BULLETIN OF THE
GREEK MATHEMATICAL SOCIETY
VOLUME 28, 1987A

COMPARISON OF RUNGE-KUTTA TYPE METHODS OF ORDER FIVE

BY

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ABSTRACT. *A criterion is proposed for determing which explicit Runge-Kutta methods of order five are the most promising as a basis for developing efficient library subroutines for solving nonstiff initial value problems. The comparison is based on the local truncation error estimate of the methods being considered, and it is applied for a class of linear first-order differential system.*

1. Introduction

Among the best methods being used today to solve initial value problems for nonstiff ordinary differential equations is generally agreed to be explicit Runge-Kutta methods. Our purpose in this paper is to develop and apply a criterion for comparing all the well known Runge-Kutta methods of order five. This criterion was originally proposed by Papageorgiou [14], but it was applied only for Runge-Kutta methods of order four.

One of the difficulties with the experimental tests of the methods is that the results depend on a variety of factors which are not inherent in the formulas and strategies that one wants to compare. Also, the cost of numerical tests, in terms of manhours and computer time, is fairly high. So it would be helpful to have an inexpensive criterion that would take into account only the essential mathematical properties of the methods and strategies that are to be used in a library subroutine.

The cost of solving a differential equation consists from two parts. The first part is the cost of evaluating the derivatives and the second, called the overhead, is the time actually spent in solving the problem after excluding the cost of evaluating the derivatives. It is difficult to measure overhead in the presence of multiprogramming, and so we are restricted in counting the cost on the function evaluations required to solve the posed problem.

So the criterion can be based on the number of function evaluations spent by each method for the integration of a differential equation over a prescribed interval, and possibly on the ratio of function evaluations betwe-

en two of these methods. This criterion is applied for the class of first-order linear diferential system of the form

$$\underline{y}' = B\,\underline{y} + \underline{c}x + \underline{d} \tag{1}$$

where B is a constant matrix whose eigenvalues are distinct, real and negative, or complex with negative real parts, and $\underline{c}$, $\underline{d}$ are constant vectors.

All the methods to be compared are of the explicit Runge-Kutta type of order five. For some of them, the local truncation error estimate is based upon a comparison of the results from two half steps and one full step. For the others, the local truncation error made in a step, is estimated by taking the step with two formulas of different accuracy and to estimate the accuracy of the lower formula by comparison, see Fehlberg [4], Verner [18].

Shampine and Watts [17] have proposed a way to compare local error estimators for the fourth-order Runge-Kutta procedures, on the basis of a different criterion and for a particular class of ordinary differential equations. Their conclusion is that an estimate proposed by Ceschino-Kuntzmann [1] is asymptotically the most accurate. Test on non-stiff systems by Enright et al. [2] and Enright and Hull [3] indicate that methods based upon Fehlberg's formulas [4, 5] are superior to others provided that the function evaluations are inexpensive (with the reservation that formulas of order five and greater cannot be used for quadrature). Jackson et al. [8] have proposed a criterion for comparing Runge-Kutta formulae of different orders. Their main conclusion is that the use of local extrapolation seems to improve the performance of some methods. In particular, a method proposed by Verner [18] and uses this technique appears to be the most promising.

In the next section we outline the proposed criterion. In section 3, all the well-knhown explicit Runge-Kutta methods of order five are briefly discussed, and an expression for the local truncation error estimate of each method is obtained applying the model differential system (1). In section 4, we present the comparison of these methods and in the last section we give the conclusions.

2. Outline of the basis of comparison

As stated above, our objective is to compare all the known to us Runge-Kutta methods of order five, in a simple way. For these methods a useful

measure of the cost is the number of function evaluations required to "solve" a problem from the class (1). By counting derivative or function evaluations, one has a way to compare methods which does not depend on the machine being used, and which is a realistic measure of the relative costs in machine time. For the better methods, the computer time required is proportional to the number of function evaluations, since the overhead per step is relatively small and is, in any event, roughly proportional to this number.

