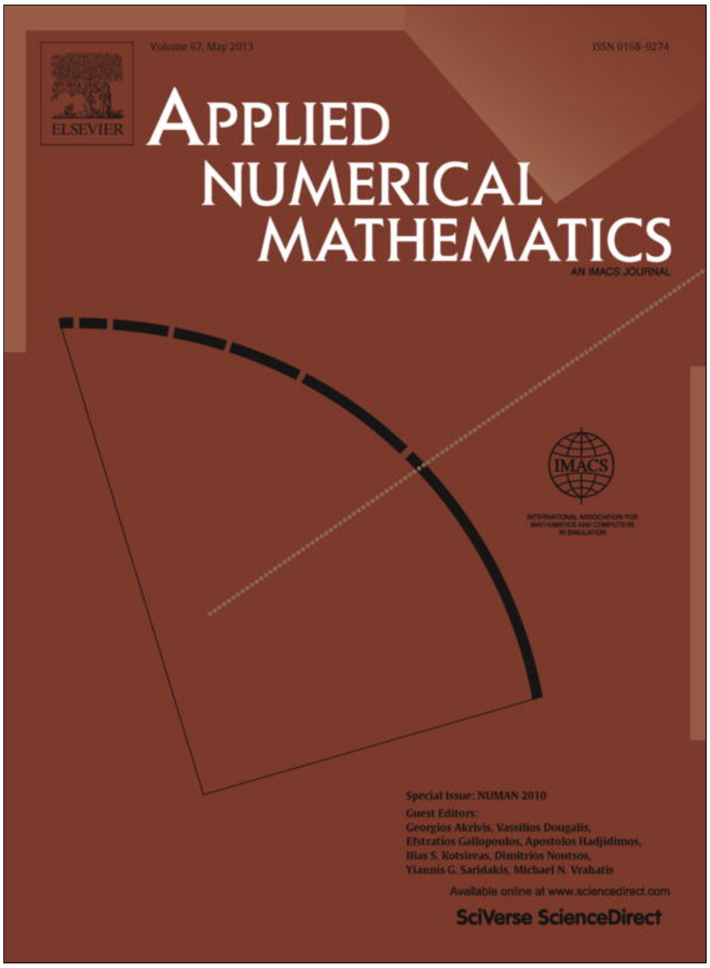
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Active and passive symmetrization of Runge–Kutta Gauss methods

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A B S T R A C T

A symmetrizer for a symmetric Runge–Kutta method is designed to preserve the asymptotic error expansion in even powers of the stepsize and to provide damping for stiff initial value problems. In this paper we study symmetrizers for the Gauss methods with two and three stages and compare the implementation in passive and active modes. In particular, we perform a detailed analysis of the Prothero–Robinson problem which provides insight into the behaviour of symmetrizers in suppressing order reduction experienced by the symmetric methods. We present numerical results on the effects of passive and active symmetrization for some stiff linear and nonlinear problems. These effects have important implications for the development of extrapolation methods based on higher order symmetric methods for the numerical solution of stiff problems. Our results show that symmetrization in both modes improves accuracy and efficiency, and can restore the classical order of the Gauss methods for stiff linear problems. We compare the two modes of symmetrization for constant stepsize and present preliminary results in a variable stepsize setting.

1. Introduction

The use of extrapolation to accelerate convergence has been known since the work of Richardson [16]. In Romberg integration [17] the application to numerical quadrature has been highly successful. The existence of asymptotic error expansions [10,18], especially those of symmetric methods, allowed extrapolation methods to be developed for ordinary differential equations. Those based on the explicit midpoint rule have had considerable success when applied to nonstiff problems (ODEX [3]). Application to stiff problems though have achieved moderate success and these have been based on the implicit midpoint or trapezoidal rules (IMPEX [8]) and the linearly implicit midpoint rule (METAN1 [2]). In these applications two features stand out – the use of the smoothing formula by Gragg [10] and the symmetry of the base methods which lead to the h^2-asymptotic error expansions of the form

$$y_n - y(x_n) = e_1 h^p + e_2 h^{p+2} + \cdots, \quad h \to 0, \tag{1}$$

where the coefficients e_i, $i = 1, 2, \ldots$, are smooth functions independent of h. Stetter [18] proved the existence of such expansions for a very general class of discretization methods for nonlinear functional equations (e.g. initial and boundary value problems for both ordinary and partial differential equations, integral and integro-differential equations). Moreover, theoretical results on the existence of an asymptotic expansion for the global error of the implicit Euler, implicit midpoint rule and implicit trapezoidal rule are given in [1] by the Vienna group. They have studied the existence of such expansions for a class of nonlinear stiff systems.

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Table 1
Maximum attainable order of symmetrizers for Gauss methods.

Stage number s	1	2	3	4	5	6	7
Classical order of $\mathscr{G}_s$	2	4	6	8	10	12	14
Maximum attainable order of $\tilde{\mathscr{G}_s}$	1	3	5	5	7	9	9

In contemplating extensions to the above-mentioned methods for stiff ordinary differential equations, we are lead to explore symmetric Runge–Kutta methods such as the Gauss and the Lobatto IIIA families of order higher than two with the idea of exploiting the h^2-asymptotic error expansion these methods possess. However there are difficulties to be overcome. The Gauss methods, for example, suffer from the phenomenon of order reduction [15,11] when applied to stiff problems. Symmetric methods, though A-stable, have weak damping properties. It is desirable in applications to stiff problems that a method provides damping and suppresses order reduction and yet, at the same time, preserves the h^2-asymptotic error expansion. Since these features are important for the development of extrapolation methods, we construct methods called *symmetrizers* [7] that are based on symmetric methods but which are themselves not symmetric and explore their properties.

Gragg [10] was the first to introduce the concept of smoothing designed to dampen the oscillatory parasitic component of the numerical solution of the explicit midpoint rule. In the late 1980s, Chan [7] generalized this concept, calling it *symmetrization*, and extended the theoretical study of extrapolation to arbitrary symmetric Runge–Kutta methods for stiff ordinary differential equations.

In this paper we study, in particular, the Gauss methods with 2 and 3 stages, $\mathscr{G}_2$ and $\mathscr{G}_3$, of classical order 4 and 6, respectively, for stiff problems. Butcher and Chan [6] have given a complete set of maximum attainable order for the symmetrizer $\tilde{\mathscr{G}_s}$ for the s-stage Gauss method, $\mathscr{G}_s$ (see Table 1). In general, a symmetrizer $\tilde{\mathscr{R}}$ has odd order $2p-1$ whenever the even order conditions up to order $2p-2$ are satisfied. The local error of $\tilde{\mathscr{R}}$ of order $2p-1$ behaves like $O(h^{2p})$. We will show in our analysis that the symmetrizer can achieve order 4 for $\tilde{\mathscr{G}_2}$ and order 6 for $\tilde{\mathscr{G}_3}$ when solving very stiff linear problems.

In a theoretical study of this phenomenon, Burrage and Chan [4] suggested that appropriate symmetrizers for $\mathscr{G}_s$ can be chosen so that the corresponding global errors behave like $O(h^{s+1})$ for $s=3$, $O(h^{s+2})$ for $s=2,4,6$ and $O(h^{s+3})$ for $s=5$.

In this paper we investigate two different ways of implementing symmetrization. In the passive mode the numerical solution of the symmetric method is propagated at every step even though symmetrization can be applied at any step. In active symmetrization, on the other hand, it is the symmetrized solution that is propagated whenever it occurs.

In Section 2 we discuss the characterization and properties of symmetry and describe the construction of symmetrizers and their passive or active implementation in Section 3. We present an analysis of the application to the model Prothero–Robinson problem in Section 4. In Section 5 we present and discuss the results of our numerical experiments and finally conclude with some remarks in Section 6.

2. Symmetry

If $\mathscr{R}$ denotes the equivalence class of Runge–Kutta methods generated by the triple (A, b, c), we write $\mathscr{R} = (A, b, c)$, where A is the Runge–Kutta matrix, b the vector of weights, c the vector of abscissas and e the vector of units. At the nth step $x_{n-1} \to x_n = x_{n-1} + h$ with stepsize h, the method is defined by

$$\begin{aligned} Y^{[n]} &= e \otimes y_{n-1} + h(A \otimes I_N) F\big(x_{n-1} + ch, Y^{[n]}\big), \\ y_n &= y_{n-1} + h\big(b^T \otimes I_N\big) F\big(x_{n-1} + ch, Y^{[n]}\big), \end{aligned} \tag{2}$$

for an initial value problem $y'(x) = f(x, y)$, $y(x_0) = y_0$, where $f : [x_0, X] \times \Re^N \to \Re^N$ and y_n is the update while $Y^{[n]}$ is the vector of internal stages with

