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A New Three-stages Fourth Order Pseudo-Runge-Kutta Method for Stiff Oodinary and Stiff Delay Differential Equations (Satu Kaedah Baru Runge-Kutta jenis 'Pseudo' Bertahap Tiga Berperingkat Empat untuk Persamaan Perbezaan Lengah Kaku dan Biasa kaku)

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Abstract : We constructed a new 3-stages fourth order pseudo-Runge-Kutta method for solving stiff ordinary and stiff delay differential equations. This method is derived by minimizing the error bound to determine the free parameters. The new method is computational cheaper than explicit Runge-Kutta method. We compared the new method with other conventional fourth order method by examples. Numerical results show that the new method is more efficient in term of accuracy compared to the standard methods.

Keywords: Pseudo-Runge-Kutta method, stiff ordinary differential equations, stiff delay differential equations

Abstrak : Kami telah membina satu kaedah baru Runge-Kutta jenis 'pseudo' bertahap 3 berperingkat empat untuk menyelesaikan persamaan perbezaan biasa kaku dan persamaan perbezaan lengah kaku. Kaedah ini diterbitkan dengan meminimumkan batas ralat untuk menentukan parameter bebas. Kaedah baru ini adalah lebih murah dari segi pengiraan berbanding dengan kaedah Runge-Kutta tersurat. Kami membandingkan kaedah baru ini dengan kaedah Runge-Kutta berperingkat empat konvensi yang lain dengan contoh. Keputusan berangka menunjukan bahawa kaedah baru ini adalah lebih efisien dari segi kejituan berbanding dengan kaedah piawai.

Katakunci: Kaedah Runge-Kutta jenis 'pseudo', persamaan perbezaan biasa jenis kaku, persamaan perbezaan lengah kaku

1. Introduction

Explicit Runge-Kutta method is probably the most popular method for numerical treatment of ordinary and delay differential equations. An *s*-stage explicit Runge-Kutta (ERK) method may be written in the form

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i K_i$$
$$K_i = f(t_n + c_i h, y_n + \sum_{j=0}^{i-1} a_{ij} K_j) \quad (1.1)$$

If $P(s)$ denotes the order that can be attained by an s-stage ERK method (1.1), Butcher [3] proved

$$P(s) = s \text{ for } s = 1, 2, 3, 4 \quad (1.2)$$

As we can see, the *s*-stage ERK method (1.1), from order one to order four requires exactly *s* functional evaluations for step.

Bryne [2] proposed a type of ERK type methods which requires fewer functional evaluations than (1.1), but have the same order of (1.1). This method is later called the pseudo-Runge-Kutta (PRK) methods. However, Bryne's method [2] is less accurate than (1.1). Many authors tried to improve the lost of accuracy of Bryne's method, Nakashima [8] introduced a pseudo-Runge-Kutta method which is cheaper than both Bryne's and ERK method (1.1), and have almost the same accuracy as (1.1) in the same order.

Based on Nakashima's idea, we construct a new three stages fourth order pseudo-Runge-Kutta method to for ordinary and delay differential equations. Compare with ERK method (1.1), the new method is still computationally cheaper.

2. Derivation of the Method

Nakashima pseudo-Runge-Kutta method (PRK) [8] can be written as follows

$$
\begin{aligned}
y_{n+1} &= y_n + h\sum_{i=0}^{s} b_i K_i \\
K_i &= f(t_n + c_i h, y_i + \lambda_i (y_n - y_{n-1}) + \sum_{j=0}^{i-1} a_{ij} K_j) \\
c_i &= \lambda_i + \sum_{j=0}^{i-1} a_{ij} \qquad i = 2, \cdots, s
\end{aligned} \tag{2.1}
$$

for $c_0 = \lambda_0 = -1$, $c_1 = \lambda_1 = 0$ and $0 \le c_s \le 1$. In [8] and [9], Nakashima proved that the pseudo-Runge-Kutta method (1.3) have the order

$$P(s) = s + 2 \text{ for } s = 2, 3, 4 \tag{2.2}$$

We found from Nakashima [8] and Shintani [12], the following eight order conditions, which are required to construct a fourth order PRK method.

