5.6

3.b

3. Use each of the Adams-Bashforth methods to approximate the solutions to the following initial-value problems. In each case, use starting values obtained from the Runge-Kutta method of order four. Compare the results to the actual values.

a. $y' = y/t - (y/t)^2$, $1 \le t \le 2$, $y(1) = 1$, with $h = 0.1$; actual solution $y(t) = \dfrac{t}{1 + \ln t}$.

b. $y' = 1 + y/t + (y/t)^2$, $1 \le t \le 3$, $y(1) = 0$, with $h = 0.2$; actual solution $y(t) = t \tan(\ln t)$.

c. $y' = -(y+1)(y+3)$, $0 \le t \le 2$, $y(0) = -2$, with $h = 0.1$; actual solution $y(t) = -3 + 2/(1 + e^{-2t})$.

d. $y' = -5y + 5t^2 + 2t$, $0 \le t \le 1$, $y(0) = 1/3$, with $h = 0.1$; actual solution $y(t) = t^2 + \frac{1}{3}e^{-5t}$.

Code is attached. Result:

time	2-step	3-step	4-step	5-step
1.0	0.000000	0.000000	0.000000	0.000000
1.2	0.221246	0.221246	0.221246	0.221246
1.4	0.486755	0.489684	0.489684	0.489684
1.6	0.805488	0.812432	0.812752	0.812752
1.8	1.185693	1.198211	1.199042	1.199432
2.0	1.637794	1.658431	1.660306	1.661318
2.2	2.175379	2.207999	2.211745	2.213479
2.4	2.816395	2.866767	2.873532	2.876278
2.6	3.584918	3.661748	3.673327	3.677724
2.8	4.513842	4.630528	4.649894	4.657003
3.0	5.649120	5.826801	5.858994	5.870610

6

6. Use all the Adams-Moulton methods to approximate the solutions to the Exercises 2(b), 2(c), and 2(d). In each case, use exact starting values and explicitly solve for w_{i+1}. Compare the results to the actual values.

2. Use all the Adams-Bashforth methods to approximate the solutions to the following initial-value problems. In each case use exact starting values and compare the results to the actual values.

a. $y' = 1 + y/t + (y/t)^2, \quad 1 \le t \le 1.5, \quad y(1) = 0,$ with $h = 0.1$; actual solution $y(t) = t\tan(\ln t)$.

b. $y' = \sin t + e^{-t}, \quad 0 \le t \le 0.5, \quad y(0) = 0,$ with $h = 0.1$; actual solution $y(t) = 2 - \cos t - e^{-t}$.

c. $y' = \frac{y+1}{t}, \quad 1 \le t \le 1.5, \quad y(1) = 1,$ with $h = 0.1$; actual solution $y(t) = 2t - 1$.

d. $y' = t^2, \quad 0 \le t \le 0.5, \quad y(0) = 0,$ with $h = 0.1$; actual solution $y(t) = \frac{1}{3}t^3$.

Code is attached. Solving for 2.a getting Results:

time	2-step	2-step(ab)	3-step	3-step-ab	4-step	4-step-ab	5-step	5-step-ab	exact
1.0	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
1.1	0.105160	0.105160	0.105160	0.105160	0.105160	0.105160	0.105160	0.105160	0.105160
1.2	0.221294	0.220871	0.221243	0.221243	0.221243	0.221243	0.221243	0.221243	0.221243
1.3	0.349231	0.348819	0.349123	0.349130	0.349121	0.349121	0.349121	0.349121	0.349121
1.4	0.489861	0.489430	0.489686	0.489669	0.489682	0.489660	0.489682	0.489682	0.489682
1.5	0.644140	0.643671	0.643883	0.643850	0.643876	0.643861	0.643875	0.643882	0.643875
1.6	0.813123	0.812599	0.812764	0.812719	0.812753	0.812742	0.812753	0.812756	0.812753
1.7	0.997993	0.997402	0.997511	0.997454	0.997495	0.997485	0.997494	0.997495	0.997494
1.8	1.200095	1.199422	1.199463	1.199394	1.199440	1.199429	1.199439	1.199439	1.199439
1.9	1.420966	1.420196	1.420149	1.420067	1.420118	1.420106	1.420116	1.420115	1.420116
2.0	1.662370	1.661484	1.661326	1.661228	1.661285	1.661271	1.661282	1.661280	1.661282
2.1	1.926341	1.925318	1.925020	1.924904	1.924966	1.924949	1.924962	1.924960	1.924962

