Numerical solution of stiff ODEs using second derivative general linear methods

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Contents

Why GLMs?

Traditional numerical methods for solving an initial value problem generally fall into two main classes: **linear multistep** (multivalue) and **Runge–Kutta** (multistage) methods.

In 1966, Butcher introduced **General Linear Methods** (GLMs) as a unifying framework for the traditional methods to study the properties of consistency, stability and convergence, and to formulate new methods with clear advantages over these classes.

Representation of GLMs

We recall general linear methods (GLMs) for the numerical solution of an autonomous system of ordinary differential equations

$$y' = f(y(x)), \quad x \in [x_0, \overline{x}], \quad y : [x_0, \overline{x}] \to \mathbb{R}^m, \quad f : \mathbb{R}^m \to \mathbb{R}^m, \tag{1}$$

where m is dimension of the system.

GLMs for ODEs can be characterized by four integers:

p the order of method; **q** the stage order;

r the number of external stages; **s** the number of internal stages.

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p the order of method; **q** the stage order;
r the number of external stages; **s** the number of internal stages.

Representation of GLMs

If h be stepsize, then the representation of GLMs takes the form

$$\begin{aligned} Y^{[n]} &= h(A \otimes I_m) f(Y^{[n]}) + (U \otimes I_m) y^{[n-1]}, \\ y^{[n]} &= h(B \otimes I_m) f(Y^{[n]}) + (V \otimes I_m) y^{[n-1]}. \end{aligned} \tag{2}$$

Here, $Y^{[n]} = [Y_i^{[n]}]_{i=1}^s$ is an approximation of stage order q to the vector

$$y(x_n + ch) = [y(x_n + c_i h)]_{i=1}^s,$$

and $f(Y^{[n])}) = [f(Y_i^{[n]})]_{i=1}^s$.

If $r = p + 1$, $y^{[n]} = [y_i^{[n]}]_{i=1}^r$ is an approximation of order p to the Nordsieck vector $y(x_n, h) = [h^{i-1} y^{(i-1)}(x_n)]_{i=1}^r$.

Why SGLMs?

One of the main directions to construct methods with higher order and extensive stability region, is the using higher derivatives of the solutions.

Although the mentioned GLMs include linear multistep methods, Runge–Kutta and many other standard methods, but for the above reasons, it thought that it could be extended to the case in which second derivatives of solution, as well as first derivatives, can be calculated. These methods were introduced by Butcher and Hojjati.

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Representation of SGLMs

A Second derivative General Linear Method (SGLM) is characterized by six matrices denoted by $A, \overline{A} \in \mathbb{R}^{s\times s}$, $U \in \mathbb{R}^{s\times r}$, $B, \overline{B} \in \mathbb{R}^{r\times s}$ and $V \in \mathbb{R}^{r\times r}$.

By denoting the second derivative stage value of step number n by $g(Y^{[n]}) = [g(Y_i^{[n]})]_{i=1}^{s}$, where $g(\cdot) = f'(\cdot)f(\cdot)$ and using of previous notations, the representation of SGLMs takes the form

$$\begin{aligned} Y^{[n]} &= h(A\otimes I_m)f(Y^{[n]}) + h^2(\overline{A}\otimes I_m)g(Y^{[n]}) + (U\otimes I_m)y^{[n-1]}, \\ y^{[n]} &= h(B\otimes I_m)f(Y^{[n]}) + h^2(\overline{B}\otimes I_m)g(Y^{[n]}) + (V\otimes I_m)y^{[n-1]}. \end{aligned} \tag{3}$$

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Representation of SGLMs

It is convenient to write coefficients of the method, that is elements of A, $\overline{A}$, U, B, $\overline{B}$ and V as a partitioned $(s+r)\times(2s+r)$ matrix

$$\left[\begin{array}{c|c|c} A & \overline{A} & U \\ \hline B & \overline{B} & V \end{array}\right].$$

Consistency and Stability

Definition 1:
An SGLM $(A, \overline{A}, U, B, \overline{B}, V)$ is 'pre-consistent' if V has an eigenvalue equal to 1 and u be a corresponding eigenvector and also $Uu = \mathrm{e}$.