Table 2.1: Fourth order Pseudo-Runge-Kutta order conditions

1.	$\tau_1^{(1)} : \sum_i b_i = 1$
2.	$\tau_1^{(2)} : \sum_i b_i c_i = \frac{1}{2}$
3.	$\tau_1^{(3)} : \sum_i b_i c_i^2 = \frac{1}{3}$
4.	$\tau_2^{(3)} : -\sum_i b_i \lambda_i + 2\sum_{ij} b_i a_{ij} c_j = \frac{1}{3}$
5.	$\tau_1^{(4)} : \sum_i b_i c_i^3 = \frac{1}{4}$
6.	$\tau_2^{(4)} : -\sum_i b_i c_i \lambda_i + 2\sum_{ij} b_i c_i a_{ij} c_j = \frac{1}{4}$
7.	$\tau_3^{(4)} : \sum_i b_i \lambda_i + 3\sum_{ij} b_i a_{ij} c_j^2 = \frac{1}{4}$

8.	$\tau_4^{(4)}: -\sum_{ij} b_i c_j^2 a_{ij} - \sum_i b_i a_{ij} \lambda_j + 2\sum_{ij} b_i a_{ij} a_{jk} c_k = 0$

By using the order condition in Table 2.1, Nakashima [8] obtained the two-stages fourth order method

$$\begin{aligned} &y(t_i + h) = y_i + h(b_0 k_0 + b_1 k_1 + b_2 k_2) \\ &k_0 = f(t_{i-1}, y_{i-1}) \\ &k_1 = f(t_i, y_i) \\ &k_2 = f(t_{i-1} + 0.7h, y_i - 2.156(y_i - y_{i-1}) + 0.833hk_0 + 2.023hk_1) \\ &b_0 = -\frac{7}{714}, b_1 = \frac{221}{714}, b_2 = \frac{500}{714} \end{aligned} \tag{2.3}$$

Similarly, we make use the order condition in Table 2.1 to construct a three-stages fourth order method. Choosing $c_3 = 1$, we have

$$\begin{aligned} &a_2 = \frac{1}{2} \\ &\lambda_2 = -2a_{20} - \frac{1}{4}, \quad \lambda_3 = -8 + 8a_{20} + \frac{9}{2}a_{32} \\ &a_{30} = \frac{7}{2} - 4a_{20} - \frac{7}{4}a_{32} \\ &b_0 = 0, \quad b_1 = \frac{1}{6}, \quad b_2 = \frac{2}{3}, \quad b_3 = \frac{1}{6} \end{aligned} \tag{2.4}$$

where a_{20} and a_{32} are free parameters which we want to determine.

According to Lambert [5], the local truncation error at t_{n+1} of the method can be defined as T_{n+1} where

$$T_{n+1} = y(t_{n+1}) - y_{n+1} \tag{2.5}$$

and $y(t_{n+1})$ is the theoretical solution and y_{n+1} is the approximated solution. We use the notation from Lotkin [6] and Ralston [11] to determine the error bounds on E for our fourth order PRK method.

$$|E| \leq CML^5 h^6 \tag{2.6}$$

Where C is the error constant in a region $\Re$ about (t_n, y_n)

$$|f(x,y)| < M \text{ and } \left| \frac{f^{i+j}(x,y)}{\partial x^i \partial y^j} \right| < \frac{L^{i+j}}{M^{j-1}} \tag{2.7}$$

where L and M are positive constants independent of t, y. We found that

$$C = \left|\frac{19}{720}\right| + \left|-\frac{31}{90} + \frac{a_{32}}{6}\right| + \left|-\frac{8}{45} + \frac{4a_{20}}{9}\right| + \left|-\frac{31}{180} + \frac{a_{32}}{12} + \frac{a_{32}}{9}\left(-\frac{3}{8} + a_{20}\right)\right| + \left|-\frac{77}{180} - \frac{2a_{20}}{9} + \frac{a_{32}}{4}\right| + \left|-\frac{31}{360} + \frac{a_{32}}{24} + \frac{a_{32}}{18}\left(-\frac{3}{8} + a_{20}\right)\right| \tag{2.8}$$