13

13. The initial-value problem

$$y' = e^y, \quad 0 \le t \le 0.20, \quad y(0) = 1,$$

has solution

$$y(t) = 1 - \ln(1 - et).$$

Applying the three-step Adams-Moulton method to this problem is equivalent to finding the fixed point w_{i+1} of

$$g(w) = w_i + \frac{h}{24}\left(9e^w + 19e^{w_i} - 5e^{w_{i-1}} + e^{w_{i-2}}\right).$$

a. With $h = 0.01$, obtain w_{i+1} by functional iteration for $i = 2, \ldots, 19$ using exact starting values w_0, w_1, and w_2. At each step, use w_i to initially approximate w_{i+1}.

b. Will Newton's method speed the convergence over functional iteration?

Code attached. Result:

time	w	y	iterations
0.00	1.000000	1.000000	0.0
0.01	1.027559	1.027559	0.0
0.02	1.055899	1.055899	0.0
0.03	1.085066	1.085066	5.0
0.04	1.115109	1.115109	5.0
0.05	1.146083	1.146083	5.0
0.06	1.178047	1.178047	5.0
0.07	1.211067	1.211066	5.0
0.08	1.245214	1.245213	5.0
0.09	1.280568	1.280568	5.0
0.10	1.317218	1.317218	5.0
0.11	1.355263	1.355263	5.0
0.12	1.394813	1.394813	5.0
0.13	1.435992	1.435991	5.0
0.14	1.478939	1.478939	5.0
0.15	1.523814	1.523813	5.0
0.16	1.570798	1.570797	5.0
0.17	1.620098	1.620097	6.0
0.18	1.671956	1.671955	6.0
0.19	1.726651	1.726649	6.0
0.20	1.784511	1.784509	6.0

b.

yes it decreases 1 iteration.

15

15. Change Algorithm 5.4 so that the corrector can be iterated for a given number p iterations. Repeat Exercise 9 with $p = 2, 3$, and 4 iterations. Which choice of p gives the best answer for each initial-value problem?

Code attached. For 3.b solved:

time	2-iteration	3-iteration	4-iteration	exact
1.0	0.000000	0.000000	0.000000	0.000000
1.2	0.221246	0.221246	0.221246	0.221243
1.4	0.489684	0.489684	0.489684	0.489682
1.6	0.812752	0.812752	0.812752	0.812753
1.8	1.199462	1.199465	1.199466	1.199439
2.0	1.661343	1.661351	1.661352	1.661282
2.2	2.213626	2.213641	2.213643	2.213502
2.4	2.876784	2.876811	2.876814	2.876551
2.6	3.678894	3.678943	3.678948	3.678475
2.8	4.659412	4.659500	4.659509	4.658665
3.0	5.875442	5.875604	5.875622	5.874100
MSE	2.6077512e-06,	3.271533e-06	3.34842e-06	0

So p=2 is the best p.

5.7

8

8. Construct an Adams Variable Step-Size Predictor-Corrector Algorithm based on the Adams-Bashforth five-step method and the Adams-Moulton four-step method. Repeat Exercise 3 using this new method.

