NUMERICAL APPROXIMATION OF TAYLOR COEFFICIENTS FOR SOLVING FIRST ORDER ODEs

István Selek
Department of Informatics, Faculty of Mechanical Engineering
Budapest University of Technology and Economics
H-1111 Budapest, Műegyetem rkp. 5. Phone: (1)-463-1170
E-mail: selek@rit.bme.hu

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INTRODUCTION

It is well-known, that differential equations are used to describe the processes of engineering, economics...etc. It is often necessary to solve a system of N first order ordinary differential equations (ODEs) of the following format:

$$y'(x) = f(y(x), x), \quad y(x_0) = y_0 \tag{1}$$

The majority of differential equations does not have an analytical solution, only a limited number of ODEs (see (1)) have an exact analytical solution. It is often the case, that even quite simple systems might have a complicated nonlinear differential equation representation, or it could be very difficult or even impossible to give the differential equations exactly. With the advent of digital computers, complex equations or systems of equations could powerfully and exactly be solved with various numerical methods. Computers can handle large amounts of data easily and quickly. Probably the most serious drawback of numerical methods is that they can only approximate the continuous solution with a series of discrete points. A large number of formulas were developed to solve these kinds of equations. Adams-Bashfort and Runge-Kutta methods are used fairly extensively nowadays. Both methods use discrete points to approximate the integral of functions from x_i to x_{i+1} where x is the variable of function.

In this paper an algorithm is proposed to approximate the Taylor series of the solution of equation (1) in given points. The proposed method can be useful for solving ODEs with continuous methods and for evaluating numerical derivatives.

THE ALGORITHM

Let us consider the differential equation (1) with its initial condition. Let us presume that the values of $y'(x)$ and $f(y(x), x)$ in x_i are known, and $f(y(x), x)$ satisfy the Lipschitz condition in every x and y_1, y_2 :

$$|f(x, y_1) - f(x, y_2)| \leq L_f |y_1 - y_2| \tag{2}$$

Where L_f is a scalar number ($L_f \in R$). Let us introduce a new variable ξ in the vicinity of x_i.

$$x = x_i + \xi \tag{3}$$

The Taylor series of $y'(x)$ in the neighbourhood of x_i is given in the following format:

$$y'(x_i) = \sum_{p=0}^{\infty} \frac{\xi^p}{p!}\, y^{(p+1)}(x_i) \tag{4}$$

When integrating equation (4) the approximate value of $y(x)$ around x_i results. Predictor methods (like Adams-Bashfort) can be based on this formula because it traces the progress in variable x. The increment of function $y(x)$ is determined by

$$\triangle y = \int_{x_i}^{x_{i+1}} y'(x)\mathrm{d}x = \sum_{p=0}^{\infty} \frac{y^{(p+1)}(x_i)}{(p+1)!}\, \xi^{p+1} \tag{5}$$

On the other hand the increment of the function can be approximated with another formula, with the use of a discrete Runge–Kutta method.

$$\triangle y = \sum_{p=1}^{\infty} \alpha_p\, k_{i,p}(\xi) \tag{6}$$

Coefficients $k_{i,p}(\xi)$ of the previous formula are calculated with

$$\begin{aligned} k_{i,1} &= \xi f(y(x_i), x_i) \\ k_{i,2} &= \xi f(x_i + A_2\xi, y(x_i) + A_2 k_{i,1}) \\ &\vdots \\ k_{i,p} &= \xi f(x_i + A_p\xi, y_(x_i) + \sum_{q=1}^{p-1} A_{p,q} k_{i,q}) \end{aligned} \tag{7}$$

where α_p and $A_{p,q}$ are constants. By using the formulas of partial differentiation, let us expand the $n^{\underline{\text{th}}}$ order differentials of $y(x)$ according to the format in (4). The results are

$$\begin{aligned} y'(x_i) &= f(y(x_i), x_i) \\ y''(x_i) &= \left.\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} f\right|_{x=x_i} \\ &\vdots \end{aligned} \tag{8}$$

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The Taylor series of $f(y(x), x)$ around x_i is determined by the following equation:

$$f(y(x_i) + k(\xi), x_i + \xi) = f(y_i, x_i) + \\ + \left.\frac{\partial f(x,y)}{\partial y}\right|_{x_i} k(\xi) + \left.\frac{\partial f(x,y)}{\partial x}\right|_{x_i} \xi + \cdots \tag{9}$$

Coefficients of equation (6) can finally be reproduced like Runge-Kutta method. After that there are two formulas available to determine function $\triangle y(x)$. Let us assume that the two formulas are equal.