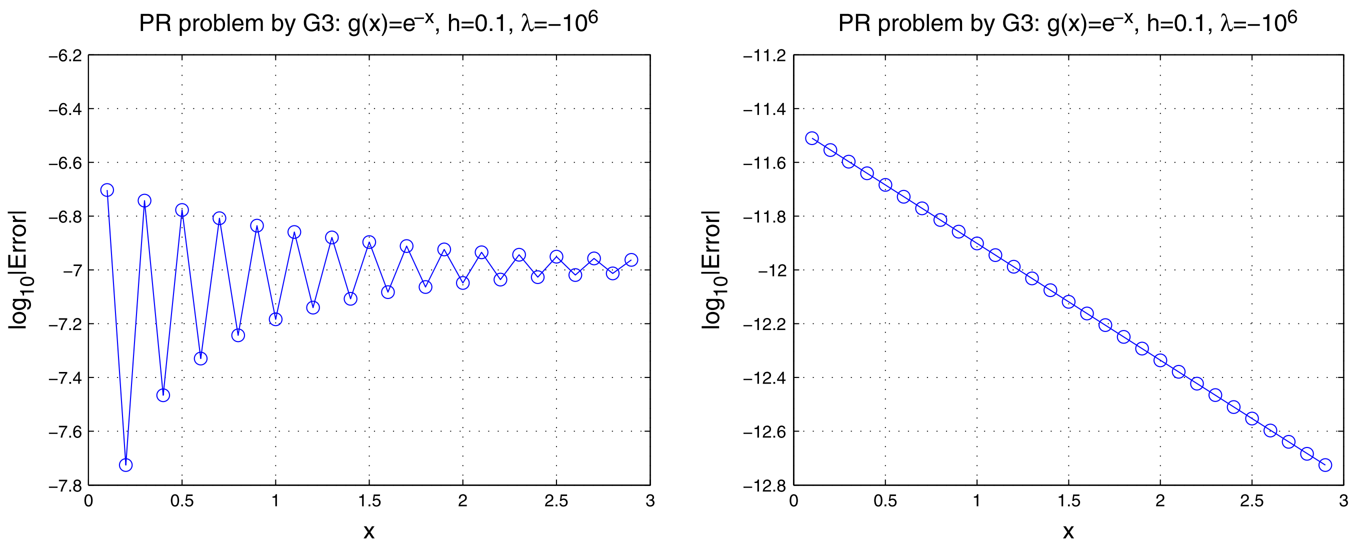
$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix}, \qquad F\big(x_{n-1} + ch, Y^{[n]}\big) = \begin{bmatrix} f(x_{n-1} + c_1 h, Y_1^{[n]}) \\ \vdots \\ f(x_{n-1} + c_s h, Y_s^{[n]}) \end{bmatrix}.$$

The method is called *symmetric* or *self-adjoint* if

$$-\mathscr{R}^{-1} = \mathscr{R}, \tag{3}$$

where $-\mathscr{R} = (-A, -b, -c)$ is the method $\mathscr{R}$ applied with stepsize $-h$, and $\mathscr{R}^{-1} = (A - eb^T, -b, c - e)$ is the inverse of $\mathscr{R}$. It follows that the adjoint of $\mathscr{R}$ is given by $-\mathscr{R}^{-1} = (eb^T - A, b, e - c) \equiv (PAP, Pb, Pc)$, and a symmetric method is therefore characterized by the symmetry conditions,

$$Pb = b, \qquad PAP = eb^T - A, \qquad Pc = e - c, \tag{4}$$



(a) $\mathscr{G}_3$ (b) $\mathscr{G}_3$ with symmetrizer

Fig. 1. Error behavior of $\mathscr{G}_3$ with symmetrizer applied to a Prothero–Robinson problem.

where P is a permutation matrix which reverses the order of the stages with its elements satisfying $p_{ij} = \delta_{i,s+1-j}$. The third condition assumes that $b^T e = 1$ and $Ae = c$ hold. The symmetry conditions (4) will be used in subsequent calculations. For example, the stability function $R(z) = 1 + zb^T(I - zA)^{-1}e$ satisfies

$$R(z)R(-z) = 1, \tag{5}$$

and therefore implies $|R(\infty)| = 1$ which means symmetric methods provide no damping for stiff problems.

In this paper, we are concerned with the Runge–Kutta methods that arise from the integration process based on Gaussian quadrature where the abscissas are given by the roots of the equation $P_s(2x-1) = 0$. Here $P_s(x)$ is the Legendre polynomial of degree s defined on the interval $[-1, 1]$. In general, an s-stage Gauss method is constructed by using the simplifying assumptions $B(s)$ and $C(s)$ [5], where

$$\begin{aligned} B(p)&: \quad b^T c^{k-1} = \frac{1}{k}, \quad k = 1, \ldots, p, \\ C(q)&: \quad Ac^{k-1} = \frac{1}{k}c^k, \quad k = 1, \ldots, q, \end{aligned} \tag{6}$$

and powers of the vector c refer to component-wise powers. In fact, $\mathscr{G}_s$ satisfies $B(2s)$ and is of classical order $2s$.

Besides the suppression of order reduction, symmetrizers can also provide damping for the oscillations that arise numerically. The stability function of $\mathscr{G}_3$, like that of the implicit midpoint rule, has the property $R(\infty) = -1$ and gives rise to the oscillatory error behavior for the Prothero–Robinson (PR) problem shown in Fig. 1(a). In a way similar to the damping that smoothing provides for the implicit midpoint rule, a generalization of smoothing (symmetrization) for $\mathscr{G}_3$ results in the error behavior shown in Fig. 1(b).

We now generalize the smoothing formula introduced by Gragg,

$$\hat{y}_n = \frac{1}{4}(y_{n-1} + 2y_n + y_{n+1}),$$

for an arbitrary symmetric Runge–Kutta method. This smoothing formula, although designed for the explicit midpoint rule, turned out to be the same for the implicit midpoint rule and implicit trapezoidal rule (see [1] and [13]). The generalized formula for symmetric Runge–Kutta methods of higher order will now involve internal stage values beyond the point x_n just as the above formula involves the update y_{n+1}.

3. Symmetrization

Let $\mathscr{R}_m = \frac{1}{m}\mathscr{R}^m$ denote the composition of m steps of an arbitrary symmetric Runge–Kutta method $\mathscr{R} \equiv (A, b, c)$ each with stepsize $h = H/m$. If the last step of $\mathscr{R}_m$ is replaced by a method $\tilde{\mathscr{R}}$, the resulting method is then denoted by $\hat{\mathscr{R}}_m = \frac{1}{m}(\mathscr{R}^{m-1} \circ \tilde{\mathscr{R}})$ as shown in Fig. 2. When $m = 1$, $\mathscr{R}_{m-1} = \mathcal{I}$, the identity method which leaves the starting value unchanged for all stepsizes and problems. Since the symmetry property $-\mathscr{R}^{-1} = \mathscr{R}$ results in $\mathscr{R}_{-m} = \mathscr{R}_m$ for all m, where $\mathscr{R}_{-m}$ is the composition of m steps of the adjoint method $-\mathscr{R}^{-1}$ with stepsize h, the method $\tilde{\mathscr{R}}$ is constructed so that $\hat{\mathscr{R}}_{-m} = \hat{\mathscr{R}}_m$ for all m. By Theorem 8.6 in [12] this preserves the h^2-asymptotic error expansion but neither $\tilde{\mathscr{R}}$ nor $\hat{\mathscr{R}}_m$ is

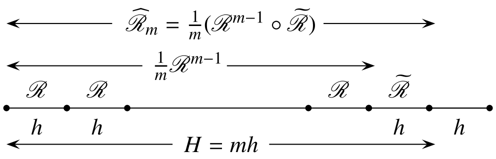


Fig. 2. Symmetrization in the m-th step.

self-adjoint. The method $\tilde{\mathscr{R}}$, called a (one-step) *symmetrizer*, must now satisfy $\tilde{\mathscr{R}} \circ (-\tilde{\mathscr{R}}^{-1}) = \mathscr{R}^2$ [7] and therefore has Butcher tableau given by

$$\tilde{\mathscr{R}} = (\tilde{A}, \tilde{b}, \tilde{c}) \equiv \left(\begin{bmatrix} A & 0 \\ eb^T & A \end{bmatrix}, \begin{bmatrix} b - Pu \\ u \end{bmatrix}, \begin{bmatrix} c \\ e + c \end{bmatrix} \right), \tag{7}$$

where the weight vector u is chosen to satisfy the damping and order conditions. We remark that the method $\tilde{\mathscr{R}}$ is the composition of two steps of $\mathscr{R}$ except that the weights are different and gives an update over one step (with stepsize h). A generalization to a composition involving four steps of $\mathscr{R}$ is possible (called a two-step symmetrizer) but will not be considered in this paper.

We suppress the Kronecker product notation for simplicity and obtain from (2) the defining equations for the symmetrized step,

$$\begin{aligned} \tilde{Y}^{[m]} &= \tilde{e} y_{m-1} + h\tilde{A}\tilde{F}\big(x_{m-1} + \tilde{c}h, \tilde{Y}^{[m]}\big), \\ \tilde{y}_m &= y_{m-1} + h\tilde{b}^T\tilde{F}\big(x_{m-1} + \tilde{c}h, \tilde{Y}^{[m]}\big) = \tilde{b}^T\tilde{A}^{-1}\tilde{Y}^{[m]} = u^T A^{-1}\big(PY^{[m]} + Y^{[m+1]}\big). \end{aligned} \tag{8}$$

Hence a symmetrizer for a Gauss method at step m depends on $Y^{[m]}$ and $Y^{[m+1]}$, the internal stage vectors for steps m and $m+1$ respectively. We remark that in the case where A is singular as for the Lobatto IIIA methods, a different way of computing the symmetrization step will have to be considered.

