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Suppressing Order Reduction on 2-Stage Gauss Method

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Abstract: The phenomenon of order reduction has been observed in higher order methods when used to solve stiff ordinary differential equation. Symmetrization is a way to prevent this phenomenon and at the same time dampening down the oscillatory behavior in the numerical solution. In this paper, we discuss the construction of two-step symmetrization for 2-stage Gauss and present the numerical results on the order accuracy of the method. It is proven that the symmetrization is able to restore the classical order behavior when solving stiff problem.

Keywords: 2-stage Gauss methods, order reduction, symmetrization.

1. Introduction

Certain higher order methods suffer the reduction of order when used to solve stiff problems. For example, 2-stage Gauss method of order-4 behaves like an order-2 method when the problem is stiff [1-6]. This is the phenomenon of order reduction. It was first observed by Prothero-Robinson (PR) [7]. The Runge-Kutta method with stepsize h for the step $\left(x_{n-1}, y_{n-1}\right) \to \left(x_n, y_n\right)$ is a one-step method defined by

$$Y_i = y_{n-1} + h\sum_{j=1}^{a} a_{ij} f\left(x_{n-1} + c_j h, Y_j\right), \quad i = 1,\ldots,s, \tag{1}$$

$$y_n = y_{n-1} + h\sum_{i=1}^{s} b_{ij} f(x_{n-1} + c_i h, Y_i). \tag{2}$$

The Prothero-Robinson problem can be written as

$$y'(x) = qy(x) + \phi(x), \quad \phi(x) = g'(x) - qg(x), \tag{3}$$

with initial condition $y(x_0) = y_0$.

When the Runge-Kutta method is used to solve the PR problem, we obtained

$$\begin{aligned} Y &= ey_{n-1} + hAF(Y) = ey_{n-1} + hA(qY + \Phi), \\ &= (I - zA)^{-1} ey_{n-1} + (I - zA)^{-1} hA\Phi, \quad z = qh \end{aligned} \tag{4}$$

where

$$Y = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_s \end{bmatrix}, \; F(Y) = \begin{bmatrix} f\left(x_{n-1} + c_1 h, Y_1\right) \\ f\left(x_{n-1} + c_2 h, Y_2\right) \\ \vdots \\ f\left(x_{n-1} + c_s h, Y_s\right) \end{bmatrix}, \; \Phi = \begin{bmatrix} \phi\left(x_{n-1} + c_1 h\right) \\ \phi\left(x_{n-1} + c_2 h\right) \\ \vdots \\ \phi\left(x_{n-1} + c_s h\right) \end{bmatrix}$$

The update is given by

$$y_n = y_{n-1} + hb^T F(Y) = R(z) y_{n-1} + hb^T (I - zA)^{-1} \Phi \tag{5}$$

where $R(z) = I + zb^T (I - zA)^{-1} e$ is the stability function.

Replacing Y, y_n and y_{n-1} by the exact values $y\left(x_{n-1} + ch\right), y\left(x_n\right)$ and $y\left(x_{n-1}\right)$ respectively yields

$$\begin{aligned} y\left(x_{n-1} + ch\right) &= \left(I - zA\right)^{-1} ey\left(x_{n-1}\right) + \left(I - zA\right)^{-1} hA\Phi \\ &\quad + \left(I - zA\right)^{-1} L_n, \\ y\left(x_n\right) &= R(z) y\left(x_{n-1}\right) + hb^T \left(I - zA\right)^{-1} \Phi \\ &\quad + zb^T \left(I - zA\right)^{-1} L_n + \ell_n, \end{aligned} \tag{6}$$

where L_n and ℓ_n are residual vectors for the internal stages and the update respectively. They have Taylor series expansions about x_{n-1} given by:

$$\begin{aligned} L_n &= \sum_{k=2}^{\infty} \frac{h^k}{k!} y^{(k)}\left(x_{n-1}\right)\left(c^k - kAc^{k-1}\right), \\ &\quad \left(Ae = c \text{ is assumed}\right), \\ \ell_n &= \sum_{k=2}^{\infty} \frac{h^k}{k!} y^{(k)}\left(x_{n-1}\right)\left(1 - kb^T c^{k-1}\right), \\ &\quad \left(b^T e = c \text{ is assumed}\right). \end{aligned} \tag{7}$$

The global error is $\varepsilon_n = R(z)\varepsilon_{n-1} + \psi_n(z)$, where $\psi_n(z)$ is the local error for the n-th step given by

$$\psi_n(z) = \ell_n + zb^T \left(I - zA\right)^{-1} L_n. \tag{8}$$

Solving the inhomogeneous difference equation, it gives

$$\varepsilon_n = \sum_{i=1}^{n} R(z)^{n-i} \psi_i(z) + R(z)^n \varepsilon_0. \tag{9}$$

The local error at step i is magnified by the stability function $R(z)^{n-i}$ and contributes to the global error at step n.