Many methods commonly in use to-day for "solving" a problem contain at least the following four components: (i) a strategy for choosing the step size; (ii) a Runge-Kutta formula to approximate the solution at each step; (iii) a formula for estimating the local truncation error at each step, and (iv) a step control algorithm for accepting or rejecting the approximation at each step. By "solving" a problem we mean that the approximation generated by the method, satisfies the acceptability criterion which depends on a tolerance parameter, ε, set by the user. This criterion determines whether or not the approximation $\underline{y}_r$ at x_r is an acceptable approximation. Most methods based upon Runge-Kutta formulas attempt to keep an estimate of the local truncation error below a specified tolerance for each step of the integration.

There are several forms of the step control algorithms used to-day in the literature. See, for example, Hull et al. [7], Gear [6], Shampine and Watts [17]. We have applied the following step control algorithm: Let us suppose that we are interested in integrating the differential system (1) over an interval [a, b]. If the maximum allowable absolute error at $x = b$ is ε, then the step-control algorithm reguires the local truncation error estimate $\underline{e}(h)$ of the method to be bounded by the tolerance ε, in the sence that the inequality

$$\| \underline{e}(h) \|_\infty \leq \frac{h\varepsilon}{b - a} \tag{2}$$

is satisfied at each step of the integration. Using (2) as an equality we can find the largest stepsize h for which (2) is satisfied.

Let us now suppose that we are interested to compare two methods, say method α and method β, and that method α requires N_α function evaluations per step, and method β, N_β function evaluations. The number of function evaluations per distance d in x required by a method, assuming

that it uses the same step length h in the subinterval d, is $fe = (d / h)N$. The ratio of function evaluations per distance d in x between the methods α and β is therefore

$$\frac{fe_\alpha}{fe_\beta} = \frac{N_\alpha\, h_\beta}{N_\beta\, h_\alpha}. \tag{3}$$

It is obvious that N_α/N_β and h_β/h_α are known for the methods being compared, and so fe_α/fe_β can be found. This ratio can be used as the basis of comparison between two of the methods.

3. Runge-kutta formulas

It is well known that an R-stage explicit Runge-Kutta formula is a scheme for calculating $\underline{y}_{r+1}$ from $\underline{y}_r$ using R function evaluations

$$\begin{aligned}
\underline{k}_1 &= \underline{f}(x_r, \underline{y}_r) \\
\underline{k}_i &= \underline{f}\Big(x_r + c_i h, \underline{y} + h \sum_{j=1}^{i-1} \alpha_{ij}\, \underline{k}_j\Big), \quad i = 1, 2, \ldots, R \\
\underline{y}_{r+1} &= \underline{y}_r + h \sum_{i=1}^{R} \beta_i\, \underline{k}_i \\
c_i &= \sum_{j=1}^{i-1} \alpha_{ij}
\end{aligned} \tag{4}$$

The constants α_{ij}, b_i, c_i are the coefficients of the formula. The method is said to be of order p if p is the largest integer such such that $\underline{T}(h) = 0(h^p)$ for any p-times differentiable function $\underline{f}(x, \underline{y})$, where $\underline{T}(h)$ is the local truncation error.

A traditional way to estimate the local error of the Runge-Kutta method of order p, arises from applying the process of defered approach to the limit, also called Richardson extrapolation [15]. With this approach we compute two approximations. The first, $\underline{y}_{r+1}$, by applying two steps of length h, and the second, $\underline{y}^*_{r+1}$, by applying one step of length 2h. The estimate of the local truncation error associated with $\underline{y}_{r+1}$ is given by

$$\underline{e} = (\underline{y}_{r+1} - \underline{y}^*_{r+1})/(2^p - 1)2. \tag{5}$$

Using this approach we have estimated the local truncation error of the Runge-Kutta methods of order five proposed by Kutta [9], Luther1 [12],

