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

M Shatalov\textsuperscript{a,\textcopyright}, I Fedotov and SV Joubert

Department of Mathematics and Statistics
Tshwane University of Technology
Pretoria, South Africa

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

\textsuperscript{a} mshatlov@csir.co.za

\textsuperscript{\textcopyright} Permanent address: Sensor Science and Technology of CSIR Manufacturing and Materials, P.O. Box 305, Pretoria 0001, South Africa
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>
<thead>
<tr>
<th>Table 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
</tr>
<tr>
<td>X</td>
</tr>
<tr>
<td>Y</td>
</tr>
</tbody>
</table>

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

**Problem A.** A linear regression fit:

$$y = a \cdot x + b$$  \hspace{1cm} (1)

where $a$, $b$ are unknown coefficients.

**Problem B.** An exponential regression fit:

$$y = \beta \cdot e^{\alpha x} \Rightarrow \ln(y) = \alpha \cdot x + \ln(\beta),$$  \hspace{1cm} (2)

which can be reduced to the previous problem by means of the logarithm where $\alpha$, $\beta$ 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):

$$y = a_1 f_1(x) + a_2 f_2(x),$$  \hspace{1cm} (3)

where $a_1$, $a_2$ are unknown coefficients.

**Problem D.** A non-linear exponential regression fit:
\[ y = a_1 e^{a_2 x} + a_4 e^{b_1 x}, \tag{4} \]

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):

\[
\begin{align*}
\frac{d^2 y}{dx^2} + c_1 \frac{dy}{dx} + c_0 y &= 0, \\
x &= x_0 = 0: \quad y(0) = \tilde{y}_0, \quad \frac{dy}{dx}\bigg|_{x=0} = \tilde{y}_1
\end{align*}
\tag{5}
\]

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 \((\frac{d^2 y}{dx^2} + c_1 \frac{dy}{dx} + c_0 y = 0)\) 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 \((c_0, c_1, \tilde{y}_0, \tilde{y}_1)\):

\[
\begin{align*}
\begin{cases}
a_i = a_i(c_0, c_1, \tilde{y}_0, \tilde{y}_1) \\
b_i = b_i(c_0, c_1, \tilde{y}_0, \tilde{y}_1)
\end{cases}
\end{align*}
\quad (i = 1, 2)
\tag{6}
\]

### 4 Solution to the problem of non-linear regression

Let us consider the ordinary differential equation of the IVP (5):
\[ \frac{d^2 y}{dx^2} + c_1 \frac{dy}{dx} + c_0 y = 0 \]  

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

\[ y + c_0 I_2(x) + c_1 I_1(x) + d_0 + d_1 x = 0 \]  

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

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

<table>
<thead>
<tr>
<th>( i )</th>
<th>( 0 )</th>
<th>( 1 )</th>
<th>( 2 )</th>
<th>( \ldots )</th>
<th>( N )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x )</td>
<td>( x_0 = 0 )</td>
<td>( x_1 )</td>
<td>( x_2 )</td>
<td>( \ldots )</td>
<td>( x_N )</td>
</tr>
<tr>
<td>( y )</td>
<td>( y_0 )</td>
<td>( y_1 )</td>
<td>( y_2 )</td>
<td>( \ldots )</td>
<td>( y_N )</td>
</tr>
<tr>
<td>( I_1(x) )</td>
<td>( 0 )</td>
<td>( I_{11} )</td>
<td>( I_{12} )</td>
<td>( \ldots )</td>
<td>( I_{1N} )</td>
</tr>
<tr>
<td>( I_2(x) )</td>
<td>( 0 )</td>
<td>( I_{21} )</td>
<td>( I_{22} )</td>
<td>( \ldots )</td>
<td>( I_{2N} )</td>
</tr>
</tbody>
</table>

where \( I_{ij} = \int_{x_0}^{x} y(\tau) d\tau \), \( I_{2j} = \int_{x_0}^{x} I_1(\tau) d\tau \). 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:

\[ F_i = \left( c_0, c_1, d_0, d_1 \right) \quad \min \sum_{j=0}^{N} \left[ y_j + c_0 I_{2j} + c_1 I_{1j} + d_0 + d_1 x_j \right]^2 \quad \rightarrow \quad \min \]  

Goal function minimization occurs when we set

\[ \frac{\partial F_i}{\partial c_0} = \frac{\partial F_i}{\partial c_1} = \frac{\partial F_i}{\partial d_0} = \frac{\partial F_i}{\partial d_1} = 0 \, . \]
This yields a system of linear algebraic equations:

\[ M \cdot [c_0, c_1, d_0, d_1]^T = N \]  \hspace{1cm} (11)

where

\[
M = \begin{bmatrix}
\sum_{j=0}^{N} I_{1j}^2 & \sum_{j=0}^{N} I_{2j} I_{1j} & \sum_{j=0}^{N} I_{2j} & \sum_{j=0}^{N} I_{2j} x_j \\
\sum_{j=0}^{N} I_{1j}^2 & \sum_{j=0}^{N} I_{1j} & \sum_{j=0}^{N} I_{1j} x_j & \sum_{j=0}^{N} I_{1j} y_j \\
N + 1 & \sum_{j=0}^{N} x_j & \sum_{j=0}^{N} x_j^2 & \sum_{j=0}^{N} x_j y_j \\
(Symm) & & & \end{bmatrix}, \quad N = (-1).
\]  \hspace{1cm} (12)