The local error at step i is given by

$$\psi_i(z) = \ell_n + zb^T\left(I - zA\right)^{-1}L_n,$$
$$= \sum_{k=2}^{\infty}\frac{h^k}{k!}y^{(k)}\left(x_{i-1}\right)\left(1 - kb^Tc^{k-1} + zb^T\left(I - zA\right)^{-1}\left(c^k - kAc^{k-1}\right)\right),$$

(10)

Note that, the simplifying assumption [8], $B(p): 1 - kb^Tc^{k-1}$ vanishes for k = 1,…, p and by $C(q): c^k - kAc^{k-1}$ vanishes for k = 1,…, q.

2. Analysis of Gauss Method

In this section we will analyse the order behavior of the symmetric methods for Gauss method.

In the nonstiff case $|\lambda| = O(1)$ or $|z| = O(h)$ as $h \to 0$, equation (10) yields

$$\psi_i(z) = \sum_{k=2}^{\infty}\frac{h^k}{k!}y^{(k)}\left(x_{i-1}\right)\left(1 - kb^Tc^{k-1} + zb^T\left(c^k - kAc^{k-1}\right) + O\left(z^2\right)\right). \tag{11}$$

In the strongly stiff case $|\lambda| = O(1/h^2)$ or $|z| = O(1/h)$ as $h \to 0$, equation (10) yields

$$\psi_i(z) = \sum_{k=2}^{\infty}\frac{h^k}{k!}y^{(k)}\left(x_{i-1}\right)\left(1 - b^TA^{-1}c^k + \frac{1}{z}b^TA^{-2}\left(c^k - kAc^{k-1}\right) + O\left(1/z^2\right)\right). \tag{12}$$

The 2-stage Gauss method satisfies the simplifying assumptions B(4) and C(2). The method is of order-4 and is given by

$$A = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} - \frac{\sqrt{3}}{6} & \frac{1}{4} \end{bmatrix},\; b = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix},\; c = \begin{bmatrix} \frac{1}{2} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} \end{bmatrix}, \tag{13}$$

where A is the Runge-Kutta matrix and b and c are vectors of weights and abscissas respectively.

In the nonstiff case, from equation (11) the local error is given by

$$\psi_i(z) = \frac{h^5}{5!36}y^{(5)}\left(x_{i-1}\right) - \frac{zh^4}{4!36}y^{(4)}\left(x_{i-1}\right) + O\left(h^6\right). \tag{14}$$

In the stiff case, from equation (11) the local error is

$$\psi_i(z) = \frac{h^3}{36}y'''\left(x_{i-1}\right) - \frac{h^3}{6z}y'''\left(x_{i-1}\right) + O\left(h^4\right). \tag{15}$$

Therefore,

$$\psi_i(z) = \begin{cases} O\left(h^5\right) & \text{if nonstiff} \\ O\left(h^3\right) & \text{if strongly stiff} \end{cases} \quad \text{as } h \to 0.$$

The stability function is given by $R(z) = \dfrac{1 + z/2 + z^2/12}{1 - z/2 + z^2/12}$

and from (9) it yields :

$$R(z) = \frac{1 + z/2 + z^2/12}{1 - z/2 + z^2/12} = \begin{cases} 1 & \text{if nonstiff} \\ 1 & \text{if strongly stiff} \end{cases} \quad \text{as } h \to 0, \tag{16}$$

$$\varepsilon_n = \begin{cases} O\left(h^4\right) & \text{if nonstiff} \\ O\left(h^2\right) & \text{if strongly stiff} \end{cases} \quad \text{as } h \to 0, \tag{17}$$

In the stiff case, 2-stage Gauss method exhibits order reduction where the method behaves like an order-2 method (see Figure 1).

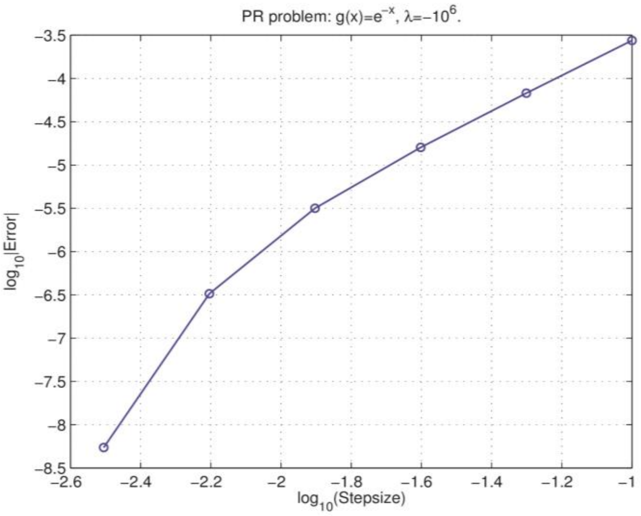

Figure 1. The phenomenon of order reduction in 2-stage Gauss method solving PR problem (3) with $g(x) = e^{-x}$, stepsize h = 0.1 and stiffness parameter $\lambda = -10^6$