$$\sum_{p=1}^{\infty} \frac{y^{(p)}(x_i)}{p\,!}\,\xi^p = \sum_{p=1}^{\infty} \alpha_p\, k_{i,p}(\xi) \tag{10}$$

By using this equation the Taylor coefficients of $y(x)$ can be taken. However, a problem arises: The formula in the left side of (10) is determined by $p^{\underline{\text{th}}}$ order functions of ξ, while the right side is determined by a first order function of ξ. As the coefficients are calculated $k_{i,p}$ has to written as a function of ξ^p. By using equation (7), let us consider a new function:

$$K_{i,p}(\xi) = f(x_i + A_p\xi, y(x_i) + \sum_{q=1}^{p-1} A_{p,q}k_{i,q}(\xi)) \tag{11}$$

Let us suppose that the Taylor coefficients up to $z^{\underline{\text{th}}}$ order ($z \in Z$) are supposed to be calculated. First the Runge-Kutta coefficients $k_{i,p}(\xi)$, α_p and $A_{p,q}$ have to be taken ($i = 1...z$, $z^{\underline{\text{th}}}$ order Runge-Kutta method). As $K_{i,p}$ is determined as the polynomial of variable ξ, the series expansion depending has to be given on ξ of $f(x_i + A_p\xi, y(x_i) + \sum_{q=1}^{p-1} A_{p,q}k_{i,q}(\xi))$ around (x_0, y_0). It can be done numerically. Let us consider h as a step of variable x, $(x_i + h = x_{i+1})$ and determine the value of $K_i(\xi)$ in points $\xi_t = th$ where $t = 0, 1, 2, ..., N$ and $N \geq z$, $(N \in Z)$. After that a set of points $\{\{\xi_t, K_{p,t}\}_{t=0}^{N}\}_{p=1}^{z}$ result. Now, let us find function $K_i(\xi)$ in the following format:

$$K_{i,p}(\xi) \approx \sum_{t=0}^{N} a_{i,p,t}\xi^t \tag{12}$$

where $a_{i,p,t}$ are unknown constant coefficients. Values of $a_{p,t}$ are determined with the help of the least squares method. After replacing the coefficients into equation (10) and equalizing the identical indices of attends, the approximation of Taylor coefficients in x_i are calculated.

$$y'(x_i) = f(y(x_i), x_i) \tag{13}$$

$$y''(x_i) = 2\sum_{m=1}^{z-1} \alpha_m a_{i,m,1} \tag{14}$$

$$y^{(n)}(x_i) = n!\sum_{m=1}^{z-1} \alpha_m a_{i,m,n-1} \tag{15}$$

Along the given order of Taylor coefficients, the precision of the proposed method can be extended, when the number of approximate points N are increased, however it is not necessary to calculate coefficients $K_{i,p}(\xi)$ up to the $z^{\underline{\text{th}}}$ order.

NUMERICAL RESULTS

In this section the performance of the method is analyzed. Two application examples are presented. The first example is the simpler one, where $K_i(\xi)$ could be written as a polynomial of variable ξ, and there is no need to use the least squares method. In the second example a more general differential equation with $f(y(x), x)$ function is examined. After the Taylor coefficients of the solution of ODEs are calculated, let us compare the results with the coefficients that were determined by the analytical solution in both examples. Let the problem be the same in both cases: the Taylor coefficients of the solution of given differential equations up to fourth order have to calculated, with the consideration of this initial condition $y(x_0 = 0) = y_0$. Let us consider the following equation as the first example

$$y'(x) = y(x)x \qquad y(0) = 1 \tag{16}$$

First let us determine the analytical solution of equation (16) by using the separation of variables method. After the conversion the result is

$$\int_{y_0}^{y} \frac{1}{y(s)}\,\mathrm{d}s = \frac{x^2}{2} \tag{17}$$

After the expansion of equation (17) the analytical solution of Eq. (16) and its derivatives are determined by the following formulas:

$$\begin{aligned} y(x) &= \exp\left(\frac{x^2}{2}\right) \\ y'(x) &= x\exp\left(\frac{x^2}{2}\right) \\ y''(x) &= \left(1+x^2\right)\exp\left(\frac{x^2}{2}\right) \\ y'''(x) &= \left(3x+x^3\right)\exp\left(\frac{x^2}{2}\right) \\ y^{(4)}(x) &= \left(3+6x^2+x^4\right)\exp\left(\frac{x^2}{2}\right) \end{aligned} \tag{18}$$

By using formulas (3), (5) and (18) the increment of $y(x)$ around $x = 0$ has the following format:

$$\triangle y = \frac{1}{2}\xi^2 + \frac{3}{24}\xi^4 + \cdots + \mathcal{O}(\xi^5) \tag{19}$$

