Global Error and Stepsize Selection in Moderately Stiff Problems

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Abstract

We consider the effect of global error on stepsize selection for moderately stiff initial-value problems, solved using explicit Runge-Kutta methods. The global error does not affect the stability of the solution, although the computational efficiency of the Runge-Kutta method is likely to be compromised. We suggest the use of the RKQ algorithm, which allows possible stepwise control of global error, as a way of countering this effect.

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1 Introduction

Numerical solutions to initial-value problems (IVPs) comprised of stiff differential equations are usually obtained using implicit, A-stable Runge-Kutta (RK) methods. Such methods are unconditionally stable, meaning that the stepsize parameter in the method does not have to be adjusted according to the degree of stiffness exhibited by the system. The only stepsize adjustments that would be present arise from local error control considerations. However, implicit methods require the solution of a set of nonlinear equations at each step (the so-called stage equations) which can be computationally expensive, particularly for systems of high dimension. For moderately stiff problems, it is feasible to use explicit RK methods; the moderate degree of stiffness mitigates somewhat against the need for very small stepsizes, and if a strict tolerance is applied in the error control, it may occur that the stepsize adjustments are driven primarily by error control requirements, rather than the need for
stability in the presence of stiffness.

Typically, we would test for stiffness by considering the eigenvalues $\lambda_j$ of the Jacobian of the system. If any eigenvalues have a negative real part, then stiffness is present; the magnitude of the eigenvalue is the associated stiffness constant. For a given explicit RK method, we adjust the stepsize $h$ so that $h\lambda_j$ lies within the stability region of that particular method. Our objective in this paper is to study the effect of global error in the numerical solution on this stepsize adjustment algorithm - after all, it is reasonable to assume that the Jacobian is, generally speaking, a function of the solution.

2 Relevant Concepts

An $n$-dimensional IVP has the form

$$y' \equiv \begin{bmatrix} y'_1 \\ \vdots \\ y'_n \end{bmatrix} = F(x,y) \equiv \begin{bmatrix} f_1 (x, y_1, \ldots, y_n) \\ \vdots \\ f_n (x, y_1, \ldots, y_n) \end{bmatrix},$$

wherein $y$ and $F$ have been implicitly defined. The Jacobian of this system is given by

$$F(x,y) \equiv \begin{bmatrix} \frac{\partial f_1}{\partial y_1} & \cdots & \frac{\partial f_n}{\partial y_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_1}{\partial y_n} & \cdots & \frac{\partial f_n}{\partial y_n} \end{bmatrix},$$

the eigenvalues of which we write as

$$\lambda_j (x,y) = \alpha_j (x,y) + \beta_j (x,y) i$$

for $j = 1, \ldots, n$. Stiffness is present when at least one eigenvalue has negative real part [1]. We will refer to such eigenvalues as stiff eigenvalues, and write

$$\lambda_j (x,y) = -\alpha_j (x,y) + \beta_j (x,y) i$$

where $\alpha_j$ is positive, for these stiff eigenvalues. The sign of $\beta_j$ does not affect this definition.

Obviously, $\lambda_j$ is a vector in the complex plane, and stiff eigenvalues lie in the left-half of the complex plane. Stepsize selection for such eigenvalues is determined from the inequality

$$h_j \leq \frac{D_j}{|\lambda_j|} = \frac{D_j}{\sqrt{\alpha_j^2 + \beta_j^2}},$$

(2)
Global error and stepsize selection in stiff problems

where $D_j$ is the distance from the origin to the boundary of the stability region of the relevant RK method, in the direction of $\lambda_j [1, 2]$. We would determine such stepsizes for all stiff eigenvalues at each RK node; the smallest of these is then chosen as the appropriate stepsize. Note that local error control also places a restriction on the stepsize [3], and it could occur that such restriction is more stringent than that in (2). In that case, the appropriate stepsize would be determined from the error control algorithm, rather than (2).

Let $y_i \equiv (y_{1,i}, \ldots, y_{n,i})$ denote the exact solution to (1) at node $x_i$, and let $w_i \equiv (w_{1,i}, \ldots, w_{n,i})$ denote the approximate numerical solution at the same node. We have

$$w_i = y_i + \Delta_i = (y_{1,i} + \Delta_{1,i}, \ldots, y_{n,i} + \Delta_{n,i}),$$

where $\Delta_i \equiv (\Delta_{1,i}, \ldots, \Delta_{n,i})$ is the global error in $w_i$.