Definition 2:
An SGLM $(A, \overline{A}, U, B, \overline{B}, V)$ is 'consistent' if it is pre-consistent with pre-consistency vector u and there exists a vector v (consistency vector) such that $B\mathrm{e} + Vv = u + v$.

Definition 3:
An SGLM $(A, \overline{A}, U, B, \overline{B}, V)$ is 'stable' if there exists a constant k such that

$$\|V^n\| \leq k, \qquad \text{for all } n = 1, 2, \cdots .$$

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Convergence

Theorem 1:
If the SGLM $(A, \overline{A}, U, B, \overline{B}, V)$ *is convergent, then it is stable.*

Theorem 2:
Let $(A, \overline{A}, U, B, \overline{B}, V)$ *denote a convergent SGLM which is, moreover, covariant with pre-consistency vector* u*. Then it is consistent.*

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Order conditions

To obtain order conditions, we assume that

$$y_i^{[n-1]} = \sum_{k=0}^{p} h^k \alpha_{ik} y^{(k)}(x_{n-1}) + O(h^{p+1}), \qquad i = 1, 2, \cdots, r.$$

The values α_{ik} must be chosen so that

$$Y_i^{[n]} = \sum_{k=0}^{p} \frac{c_i^k}{k!} h^k y^{(k)}(x_{n-1}) + O(h^{q+1}), \qquad i = 1, 2, \cdots, s,$$

and

$$y_i^{[n]} = \sum_{k=0}^{p} h^k \alpha_{ik} y^{(k)}(x_n) + O(h^{p+1}), \qquad i = 1, 2, \cdots, r,$$

for the same numbers α_{ik}.

Order Conditions

Theorem 4: *An SGLM has order p and stage order $q = p$ iff*

$$e^{cz} = zAe^{cz} + z^2\overline{A}e^{cz} + Uw + O(z^{p+1}), \qquad (4)$$

$$e^{z}w = zBe^{cz} + z^2\overline{B}e^{cz} + Vw + O(z^{p+1}). \qquad (5)$$

where the exp *function is applied component-wise to a vector and $w = w(z)$ is a vector with elements given by*

$$w_i = \sum_{k=0}^{p} \alpha_{ik} z^k, \qquad i = 1, 2, \cdots, r.$$

Let us to denote $\alpha_k = [\alpha_{1k} \;\; \alpha_{2k} \;\; \cdots \;\; \alpha_{rk}]^T$ for $k = 0, 1, \cdots, p$.

Corollary: *For the case of $U = I_s$ in an SGLM with $p = q$, the vectors α_k have the form*

$$\alpha_0 = \mathrm{e}, \;\; \alpha_1 = c - A\mathrm{e}, \;\; \alpha_k = \frac{c^k}{k!} - \frac{Ac^{k-1}}{(k-1)!} - \frac{\overline{A}c^{k-2}}{(k-2)!}, \quad k = 2, 3, \ldots, p,$$

where $\mathrm{e} = [1, 1, \ldots, 1]^T \in \mathbb{R}^s$.

Stability matrix and RKS property

The stability matrix of SGLMs is obtained by applying these methods to the standard test problem of Dahlquist $y' = qy$, where q is a (possibly complex) number, which it is

$$M(z) = V + \left(zB + z^2\overline{B}\right)\left(I - zA - z^2\overline{A}\right)^{-1}U.$$

Definition 5: If the characteristic polynomial of $M(z)$, known as the stability function, has the special form

$$p(w, z) = det\left(wI - M(z)\right) = w^{r-1}\left(w - R(z)\right),$$

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Types of SGLMs

We divide SGLMs into four types, depending on the nature of the differential system to be solved and the computer architecture that is used to implement these methods.