By using the symmetry conditions (4), the stability function of $\tilde{\mathscr{R}}$ can be shown to be given by

$$\tilde{R}(z) = 1 + z\tilde{b}^T(\tilde{I} - z\tilde{A})^{-1}\tilde{e} = R(z)\big(1 + 2z^2u^T\big(I - z^2A^2\big)^{-1}c\big). \tag{9}$$

Hence $\tilde{R}(\infty) = R(\infty)(1 - 2u^T A^{-1}e)$ and $\tilde{R}(\infty) = 0$ gives the damping condition

$$u^T A^{-1} e = \frac{1}{2}, \tag{10}$$

since A is nonsingular for Gauss methods. In the case of $\tilde{\mathscr{G}}_2$, the remaining parameter in u is chosen to satisfy the condition for order 3, namely,

$$u^T c = 0. \tag{11}$$

This yields $u = [\frac{\sqrt{3}+1}{24}, -\frac{\sqrt{3}-1}{24}]^T$ and therefore (8) becomes

$$\tilde{y}_m = \left(\frac{1}{4} + \frac{\sqrt{3}}{6}\right)\big(Y_1^{[m+1]} + Y_2^{[m]}\big) + \left(\frac{1}{4} - \frac{\sqrt{3}}{6}\right)\big(Y_1^{[m]} + Y_2^{[m+1]}\big). \tag{12}$$

The stability function is given by

$$\tilde{R}(z) = \frac{1 - \frac{1}{12}z^2}{\big(1 - \frac{1}{2}z + \frac{1}{12}z^2\big)^2}. \tag{13}$$

For $\tilde{\mathscr{G}}_3$ the fulfillment of (10) and (11) leaves one further parameter to be determined. The conditions for order 5 are $u^T c^3 = 0$ and $u^T Ac^2 = 0$. Since $C(3)$ holds for $\mathscr{G}_3$ these two conditions are equivalent and $\tilde{\mathscr{G}}_3$ will be of order 5 if we choose

$$u^T c^3 = 0. \tag{14}$$

This yields $u = [\frac{13+3\sqrt{15}}{360}, -\frac{1}{45}, \frac{13-3\sqrt{15}}{360}]^T$,

$$\tilde{y}_m = \left(\frac{1}{4} + \frac{\sqrt{15}}{15}\right)\big(Y_1^{[m+1]} + Y_3^{[m]}\big) + \left(\frac{1}{4} - \frac{\sqrt{15}}{15}\right)\big(Y_1^{[m]} + Y_3^{[m+1]}\big), \tag{15}$$

and the stability function

$$\tilde{R}(z) = \frac{1 - \frac{1}{20}z^2 + \frac{1}{600}z^4}{\left(1 - \frac{1}{2}z + \frac{1}{10}z^2 - \frac{1}{120}z^3\right)^2}. \tag{16}$$

We can obtain a second symmetrizer of order 3 if, instead of (14), we choose

$$u^T A^{-1} c^4 = 0, \tag{17}$$

which gives $u = [\frac{43+9\sqrt{15}}{1224}, -\frac{4}{153}, \frac{43-9\sqrt{15}}{1224}]^T$,

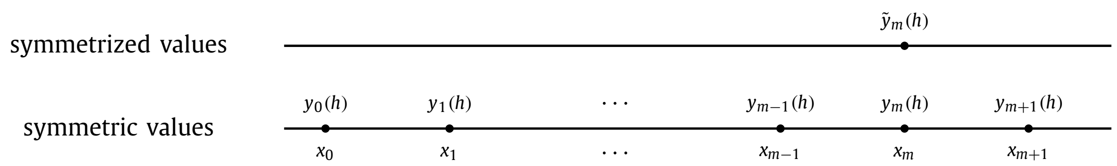
$$\tilde{y}_m = \left(\frac{55}{204} - \frac{7\sqrt{15}}{102}\right)\left(Y_1^{[m]} + Y_3^{[m+1]}\right) + \left(\frac{55}{204} + \frac{7\sqrt{15}}{102}\right)\left(Y_1^{[m+1]} + Y_3^{[m]}\right) - \frac{2}{51}\left(Y_2^{m]} + Y_2^{[m+1]}\right), \tag{18}$$

and the stability function

$$\tilde{R}(z) = \frac{1 - \frac{1}{20}z^2 + \frac{11}{5100}z^4}{\left(1 - \frac{1}{2}z + \frac{1}{10}z^2 - \frac{1}{120}z^3\right)^2}. \tag{19}$$

3.1. Passive symmetrization

When symmetrization occurs at a point the symmetrized value is not propagated in the passive mode; the symmetric solutions of the base method are propagated without invoking previously computed symmetrized values. In this mode, we compute many steps with the symmetric method, storing at each step the update as well as the internal stage values $Y^{[m]}$ and $Y^{[m+1]}$, and calculating the symmetrized value according to (8) whenever it is desired. Schematically, we have



3.2. Active symmetrization

In the active mode, the symmetrized value is propagated whenever it is computed. There are many different active options. When symmetrization is applied at every step the method is equivalent to $\hat{\mathscr{R}}_1 = \tilde{\mathscr{R}}$ as defined by (7). Another option, for example, is to apply symmetrization at every alternate step. In this case the basic method is $\hat{\mathscr{R}}_2 = \frac{1}{2}(\mathscr{R} \circ \tilde{\mathscr{R}})$, where the composition of the $3s$ stages is given by

$$\mathscr{R} \circ \tilde{\mathscr{R}} = (\hat{A}, \hat{b}, \hat{c}) \equiv \left(\begin{bmatrix} A & 0 & 0 \\ eb^T & A & 0 \\ eb^T & eb^T & A \end{bmatrix}, \begin{bmatrix} b \\ b - Pu \\ u \end{bmatrix}, \begin{bmatrix} c \\ e + c \\ 2e + c \end{bmatrix} \right). \tag{20}$$

The stability function is then given by $\hat{R}_2(z) = R(z/2)\tilde{R}(z/2)$. We note that $\hat{\mathscr{R}}_1$ in each step involves solving two sets of implicit systems of equations whereas $\hat{\mathscr{R}}_2$ requires three. However, we have observed that $\hat{\mathscr{R}}_2$ is more efficient than $\hat{\mathscr{R}}_1$ for both $\mathscr{G}_2$ and $\mathscr{G}_3$ (see Fig. 3 and Section 4.1).

4. Analysis of the Prothero–Robinson problem

The Prothero–Robinson (PR) problem [15] is defined by

$$y'(x) = \lambda\big(y(x) - g(x)\big) + g'(x) = \lambda y(x) + \phi(x), \qquad y(x_0) = g(x_0), \quad \lambda \in \mathbb{C},\ \Re(\lambda) < 0, \tag{21}$$

where $\phi(x) = g'(x) - \lambda g(x)$ and g is a smooth function. The problem is stiff when $|\lambda|$ is large but the exact solution will remain $y(x) = g(x)$ irrespective of the degree of stiffness. We will compare the global error after n steps of passive symmetrization at step n with active symmetrization at each of the n steps.

It is easy to show that the global error of the numerical solution after n steps consists of the sum of local errors modified by the stability function and is given by (see [11])

$$\epsilon_n = y_n - y(x_n) = \sum_{i=1}^{n} R(z)^{n-i}\psi_i(z), \tag{22}$$

where $\psi_i(z)$ is the local error for the i-th step given by

$$\psi_i(z)=\sum_{k=2}^{\infty}\frac{h^k}{k!}\left(1-kb^Tc^{k-1}+zb^T(I-zA)^{-1}\left(c^k-kAc^{k-1}\right)\right)g^{(k)}(x_{i-1}). \tag{23}$$

The term $1-kb^Tc^{k-1}$ vanishes for $k=1,\dots,p$ if $B(p)$ holds, while c^k-kAc^{k-1} vanishes for $k=1,\dots,q$ if $C(q)$ holds. $\mathscr{G}_2$ has classical order 4 and stage order 2 since $B(4)$ and $C(2)$ hold while $\mathscr{G}_3$ has classical order 6 and stage order 3 since $B(6)$ and $C(3)$ hold. For $\mathscr{G}_2$ we have $\psi_i(z)=O(h^3)$ as $h\to 0$ and $z\to\infty$. However, $R(z)\to 1$, and the sum over the local error terms in the global error introduces a factor n which results in the global error behaving like $O(h^2)$. This is the phenomenon of order reduction where the error behavior of the method for stiff problems is governed by the stage order. For $\mathscr{G}_3$ both the local and global error behaves like $O(h^4)$ because $R(\infty)=-1$ results in the cancellation of consecutive terms.

We now investigate the effect of symmetrization on the methods $\mathscr{G}_2$ and $\mathscr{G}_3$.

4.1. Active symmetrization by $\hat{\mathscr{R}}_1$ or $\hat{\mathscr{R}}_2$

In the case of active symmetrization at every step, $\hat{\mathscr{R}}_1=\tilde{\mathscr{R}}$, as given by (7). The stability function $R(z)$ in (22) is replaced by $\tilde{R}(z)$ and (23) is replaced by

$$\tilde{\psi}_i(z)=\sum_{k=2}^{\infty}\frac{h^k}{k!}\left(1-k\tilde{b}^T\tilde{c}^{k-1}+z\tilde{b}^T(\tilde{I}-z\tilde{A})^{-1}\left(\tilde{c}^k-k\tilde{A}\tilde{c}^{k-1}\right)\right)\tilde{y}^{(k)}(x_{i-1}). \tag{24}$$

When the problem is stiff (that is, $|\lambda|\sim O(1/h^2)$), then $|z|=|\lambda|h\sim O(1/h)\to\infty$ as $h\to 0$, the local error for $\tilde{\mathscr{G}}_2$ becomes

$$\begin{aligned}\tilde{\psi}_i(z)=&\frac{h^3}{6}\tilde{y}'''(x_{i-1})\left(1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^3-\frac{1}{z}\tilde{b}^T\tilde{A}^{-2}\left(\tilde{c}^3-3\tilde{A}\tilde{c}^2\right)+O\left(1/z^2\right)\right)\\&+\frac{h^4}{24}\tilde{y}^{(4)}(x_{i-1})\left(1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^4+O(1/z)\right)+O\left(h^5\right).\end{aligned}$$

Now we have for $k\leqslant 4$, $1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^k=(1-2u^TA^{-1}e)(1-b^TA^{-1}c^k)-2k(k-1)u^Tc-2\binom{k}{4}u^TA^{-1}c^4$. By (10) and (11), $1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^3=0$ while $1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^4=-2u^TA^{-1}c^4=\frac{1}{36}$. Since $\tilde{b}^T\tilde{A}^{-2}(\tilde{c}^3-3\tilde{A}\tilde{c}^2)=\frac{1}{6}$, the leading error term in $\tilde{\psi}_i(z)$ is $O(h^4)$ and is independent of stiffness, provided that $|\lambda|\sim O(1/h^2)$. Moreover, since $\tilde{R}(z)=O(1/z^2)$ as $z\to\infty$, the contributions to the global error at step n due to the local errors at all steps except the last are dampened by the stability function. The global error at step n is therefore essentially determined by the local error at step n and is $O(h^4)$, thus suppressing order reduction and restoring the classical order of the basic symmetric method.