Our objective is to minimize the right hand side of (2.8). Using a special command of *Mathematica* 5.0, we found that the bound of C is minimized when $a_{20} = \frac{2}{5}$ and $a_{32} = \frac{31}{15}$.

```
bound = 19/720 + Abs[-31/90 + 1/6 a[32]] + Abs[-8/45 + 4/9 a[20]] + Abs[-31/180 + 1/12 a[32] + 1/9 a[32] (-3/8 + a[20])]
  + Abs[-77/180 - 2/9 a[20] + 1/4 a[32]] + Abs[-31/360 + 1/24 a[32] + 1/18 a[32] (-3/8 + a[20])]
Minimize[bound, {a[20], a[32]}]
  {7/200, {a[20] → 2/5, a[32] → 31/15}}
```

Substituting the value a_{20} and a_{32} into (2.4), the new three- stages fourth order pseudo Runge-Kutta method is

$$y(t_i + h) = y_i + \frac{h}{6}(k_1 + 4k_2 + k_3)$$

where

$$\begin{aligned}
k_0 &= f(t_{i-1}, y_{i-1}) \\
k_1 &= f(t_i, y_i) \\
k_2 &= f(t_{i-1} + \frac{h}{2}, y_i - \frac{21}{20}(y_i - y_{i-1}) + \frac{2}{5}hk_0 + \frac{23}{20}hk_1) \\
k_3 &= f(t_{i-1} + h, y_i + \frac{9}{2}(y_i - y_{i-1}) - \frac{103}{60}hk_0 - \frac{77}{20}hk_1 + \frac{31}{15}hk_2)
\end{aligned} \tag{2.9}$$

The local truncation error for formula (2.9) satisfies

$$|E| \le 0.035ML^5h^6 \tag{2.10}$$

is found to be smaller than the local truncation error for Nakashima's fourth order method.

3. Stability Analysis

To determine the stability function of the new method, we applied the famous Dahlquist's test equation

$$y' = f(x, y) = \lambda y \tag{3.1}$$

to formula (2.9). The stability polynomial for the new pseudo-Runge-Kutta method is

$$y_{i+i} = y_i + \frac{7}{60}h\lambda y_{i-1} + \frac{53}{60}h\lambda y_i + \frac{77}{225}h^2\lambda^2 y_{i-1} + \frac{97}{900}h^2\lambda^2 y_i + \frac{31}{225}h^3\lambda^3 y_{i-1} + \frac{713}{1800}h^3\lambda^3 y_i \tag{3.2}$$

On assuming $h\lambda = z$, $y_{i+1} = \zeta$, $y_i = \zeta^0$ and $y_{i-1} = \zeta^{-1}$ equation (3.2) becomes

$$\zeta^2 - \zeta\left(1 + \frac{53}{60}z + \frac{97}{900}z^2 + \frac{713}{1800}z^3\right) + \frac{7}{60}z - \frac{77}{225}z^2 - \frac{31}{225}z^3 = 0 \tag{3.3}$$

Solving equation (3.3) we have two roots

$$\begin{aligned} \zeta_1 &= \frac{1}{2} + \frac{53}{120}z + \frac{97}{1800}z^2 + \frac{713}{3600}z^3 + \frac{1}{3600}\alpha \\ \zeta_2 &= \frac{1}{2} + \frac{53}{120}z + \frac{97}{1800}z^2 + \frac{713}{3600}z^3 - \frac{1}{3600}\alpha \end{aligned} \tag{3.4}$$

where

$$\alpha = \sqrt{3240000 + 7236000z + 7661700z^2 + 469320z^3 + 2304976z^4 + 276644z^5 + 508369z^6}$$

According to [9] and [14], $|\zeta_1| \le 1$ and $|\zeta_2| \le 1$ are two stability functions for the new PRK method. By taking $z = x + yi$, we plot the stability region using MAPLE package. The shaded region is the region which satisfies the condition $|\zeta_1| \le 1$ and $|\zeta_2| \le 1$. The stability region for the new method is given in Figure 3.1.