- For type 1 or 2 methods, matrices A and $\overline{A}$ have the form

$$A = \begin{bmatrix} \lambda & & & \\ a_{21} & \lambda & & \\ \vdots & \vdots & \ddots & \\ a_{s1} & a_{s2} & \cdots & \lambda \end{bmatrix}, \quad \overline{A} = \begin{bmatrix} \mu & & & \\ \overline{a}_{21} & \mu & & \\ \vdots & \vdots & \ddots & \\ \overline{a}_{s1} & \overline{a}_{s2} & \cdots & \mu \end{bmatrix},$$

  where $\lambda = \mu = 0$ or $\lambda > 0$, $\mu < 0$, respectively.
- For type 3 or 4 methods, $A = \lambda I$ and $\overline{A} = \mu I$, where $\lambda = \mu = 0$ or $\lambda > 0$, $\mu < 0$, respectively.

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Types of SGLMs (cont'd)

An obvious extension to the idea of type 4 methods is to allow the matrices A and $\overline{A}$ to be

$$A = \operatorname{diag}\left\{\underbrace{\lambda_1, \cdots, \lambda_1}_{k_1\ times}, \underbrace{\lambda_2, \cdots, \lambda_2}_{k_2\ times}, \cdots, \underbrace{\lambda_d, \cdots, \lambda_d}_{k_d\ times}\right\},$$

$$\overline{A} = \operatorname{diag}\left\{\underbrace{\mu_1, \cdots, \mu_1}_{k_1\ times}, \underbrace{\mu_2, \cdots, \mu_2}_{k_2\ times}, \cdots, \underbrace{\mu_d, \cdots, \mu_d}_{k_d\ times}\right\},$$

(generalized type 4) where $\sum_{i=1}^{d} k_i = s$ and $\lambda_i \neq \lambda_j$, $\mu_i \neq \mu_j$ for $i \neq j$.

Order barriers

- Let p be the order of an SGLM of type 2 with RKS property. Then

$$p \leq \begin{cases} 2s+2, & \text{if} \quad \mu < -\frac{\lambda^2}{4}, \\ 2s+1, & \text{if} \quad \mu \geq -\frac{\lambda^2}{4}, \end{cases}$$

where s is the number of internal stages.

- The orders of types 3 and 4 SGLMs with RKS property cannot exceed two and four respectively.

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Order barriers (cont'd)

- Let p be the order of a SGLM of generalized type 4 with RKS property. Then

$$p \leq \begin{cases} 4d & \forall j = 1, 2, \cdots, d: \quad \mu_j < -\frac{\lambda_j^2}{4}, \\ 4d - 2\ell + 1 & \forall i = 1, 2, \cdots, \ell,\ s.t.\ j_i \in \{1, \cdots, d\}: \quad \mu_{j_i} \geq -\frac{\lambda_{j_i}^2}{4}, \end{cases}$$

where $\ell \leq d$ and $j_{i_1} \neq j_{i_2}$ for $i_1 \neq i_2$.

Methods with $r = s = 1$

$$
\begin{aligned}
Y^{[n]} &= h\lambda f(Y^{[n]}) + h^2\big(\tfrac{1}{6} - \tfrac{1}{2}\lambda\big) g(Y^{[n]}) + y^{[n-1]}, \\
y^{[n]} &= hf(Y^{[n]}) + h^2\big(\tfrac{1}{2} - \lambda\big) g(Y^{[n]}) + y^{[n-1]},
\end{aligned}
\tag{6}
$$

where

$$Y^{[n]} = y(x_{n-1} + c_1 h) + O(h^4),$$

with c_1 as a free parameter.

This method is A-stable of maximal order $p = q = 3$, if $\lambda \geq \frac{\sqrt{3}+1}{\sqrt{3}}$.

Methods with $r = s = 2$

Pairs of (λ, μ) values in domain $[0, 2] \times [-1, 0]$ giving A-stability are shown in the following Figure.

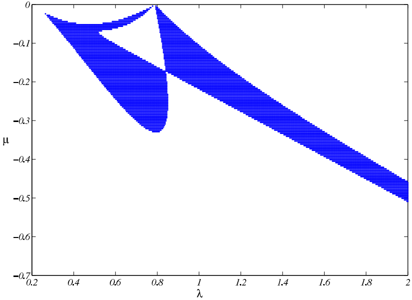

Figure: A-stable choices of (λ, μ) in domain $[0, 2] \times [-1, 0]$ for $s = 2$ and $p = 3$.