3. Use the Adams Variable Step-Size Predictor-Corrector Algorithm with tolerance $TOL = 10^{-6}$, $hmax = 0.5$, and $hmin = 0.02$ to approximate the solutions to the given initial-value problems. Compare the results to the actual values.

a. $y' = y/t - (y/t)^2, \quad 1 \le t \le 4, \quad y(1) = 1$; actual solution $y(t) = t/(1 + \ln t)$.

b. $y' = 1 + y/t + (y/t)^2, \quad 1 \le t \le 3, \quad y(1) = 0$; actual solution $y(t) = t \tan(\ln t)$.

c. $y' = -(y+1)(y+3), \quad 0 \le t \le 3, \quad y(0) = -2$; actual solution $y(t) = -3 + 2(1 + e^{-2t})^{-1}$.

d. $y' = (t + 2t^3)y^3 - ty, \quad 0 \le t \le 2, \quad y(0) = \frac{1}{3}$; actual solution $y(t) = (3 + 2t^2 + 6e^{t^2})^{-1/2}$.

Code attached. Some Result on solving 3.b:

i	time	w	h	exact
0.0	1.000000	0.000000	0.050000	0.000000
1.0	1.050000	0.051270	0.050000	0.051270
2.0	1.100000	0.105160	0.050000	0.105160
3.0	1.150000	0.161781	0.050000	0.161781
4.0	1.200000	0.221243	0.050000	0.221243
6.0	1.300000	0.349121	0.050000	0.349121
7.0	1.350000	0.417759	0.050000	0.417759
8.0	1.400000	0.489682	0.050000	0.489682
9.0	1.450000	0.565011	0.050000	0.565011
9.0	1.450000	0.565011	0.080090	0.565011
10.0	1.530090	0.693095	0.080090	0.693096
11.0	1.610181	0.830814	0.080090	0.830814
12.0	1.690271	0.978788	0.080090	0.978788
13.0	1.770361	1.137704	0.080090	1.137704
15.0	1.930542	1.491511	0.080090	1.491511
16.0	2.010632	1.688208	0.080090	1.688208
17.0	2.090722	1.899490	0.080090	1.899490
18.0	2.170813	2.126562	0.080090	2.126562
18.0	2.170813	2.126562	0.066430	2.126562
19.0	2.237243	2.327853	0.066430	2.327853
20.0	2.303673	2.541808	0.066430	2.541809
21.0	2.370103	2.769394	0.066430	2.769395
22.0	2.436533	3.011687	0.066430	3.011688
23.0	2.502963	3.269888	0.054655	3.269889
24.0	2.557618	3.495195	0.054655	3.495196
25.0	2.612273	3.733012	0.054655	3.733013
26.0	2.666928	3.984259	0.054655	3.984260
27.0	2.721583	4.249950	0.054655	4.249952
28.0	2.776238	4.531214	0.045740	4.531215
29.0	2.821978	4.779473	0.045740	4.779474
30.0	2.867718	5.040321	0.045740	5.040323
31.0	2.913458	5.314647	0.045740	5.314649
32.0	2.959198	5.603427	0.045740	5.603428
33.0	3.004938	5.907735	-0.001235	5.907737
34.0	3.003704	5.899308	-0.001235	5.899310
35.0	3.002469	5.890892	-0.001235	5.890894
36.0	3.001235	5.882489	-0.001235	5.882491
37.0	3.000000	5.874098	-0.001235	5.874100
38.0	2.998765	5.865719	-0.001235	5.865721

5.9

2.b

2. Use the Runge-Kutta method for systems to approximate the solutions of the following systems of first-order differential equations and compare the results to the actual solutions.

a. $u_1' = u_1 - u_2 + 2, \quad u_1(0) = -1;$
$u_2' = -u_1 + u_2 + 4t, \quad u_2(0) = 0; \quad 0 \le t \le 1; \quad h = 0.1;$
actual solutions $u_1(t) = -\frac{1}{2}e^{2t} + t^2 + 2t - \frac{1}{2}$ and $u_2(t) = \frac{1}{2}e^{2t} + t^2 - \frac{1}{2}$.