3 Theoretical Analysis

Let us write

$$\lambda_{j,i} (x_i, w_i) = -\alpha_{j,i} (x_i, w_i) + \beta_{j,i} (x_i, w_i) \mathbf{i}$$

for stiff eigenvalues at $x_i$, as functions of the numerical solution $w_i$. A Taylor expansion about $y_i$ gives

$$\lambda_{j,i} (x_i, w_i) = -\alpha_{j,i} (x_i, y_i) + \beta_{j,i} (x_i, y_i) \mathbf{i}$$

$$+ \sum_{k=1}^{n} \Delta_{k,i} \left( -\frac{\partial \alpha_{j,i}}{\partial y_k} \bigg|_{y_i} + \mathbf{i} \frac{\partial \beta_{j,i}}{\partial y_k} \bigg|_{y_i} \right) + \ldots. \quad (3)$$

This gives

$$\lambda_{j,i}^2 (x_i, w_i) = \lambda_{j,i} (x_i, w_i) \lambda_{j,i}^* (x_i, w_i)$$

$$\approx \alpha_{j,i}^2 (x_i, y_i) + \beta_{j,i}^2 (x_i, y_i) + 2\alpha_{j,i} \sum_{k=1}^{n} \Delta_{k,i} \frac{\partial \alpha_{j,i}}{\partial y_k} \bigg|_{y_i} + 2\beta_{j,i} \sum_{k=1}^{n} \Delta_{k,i} \frac{\partial \beta_{j,i}}{\partial y_k} \bigg|_{y_i}$$

$$= \lambda_{j,i}^2 (x, y_i) + E_{j,i}$$

in which we have implicitly defined the error term $E_{j,i}$. In the second line above, we have ignored higher-order terms.

We now have

$$h_{j,i} \leq \frac{D_{j,i}}{\sqrt{\lambda_{j,i}^2 (x, y_i) + E_{j,i}}} = \frac{D_{j,i}}{\sqrt{\lambda_{j,i}^2 (x, y_i)}} \left( 1 - \frac{E_{j,i}^2}{2} + \frac{3E_{j,i}^2}{8} + \ldots \right)$$
where $E'_{j,i} \equiv E_{j,i}/\lambda^2_{j,i}(x,y_i)$. Hence,

$$h_{j,i} \lesssim \frac{D_{j,i}}{|\lambda_{j,i}(x,y_i)|} - \frac{D_{j,i}E'_{j,i}}{2|\lambda_{j,i}(x,y_i)|} + \frac{3D_{j,i}E^2_{j,i}}{8|\lambda_{j,i}(x,y_i)|},$$

(4)

ignoring higher-order terms. Clearly, as $E'_{j,i} \to 0$, so we recover (2). The last two terms are a modification to the stepsize condition due to the presence of global error in the numerical solutions that appear in the Jacobian.

## 4 Discussion

Firstly, we note that the stepsize condition always results in a stepsize such that $h_{j,i}\lambda_{j,i}(x,w_i)$ lies within the region of stability of the RK method, irrespective of the magnitude of the global error. This result is both important and pleasing, because it means that the presence of global error in the Jacobian will not compromise the stability of the computation (as long as the stepsize condition is enforced).

Secondly, we see from (3) that the error terms could be positive or negative. This means that $\lambda_{j,i}(x,w_i)$ might lie outside the region of stability, even though $\lambda_{j,i}(x,y_i)$ is within it. This would lead to a stepsize adjustment even though, strictly speaking, it is not required. This effect is reflected in (4) where, if the second-order term is negligible and $E'_{j,i} > 0$, $h_{j,i}$ will be smaller than $D_{j,i}/|\lambda_{j,i}(x,y_i)|$. Smaller stepsizes means more nodes on the interval of integration, which reduces the computational efficiency of the method. On the other hand, the signs of the error terms could be such that $h_{j,i}$ is found to be larger than $D_{j,i}/|\lambda_{j,i}(x,y_i)|$. This could possibly lead to a local error larger than the imposed tolerance, which would then result in a stepsize adjustment, based on error control considerations, and a consequent recomputation of that step - another source of computational inefficiency.

Lastly, if the system is weakly stiff ($(\lambda_{j,i}(x,y_i) < 1)$ then $E'_{j,i}$ could be relatively large. This could affect the RHS of (4) quite substantially, in the ways already discussed. The only mitigation against such effects are to ensure that the global error is always small. This is not always a consequence of local error control - in fact, it is usually not [4] - and so we would suggest the possible use of the RKQ algorithm as the preferred method of solution. The reader is referred to our previous work for appropriate detail [5, 6, 7, 8]; it suffices to say here that RKQ (more properly, RK_qvQz) uses three RK methods of orders $r, v$ and $z$ in an attempt to provide stepwise control of both local and global error.
5 Conclusion

We have investigated the effect of global error on stepsize adjustment for moderately stiff initial-value problems, solved using explicit Runge-Kutta methods. We find that global error will not affect the stability of the solution, but is likely to reduce the computational efficiency of the Runge-Kutta method. We have proposed that the use of the RKQ algorithm, which can facilitate stepwise control of global error, could be preferable to mere local error control alone when solving moderately stiff problems.

References


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