Methods with $r = s = 2$ (cont'd)

The coefficients for the method with $(\lambda, \mu) = (\frac{2}{5}, -\frac{1}{12})$ and $c = [0 \;\; 1]^T$ are

$$\left[\begin{array}{cc|cc|cc} \frac{2}{5} & 0 & -\frac{1}{12} & 0 & 1 & 0 \\ a_{21} & \frac{2}{5} & -\frac{2}{5}a_{21} + \frac{5}{9} & -\frac{1}{12} & 0 & 1 \\ \hline \frac{81}{100} + \frac{1}{10}a_{21} & \frac{9}{100} & \frac{1}{18} - \frac{1}{25}a_{21} & 0 & \frac{9}{10} & \frac{1}{10} \\ \frac{171}{100} - \frac{4}{5}a_{21} & \frac{19}{100} - \frac{1}{10}a_{21} & \frac{41}{90} - \frac{49}{100}a_{21} & \frac{2}{45} - \frac{1}{20}a_{21} & \frac{9}{10} & \frac{1}{10} \end{array}\right],$$

with the free parameter a_{21}. If we select $a_{21} = \frac{55}{27}$, the method will be L-stable.

Methods with $r = s = 1$

$$
\begin{aligned}
Y^{[n]} &= \tfrac{1}{2}hf(Y^{[n]}) - \tfrac{1}{12}h^2 g(Y^{[n]}) + y^{[n-1]}, \\
y^{[n]} &= hf(Y^{[n]}) + y^{[n-1]},
\end{aligned}
\tag{7}
$$

where

$$
Y^{[n]} = y(x_{n-1} + c_1 h) + O(h^4),
$$

with c_1 as a free parameter. This methods is A-stable.

Methods with $r = s = 2$

The only method in this class with A-stability property is

$$\left[\begin{array}{cc|cc|cc} \frac{1}{2} & 0 & -\frac{1}{12} & 0 & 1 & 0 \\ 1 & \frac{1}{2} & 0 & -\frac{1}{12} & 0 & 1 \\ \hline 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right].$$

We note that this method is not a genuine $r = s = 2$ SGLM, because it reduces to the $r = s = 1$ SGLM given by (7).

Implemented methods

In what follows, we describe details of the implemented methods:

- **Method 1:** SGLM-maximal order 3 (6) with $\lambda = \frac{5}{3}$, $c_1 = 1$,
- **Method 2:** SGLM-maximal order 4 (7) with $c_1 = 1$,
- **Method 3:** SDIRK order 3,
- **Method 4:** SDIRK order 4.

Stiff problems

I. The non-linear stiff system of ODEs

$$\begin{cases} y_1' = -10004y_1 + 10000y_2^4, & y_1(0) = 1, \\ y_2' = y_1 - y_2(1 + y_2^3), & y_2(0) = 1, \end{cases}$$

with the exact solution $y_1(x) = \exp(-4x)$ and $y_2(x) = \exp(-x)$. This problem is stiff with approximately stiffness ratio 10^4 near to $x = 0$.

II. The Robertson chemical kinetics problem

$$\begin{cases} y_1' = -0.04y_1 + 10^4 y_2 y_3, & y_1(0) = 1, \\ y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2, & y_2(0) = 0, \\ y_3' = 3 \times 10^7 y_2^2, & y_3(0) = 0. \end{cases}$$

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Numerical results for problem I

Table: The global error at the end of the interval of integration $[0, 1]$ for problem I.

h	2^{-1}	2^{-2}	2^{-3}	2^{-4}	2^{-5}
Method 1	$2.88E-03$	$4.41E-04$	$6.20E-05$	$8.28E-06$	$1.07E-06$
$R(h)$		6.53	7.11	7.49	7.74
Method 2	$3.34E-05$	$2.08E-06$	$1.29E-07$	$8.05E-09$	$5.03E-10$
$R(h)$		16.06	16.12	16.02	16.00

Note that $R(h) = Err(h)/Err(h/2)$.