b. $u_1' = \frac{1}{9}u_1 - \frac{2}{3}u_2 - \frac{1}{9}t^2 + \frac{2}{3}, \quad u_1(0) = -3;$
$u_2' = u_2 + 3t - 4, \quad u_2(0) = 5; \quad 0 \le t \le 2; \quad h = 0.2;$
actual solutions $u_1(t) = -3e^t + t^2$ and $u_2(t) = 4e^t - 3t + 1$.

c. $u_1' = u_1 + 2u_2 - 2u_3 + e^{-t}, \quad u_1(0) = 3;$
$u_2' = u_2 + u_3 - 2e^{-t}, \quad u_2(0) = -1;$
$u_3' = u_1 + 2u_2 + e^{-t}, \quad u_3(0) = 1; \quad 0 \le t \le 1; \quad h = 0.1;$
actual solutions $u_1(t) = -3e^{-t} - 3\sin t + 6\cos t, \quad u_2(t) = \frac{3}{2}e^{-t} + \frac{3}{10}\sin t - \frac{21}{10}\cos t - \frac{2}{5}e^{2t}$,
and $u_3(t) = -e^{-t} + \frac{12}{5}\cos t + \frac{9}{5}\sin t - \frac{2}{5}e^{2t}$.

d. $u_1' = 3u_1 + 2u_2 - u_3 - 1 - 3t - 2\sin t, \quad u_1(0) = 5;$
$u_2' = u_1 - 2u_2 + 3u_3 + 6 - t + 2\sin t + \cos t, \quad u_2(0) = -9;$
$u_3' = 2u_1 + 4u_3 + 8 - 2t, \quad u_3(0) = -5; \quad 0 \le t \le 2; \quad h = 0.2;$
actual solutions $u_1(t) = 2e^{3t} + 3e^{-2t} + t, \quad u_2(t) = -8e^{-2t} + e^{4t} - 2e^{3t} + \sin t$, and $u_3(t) = 2e^{4t} - 4e^{3t} - e^{-2t} - 2$.

Code attached. Result:

t	u0	u1	u0_actual	u1_actual
0.0	-3.000000	5.000000	-3.000000	5.000000
0.2	-3.624089	5.275600	-3.624208	5.285611
0.4	-4.313589	5.745058	-4.315474	5.767299
0.6	-5.100691	6.451294	-5.106356	6.488475
0.8	-6.024712	7.446730	-6.036623	7.502164
1.0	-7.133675	8.795396	-7.154845	8.873127
1.2	-8.486232	10.575497	-8.520351	10.680468
1.4	-10.154026	12.882552	-10.205600	13.020800
1.6	-12.224557	15.833229	-12.299097	16.012130
1.8	-14.804698	19.570026	-14.908942	19.798590
2.0	-18.024986	24.266989	-18.167168	24.556224

Discussion Question 1

1. The system below describes the chemical reaction of Robertson. This is considered to be a "stiff" system of ODEs. Can Algorithm 5.7 be applied to this system on $0 \le x \le 40$ with good results? Why or why not?

$$y_1' = -0.04y_1 + 10^4 y_2 y_3$$
$$y_2' = -0.04y_1 - 10^4 y_2 y_3 - 3 * 10^7 y_2^2$$
$$y_3' = 3 * 10^7 y_2^2$$

Yes.

The above equation provides a short interval [0, 40]. Then it has no difficult to integrate. 10^11 , the integration will fail If the intervals are very large to integrate it. The algorithm 5.9 is used to approximate the solution on the above ordinary differential equation system. It satisfied the end points, number of equations, integers and initial conditions. Therefore, the approximations YI and hat the (N+1) values of t. The sets of ODEs are bringing about from the time- based integration of great chemical reaction mechanisms. Here, the difficulty rises from the living of exact slow and exact fast reactions. Hence, the algorithm applied to this system will give good results.