Now the Taylor coefficients are calculated numerically and $\triangle y$ is written. As the Taylor series up to fourth order is to be calculated by using formula (11) the Runge-Kutta equation has the following form:

$$\triangle y = \frac{1}{6}k_{0,1}+\frac{2}{6}k_{0,2}+\frac{2}{6}k_{0,3}+\frac{1}{6}k_{0,4}+...+\mathcal{O}(\xi^5) \quad (20)$$

where,

$$\begin{aligned}
k_{0,1} &= \xi K_{0,1}(\xi) = \xi f(x_0, y_0) \\
k_{0,2} &= \xi K_{0,2}(\xi) = \xi f(x_0 + \frac{\xi}{2}, y_0 + \frac{k_{0,1}}{2}) \\
k_{0,3} &= \xi K_{0,3}(\xi) = \xi f(x_0 + \frac{\xi}{2}, y_0 + \frac{k_{0,2}}{2}) \\
k_{0,4} &= \xi K_{0,4}(\xi) = \xi f(x_0 + \xi, y_0 + k_{0,3})
\end{aligned}$$

and $f(y,x) = xy$. By using the values of x_0 and y_0 and the form of $k_{0,p}$, $K_{0,p}(\xi)$ functions could be calculated. The formulas of these functions are

$$\begin{aligned}
K_{0,1}(\xi) = 0\cdot 1 = 0 \quad &, \quad k_{0,1} = 0 \\
K_{0,2}(\xi) = \frac{\xi}{2}\cdot 1 = \frac{\xi}{2} \quad &, \quad k_{0,2} = \frac{\xi^2}{2} \\
K_{0,3}(\xi) = \frac{\xi}{2}\left(1+\frac{\xi^2}{4}\right) \quad &, \quad k_{0,3} = \frac{\xi^2}{2}+\frac{\xi^4}{8} \\
K_{0,4}(\xi) = \xi\left(1+\frac{\xi^2}{2}+\frac{\xi^4}{8}\right) \quad &, \quad k_{0,4} = \xi^2+\frac{\xi^4}{2}+\frac{\xi^6}{8}
\end{aligned}$$

By using formula (20) the numerical approximation of $\triangle y$ is determined by a following equation:

$$\triangle y = \frac{1}{2}\xi^2 + \frac{3}{24}\xi^4 + \cdots + \mathcal{O}(\xi^5) \quad (21)$$

Comparing the given result to the analytical form of $\triangle y$ it is evident, that the two expressions are equal. It was easy to see that how to write $K_{0,p}$ as a polynomial of variable ξ and the basis of the method. In the next example let us consider the following equation:

$$y'(x) = y(x)\cos(x) \qquad y(0) = 1 \quad (22)$$

The analytical solution of equation (22) is determined by the following form:

$$y(x) = C\exp(\sin(x)) \quad (23)$$

By using the initial conditions $C = 1$ results. Let us write the derivatives of $y(x)$ in the point $x = 0$:

$$\begin{aligned}
y'(0) &= \Big[\cos(x)\exp(\sin(x))\Big]_{x=0} = 1 \\
y''(0) &= \Big[\left(\sin(x)+\cos(x)^2\right)\exp(\sin(x))\Big]_{x=0} = 1 \\
y^{(3)}(0) &= \Big[(-\cos(x) - 3\sin(x)\cos(x) + \\
&\quad + \cos(x)^3\Big)\exp(\sin(x))\Big]_{x=0} = 0 \\
y^{(4)}(0) &= \Big[\Big(\sin(x) + 3\sin(x)^2 - 4\cos(x)^2 + \\
&\quad -6\sin(x)\cos(x)^2 + \cos(x)^4\Big) \\
&\quad \exp(\sin(x))\Big]_{x=0} = -3
\end{aligned}$$

By using these results the Taylor series of $y(x)$ around $x = 0$ has the following form:

$$y(x) = 1 + \xi + \frac{1}{2}\xi^2 - \frac{3}{24}\xi^4 + \cdots + \mathcal{O}(\xi^5) \quad (24)$$

As the Taylor coefficients are calculated numerically, the $K_{0,p}$, $(p = 1,2,3,4)$ coefficients in the Runge-Kutta method have to be written as a polynomial of variable ξ. In the first example it is easy to write $K_{0,1}$. It is known that $f(x,y) = y\cos(x)$, by using this the first coefficient can be calculated.