Numerical results for problem I (cont'd)

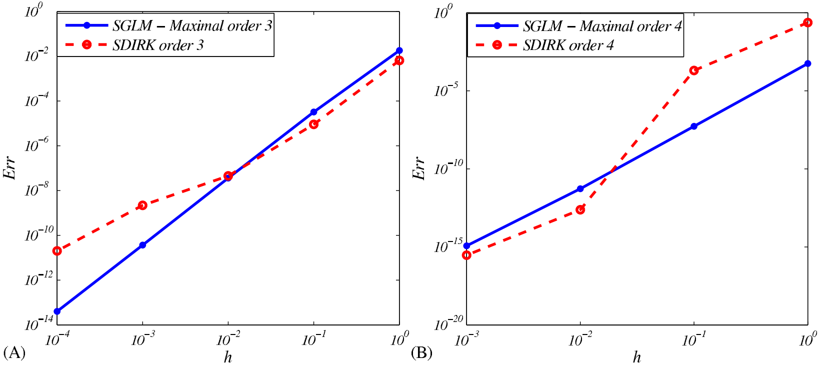

Figure: Errors versus stepsize for problem I: (A) solved by Method 1 and Method 3, (B) solved by Method 2 and Method 4.

Numerical results for problem II

Table: Numerical results for Robertson problem solved by Methods 1 and 3.

x	ns	Method 1 $[y_1, y_2, y_3]^T$	Method 1 $nfe + nge$	Method 3 $[y_1, y_2, y_3]^T$	Method 3 nfe
0.4	400	$9.851721150 \times 10^{-1}$ $3.386395399 \times 10^{-5}$ $1.479402101 \times 10^{-2}$	2×819	$9.851721139 \times 10^{-1}$ $3.386395379 \times 10^{-5}$ $1.479402211 \times 10^{-2}$	2813
4	4000	$9.055186791 \times 10^{-1}$ $2.240475693 \times 10^{-5}$ $9.445891614 \times 10^{-2}$	2×8019	$9.055186786 \times 10^{-1}$ $2.240475688 \times 10^{-5}$ $9.445891662 \times 10^{-2}$	28013
40	40000	$7.158270688 \times 10^{-1}$ $9.185534768 \times 10^{-6}$ $2.841637457 \times 10^{-1}$	2×80019	$7.158270687 \times 10^{-1}$ $9.185534765 \times 10^{-6}$ $2.841637457 \times 10^{-1}$	252770
400	400000	$4.505186685 \times 10^{-1}$ $3.222901442 \times 10^{-6}$ $5.494781086 \times 10^{-1}$	2×800019	$4.505186685 \times 10^{-1}$ $3.222901442 \times 10^{-6}$ $5.494781086 \times 10^{-1}$	2412770

Numerical results for problem II (cont'd)

Table: Numerical results for Robertson problem solved by Methods 2 and 4.

x	ns	Method 2 $[y_1, y_2, y_3]^T$	Method 2 $nfe + nge$	Method 4 $[y_1, y_2, y_3]^T$	Method 4 nfe
0.4	400	$9.851721139 \times 10^{-1}$ $3.386395379 \times 10^{-5}$ $1.479402217 \times 10^{-2}$	2×809	$9.851721139 \times 10^{-1}$ $3.386395379 \times 10^{-5}$ $1.479402218 \times 10^{-2}$	3618
4	4000	$9.055186786 \times 10^{-1}$ $2.240475688 \times 10^{-5}$ $9.445891665 \times 10^{-2}$	2×8009	$9.055186786 \times 10^{-1}$ $2.240475688 \times 10^{-5}$ $9.445891666 \times 10^{-2}$	36018
40	40000	$7.158270687 \times 10^{-1}$ $9.185534765 \times 10^{-6}$ $2.841637457 \times 10^{-1}$	2×80009	$7.158270687 \times 10^{-1}$ $9.185534765 \times 10^{-6}$ $2.841637457 \times 10^{-1}$	332593
400	400000	$4.505186685 \times 10^{-1}$ $3.222901442 \times 10^{-6}$ $5.494781086 \times 10^{-1}$	2×800009	$4.505186685 \times 10^{-1}$ $3.222901442 \times 10^{-6}$ $5.494781086 \times 10^{-1}$	3212593

Thank you for your attention