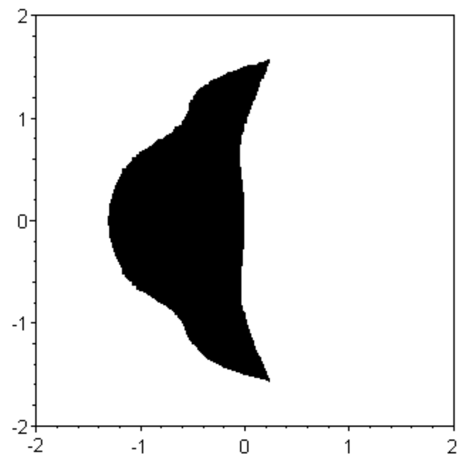

Figure 3.1: Stability Region for new 3-stages fourth order PRK method with minimize error bound

4. Solving Stiff Ordinary and Stiff Delay Differential Equations

It is known that the first order stiff differential equation

$$\left.\begin{aligned} y'(t) &= f(t, y(t)) \\ y(t_0) &= y_0 \end{aligned}\right\} \tag{4.1}$$

can be solved directly using (2.1). Similarly, (2.1) can be adapted to solve any first stiff delay differential equation in the form

$$\left.\begin{array}{ll} y'(t) = f(t, y(t), y(t-\tau)) & t \geq t_0 \\ y(t) = \varphi(t) & t \leq t_0 \end{array}\right\} \qquad (4.2)$$

where $\varphi(t)$ is the initial function, $\tau(t,y(t))$ is the delay argument and $y(t-\tau)$ is the solution of the delay term. The idea is generalized (2.1) in to the form

$$\begin{aligned} y_{i+1} &= y_i + h\sum_{i=0}^{s} b_i K_i \\ K_i &= f(t_i + c_i h, y_i + \lambda_i (y_i - y_{i-1}) + \sum_{j=0}^{i-1} a_{ij} K_j, y(t_n + c_i h - \tau)) \end{aligned} \qquad (4.3)$$

When solving (4.2), one difficulty is to approximate the delay term, $y(t_n + c_i h - \tau)$ on $[t_i, t_j]$ .However, the delay term can still be approximated using previously computed values of $y(t)$ using interpolation method. Here, we choose to use three-point Hermite divided-difference interpolation to approximate the delay term.

5. Numerical Results

We have written experimental program in MAPLE to solve stiff ordinary and stiff delay differential equations using formula (2.9) and other fourth order method. The test problems below were obtained form Yaacob et al. [14].

Problem 1: First order stiff ordinary differential equation

$$y'(t) = -100y + 99e^{2t}$$
$$y(0) = 0$$

Exact solution: $y(t) = \frac{33}{34}(e^{2t} - e^{-100t})$

Results are given for $t \in [0,1]$

Problem 2: Second order stiff ordinary differential equation

$$y''(t) + 101y'(t) + 100y(t) = 0$$
$$y(0) = 1.01, \quad y'(0) = -2$$

Exact solution: $y(t) = 0.01e^{-100t} + e^{-t}$

Results are given for $t \in [0,1]$

Problem 3: Stiff delay differential equation

$$y'(t) = py(t) - y(t-\tau)e^{(p-1)}$$
$$y(t) = e^{(p-1)t}, \quad t \leq 0$$
$$\tau = 1, \quad p = -24, \quad -100$$

Exact solution: $y(t) = e^{(p-1)t}$
Results are given for $t \in [0,2]$

We solved stiff ordinary and stiff delay differential equations using the new fourth order PRK method (2.9), Nakashima's fourth order PRK method and classical fourth order ERK method. The necessary value y_1 for PRK method are computed by the classical fourth order ERK method. Numerical results are given from Table 5.1 to 5.7.