In the case of active symmetrization at every alternate step using $\hat{\mathscr{R}}_2=\frac{1}{2}(\mathscr{R}\circ\tilde{\mathscr{R}})$ as given by (20), we have for $k\leqslant 4$,

$$1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^k=\left(1-2u^TA^{-1}e\right)\left(1-\frac{1}{2^k}R(\infty)b^TA^{-1}c^k-\frac{1}{2^k}b^TA^{-1}(e+c)^k\right)-\binom{k}{2}u^Tc-\frac{1}{8}\binom{k}{4}u^TA^{-1}c^4.$$

Again by (10) and (11), $1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^3=0$ while $1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^4=-\frac{1}{8}u^TA^{-1}c^4=\frac{1}{576}$. Taking into account that each step of $\hat{\mathscr{R}}_2$ involves 3/2 times the computations compared with $\hat{\mathscr{R}}_1$, the coefficient of h^4 is smaller by a factor $(\frac{3}{4})^4$. Hence we use $\hat{\mathscr{R}}_2$ for comparison with the passive case.

For $\tilde{\mathscr{G}}_3$ the terms in (24) vanish for k up to 3 and, since $1-\tilde{b}^T\tilde{A}^{-1}\tilde{c}^4=-2u^TA^{-1}c^4$ vanishes for the order-3 symmetrizer but not for the order-5 symmetrizer, we have

$$\tilde{\psi}_i(z)=\begin{cases}O(h^4) & \text{for the symmetrizer of order 5,}\\ O(h^6) & \text{for the symmetrizer of order 3,}\end{cases}\qquad\text{since } |z|=|\lambda|h\sim O(1/h)\text{ as } h\to 0.$$

The global error for $\tilde{\mathscr{G}}_3$, as for $\tilde{\mathscr{G}}_2$, behaves like the local error at the last step.

4.2. Passive symmetrization after $n-1$ steps

In passive symmetrization at step n, the global error becomes

$$\tilde{\epsilon}_n=\tilde{R}(z)\epsilon_{n-1}+\tilde{\psi}_n(z), \tag{25}$$

where $\tilde{R}(z)$ is given by (13) for $\tilde{\mathscr{G}}_2$ and either (16) or (19) for $\tilde{\mathscr{G}}_3$; $\tilde{\psi}_n(z)$ is the local error at step n, and ϵ_{n-1} is the global error of the symmetric solution up to step $n-1$. When $z\to\infty$, $\tilde{R}(z)=O(1/z^2)$ and therefore dampens the global error ϵ_{n-1} so that the global error $\tilde{\epsilon}_n$ behaves essentially like the local error $\tilde{\psi}_n(z)$. Just as in the analysis given in Section 4.1 the local and global errors behave as follows:

$$\tilde{\epsilon}_n\sim\tilde{\psi}_n(z)=\begin{cases}O(h^4) & \text{for } \tilde{\mathscr{G}}_2 \text{ and the order-5 } \tilde{\mathscr{G}}_3,\\ O(h^6) & \text{for the order-3 } \tilde{\mathscr{G}}_3.\end{cases}$$

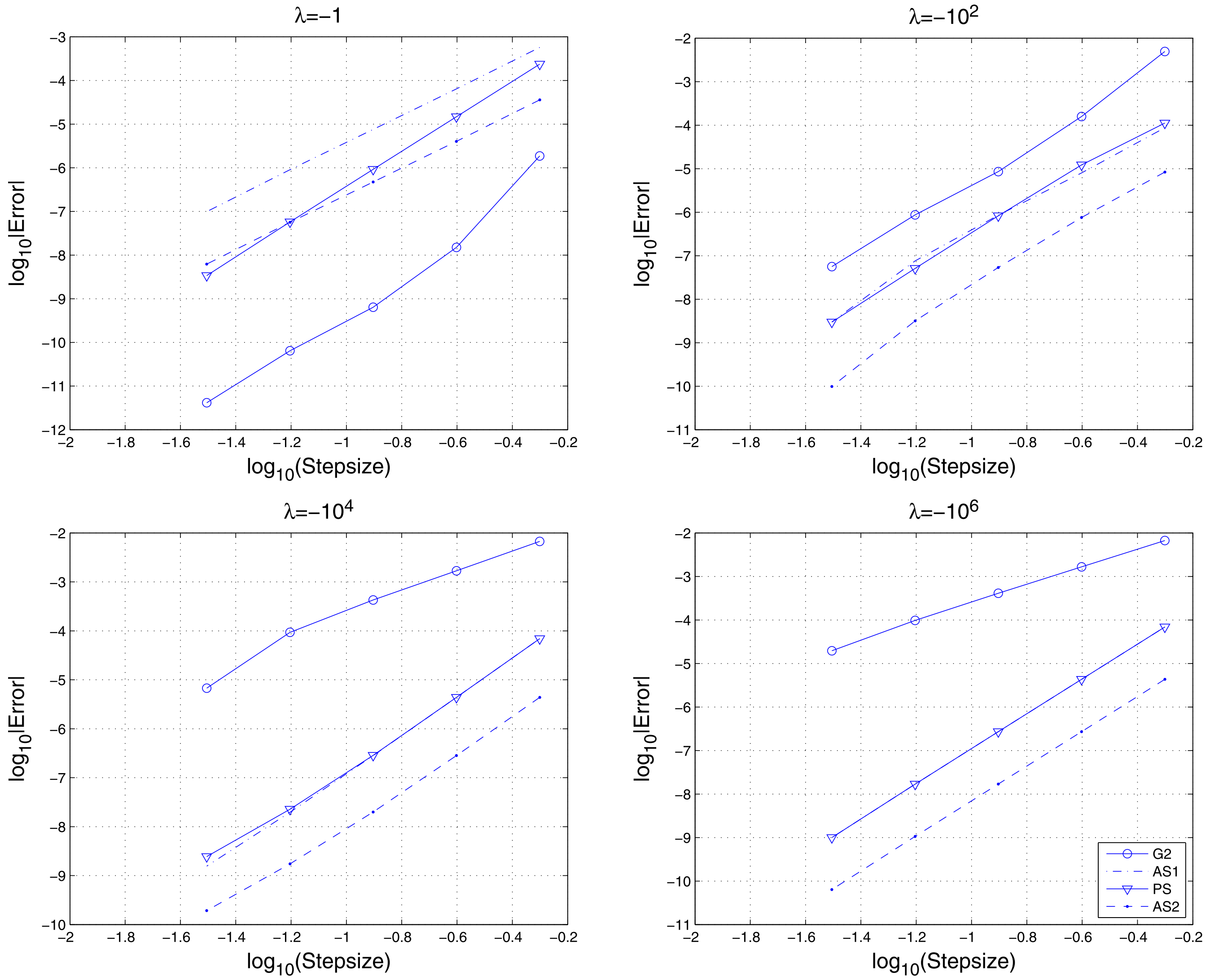


Fig. 3. PR problem for $g(x) = \sin(x)$: Order behavior of $\mathscr{G}_2$ with active and passive symmetrization for different λ values at $X = 5$.

Since damping in both the active and passive modes results in the global error being determined by essentially the local error in the last step and therefore having essentially the same value for stiff linear problems, we investigate whether the situation is similar for stiff nonlinear problems. If both modes are equally efficient we can then conclude that passive symmetrization is to be preferred.

4.3. Numerical results on order behavior

This explains the restoration of the classical order behavior of Gauss methods with symmetrizer in passive and active modes for a very stiff PR problem with $g(x) = \sin(x)$. To confirm these theoretical results, we have performed numerical experiments on the PR test problem. The plots in Fig. 3 show the numerical results for $\mathscr{G}_2$ with active and passive symmetrization for different values of the stiffness parameter λ. When the problem is nonstiff (e.g. $\lambda = -1$), the plots show order-3 behavior for active symmetrization and order-4 behavior for passive symmetrization. This is true of the active case because we are applying (7) with $\tilde{\mathscr{R}} = \tilde{\mathscr{G}}_2$ which is of order 3. In the passive case it is true because we are applying an order-3 symmetrizer locally at the end of the step and the global order will show order-4 behavior. As for the mildly stiff case (e.g. $\lambda = -10^2$ and $\lambda = -10^4$) we observe that $\mathscr{G}_2$ will start to show order reduction from 4 to 2 and will recover its classical order as the stepsize is further reduced. We can also observe that the symmetrizer will start to have an effect here. When the problem is very stiff (e.g. $\lambda = -10^6$), the symmetrizer is more accurate compared to the base method. Another interesting observation is that the active symmetrization using $\hat{\mathscr{R}}_1$ will behave like passive symmetrization and give order-4 behavior (see Section 4.1). Moreover, there seems to be an improvement in accuracy when active symmetrization is applied at every alternate step, $\hat{\mathscr{R}}_2$. The behavior of $\mathscr{G}_3$ for $\lambda = -1$ to $\lambda = -10^6$ is similar to that for $\mathscr{G}_2$. Therefore when applied with extrapolation, the global error of $\tilde{\mathscr{G}}_2$ and $\tilde{\mathscr{G}}_3$ can be expected to behave like $O(h^6)$ and $O(h^8)$ respectively. Since we