3. Symmetrized Method

Symmetrization is a generalization of smoothing introduced by Chan [9]. The main ideas of the construction are to dampen down the oscillations in the numerical solution and to suppress order reduction of higher order methods in solving stiff problems. The one-step symmetrizer is a composition of two-symmetric methods with appropriate weights [10-12]. The one-step symmetrizer has been constructed by Gorgey and Chan [12], and proven to preserve the classical order of particular members of the Gauss and Lobatto IIIA family of members.

Two-step symmetrization of the order-2 symmetric methods provides promising results particularly in terms of accuracy and efficiency [13]. Thus, we wish to examine the effects of two-step symmetrization applied to higher order symmetric method and compare the accuracy and efficiency with the one-step symmetrization and the base method itself.

3.1Two-step Symmetrization of 2-stage Gauss Method

The method is the composition of four steps of the 2-stage Gauss method (13). The symmetrized matrix, the vectors of weights and abscissas are given by

$$\tilde{A} = \begin{bmatrix} A & 0 & 0 & 0 \\ eb^T & A & 0 & 0 \\ eb^T & eb^T & A & 0 \\ eb^T & eb^T & eb^T & A \end{bmatrix},\; \tilde{b} = \begin{bmatrix} b^T - v^TP \\ b^T - u^TP \\ u^T \\ v^T \end{bmatrix} \text{ and}$$

$$\tilde{c} = \begin{bmatrix} c \\ e+c \\ 2e+c \\ 3e+c \end{bmatrix}, \quad (18)$$

where P is the permutation matrix and vectors u and v are chosen to satisfy damping condition, $\tilde{R}(\infty)=0 \rightarrow u^T A^{-1}e + R(\infty)v^T A^{-1}e = \frac{1}{2}$ and order-3 condition obtained from the simplifying assumption [8], $u^T c + v^T(e+c) = 0$. The symmetrizer, however, cannot attain order-4 as the conditions $u^T c^3 + v^T(e+c)^3 = 0$ and $(u^T + v^T)(c^3 - 3Ac^2) = 0$ cannot be satisfied simultaneously. Solving all these equations, we obtain the following values for the parameters:

$$u_1 = \frac{29+27\sqrt{3}}{576},\ u_2 = \frac{29-27\sqrt{3}}{576},\ v_1 = \frac{-5-\sqrt{3}}{1728} \text{ and } v_2 = \frac{-5+9\sqrt{3}}{1728}. \quad (19)$$

The symmetrization can be applied in active and passive implementations [14]. Thus, we will analyze the implementation in both modes to determine the order of the method when solving nonstiff and stiff cases.

3.2 Active and Passive Symmetrization

Symmetrization can be done either in active or passive modes. In active symmetrization, the symmetrized values are used as starting values for subsequent computations whenever it is computed, that is, the symmetrized values are used in propagating the numerical solution. In passive symmetrization the symmetrized values are computed whenever desired.

The analysis of two-step symmetrization is similar to the analysis of Gauss method in Section 2 except that now it involves two-step. The global error is given by

$$\varepsilon_n = \sum_{i=1}^{n} \tilde{R}(z)^{n-i}\tilde{\psi}_i(z), \quad (20)$$

and the local error by

$$\tilde{\psi}_i(z) = \sum_{k=2}^{\infty} \frac{h^k}{k!} y^{(k)}(x_{i-1}) \left(2^k - k\tilde{b}^T\tilde{c}^{k-1} + z\tilde{b}^T\left(\tilde{I}-z\tilde{A}\right)^{-1}\left(\tilde{c}^k - k\tilde{A}\tilde{c}^{k-1}\right)\right). \quad (21)$$

We remark that for the active symmetrization, in the nonstiff case, since $\tilde{R}(\infty) = O(1)$ as $z \rightarrow 0$ the sum in (20) contributes the factor n to the local error terms and this leads to the cancellation of one power of h in the lowest order term $\tilde{\psi}_i$; in the strongly stiff case, the global error is determined by the local error at the last step which is unaffected by the damping of the stability function. Whereas the global error of the symmetrizer applied in the passive mode will behave like the local error $\tilde{\psi}_n$ at the n-step.

4. Results and Discussion

In this section we investigate the order accuracy of 2-stage Gauss method on the PR problem by calculating the slope of the log-log plot of absolute error versus stepsize. We use different values of stiff parameter to examine the behaviour of the methods. Table 1 shows the abbreviation used in the following discussion.