$$K_{0,1} = 1\cos(0) = 1 \quad , \quad k_{0,1} = \xi \quad (25)$$

Let us say that $K_{0,1}$ does not depend on variable ξ. In the next step let us consider a stepsize $h = 0.1$ and the number of interpolation points $N = 6$. Let us determine $K_{0,2}(\xi)$ in given points (See in Table 1), where

$$K_{0,2} = f(x_0 + \frac{\xi}{2}, y_0 + \frac{k_{0,1}}{2}) \quad (26)$$

and the values of $K_{0,2}(\xi)$:

Table 1: The values of $K_{0,2}(\xi)$ in given points

ξ	$K_{0,2}(\xi)$
0.0	1
0.1	1.04868
0.2	1.09450
0.3	1.13708
0.4	1.17608
0.5	1.21114

To determine the polynomial the points have to be interpolated and the method of least squares has to be used. The format of the approximate polynomial is the same as in the previous section in equation (11). According to the method of least squares the coefficients of the approximate polynomial of $K_{0,2}(\xi)$ have the following format (The values of coefficients up to fifth order are shown in Table 3):

$$K_{0,2} \approx 1 + 0.5\xi - 0.125\xi^2 + 0.0625\xi^3 + \ldots \quad (27)$$

By using this result up to the third order the value of $k_{0,2}$ is obtained.

$$k_{0,2} = \xi + 0.5\xi^2 - 0.125\xi^3 + 0.0625\xi^4 \tag{28}$$

Substituting the given $k_{0,2}$ to $K_{0,3} = f(x_0 + \frac{\xi}{2}, y_0 + \frac{k_{0,2}}{2})$ and resuming the method $k_{0,3}$ is

$$\begin{aligned} K_{0,3}(\xi) &\approx 1 + 0.5\xi - 0.1249\xi^2 + 0.1241\xi^3 + \ldots \\ k_{0,3}(\xi) &= \xi + 0.5\xi^2 + 0.1249\xi^3 - 0.1241\xi^4 \end{aligned}$$

and $k_{0,4}$

$$\begin{aligned} K_{0,4}(\xi) &\approx 1 + 1.0001\xi - 0.0022\xi^2 + 0.3572\xi^3 + \ldots \\ k_{0,4}(\xi) &= \xi + 1.0001\xi^2 - 0.0022\xi^3 + 0.3572\xi^4 \end{aligned}$$

as a polynomial of variable ξ. (Table 2 shows the values of $K_{0,3}(\xi)$ and $K_{0,4}(\xi)$)

Table 2: The values of $K_{0,3}(\xi)$ and $K_{0,4}(\xi)$ in given points

ξ	$K_{0,3}(\xi)$	$K_{0,4}(\xi)$
0.0	1	1
0.1	1.05111	1.09959
0.2	1.10390	1.19646
0.3	1.15741	1.28718
0.4	1.21057	1.36760
0.5	1.26223	1.43296

Figure 1 shows the values of $K_{i,p}$ in discrete points, and their numerical approximations with a polynomial of ξ. The forms of approximate polynomials can be seen in Table 3.

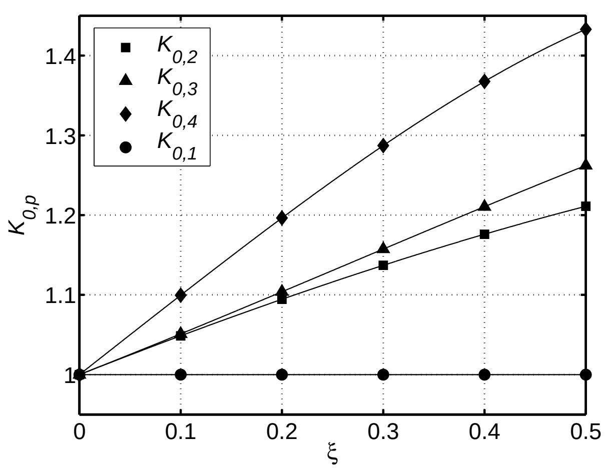

Figure 1: The numerical approximation of $K_{i,p}(\xi)$ functions

By using formula (14) the numerical approximation of Taylor coefficients is determined by the following forms:

$$\begin{aligned} y'(0) &\approx \left(\frac{1}{6} + \frac{2}{6} + \frac{2}{6} + \frac{1}{6}\right) = 1 \\ y''(0) &\approx 2\left(\frac{2}{6}0.5 + \frac{2}{6}0.5 + \frac{1}{6}1.0001\right) = \\ &= 2 \cdot 0.50001 = 1.0002 \\ y'''(0) &\approx 6\left(-\frac{2}{6}0.125 + \frac{2}{6}0.1249 - \frac{1}{6}0.0022\right) = \\ &= 6 \cdot -0.0004 = -0.0024 \\ y^{(4)} &\approx 24\left(-\frac{2}{6}0.0625 - \frac{2}{6}1.241 - \frac{1}{6}0.3572\right) = \\ &= 24 \cdot -0.1217 = -2.9208 \end{aligned}$$

The analytical and numerical solutions are compared, see Table 4, 5 and 6. These tables contain the Taylor coefficients along with the value of h. The tables show that when decreasing the stepsize h the error of Taylor coefficients is also decreasing along given conditions.