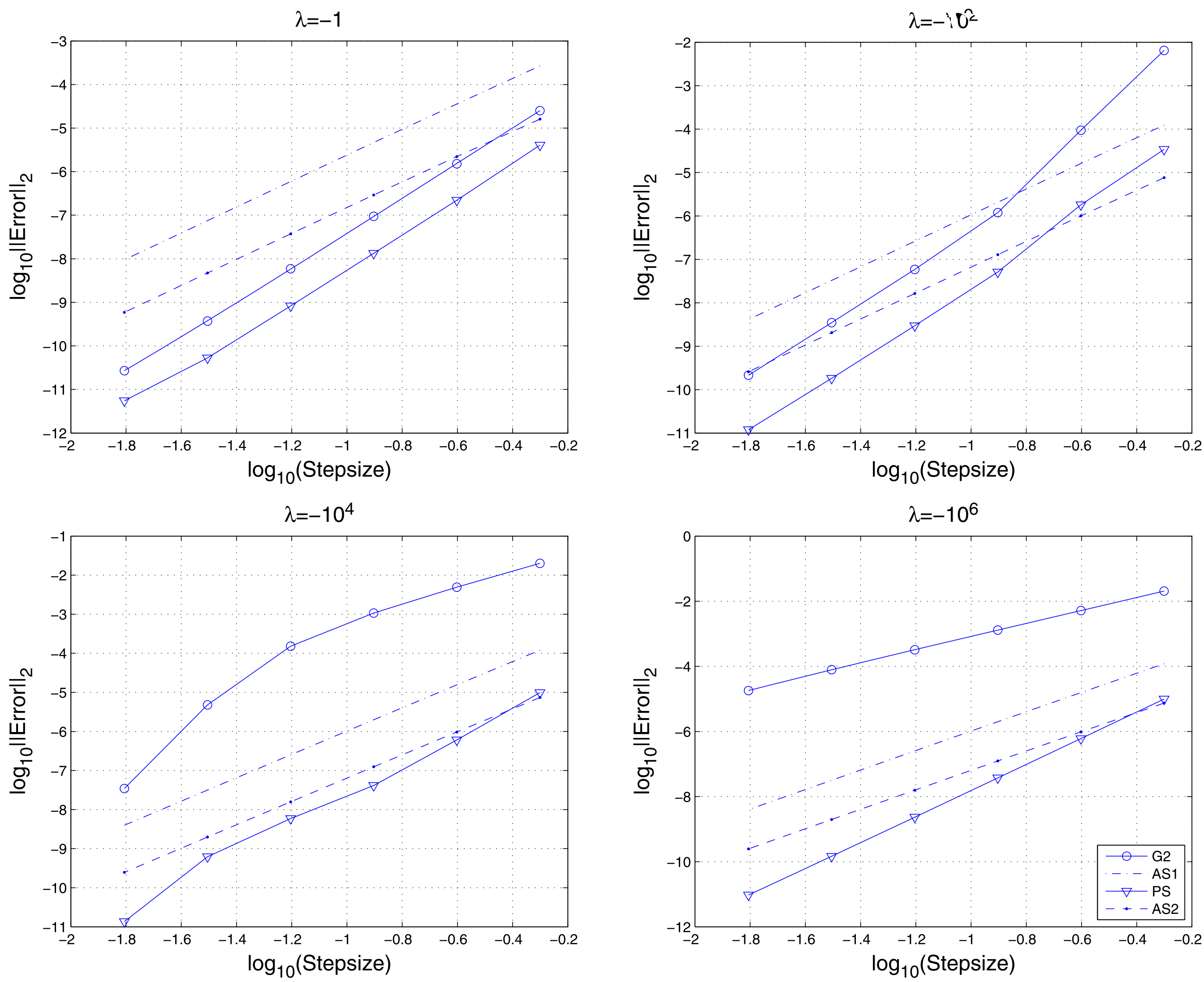


Fig. 4. Kaps problem (Problem 2): Order behavior of $\mathscr{G}_2$ with active and passive symmetrization for different λ values at $X = 3$.

have observed that active symmetrization applied at every alternate step gives smaller error than active symmetrization applied at every step, the following numerical results will only be given for $\hat{\mathscr{R}}_2$ in the active mode.

The order behavior of the methods for nonlinear problems is difficult to analyze theoretically. Nevertheless, it is interesting to determine the behavior of symmetrizers for these problems experimentally. We choose the Kaps problem (26) as a test problem. Numerical results are given in Figs. 4–6. When the problem is nonstiff (e.g. $\lambda = -1$), the order behavior of active as well as passive symmetrization is similar to the PR case for both $\tilde{\mathscr{G}}_2$ and $\tilde{\mathscr{G}}_3$. The irregular behavior of $\tilde{\mathscr{G}}_3$ seen in Figs. 5 and 6 as the stepsize decreases is due to roundoff error. In the mildly stiff case we observe that $\mathscr{G}_2$ and $\mathscr{G}_3$ will exhibit order reduction from 4 to 2 and from 6 to 4 respectively. Meanwhile passive and active symmetrization of $\mathscr{G}_2$ and $\mathscr{G}_3$ show order behavior similar to the PR case. When the problem is stiff (e.g. $\lambda = -10^6$), active symmetrization of $\mathscr{G}_2$ shows order-3 behavior while passive symmetrization still gives order-4 behavior (see Fig. 4). However for $\mathscr{G}_3$, active symmetrization gives order-4 behavior with the order-5 symmetrizer and order-3 behavior with the order-3 symmetrizer (see Fig. 5 and Fig. 6). This is completely different from the PR case where the classical order is restored. On the other hand, passive symmetrization still gives order-4 behavior with both the order-3 and the order-5 symmetrizer. We note that similar order behavior was observed for the Oregonator problem given in [11] for short intervals using constant stepsize. The summary of the order behavior for the linear and nonlinear Kaps problem is given in Table 2.

5. Further numerical examples and efficiency considerations

We now present the results of numerical experiments for $\mathscr{G}_2$ and $\mathscr{G}_3$ with active and passive symmetrization/extrapolation on linear and nonlinear problems. The main aim in this paper is to investigate the performance of active and passive symmetrization. In our experiments we carry out extrapolation with stepsizes h and $h/2$. For constant stepsize we perform passive extrapolation where the extrapolated values are not propagated. This is because we have found this mode to be more efficient than the active mode in which the extrapolated values are propagated. However, the opposite is the case in

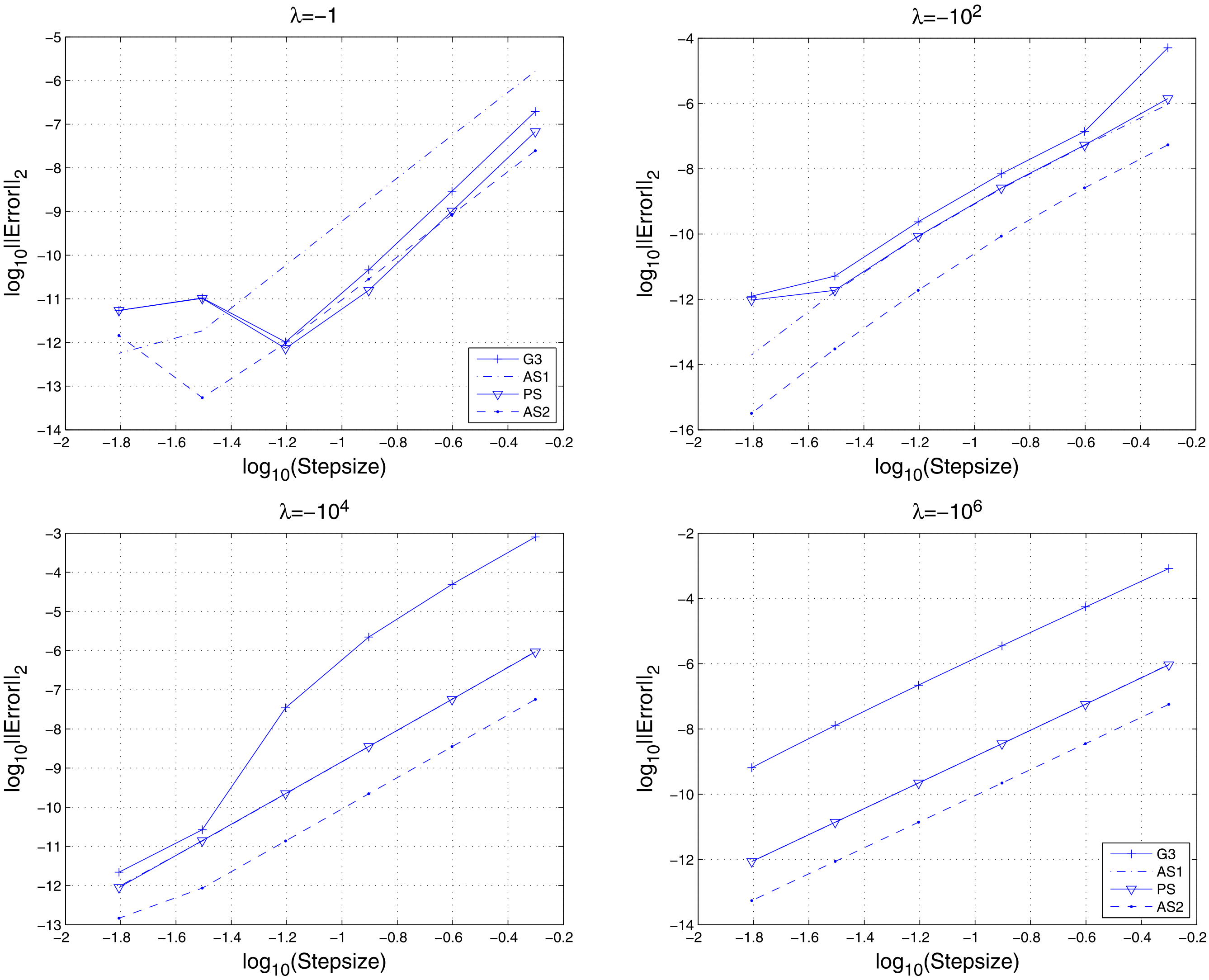


Fig. 5. Kaps (Problem 2): Order behavior of $\mathcal{G}_3$ with active and passive symmetrization for different λ values at $X = 3$ using order-5 symmetrizer.

