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Taylor Series Based Computations and MATLAB ODE Solvers Comparisons

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Abstract. The paper is a part of student cooperation in AKTION project (Austria-Czech). Taylor series method for solving differential equations represents a non-traditional way of a numerical solution. Even though this method is not much preferred in the literature, experimental calculations done at the Department of Intelligent Systems of the Faculty of Information Technology of TU Brno have verified that the accuracy and stability of the Taylor series method exceeds the currently used algorithms for numerically solving differential equations.

The paper deals with possibilities of numerical solution of Initial Value Problems of Ordinary Differential Equations (ODEs) - using the Taylor series method with automatic computation of higher Taylor series terms.

The explicit and implicit scheme of Taylor series method is compared with numerical solvers implemented in MATLAB software [1]. The computation time and accuracy of our approach are compared with that of MATLAB ode solvers on a set of ODEs test examples [2].

Keywords: Differential equations, Taylor series method, Stiff systems, TKSL, MATLAB PACS: 02,89

INTRODUCTION

The "Modern Taylor Series Method" (MTSM) is used for numerical solution of differential equations. The MTSM is based on a recurrent calculation of the Taylor series terms for each time interval. Thus the complicated calculation of higher order derivatives (much criticised in the literature) need not be performed but rather the value of each Taylor series term is numerically calculated. Solving the convolution operations is another typical algorithm used.

An important part of the MTSM is an automatic integration order setting, i.e. using as many Taylor series terms as the defined accuracy requires. Thus it is usual that the computation uses different numbers of Taylor series terms for different steps of constant length.

The MTSM has been implemented in TKSL software [3]. Some articles that are focused on the MTSM were published last years [4, 5].

There are several papers that focus on computer implementations of the Taylor series method in different context "a variable order and variable step" (see, for instance, [6, 7]). Another more detailed description of a variable step size version and software implementation of the Taylor series method can be seen in [8]. The stability domain for several Taylor methods is presented in [9]. Promising A-stable combination of implicit Taylor series method with Trapezoidal rule is described in [10].

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EXPLICIT SOLVERS

The best-known and most accurate method of calculating a new value of a numerical solution of ordinary differential equation y' = f(t, y), $y(0) = y_0$ is to construct the Taylor series [11, 12].

The *n*-th order method (ORD = n) uses *n* Taylor series terms in the explicit form

$$y_{i+1} = y_i + h \cdot f(t_i, y_i) + \frac{h^2}{2!} \cdot f^{[1]}(t_i, y_i) + \dots + \frac{h^n}{n!} \cdot f^{[n-1]}(t_i, y_i), \quad ORD = n.$$
(1)
(2)

Benchmark set of ordinary differential equations [2] was used for tests. Following comparisons of entire "non-stiff package", except for non-continuous equations F1 - F5 have been completed. Simulated interval (t_{max}) was set to 100 seconds, minimal integration time step (h) was set to 1 second.

MTSM (based on explicit Taylor series form (2)) was compared with MATLAB explicit **ode** solvers. It was found that the best MATLAB solver for our set of test examples was **ode45** solver. Results of computation times comparisons for MTMS (**expTay**) ORD = 10 can be seen in Tab. 1 (every time is taken from 50 runs of computations). Ratios of computation times

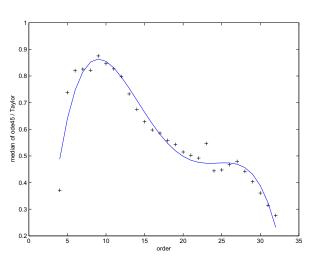
$$ratio_{1e} = \frac{ode45}{expTay}, \quad ratio_{2e} = \frac{expTay}{ode45}$$

can be seen in Tab. 1 (the bold numbers represents faster solutions of computations).

Median time of all examples for different order of MTSM can be seen in figure right to Tab. 1.

TABLE 1.	Comparison of ode45	and explicit Taylor ($ORD = 10$)
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	ode45 [s]	expTay [s]	ratio _{1e}	ratio2e
	[5]	[8]	rano _{1e}	runo _{2e}
A1	0.0118	0.0053	2.2108	0.4523
A2	0.0047	0.0055	0.8541	1.1708
A3	0.0304	0.0164	1.8603	0.5375
A4	0.0048	0.0050	0.9571	1.0448
A5	1.8295	0.0349	52.3957	0.0191
B1	0.0485	0.0315	1.5404	0.6492
B2	0.0222	0.0086	2.5713	0.3889
B3	0.0104	0.0064	1.6132	0.6199
B4	0.0365	1.0375	0.0351	28.4578
B5	0.0240	0.0032	7.4430	0.1344
C1	0.0165	0.0123	1.3407	0.7459
C2	0.0710	0.4187	0.1696	5.8964
C3	0.0378	0.0216	1.7494	0.5716
C4	0.0552	0.0918	0.6012	1.6633
D1	0.0553	0.7054	0.0784	12.7506
D2	0.0603	0.6933	0.0870	11.4892
D3	0.0716	0.7111	0.1007	9.9329
D4	0.0932	0.7062	0.1320	7.5786
D5	0.1269	1.9798	0.0641	15.6022
E1	0.0259	0.0552	0.4693	2.1308
E2	0.0581	0.0564	1.0302	0.9707
E3	0.0271	0.1009	0.2682	3.7290
E4	0.0042	0.0050	0.8381	1.1932
E5	0.0129	0.0338	0.3811	2.6243
median			0.9595	3.2340



IMPLICIT SOLVERS

There are some peculiar systems of differential equations, which cannot be solved by commonly used (explicit) numerical methods - *the stiff systems*. While the definition of this kind of systems is intuitively clear to the mathematicians the exact definition has not been yet specified [13].