We observe that in the nonstiff case with $\lambda = -1$ (Figure 2), the base method G2, 2PS and 1PS are of order-4 while the symmetrizers in active mode (1AS and 2AS) are of order-3. In this case, the base method lies at the bottom of the figure indicating that it is most accurate. However, as the stiffness parameter increases, we observe that the symmetrizers (both one-step and two-step) lie at the bottom of the graph indicating that it is more accurate than the base method with 2AS giving the most accurate behavior in mildly to strongly stiff cases (Figure 3-5). We also note that the base method experiences order reduction with order-2 behaviour in the strongly stiff case as shown in Figure 5. However, all symmetrizers are able to suppress order reduction. The one-step symmetrizers (1PS and 1AS) restore the classical order-4 behaviour of the method and the two-step symmetrizers (2PS and 2AS) have super-convergent order-6 behaviour and are the most accurate methods for this particular problem.

Table 1. Notation for Numerical Experiments

Abbreviation	Definition
G2	2-stage Gauss (base method)
1AS	one-step active symmetrization
2AS	two-step active symmetrization
1PS	one-step passive symmetrization
2PS	two-step passive symmetrization

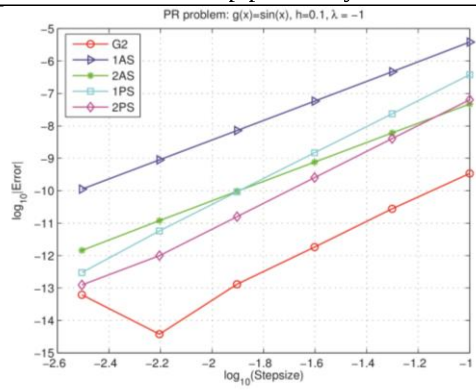

Figure 2. Order behavior of 2-stage Gauss and the symmetrizers solving PR problem for nonstiff case with $\lambda = -1$

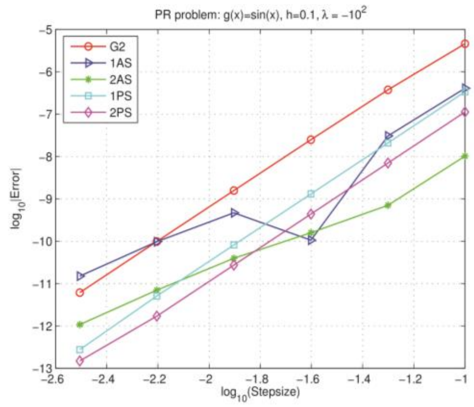

Figure 3. Order behavior of 2-stage Gauss and the symmetrizers solving PR problem for mildly stiff case with $\lambda = -10^2$

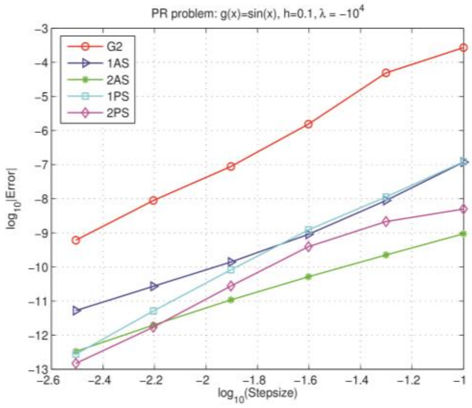

Figure 4. Order behavior of 2-stage Gauss and the symmetrizers solving PR problem for mildly stiff case with $\lambda=-10^4$

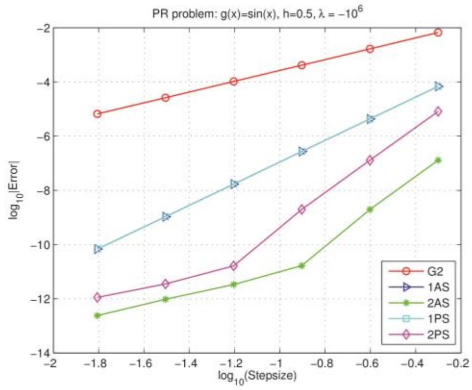

Figure 5. Order behavior of 2-stage Gauss and the symmetrizers solving PR problem for strongly stiff case with $\lambda=-10^6$

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6. Conclusion

The numerical results on the order behaviour of the 2-stage Gauss method, one-step symmetrization, and two-step symmetrization on the PR problem have proven that the symmetrizers are able to suppress order reduction in the strongly stiff cases. The one-step symmetrization restores the classical order-4 of the method and the two-step symmetrization in both modes shows superconvergent order-6 behaviour in this particular case. Moreover, the symmetrizers seem to be advantageous in terms of accuracy in the mildly to strongly stiff cases of linear PR problem. It is of interest to investigate the performance of the symmetrizers in other nonlinear problems and also when apply with extrapolation.

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