Table 2
Summary of order for $\mathcal{G}_2$ and $\mathcal{G}_3$ with passive ($\tilde{p}$) and active ($\hat{p}$) symmetrization for linear scalar problems and nonlinear Kaps problem.

		Nonstiff case, $\lambda = -10$			Stiff case, $\lambda = -10^6$		
		p	$\tilde{p}$	$\hat{p}$	p	$\tilde{p}$	$\hat{p}$
Linear scalar problems							
$\mathcal{G}_2$		4	4	3	2	4	4
$\mathcal{G}_3$	Eq. (15)	6	6	5	4	4	4
	Eq. (18)	6	4	3	4	6	6
Nonlinear Kaps problem							
$\mathcal{G}_2$		4	4	3	2	4	3
$\mathcal{G}_3$	Eq. (15)	6	6	5	4	4	4
	Eq. (18)	6	4	3	4	4	3

the variable stepsize setting and we therefore present results for active extrapolation. We leave the detailed study of active and passive extrapolation to another paper.

Since analysis of the PR problem suggests improvement in the accuracy of symmetric methods when applied with symmetrization, the interest is in the efficiency of the two modes for more general problems. In our experiments, passive and active symmetrization applied with extrapolation are performed separately. Efficiency is measured using CPU time. We have also computed efficiencies using the number of function evaluations and found similar results. Hence all our numerical results are presented using CPU time. We have implemented compensated summation in our computations to minimize roundoff error. All the nonlinear equations are solved using simplified Newton as in [11] on page 119. The experiments are for six problems. We use constant stepsize for Problems 1–2 and variable stepsize for Problems 3–5 with the standard

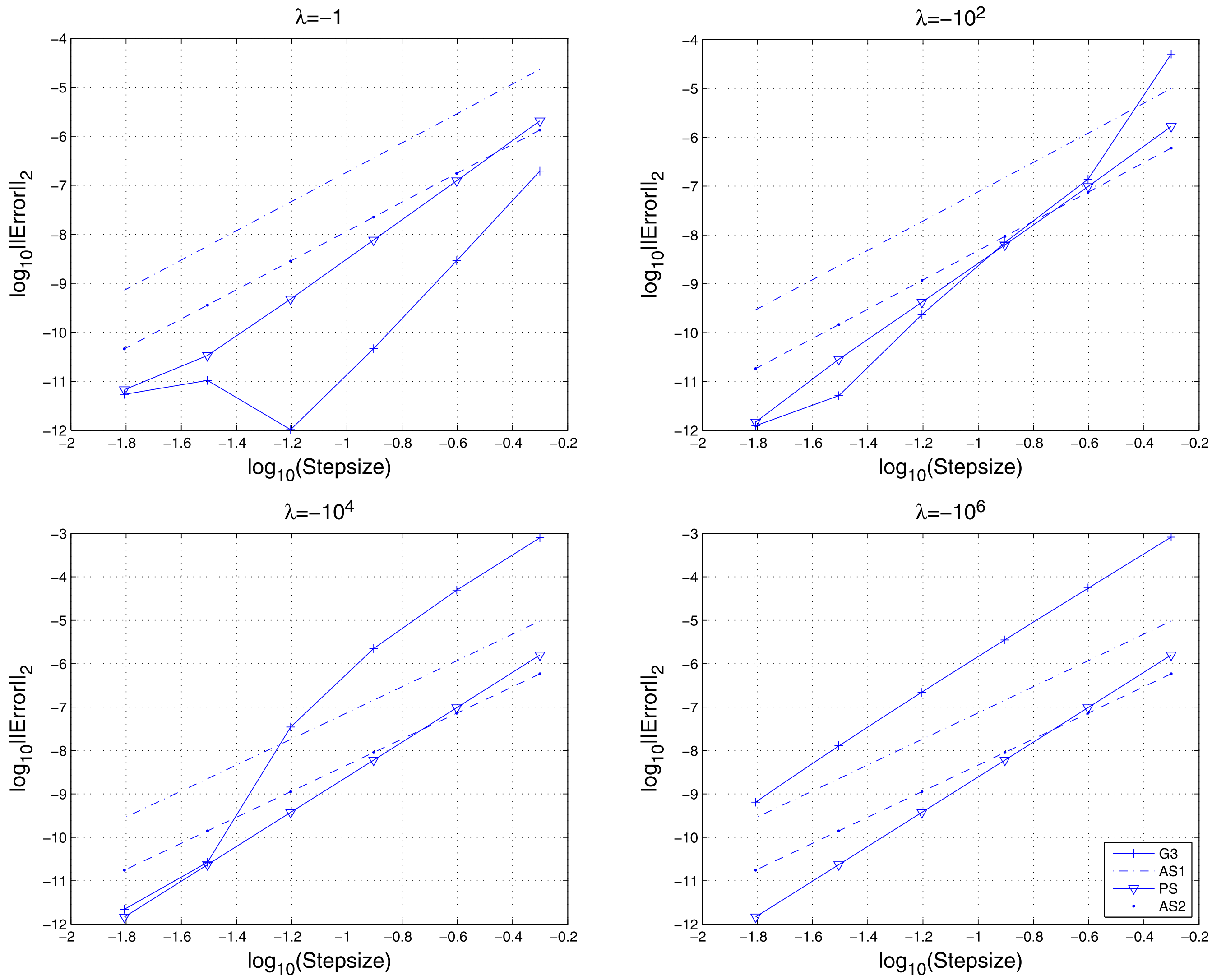


Fig. 6. Kaps (Problem 2): Order behavior of $\mathscr{G}_3$ with active and passive symmetrization for different λ at $X = 3$ using order-3 symmetrizer.

Table 3
Notation for numerical experiments.

G_s	$s = 2, 3$, s-stage Gauss method
PS	Passive symmetrization
ASj	Active symmetrization with $j = 1$ at every step and $j = 2$ at every alternate step
	A last X attached to PS or ASj means with extrapolation

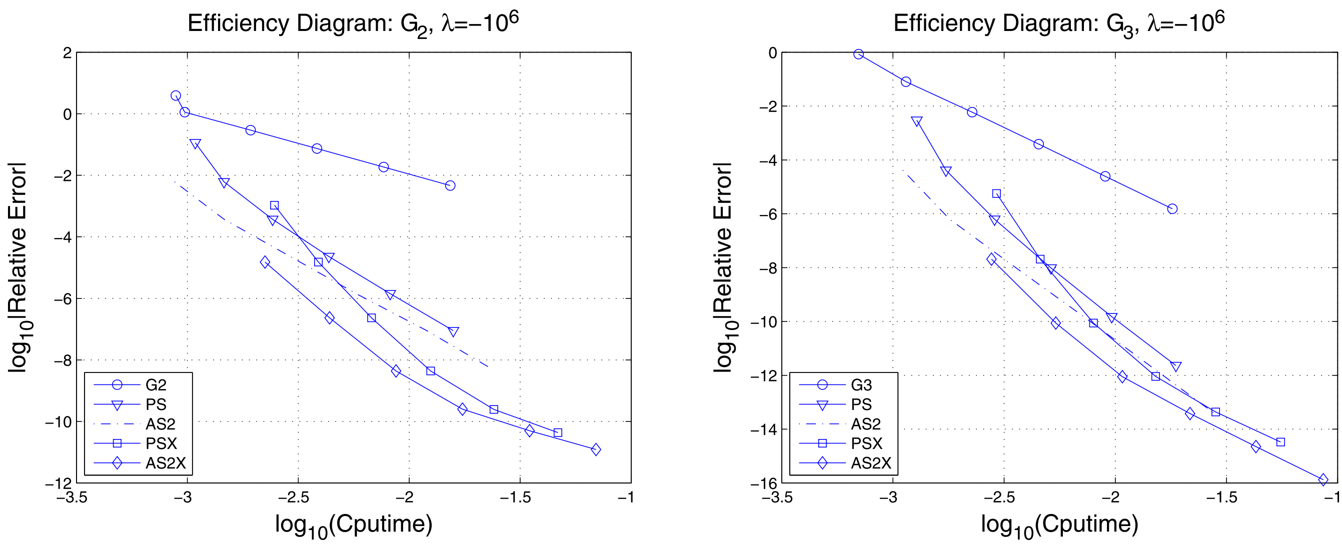
stepsize control as given in [11]. In the variable stepsize setting the local errors are estimated using the difference between the approximations for the base method and the symmetrizer. These three problems are solved with the tolerances $tol = 10^{-i}, i = 5, \dots, 12$. The notation we use in all the numerical experiments is given in Table 3.

