linear regression, which is linear with regards to coefficients (***Problem C***):

$$y = a_1 f_1(x) + a_2 f_2(x), \qquad \text{(where } a_1, a_2 \text{ are } \textit{unknowns}\text{).} \tag{17}$$

To solve this problem we enlarge table 1 as follows:

Table 3

i	0	1	2	…	*N*
x	$x_0 = 0$	x_1	x_2	…	x_N
y	y_0	y_1	y_2	…	y_N
$f_1(x)$	f_{10}	f_{11}	f_{12}	…	f_{1N}
$f_2(x)$	f_{20}	f_{21}	f_{22}	…	f_{2N}

where $f_{1j} = e^{b_1 x_j}$, $f_{2j} = e^{b_2 x_j}$ ($j = 0,1,\ldots,N$).

The goal function for this problem according to the lease squares method is:

$$F_2(a_1, a_2) = \frac{1}{2}\sum\left[a_1 f_{1i} + a_2 f_{2i} - y_i\right]^2 \quad \to \quad \min . \tag{18}$$

Goal function minimization occurs when we set:

$$\frac{\partial F_1}{\partial a_1} = \frac{\partial F_1}{\partial a_2} = 0 . \tag{19}$$

This is yields a linear system of linear algebraic equations:

$$M_2 \cdot \left[a_1, a_2\right]^T = N_2 \tag{20}$$

where

$$M_2 = \begin{bmatrix} \sum\limits_{j=0}^{N} f_{1j}^2 & \sum\limits_{j=0}^{N} f_{1j} f_{2j} \\ (Symm) & \sum\limits_{j=0}^{N} f_{2j}^2 \end{bmatrix}, \qquad N_2 = \begin{bmatrix} \sum\limits_{j=0}^{N} f_{1j} y_j \\ \sum\limits_{j=0}^{N} f_{2j} y_j \end{bmatrix}. \tag{21}$$

The non-linear exponential regression ***Problem D*** is solved by means of conversion of the initial problem to the equivalent IVP, problem with unknown coefficients of the linear ordinary differential equation and unknown initial conditions. This method is applicable to a broad class of interpolation and extrapolation problems. It is very simple and could be realised in any CAS such as DERIVE, Mathcad or Mathematica.

5 Example

Let us consider function $y = a_1 e^{b_1 \cdot x} + a_2 e^{b_2 \cdot x}$ with $a_1 = 100.41$, $a_2 = 9.77$, $b_1 = -1.3$, $b_2 = -0.21$ in the interval $x \in [0, 8]$ and calculate its values at $N + 1 = 101$ points. This data produced using Mathcad 12 in the following table is considered to be "statistics".

Table 4

	0	1	2	3	4	5	6	7
x	0	0.08	0.16	0.24	0.32	0.4	0.48	0.56
y	110.18	99.882	90.61	82.261	74.741	67.967	61.863	...

Numerical integration can be used on the "statistics" or, alternately, one may fit a cubic spline through the "statistics" to obtain a function that can be integrated using Mathcad. A graph of this cubic spline follows in Figure 1.

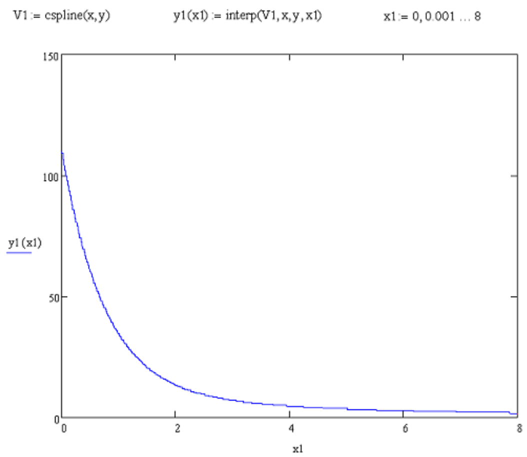

Figure1: A cubic spline fitted to the "statistics"

After calculating tables 2 and 3, a non-linear exponential regression fit $Y(x) = \overline{a}_1 e^{\overline{b}_1 \cdot x} + \overline{a}_2 e^{\overline{b}_2 \cdot x}$ is determined. The results are as follows (with five decimal place accuracy):

$$\begin{bmatrix} \overline{a}_1 \\ \overline{a}_2 \\ \overline{b}_1 \\ \overline{b}_2 \end{bmatrix} = \begin{bmatrix} 100.40998 \\ 9.77003 \\ -1.30000 \\ -0.21000 \end{bmatrix}, \qquad \begin{bmatrix} a_1 \\ a_2 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 100.41000 \\ 9.77000 \\ -1.30000 \\ -0.21000 \end{bmatrix}$$

The graphs of the functions y(x) and Y(x) and absolute error in the logarithmic scale follow in Figure 2.

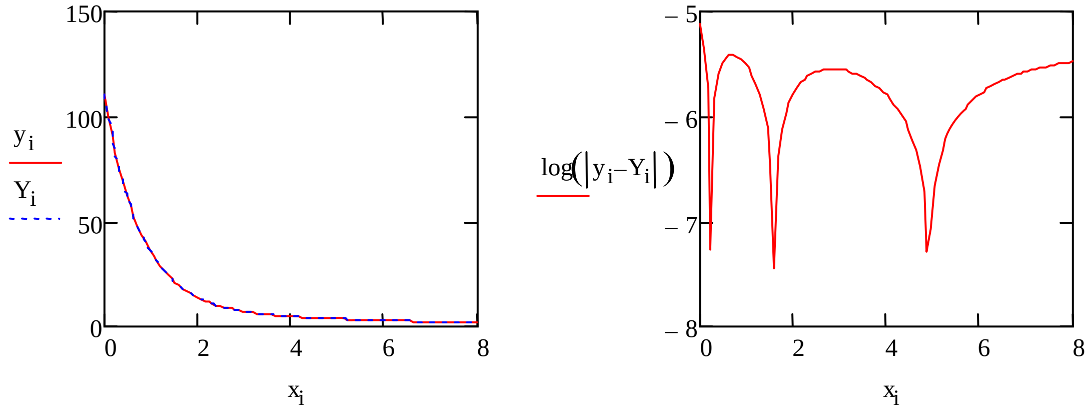

Figure 2: Graphs of the functions and the logarithm of absolute error

6 Conclusion

1. A novel method of non-linear regression is developed which reduces the regression problem to the identification of an IVP. That is, the non-linear exponential regression ***Problem D*** is solved by means of converting the initial problem to an equivalent IVP with unknown coefficients of the linear ordinary differential equation and unknown initial conditions.
2. In the formulated algorithm, two goal functions are constructed which reduce the problem to a corresponding system of linear algebraic coefficients.
3. The formulated algorithm may be used for both interpolation and extrapolation of functions.
4. All steps of the algorithm may be formulated in ***DERIVE*** or some other suitable CAS.
5. Because of the availability of CAS such as ***DERIVE*,** this method can be taught to undergraduate students that have completed a first course in ODE.

References

[1] I. Fedotov and M. Shatalov (2007). “On identification of dynamical systems parameters from experimental data”, *RGMIA, Victoria University (Melbourne)*, 10(1), Issue 2: pp. 106-116.

[2] N.R. Draper and H. Smith (1981). *Applied Regression Analysis, Second Edition.* New York: John Wiley & Sons.