Table 3: The forms of approximate polynomials

	ξ^0	ξ^1	ξ^2	ξ^3	ξ^4	ξ^5
$K_{0,1}$	1	0	0	0	0	0
$K_{0,2}$	1	0.5	-0.125	-0.0625	0.0026	0.0013
$K_{0,3}$	1	0.5	0.1249	-0.1241	-0.063	0.0156
$K_{0,4}$	1	1.0	-0.002	-0.3572	-0.400	0.1006

Table 4: $h = 0.5$

	$y'(0)$	$y''(0)$	$y'''(0)$	$y_{(4)}(0)$
Analytical	1	1	0	-3
Numerical	1	0.9644	0.4141	-4,8992

Table 5: $h = 0.1$

	$y'(0)$	$y''(0)$	$y'''(0)$	$y_{(4)}(0)$
Analytical	1	1	0	-3
Numerical	1	1.0002	-0.0024	-2.9208

Table 6: $h = 0.01$

	$y'(0)$	$y''(0)$	$y'''(0)$	$y_{(4)}(0)$
Analytical	1	1	0	-3
Numerical	1	1	$-5 \cdot 10^{-7}$	-3

CONCLUSIONS

A general algorithm designed for the approximation of Taylor coefficients of the solution of first order ODEs has been presented. This method gives a continuous approximation, it can approximate the solution with a $z^{\underline{\text{th}}}$ order polynomial in any points where the function of solution is interpretable. The presented method based on the standard Runge-Kutta method, but it takes the constants used by RK as a function of a local variable. Therefore the main difference between this method to other standard methods for example discrete Runge-Kutta, Adams-Bashfort, Adams-Moulton etc. while the standard methods give a discrete approximation point by point this method approximate the function of solution by a continuous polynom in given points it is show more information the behavior of the solution in the neighborhood of approximated points. This method only the first step to the simulation it can take as a predictor method so it can be decisive the integration with variable stepsize to determine the value of the stepsize or the order of approximation. The method can be useful in determining the derived functions of solution up to $z^{\underline{\text{th}}}$ order.

REFERENCES

A. Coddington; N. Levinson. 1955. *Theory of Ordinary Differential Equations.* McGraw-Hill, New York.

E. Hairer; S.P. Norsett; G.Wanner. 1987. *Solving Ordinary Differential Equations, I. Nonstiff Problems.* Springer, Berlin.

Halász Gábor; Huba Antal. 2003. *Műszaki mérések.* Műegyetemi Kiadó, Budapest, ISBN 963-420-744-8

P. Henrici. 1962. *Discrete Variable Methods in Ordinary Differential equations*, Wiley, New York.

Peter Henrici. 1985. *Numerikus Analízis.* Műszaki könyvkiadó, Budapest, ISBN 963-10-6419-0

P. Davis. 1961. *Interpolation and approximation.* Blaisdell, Waltham.

P.N. Brown, G.D. Byrne, A:C: Hindmarsh, VODE. 1989. "A variable coefficient ODE solver." *SIAM J. Sci. Stat. Comp.* **10**, 1038-1051

Stoher József; Bulirsch Roland. 2002. *Introduction to numerical analysis.* Springer, New York. ISBN 0-387-95452-X

Stoyan Gisbert; Takó Galina. 1995. *Numerikus Módszerek II.* ELTE-TypoTEX, Budapest. ISBN 963-7546-53-7

W.H. Enright, K.R. Jackson, S.P. Norsett and P.G. Thomsen. 1986. "Interpolants for Runge-Kutta formulae." *ACM Trans. Math. Software* **12**, 193-218

AUTHOR BIOGRAPHY

ISTVÁN SELEK received the M.Sc degree in mechanical engineering with a major in applied mechanics and machine design from the Faculty of Mechanical Engineering Budapest University of Technology and Economics (BUTE) in 2003. In 2003 he began his Ph.D. studies in BUTE. His primary research interest is the simulation of highly nonlinear processes with time delays, by using Soft Computing methods.