Similarly like explicit Taylor series the implicit form of the n-th order method (ORD = n) can be expressed in the form

$$y_{i+1} = y_i + h \cdot f(t_{i+1}, y_{i+1}) - \frac{h^2}{2!} \cdot f'(t_{i+1}, y_{i+1}) - \dots - \frac{(-h)^n}{n!} \cdot f^{(n-1)}(t_{i+1}, y_{i+1}), \quad ORD = n.$$
(3)

Stiff Problems

Implicit Taylor Series Method with Recurrent Calculation of Taylor Series Terms and Newton Method (ITMRN) based on (3) was implemented in MATLAB. Stability and accuracy of the ITMRN computation of ODEs were analyzed.

Benchmark set of ordinary differential equations [2] was used for tests. Comparisons of entire "stiff package" equations A1, A3, A4, B1-B5 where analytic solution is well-known (obtained from Maple software [14]) have been completed. Simulated interval was used from article, integration time step was set to time interval (just 1 integration step was needed).

TABLE 2. Comparison of MATLAB stiff ode solvers and ITMRN

	ode15s [s]	impTay1 [s]	impTay2 [s]	impTay3 [s]	ratio _{1i}	ratio _{2i}	ratio _{3i}	Error(y) (ORD)
A1	0.0538	0.0022	0.0023	0.0015	34.1588	58.8119	36.5149	3.2468×10 ⁻⁵ (10)
A3	0.0722	0.0023	0.0024	0.0015	45.9286	83.017842	50.9011	1.064661×10 ⁻⁵ (10)
A4	0.0920	0.0129	0.0069	0.0037	24.6389	67.185681	28.1318	3.063018×10 ⁻⁵ (6)
B1	0.5533	0.0012	0.0010	0.00063	872.6757	12678.4996	7307.7485	0.7003512×10^{-5} (3)
B2	0.0608	0.0043	0.0044	0.0026	22.9871	59.6822	28.7128	3.248772×10^{-5} (10)
B3	0.0651	0.0043	0.0045	0.0027	23.5398	63.9215	30.2985	3.248772×10^{-5} (10)
B4	0.1377	0.0044	0.0046	0.0027	50.4536	228.7384	105.1956	3.248772×10^{-5} (10)
B5	1.4354	0.0044	0.0045	0.0027	525.8835	1388.9469	594.2142	3.248772×10 ⁻⁵ (10)

Three types of ITMRN were implemented:

- Implicit Taylor series method + Newton's method where Jacobian matrix was computed using **differential** formulae impTay1 in Tab. 2
- Implicit Taylor series method + Newton's method where Jacobian matrix was computed with **symbolic opera**tions (analytically) - **impTay2** in Tab. 2
- Implicit Taylor series method + Newton's method where Jacobian matrix was computed using **Broyden's method** - **impTay3** in Tab. 2

Absolute error ||Error(y)|| in Tab. 2 of numerical solution is defined as difference between numerical y_i and analytical $y(t_i)$ solution

$$||\text{Error}(y)|| = ||y_i - y(t_i)||,$$
(4)

where $t_i = h \cdot i$ (for ITMRN and our test examples in Tab. 2 - i = 1 and $h = t_{max}$). Maximum absolute error in our tests is set to 10^{-4} . Absolute error is completed with information of (*ORD*) used.

Time of computations of **ode15**, **impTay1**, **impTay2**, **impTay3** are presented for test equations in Tab. 2. Ratios of computation times for others MATLAB implicit solvers

$$ratio_{1i} = \frac{ode15s}{impTay3}, \quad ratio_{2i} = \frac{ode25s}{impTay3}, \quad ratio_{3i} = \frac{ode23tb}{impTay3},$$

can be also seen in Tab. 2.

Condition number of Jacobian matrix in Newton iteration method becomes higher, that is why multiple arithmetic is needed for higher order and higher integration step size.³

CONCLUSIONS

Ten Taylor series terms (ORD = 10) of explicit Taylor series proved to be the best method for the given set of "nonstiff" ODEs. As expected, a solution of linear systems of ODEs using higher order Taylor series (and corresponding higher integration time step) was faster than that of low order Taylor series method (lower integration step).

Multiple arithmetic for higher order of implicit Taylor series method (and higher integration step) must be used as condition number of Jacobian matrix in Newton iteration method becomes higher.

Detailed information will be given during the ICNAAM 2013 conference.

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 $^{^{3}}$ The special data type vpa (variable precision arithmetic) in MATLAB is implemented or for C/C++ programs GMP library [15] should be used (this library is used in TKSL software).