Problem 1.

$$y' = \lambda y + e^{-x}, \qquad y(0) = -\frac{1}{1+\lambda}, \qquad \lambda \in (-\infty, -2], \qquad y(x) = -\frac{1}{1+\lambda} e^{-x}.$$

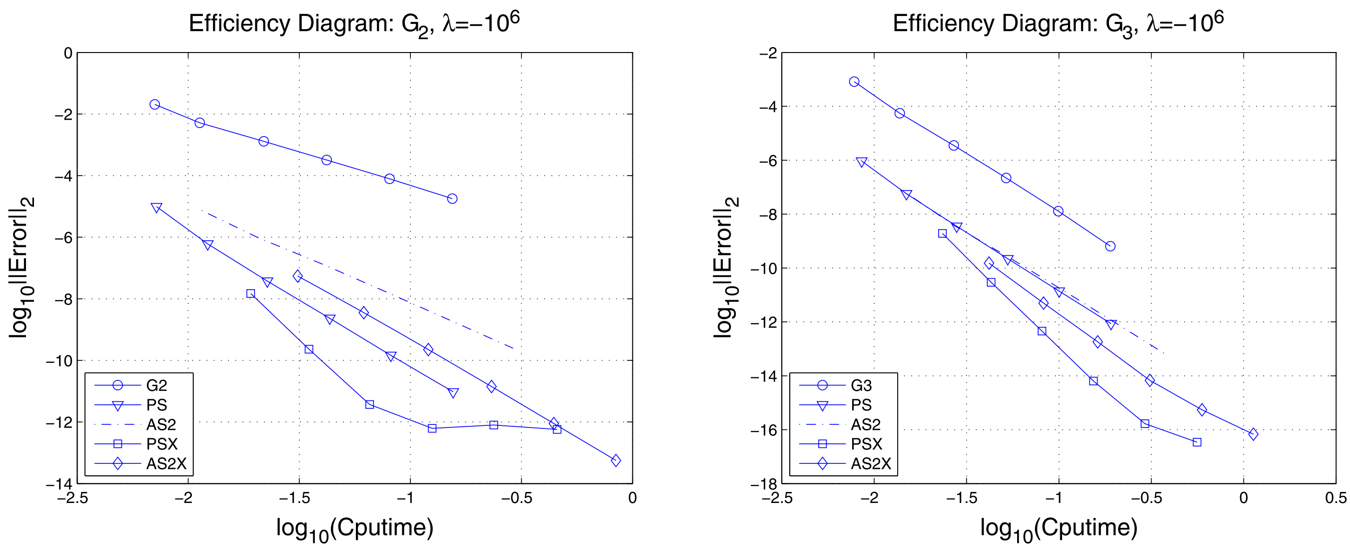
We integrated to $X = 3$ with stepsize $h = 3$ and $\lambda = -10^6$.

Problem 1 is a linear problem given in [9]. Fig. 7 shows the efficiency diagram for $\mathscr{G}_2$ and $\mathscr{G}_3$ with passive and active symmetrization/extrapolation for the very stiff case (that is, $\lambda = -10^6$). We observe that with both methods, the symmetrizer restores the classical order behavior and therefore allows extrapolation to improve accuracy. Moreover, although active symmetrization requires more computational time, it seems to be slightly more efficient than passive symmetrization. We have performed tests with the λ values, $\lambda = -1$, $\lambda = -10^2$ and $\lambda = -10^4$ and the observation is similar to that for the Prothero–Robinson test problem given in Fig. 3.



(a) $\mathcal{G}_2$ (b) $\mathcal{G}_3$

Fig. 7. Problem 1: The efficiency diagram of $\mathcal{G}_2$ and $\mathcal{G}_3$ with passive and active symmetrization and extrapolation for $\lambda = -10^6$ and $h = 3$ at $X = 3$.



(a) $\mathcal{G}_2$ (b) $\mathcal{G}_3$

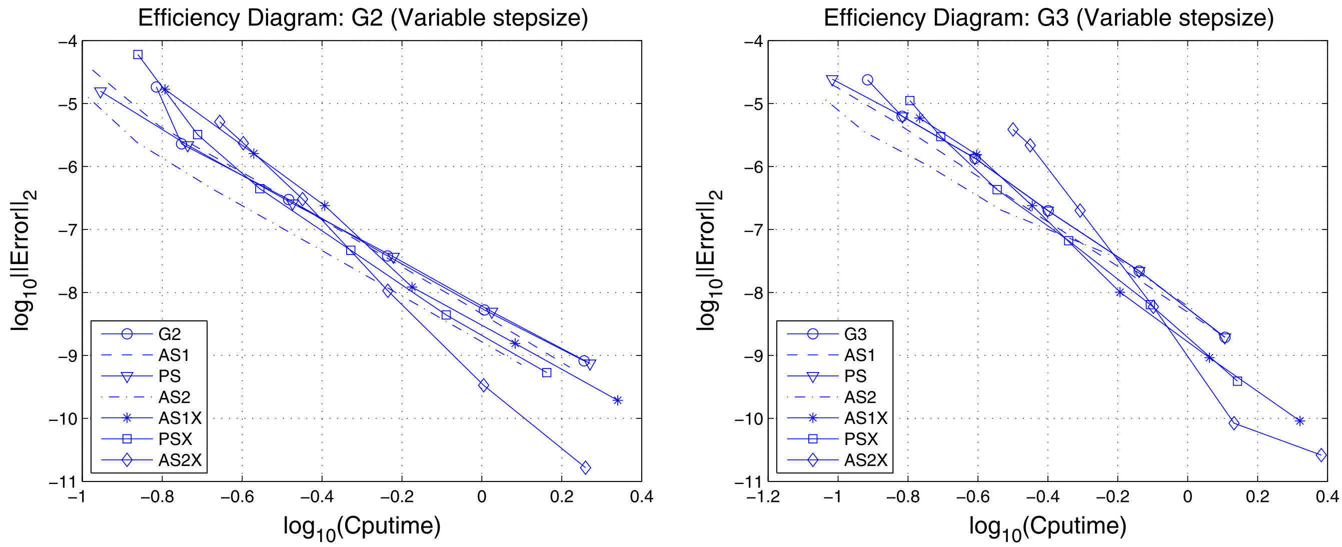
Fig. 8. Problem 2 (Kaps): The efficiency diagram of $\mathcal{G}_2$ and $\mathcal{G}_3$ with passive and active symmetrization and extrapolation for $\lambda = -10^6$ and $h = 1$ at $X = 3$. We use the order-5 symmetrizer for $\mathcal{G}_3$.

Problem 2 *(Kaps).*

$$\begin{aligned} y_1' &= (\lambda - 2)y_1 - \lambda y_2^2, \quad y_1(0) = 1, \\ y_2' &= y_1 - y_2(1 + y_2), \quad y_2(0) = 1, \end{aligned} \tag{26}$$

with $y_1(x) = e^{-2x}$ and $y_2(x) = e^{-x}$. We integrated to $X = 3$ with stepsize $h = 1$ and $\lambda = -10^6$.

Problem 2 is a well-known two-dimensional nonlinear problem. Fig. 8 shows the efficiency diagram for $\mathcal{G}_2$ and $\mathcal{G}_3$. For this value of the stiffness parameter (i.e. $\lambda = -10^6$), we observe that passive symmetrization of $\mathcal{G}_2$ is more efficient than active symmetrization because the global error in the passive case behaves like $O(h^4)$ in contrast to the $O(h^3)$ behavior in the active case (refer Fig. 8(a)). Therefore with extrapolation the global error for passive symmetrization behaves like $O(h^6)$. On the other hand, neither passive nor active symmetrization improves the order behavior of $\mathcal{G}_3$ (see Fig. 5). However, in Fig. 8(b) we see that the global error of $\mathcal{G}_3$ with symmetrization is much smaller than without. In addition, extrapolation gives order-6 behavior and greater accuracy in both cases. Symmetrization in the active mode is more efficient than in the passive mode for $\mathcal{G}_3$, an effect opposite to that for $\mathcal{G}_2$.



(a) $\mathscr{G}_2$ (b) $\mathscr{G}_3$

Fig. 9. Problem 3 (HIRES): The efficiency diagram of $\mathscr{G}_2$ and $\mathscr{G}_3$ with passive and active symmetrization and extrapolation using initial stepsize $h = 0.01$ at $X = 321.8122$. We use the order-5 symmetrizer for $\mathscr{G}_3$.

Problem 3 *(HIRES).* HIRES or 'High Irradiance RESponse' is a nonlinear system of 8 dimensions. It is an example of a mildly stiff problem. The mathematical model is given in Hairer and Wanner [11]. The initial value is given by $y_0 = [1, 0, 0, 0, 0, 0, 0, 0.0057]^T$. We integrated to $X = 321.8122$ using the initial stepsize $h = 0.01$. Since this is a problem of dimension 8, it is hard to obtain the exact solution. The reference solution is obtained by RADAU5 using a very small tolerance [14]:

$$\begin{aligned}
y_1' &= -1.71y_1 + 0.43y_2 + 8.32y_3 + 0.0007, \\
y_2' &= 1.71y_1 - 8.75y_2, \\
y_3' &= -10.03y_3 + 0.43y_4 + 0.035y_5, \\
y_4' &= 8.32y_2 + 1.71y_3 - 1.12y_4, \\
y_5' &= -1.745y_5 + 0.43y_6 + 0.43y_7, \\
y_6' &= -280y_6y_8 + 0.69y_4 + 1.71y_5 - 0.43y_6 + 0.69y_7, \\
y_7' &= 280y_6y_8 - 1.81y_7, \\
y_8' &= -y_7'.
\end{aligned}$$

