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A CLASS OF SINGLE STEP METHODS WITH A LARGE INTERVAL OF ABSOLUTE STABILITY*[1)2)]

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Abstract

In this paper, a class of integration formulas is derived from the approximation so that the first derivative can be expressed within an interval $[nh, (n+1)h]$ as

$$\frac{dy}{dt} = -P(y - y_n) + f_n + Q_n(t).$$

The class of formulas is exact if the differential equation has the shown form, where P is a diagonal matrix, whose elements

$$-p_j = \frac{\partial}{\partial y_j} f_j(t_n, y_n), \quad j = 1, \cdots, m$$

are constant in the interval $[nh, (n+1)h]$, and $Q_n(t)$ is a polynomial in t.

Each of the formulas derived in this paper includes only the first derivative f and

$$\frac{\partial}{\partial y_j} f_j(t_n, y_n).$$

It is identical with a certain Runge-Kutta method as P tends to zero and thus correct to the order of such Runge-Kutta method. In particular, when $Q_n(t)$ is a polynomial of degree two, one of our formulas is an extension of Treanor's method, and possesses better stability properties. Therefore the formulas derived in this paper can be regarded as a modified or an extended form of the classical Runge-Kutta methods. Preliminary numerical results indicate that our fourth order formula is superior to Treanor's in stability properties.

§1. Introduction

It is well known that the classical Runge-Kutta method, generally very satisfactory for non-stiff systems, fails badly in handling stiff systems. Thus, it is desirable to have a class of explicit formulas which can handle stiff systems (at least some special stiff systems) but which can provide proper speed and accuracy, of course, where a little special treatment is required.

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In many practical applications, one encounters systems of ordinary differential equations which can often be expressed approximately as

$$y' = -P(y - y_n) + f_n + \tilde{Q}_n(t, y),$$

where P is a diagonal matrix, $p_j = -\partial f_j/\partial y_j$ is a large quantity, $\tilde{Q}_n(t, y)$ is a function of t and y varies slowly and thus can be approximated by a polynomial $Q_n(t)$ in t. By virtue of this fact Treanor has proposed a modified Runge-Kutta method in [1], however, the interval of absolute stability is still small for handling stiff systems [2], [3]. Though the approach we will use is almost the same as Treanor's, one of the formulas we will provide, when $Q_n(t)$ is a polynomial of degree two, is really an extension of Treanor's method and possesses even better stability properties. Therefore, our formulas may also be regarded as a modified or an extended form of the classical Runge-Kutta methods.

Finally, eleven test problems arising mainly in chemistry from [4], [5] are chosen for numerical experiment. Preliminary numerical results indicate that our fourth order formula is superior to Treanor's in stability properties. However, just like Treanor's method, generally speaking our formulas are suitable only for the cases in which the main diagonal elements of the Jacobian matrix are large and the off-diagonal elements are comparatively small.

§2. Derivation of Integration Formulas

In this section a class of numerical integration formulas of the stiff initial value problem

$$\begin{cases} y' = f(t, y), \\ y|_{t=0} = y_0 \end{cases} \tag{1}$$

will be derived.

Assume that the equations of (1) at point (t_n, y_n) can be expressed approximately as

$$y' = -P(y - y_n) + f_n + Q_n(t), \tag{2}$$

where P is a diagonal matrix with elements

$$-p_j = \frac{\partial}{\partial y_j} f_j(t_n, y_n), \quad j = 1, 2, \cdots, m$$

and $Q_n(t)$ is a polynomial in t containing unknown parameters which are determined in the course of the integration.

To simplify notation, we restrict our discussion to the scalar equation, and set

$$F_0(h) = e^{-ph}, \quad F_l(h) = \frac{F_{l-1}(h) - \dfrac{1}{(l-1)!}}{(-ph)}, \quad l = 1, 2, \cdots. \tag{3}$$

Now the formulas for different $Q_n(t)$ are derived as follows. First of all we consider the simplest case, namely Eq. (1) can be expressed approximately in the interval $[nh, (n+1)h]$ as

$$y' = -p(y - y_n) + f_n + A(t - t_n). \tag{2.1}$$

Then the ordinary differential equation

$$y' = -p(y - y_n) + f_n,$$