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

\[ M \cdot [c_0, c_1, d_0, d_1]^T = N. \]  \hspace{1cm} (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:

\[ \tilde{y}_0 = -d_0, \quad \tilde{y}_1 = -d_1 + c_1 d_0 \]  \hspace{1cm} (14)

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

\[ \lambda^2 + c_1 \lambda + c_0 = 0. \]  \hspace{1cm} (15)

Hence the eigenvalues of the ODE are:

\[ \lambda_{1,2} = -\frac{c_1}{2} \pm \sqrt{\left(\frac{c_1}{2}\right)^2 - c_0}. \]  \hspace{1cm} (16)

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

\[ y = a_1 f_1(x) + a_2 f_2(x), \quad \text{(where } a_1, a_2 \text{ are unknowns).} \]  \hspace{1cm} (17)
To solve this problem we enlarge table 1 as follows:

<table>
<thead>
<tr>
<th>$i$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>...</th>
<th>$N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x$</td>
<td>$x_0 = 0$</td>
<td>$x_1$</td>
<td>$x_2$</td>
<td>...</td>
<td>$x_N$</td>
</tr>
<tr>
<td>$y$</td>
<td>$y_0$</td>
<td>$y_1$</td>
<td>$y_2$</td>
<td>...</td>
<td>$y_N$</td>
</tr>
<tr>
<td>$f_1(x)$</td>
<td>$f_{10}$</td>
<td>$f_{11}$</td>
<td>$f_{12}$</td>
<td>...</td>
<td>$f_{1N}$</td>
</tr>
<tr>
<td>$f_2(x)$</td>
<td>$f_{20}$</td>
<td>$f_{21}$</td>
<td>$f_{22}$</td>
<td>...</td>
<td>$f_{2N}$</td>
</tr>
</tbody>
</table>

where $f_{ij} = e^{h_{ij}}, f_{2j} = e^{h_{2j}}$ ($j = 0, 1, \ldots, N$).

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

$$ F_2(a_1, a_2) = \frac{1}{2} \sum [a_1 f_i + a_2, f_{2i} - y_i]^2 \rightarrow \text{min}. \quad (18) $$

Goal function minimization occurs when we set:

$$ \frac{\partial F_2}{\partial a_1} = \frac{\partial F_2}{\partial a_2} = 0. \quad (19) $$

This yields a linear system of linear algebraic equations:

$$ M_2 \cdot [a_1, a_2]^T = N_2 \quad (20) $$

where

$$ M_2 = \begin{bmatrix} \sum_{j=0}^{N} f_{ij}^2 & \sum_{j=0}^{N} f_{ij} f_{2j} \\ \sum_{j=0}^{N} f_{ij} f_{2j} & \sum_{j=0}^{N} f_{2j}^2 \end{bmatrix}, \quad N_2 = \begin{bmatrix} \sum_{j=0}^{N} f_{ij} y_j \\ \sum_{j=0}^{N} f_{2j} y_j \end{bmatrix}. \quad (21) $$

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 \( y = a_1 e^{b_1 x} + a_2 e^{b_2 x} \) 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".

\[
\begin{array}{cccccccc}
\hline
x & 0 & 0.08 & 0.16 & 0.24 & 0.32 & 0.4 & 0.48 & 0.56 \\
y & 110.18 & 99.882 & 90.61 & 82.261 & 74.741 & 67.967 & 61.863 & \ldots \\
\hline
\end{array}
\]

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.

After calculating tables 2 and 3, a non-linear exponential regression fit \( Y(x) = a_1 e^{b_1 x} + a_2 e^{b_2 x} \) is determined. The results are as follows (with five decimal place accuracy):

\[
\begin{bmatrix}
\bar{a}_1 \\
\bar{a}_2 \\
\bar{b}_1 \\
\bar{b}_2 \\
\end{bmatrix}
= 
\begin{bmatrix}
100.40998 \\
9.77003 \\
-1.30000 \\
-0.21000 \\
\end{bmatrix}, \quad
\begin{bmatrix}
a_1 \\
a_2 \\
b_1 \\
b_2 \\
\end{bmatrix}
= 
\begin{bmatrix}
100.41000 \\
9.77000 \\
-1.30000 \\
-0.21000 \\
\end{bmatrix}
\]

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