Below are the notations used:

ERK44 : Classical four-stages fourth order ERK method
PRK24 : Nakashima two-stages fourth order PRK method
NPRK34 : New three-stages fourth order PRK method
MAXERR : Maximum error | $y(x_i)$ - y_i |
N : Number of steps

Table 5.1: Numerical solutions for Problem 1 (N=1024)

t	ERK44	PRK24	NPRK34	Exact solution
t_1	0.09220039164	0.09220039164	0.09220039164	0.0922004627
t_{100}	1.179879515	1.179879511	1.179879515	1.179879515
t_{500}	2.577215460	2.577215459	2.577215459	2.577215460
t_{1000}	6.843313452	6.843313451	6.843313450	6.83313450

Table 5.2: Numerical solutions for Problem 2 (N=1024)

t	ERK44	PRK24	NPRK34	Exact solution
t_1	1.008045921	1.008045921	1.008045921	1.008093520
t_{100}	0.9058492288	0.9012273836	0.9060597563	0.9069611918
t_{500}	0.6124463697	0.6072750189	0.6126817503	0.6136802512
t_{1000}	0.3754774562	0.3707503107	0.3756929975	0.3766034507

Table 5.3: Numerical solutions for Problem 3, $p = -100$ (N=800)

t	ERK44	PRK24	NPRK34	Exact solution
t_1	0.776864167005	0.776864167005	0.776864167005	0.776856212839
t_{400}	1.37818075(-44)	1.49941447(-44)	1.36390191(-44)	1.36853947(-44)
t_{600}	1.62271317(-66)	1.87469021(-66)	1.58182480(-66)	1.60098031(-66)
t_{800}	1.91441879(-88)	2.37386785(-88)	1.82606483(-88)	1.87290028(-88)

Table 5.4: Maximum absolute errors for Problem 1

N	Method	MAXERR
128	ERK44	2.0774 (-3)
	PRK24	**
	NPRK34	2.0774 (-3)
256	ERK44	9.4740 (-5)
	PRK24	1.0772 (-3)
	NPRK34	6.8991 (-5)
512	ERK44	5.0920 (-6)
	PRK24	3.5510 (-5)
	NPRK34	2.2245 (-6)
1024	ERK44	2.9361 (-7)
	PRK24	1.7240 (-5)
	NPRK34	7.1061 (-7)

Table 5.5: Maximum absolute errors for Problem 2

N	Method	MAXERR

	ERK44	1.3246 (-2)
	PRK24	**
128	NPRK34	4.9502 (-3)
	ERK44	5.3263 (-3)
	PRK24	**
256	NPRK34	2.5041 (-3)
	ERK44	2.5326 (-3)
	PRK24	2.7955 (-2)
512	NPRK34	1.7685 (-3)
	ERK44	1.2339 (-3)
	PRK24	6.4053 (-3)
1024	NPRK34	9.9851 (-4)

Table 5.6: Maximum absolute errors for Problem 3 ($p = -24$)

N	Method	MAXERR
	ERK44	7.4423 (-7)
	PRK24	4.9278 (-6)
400	NPRK34	2.1925(-7)
	ERK44	4.4201 (-8)
	PRK24	2.6823 (-7)
800	NPRK34	8.5393 (-9)

Table 5.7: Maximum absolute errors for Problem 3 ($p = -100$)

N	Method	MAXERR
	ERK44	2.9589 (-4)
	PRK24	6.7648 (-3)
400	NPRK34	2.4448 (-4)
	ERK44	1.4973 (-5)
	PRK24	1.1934 (-4)
800	NPRK34	7.9542 (-6)

6. Conclusion

We derived a three-stages fourth order pseudo-Runge-Kutta method, namely NPRK34 method, based on Nakashima’s idea [7] to solved stiff ordinary and stiff delay differential equations.

The numerical results show that Nakashima’s fourth order PRK method is not suitable to solve stiff ordinary and delay problems. According to the numerical results presented in Table 5.1 to 5.3, the error produce by Nakashima’s method is larger compare to other fourth order method. Furthermore, Nakashima’s method does not able to solve problem 1 for N = 128 and problem 2 for N = 128 and N = 256, that is, the error extremely large. The failure is indicated by a “ ** ” in place of a number in Table 5.1 and 5.2.

From the numerical results, the NPRK34 method is more accurate compare with classical fourth order ERK method and Nakashima’s method. In addition, the NPRK34 method is computational cheaper than other fourth order ERK method. Therefore we recommend it for use in the computation of stiff ordinary and stiff delay differential equation problems.

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