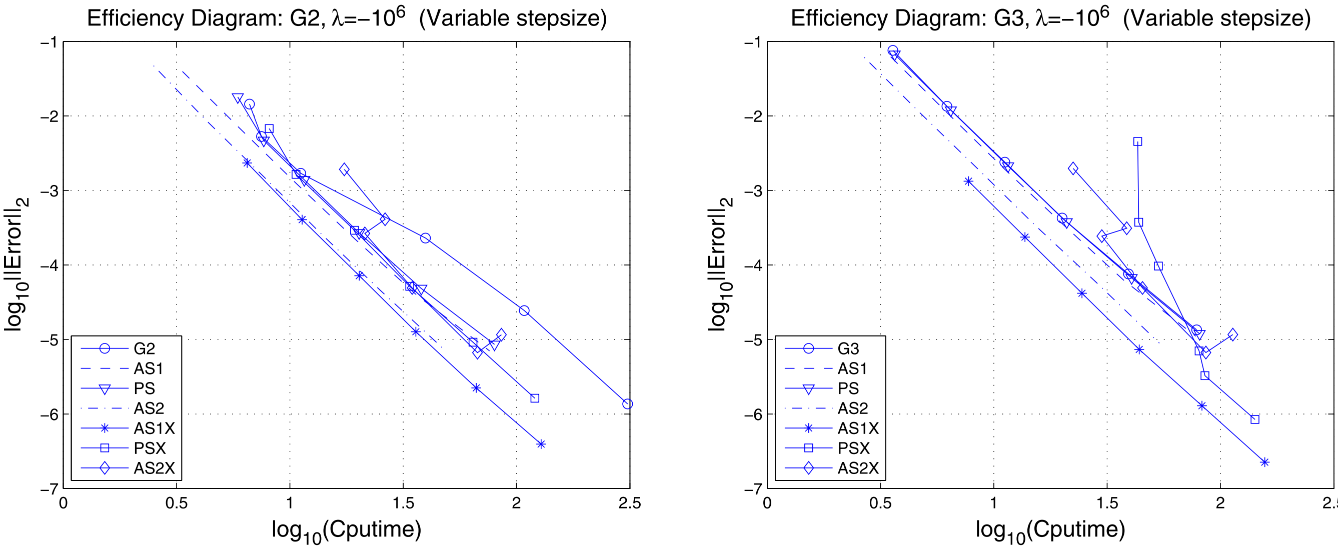
The numerical results for Problem 3 are given in Fig. 9 using variable stepsize control. For this mildly stiff problem we observed that symmetrization of $\mathscr{G}_2$ is slightly more efficient in the active than in the passive mode. Furthermore, active symmetrization with extrapolation is also observed to give greater accuracy than passive symmetrization with extrapolation. In the constant stepsize setting we found that symmetrization at every alternate step (AS2) is more efficient than at every step (AS1) over many test problems. Referring to Fig. 9 we observe that AS2 still gives greater accuracy than AS1 when variable stepsize is used for this problem. In general it is still uncertain which of the active symmetrization is more efficient in the variable stepsize setting. Similar results are obtained for $\mathscr{G}_3$.

Problem 4.

$$\begin{aligned}
y_1' &= -y_2 - \lambda y_1(1 - y_1^2 - y_2^2), \quad y_1(0) = 1, \\
y_2' &= y_1 - \rho\lambda y_2(1 - y_1^2 - y_2^2), \quad y_2(0) = 0,
\end{aligned}$$

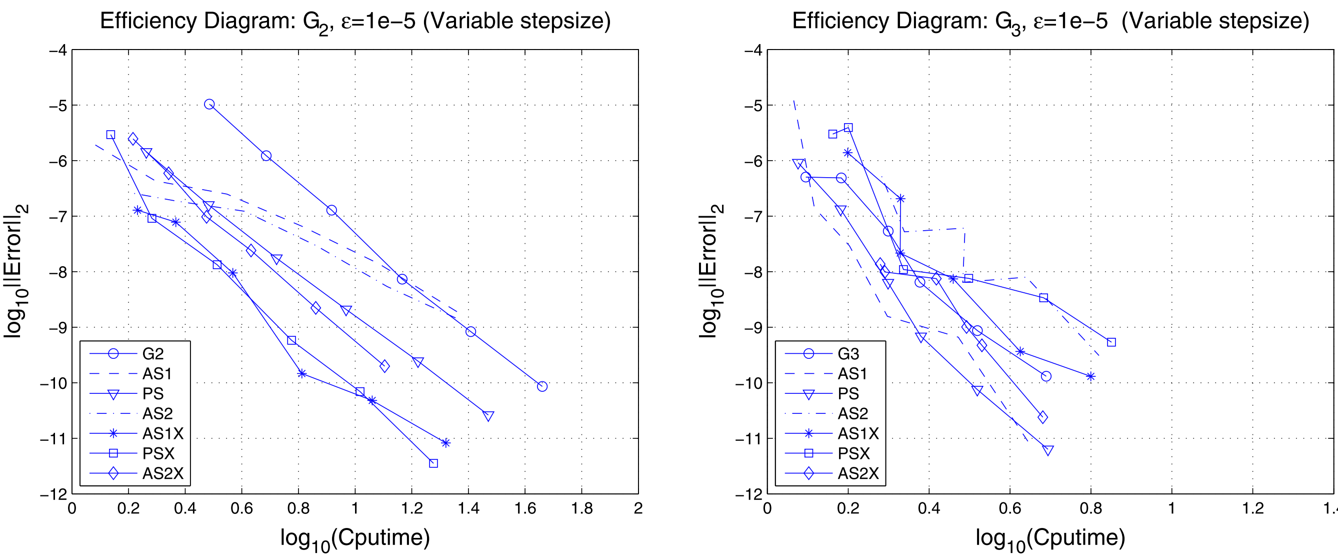
with $\rho = 1$. We integrated to $X = 7$ with $h = 0.005$ and $\lambda = -10^6$.

Problem 4 has a smooth invariant manifold and the solution lies on the unit circle. Numerical results are presented in Fig. 10. We observe that $\mathscr{G}_2$ is more efficient when applied with symmetrization in either mode. Moreover, in this problem we observe that the extrapolation AS1X is more efficient than AS2X and PSX. Similar results are seen for $\mathscr{G}_3$.



(a) $\mathscr{G}_2$ (b) $\mathscr{G}_3$

Fig. 10. roblem 4: The efficiency diagram of $\mathscr{G}_2$ and $\mathscr{G}_3$ with passive and active symmetrization and extrapolation using initial stepsize $h = 0.005$ at $X = 7$. We use the order-5 symmetrizer for $\mathscr{G}_3$.



(a) $\mathscr{G}_2$ (b) $\mathscr{G}_3$

Fig. 11. Problem 5: The efficiency diagram of $\mathscr{G}_2$ and $\mathscr{G}_3$ with passive and active symmetrization and extrapolation using initial stepsize $h = 0.001$ at $X = 2$. We use the order-5 symmetrizer for $\mathscr{G}_3$.

Problem 5 *(Van der Pol).* Van der Pol is a system of ODEs of dimension 2 that describes the behavior of nonlinear circuits [11]. The parameter ϵ is a stiffness parameter. The problem becomes more stiff by decreasing the value of ϵ.

$$y_1' = y_2, \qquad y_1(0) = 2,$$
$$y_2' = \frac{1}{\epsilon}\big((1 - y_1^2)y_2 - y_1\big), \qquad y_2(0) = 0.$$

We integrated to $X = 2$ with $h = 0.001$ and $\epsilon = 10^{-5}$.

The numerical results for Problem 5 is given in Fig. 11. For $\mathscr{G}_2$ we observed that passive symmetrization is more efficient than the active symmetrization. However, with extrapolation both passive and active symmetrization are equally efficient. Another observation is that AS1X is more efficient than AS2X. This is contrary to the constant stepsize setting and the results observed in Problem 3. On the other hand, for $\mathscr{G}_3$ we observed that passive symmetrization is more advantageous than active symmetrization. However, it is hard to observe the efficiency of symmetrization with extrapolation and it can be due to the roundoff error. Nevertheless, symmetrization performed better than the base methods.

6. Conclusion

In this paper our experimental results show that a Gauss method is more accurate and efficient when applied with a symmetrizer in either mode. The results also show that symmetrization can restore the classical order in solving stiff linear scalar problems and that extrapolation improves both accuracy and efficiency. Symmetrization in the passive mode seems to be marginally more efficient than in the active mode for this type of problem. The feasibility of basing an extrapolation method on higher order symmetric Runge–Kutta methods with symmetrizers appears promising at least for linear problems using fixed stepsize.

In the case of nonlinear problems our experiments on fixed stepsize show that passive symmetrization/extrapolation is more efficient than active symmetrization/extrapolation. On the other hand, in a variable stepsize setting, extrapolation of active symmetrization is more efficient than that of passive symmetrization. In our variable stepsize experiments, the code used is preliminary since some important features such as error estimation, stepsize control and starting values have yet to be refined.

A drawback of symmetrization is the need to compute beyond the current step. If computation cannot proceed beyond the endpoint then the symmetrized value there has to be estimated by some other means. For example, if the symmetrized values $\hat{y}_{n-i}$ for $i = 1, \ldots, 5$ have been computed, then using the interpolating polynomial,

$$p(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4,$$

where the coefficients are determined by $p(ih) = \hat{y}_{n-i}$, we can estimate the symmetrized value at x_n without additional cost by

$$\hat{y}_{est} = a_0 = 5\hat{y}_{n-1} - 10\hat{y}_{n-2} + 10\hat{y}_{n-3} - 5\hat{y}_{n-4} + \hat{y}_{n-5}.$$

If additional symmetrized values are computed in the last step $x_{n-1} \to x_{n-1} + h$ using stepsize $h/5$ at $x_{n-i/5} = x_{n-1} + \frac{1}{5}(5 - i)h$, $i = 1, \ldots, 4$, then a better estimate can be obtained by

$$\hat{y}_{est} = 5\hat{y}_{n-1/5} - 10\hat{y}_{n-2/5} + 10\hat{y}_{n-3/5} - 5\hat{y}_{n-4/5} + \hat{y}_{n-1}.$$

In the future we hope to report on a study of symmetrization and extrapolation in a wider context with a more practical code.

Acknowledgement

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