Luther2 [12], Nyström [13], Sarafyan [16] and Lawson [11] which have been considered in our comparison. These methods are all six-stage methods, and their local truncation error estimate is given by

$$\underline{e} = (\underline{y}_{r+1} - \underline{y}^*_{r+1})/62. \tag{6}$$

It is easily verified that for these methods twelve function evaluations are required to obtain the fifth-order value of $\underline{y}_{r+1}$, and five more function evaluations to obtain $\underline{y}^*_{r+1}$. Thus their sixth-order local truncation error estimates use 8½ function evaluations if the step is acceptable, while an unacceptable step results in a loss of eleven function evaluations before the computations are recycled. Fehlberg [4] has proposed an eight-stage fifth-order procedure. He arrives at the formula by deriving formulae of order five and six, and using their difference as an estimate of the error in the fifth-order formula. So it uses eight function evaluations per step if the step is acceptable and if the step is unacceptable, seven function evaluations are lost. Finally, Verner [18], has derived in an analogous way an eight-stage fifth-order method where again eight function evaluations are spent if the step is acceptable, and seven function evaluations are lost if the step is unacceptable.

By applying the model differential equation (1) to any Runge-Kutta type method of order five, it can be shown that all the various local truncation error estimates have a leading term of the form

$$\underline{e} = \gamma h^6 B^4 \{B^2 \underline{y} + (Bx + I)\underline{c} + B\underline{d}\} \tag{7}$$

where γ is a real constant varying from method to method and I the unit matrix. A table indicating the values of this constant for the methods being considered is presented in the next section.

4. Comparison of the methods

The methods being compared can be separated in two classes. The first consists of methods which estimate the local truncation error estimate in one step, and the second, of methods which estimate the local error accumulated in two steps. The methods of Fehlberg and Verner fall in the first class and we shall denote them by FEH, VER respectively. The methods of Kutta, Nyström, Sarafyan, Lawson, Luther1, and Luther2 which we shall denote by KUT, NYS, SAR, LAW, LUT1 and LUT2 respectively

fall in the second. In order to make the latter methods equivalent for comparison to the first, we can assume that their local error estimate in a single step can be approximated by the half of the local error estimate accumulated in two steps, provided that the propagation of the error is stable.

The acceptability criterion (2) using the form (7) becomes

$$\|\gamma h^6 B^4 \{B^2 \underline{y} + (Bx + I)\underline{c} + B\underline{d}\}\|_\infty \leq \frac{h\varepsilon}{b - a}. \tag{8}$$

Since the eigenvalues of B have been assumed distinct, it is well known that there exists a non-singular matrix H such that

$$H^{-1}BH = \Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$$

where λ_i, $i = 1, 2, \ldots, n$ are the eigenvalues of B. Then equation (7) is equivalent to the equation

$$H^{-1}\underline{e} = \gamma h^6 H^{-1} B^4 \{B^2 H H^{-1}\underline{y} + (Bx + I)HH^{-1}\underline{c} + BHH^{-1}\underline{d}\}.$$

Using the above transformation we define the new vectors $\underline{e}^* = H^{-1}\underline{e}$, $\underline{y}^* = H^{-1}\underline{y}$, $\underline{c}^* = H^{-1}\underline{c}$, $\underline{d}^* = H^{-1}\underline{d}$, which will grow or decay if and only if the original vectors do, Lambert [10] page 221. Then we finally get in component form the expression

$$e_i^* = \gamma h^6 \lambda_i^5 \{\lambda_i y_i^* + (x + \lambda_i^{-1})c_i^* + d_i^*\} \quad (i = 1, 2, \ldots, n) \tag{9}$$

