Evaluating The Parameters of Implicit Runge-Kutta Methods Using Optimization Methods

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Abstract

In this paper, evaluating the parameters of implicit Runge-Kutta methods using the least square optimization method have been introduced, which is used for solving the nonlinear system of algebraic equations resulting from the derivation of any R-stages fully implicit Runge-Kutta method.

Introduction

Solution of ordinary differential equations is of great importance in applied mathematics field, since such type of equations may be sometimes are so difficult to be solved analytically. Therefore, numerical methods are needed with a sophisticated accuracy [3].

One of the most popular methods used for solving ordinary differential equations is the Runge-Kutta method, which are of higher order methods and low stages. The general form of R-stages implicit Runge-Kutta methods is given by [6], [7]:

$$y_{n+1} = y_n + h\sum_{i=1}^{R} C_i K_i$$

where:

$$K_i = f(x_n + ha_i, y_n + h\sum_{j=1}^{R} b_{ij} K_j)$$

$$a_i = \sum_{j=1}^{k} b_{ij}$$

and C_i, a_i and b_{ij} are constants to be calculated.

For convenience, we design the process by an array as follows:

a_1	b_{11}	b_{12}	$\dots$	b_{1R}
a_2	b_{21}	b_{22}	$\dots$	b_{2R}
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
a_R	b_{R1}	b_{R2}	$\dots$	b_{RR}
	C_1	C_2	$\dots$	C_R

When it is desirable to remark that:

1. If $b_{ij} = 0$, for every $(i < j)$, then the method is called semi-explicit Runge-Kutta method.
2. If $b_{ij} = 0$, for every $(i \le j)$ and $b_{ii} = 0$, then the method is called explicit Runge-Kutta method.
3. Otherwise it is called an implicit Runge-Kutta method.

Also, one of the basic consequences of the theory of Runge-Kutta methods that the maximum error term in R-stages Runge-Kutta methods is of order $p = R$ in explicit Runge-Kutta method, $p = R + 1$ in semi-explicit Runge-Kutta methods and $p = 2R$ in implicit Runge-Kutta method [5].

Hence the implicit methods are more accurate than the other methods, but are so difficult to be derives and use in the numerical applications.

In this paper, the utility of least square optimization methods will be improved to solve the resulting non-linear system in order to evaluate the constants of the method.

Derivation of Implicit Runge-Kutta Method

For simplicity and as an illustration purpose, we consider 2 stages implicit Runge-Kutta method with maximum possible order.

$$y_{n+1} = y_n + h(C_1K_1 + C_2K_2)$$

Where:

$$K_1 = f(x_n + ha_1, y_n + b_{11}hK_1 + b_{12}hK_2)$$

$$K_2 = f(x_n + ha_2, y_n + b_{21}hK_1 + b_{22}hK_2)$$

and

$$a_1 = b_{11} + b_{12}, \quad a_2 = b_{21} + b_{22}$$

Following [2] and [3], we can derive the two-stages implicit Runge-Kutta method of order (4) if:

[illegible] $= 1$

[illegible] $= \frac{1}{2}$

[illegible] $= \frac{1}{?}$

[illegible] $= \frac{1}{?}$

[illegible] $= \frac{1}{?}$

[illegible]

[illegible] $= \frac{1}{?}$

[illegible] $= \frac{1}{4}$

The last system is a system of non-linear algebraic equations that constitute some function such that the critical points of the implicit Runge-Kutta method of order $p = 4$. The solution and the evaluation of these constants is of great importance.

The modified "approach" is the minimization approach which is to minimize the problem equivalent to the solution of the related to above nonlinear system of algebraic equations.

The procedure of constructing the objective function is as follows:

1. Rewriting the constitution equations of the non-linear system in such a way that each equation equals zero.
2. Squaring each equation of non-linear system resulting from step (1).
3. Constructing the objective function in terms of the constants of the implicit Runge-Kutta methods C_1, C_2, a_1, a_2, etc., by adding the resulting eight equations from step (2). That is:

$$f(C_1, C_2, \ldots, b_{22}) = f_1^2 + f_2^2 + \ldots + f_8^2 \qquad (2)$$

where:

$$f_1 = C_1 + C_2 - 1$$

$$f_2 = C_1 a_1 + C_2 a_2 - \frac{1}{2}$$

$$f_3 = C_1(b_{11}a_1 + b_{12}a_2) + C_2(b_{21}a_1 + b_{22}a_2) - \frac{1}{6}$$

$$f_4 = C_1 a_1^2 + C_2 a_2^2 - \frac{1}{3}$$

$$f_5 = (C_1 b_{11} + C_2 b_{21})(b_{11}a_1 + b_{12}a_2) + (C_1 b_{12} + C_2 b_{22})(b_{21}a_1 + b_{22}a_2) - \frac{1}{24}$$

$$f_6 = C_1 a_1(b_{11}a_1 + b_{12}a_2) + C_2 a_2(b_{21}a_1 + b_{22}a_2) - \frac{1}{8}$$

$$f_7 = C_1(b_{11} a_1^2 + b_{12} a_2^2) + C_2(b_{21} a_1^2 + b_{22} a_2^2) - \frac{1}{12}$$

$$f_8 = C_1 a_1^3 + C_2 a_2^3 - \frac{1}{4}$$

Hence minimizing (2) gives the critical points, which solve the nonlinear system of algebraic equations.

It is of advantage to notice that the objective function f will surly minimized since it is a sum of quadratic functions in which each of them equals zero. Hence the minimum of the objective function mast tends to zero.

Numerical Results

The results of carrying on a computer program for minimizing equation (2) with the initial values (0.1, 0.2, …, 0.6) for the variables (C_1, C_2, b_{11}, b_{12}, b_{21} and b_{22}) respectively gives the following:

	0.250051	0.5386741
	-3.869956×10^{-2}	0.2499921
	0.5004003	0.499881

Also, carrying another excusion to the computer program, with initial values (1, 2, 3, 4, 5, 6) gives:

	0.2500022	0.538694
	-3.869695×10^{-2}	0.24999103
	0.5000081	0.4989014

Which are accurate in comparison with the analytical results obtained in other literatures [4], [5].

	0.25	0.5386751
	−0.0386751	0.25
	0.5	0.5

Which shows that the minimizing problem has a unique solution to the linear system.

Remark

Other R-stages method could be derived similarly as in 2-stages implicit Runge-Kutta methods, as it is illustrated above.

References

1. Beveridge C. R., and Schechter, R. S., Optimization Theory and Practices, 1988.
2. Bunday, B. D., Basic Optimization Methods,Edward Arnold publishers Ltd,1985.
3. Butcher, J. C., The Numerical Analysis of Ordinary Differential Equations,John wiley & sons,New York,1987.
4. Dormand, J. R., and Prince, P. J., Runge-Kutta Triples, Computers Math. Applic., 12 A(9): 1007-1017, 1986.
5. Gladwell, I., Shanpine, L. F., Bace, L. S., , Practical Aspects of Interpolation in Use Runge-Kutta Codes, 1987.
6. Hall, G. and Watt, J. M., Modern Numerical Methods for Ordinary Differential Equations, oxford university press,1976.
7. Lambert, J. D., Computational Methods in Ordinary Differential Equations ,John wiley & sons,1981.

الخلاصة

في هذا البحث، تم حساب المعاملات الوسيطية لاشتقاق طريقة رانج-كوتا الضمنية من الرتبة الثانية و الرابعة وذلك باستخدام أسلوب طريقة المربعات الصغرى لحل نظام من المعادلات الغير خطية الجبرية الناتجة من اشتقاق الصيغة العامة لهذه الطريقة.