AN OPTIMAL \((m+3)[m+4]\) RUNGE KUTTA ALGORITHM

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Abstract. Recurrent power series methods are particularly applicable to problems in celestial mechanics since the Taylor coefficients may be expressed by recurrence relations. However, as the number of Taylor coefficients increases as is often necessary because of accuracy requirements, the computing time grows prohibitively large. In order to avoid this unfavorable situation, Dr. E. Fehlberg introduced in 1960 Runge-Kutta methods that use the first \(m\) Taylor coefficients obtained by recursive relations, or some other technique.

Optimal \(m\)-fold Runge-Kutta methods are introduced. Embedded methods of order \((m+3)[m+4]\) and \((m+4)[m+5]\) are presented which have coefficients that produce minimum local truncation errors for the higher order pair of solutions of the method, as well as providing a near maximum absolute stability region. It is emphasized that the methods are formulated such that the higher order pair of solutions is to be utilized. These optimal methods are compared to the existing \(m\)-fold methods for several test problems. The numerical comparisons show that the optimal methods are more efficient. It is stressed that these optimal methods are particularly efficient when \(m\) is small.

1. Introduction

Recurrent power series methods are readily applicable to problems in celestial mechanics because the Taylor coefficients may be expressed by simple recurrence relations. However, as the number of the Taylor coefficients increases, as is often necessary to increase the order of the Taylor sum approximation for accuracy requirements, the computing time grows prohibitively large. In order to avoid this unfavorable situation, Fehlberg (1960) introduced Runge-Kutta methods that use the first \(m\) Taylor coefficients obtained by recursive relations, or by some other technique. Explicit Runge-Kutta methods have the unfavorable characteristic of requiring a large number of function evaluations for a high order method. Remembering that Runge-Kutta methods are reformulations of a Taylor sum, it will be advantageous to utilize a low order method to decrease the number of function evaluations, and thereby reduce the computing time.

The \(m\)-fold methods of Fehlberg combine the advantages of both the recurrent power series and Runge-Kutta methods. First, \(m\) Taylor coefficients are computed where the computing time is minimal. Then, these \(m\) derivatives are introduced into a Runge-Kutta algorithm of order \(p\) that requires a low number of function evaluations. Thus the algorithm has an accuracy of order \(m+p\).

An embedded method of order \((m+3)[m+4]\) is introduced having coefficients with a minimum local truncation error for the higher order solution of the pair. Thus, a method of order \([m+4]\) is available in conjunction with a lower order method \((m+3)\). The difference between the two solutions will be of order \([m+4]\). This information provides an estimate of the local error of the method for a step control procedure. It
is emphasized that this algorithm is formulated such that the higher order solution is to be utilized.

2. Runge Kutta Algorithm

Consider a system of first-order differential equations with the initial conditions given,
\[
\frac{dx}{dt} = f(t, x), \quad x(t_0) = x_0.
\]

Introduce a new variable \( y \),
\[
y = x - \sum_{v=1}^{m+1} X_v(t - t_0)^v,
\]
where the \( X_v \) are the \( v \)th coefficients of the Taylor sum
\[
x(t) = \sum_{v=0}^{m+1} X_v(t - t_0)^v.
\]

Upon differentiating,
\[
\frac{dy}{dt} = f - \sum_{v=0}^{m+1} vX_v(t - t_0)^{v-1} = g(t, y).
\]

A Runge-Kutta algorithm will be developed for the system of equations
\[
\frac{dy}{dt} = g(t, y).
\]

At \( t = t_0, x(t_0) = y(t_0) = y_0 \), and \( g(t_0, y_0) = 0 \).

The Runge-Kutta algorithm for this new system will be
\[
y(t_0 + h) = y_0 + h \sum_{k=1}^{3} C_k g_k + O(h^{m+4})
\]
\[
\dot{y}(t_0 + h) = y_0 + h \sum_{k=1}^{4} \dot{C}_k g_k + O(h^{m+5}),
\]
where
\[
g_1 = g(t_0 + \alpha_1 h, y_0)
\]
\[
g_k = g\left(t_0 + \alpha_k h, y_0 + h \sum_{\lambda=1}^{k-1} \beta_{k\lambda} g_\lambda\right), \quad k = 2, 3, 4.
\]

The error estimate, \( \text{Err} \), is defined as
\[
\text{Err} = y - \dot{y},
\]
which is of order \([m+4]\).

The parameters \( \alpha, \beta, C, \) and \( \dot{C} \) have to satisfy the following equations of condition which are generated by comparing the coefficients of the Taylor expansions of the solution of the differential equation with the coefficients of the algorithm.