It follows that for each $i = 1, 2, \ldots, n$, (8) can be substituted by

$$|\gamma h^6 \lambda_i^5 \{\lambda_i y_i^* + (x + \lambda_i^{-1})\, c_i^* + d_i^*| \leq \frac{h\varepsilon}{b - a}$$

and for some i the maximum acceptable value of h for each method is given by

$$h = \sqrt[5]{\frac{|\gamma|^{-1}}{b - a} \cdot \frac{\varepsilon}{\lambda_i^4} \cdot \frac{1}{|\lambda_i y_i^* + (x + \lambda_i^{-1})c_i^* + d_i^*|}}. \tag{10}$$

So for two methods say α and β, the ratio $h_\alpha/h_\beta = \sqrt[5]{|\gamma_\beta|/|\gamma_\alpha|}$ and equation (3) takes the form

$$\frac{fe_\alpha}{fe_b} = \frac{N_\alpha}{N_\beta} \cdot \sqrt[5]{|\gamma_\beta|/|\gamma_\alpha|} \tag{11}$$

which can be easily calculated.

The following Table I indicates the numerical value γ for each method, the number of function evaluations which each method spends for an accepted step, the number of function evaluatins which each method loses with a rejected step and the type of the error estimate for each method. Using (11) and the data of Table I, we compute the ratio of function evaluations between Verner's method and the others, and how many more function evaluations in % per distance in x each method needs if it is compared with Verner's method. The results of these computations can be found in Table II.

TABLE I

Constant γ	Func. Evals. Per. Acced. Step	Func. Evals. Per Reject. Step	Type of Error Estimate
$\gamma_{FEH} = 1/2160$	8	7	Formula pair
$\gamma_{VER} = 1/3240$	8	7	Formula pair
$\gamma_{KUT} = 1/1440$	8½	11	1-step-two-½steps
$\gamma_{LUT1} = 13/5760$	8½	11	1-step-two-½steps
$\gamma_{NYS} = 1/1440$	8½	11	1-step-two-½steps
$\gamma_{LAW} = 7/23040$	8½	11	1-step-two-½steps
$\gamma_{LUT2} = 1/576$	8½	11	1-step-two-½steps
$\gamma_{SAR} = 613/78120$	8½	11	1-step-two-½steps

TABLE II

Methods	$F_{EVER}/F_{EOTHERS}$	%, more fun. eval. of Meth. compared with Verner's
LAWSON	0.9441	5.59
FEHLBERG	0.9221	7.79
KUTTA	0.8003	19.97
NYSTRÖM	0.8003	19.97
LUTHER2	0.663	33.73
LUTHER1	0.6322	36.78
SARAFYAN	0.4927	50.73

5. Conclusions

From the above we can verify that the best method for the class of diffe-

rential equations (1) in terms of the number of function evaluations is Verner's method. Also it is clear that Lawson's method is very comparable with Verner's method. Fehlberg's method although seems comparable with the others it has the shortcoming that if it is applied to a quadrature problem, the error estimate is identically zero, see Jackson et al. [8].

The selection of the step size depends not only on the accuracy, but also on the stability of the method. We cannot state precisely the interaction of accuracy and stability when the step h is to be selected, but computational experience indicates that stability plays an essential role. This is true, especially for those values of the tolerance ε which correspond to low accuracies, when there are eigenvalues of the matrix B "sufficiently large" in absolute value. When the eigenvalues of B are not "sufficiently large" then, the accuracy plays the essential role. So in the first case, since the interval of absolute stadility of Verner's method is smaller than the inerval of Lawson's, the latter selects larger steps and, therefore the number of steps that Lawson's method needs, for the integration of a specific equation over a given interval, is smaller than the number of steps which Verner's method needs. So the total number of function evaluations which are spent by Lawson's method, is very comparable with the total number of function evaluations which are spent by Verner's method. In the case where the accuracy plays the essential role in the selection of h, Verner's method is the best. Computational experience indicates that the inverse holds for values of ε which correspond to high accuracies.

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(Received by the editors, September 10, 1986)

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