5.10

2

2. For the Adams-Bashforth and Adams-Moulton methods of order four,

a. Show that if $f = 0$, then

$$F(t_i, h, w_{i+1}, \ldots, w_{i+1-m}) = 0.$$

b. Show that if f satisfies a Lipschitz condition with constant L, then a constant C exists with

$$|F(t_i, h, w_{i+1}, \ldots, w_{i+1-m}) - F(t_i, h, v_{i+1}, \ldots, v_{i+1-m})| \le C \sum_{j=0}^{m} |w_{i+1-j} - v_{i+1-j}|.$$

a.

Adams-Bashforth 4^{th}order:

$$w_{i+1} = w_i + F(t_i, h, w_{i+1}, w_i, w_{i-1}, w_{i-2}, w_{i-3})$$

$$F(t_i, h, w_{i+1}, w_i, w_{i-1}, w_{i-2}, w_{i-3})$$

$$= \frac{h}{24} [\, 55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})]$$

If f=0 then F=0.

Adams-Moulton 4^{th}order:

$$w_{i+1} = w_i + F(t_i, h, w_{i+1}, w_i, w_{i-1}, w_{i-2})$$

$$F(t_i, h, w_{i+1}, w_i, w_{i-1}, w_{i-2})$$
$$= \frac{h}{24}\ [\ 9f(t_{i+1}, w_{i+1}) +\ 19f(t_i, w_i) - f(t_{i-1}, w_{i-1}) +\ f(t_{i-2}, w_{i-2})]$$

If f=0 then F=0.

b.

f satisfies Lipschitz condition:

$$|f(t, w_1) -\ f(t, w_2)| \leq\ L|w_1 -\ w_2|$$

Adams-Bashforth:

$$\begin{aligned}
&|F(t_i, h, w_{i+1}, w_i, w_{i-1}, w_{i-2}, w_{i-3})\ -\ F(t_i, h, v_{i+1}, v_i, v_{i-1}, v_{i-2}, v_{i-3})| \\
&\quad = \frac{h}{24}\ |[\ 55f(t_i, w_i) -\ 59f(t_{i-1}, w_{i-1}) +\ 37f(t_{i-2}, w_{i-2}) -\ 9f(t_{i-3}, w_{i-3})] \\
&\quad -\ [\ 55f(t_i, v_i) -\ 59f(t_{i-1}, v_{i-1}) +\ 37f(t_{i-2}, v_{i-2}) -\ 9f(t_{i-3}, v_{i-3})]| \\
&\quad \leq \frac{55h}{24}|f(t_i, w_i) - (t_i, v_i)| + \frac{59h}{24}|f(t_{i-1}, w_{i-1}) - (t_{i-1}, v_{i-1})| \\
&\quad + \frac{37h}{24}|f(t_{i-2}, w_{i-2}) - (t_{i-2}, v_{i-2})| + \frac{9h}{24}|f(t_{i-3}, w_{i-3}) - (t_{i-3}, v_{i-3})| \\
&\quad \leq \frac{55h}{24}L_1|w_i - v_i| + \frac{59h}{24}L_2|w_{i-1} - v_{i-1}| + \frac{37h}{24}L_3|w_{i-2} - v_{i-2}| + \frac{9h}{24}L_4|w_{i-3} - v_{i-3}|
\end{aligned}$$

Take C as below:

$$C = \max\left(\frac{55h}{24}L_1, \frac{59h}{24}L_2\ , \frac{37h}{24}L_3, \frac{9h}{24}L_4\right)$$

Then:

$$F(t_i, h, w_{i+1}, w_i, w_{i-1}, w_{i-2}, w_{i-3})\ -\ F(t_i, h, v_{i+1}, v_i, v_{i-1}, v_{i-2}, v_{i-3})| \leq C\sum_{j=0}^{4}\left|w_{i+1-j} - v_{i+1-j}\right|$$

Adams-Moulton:

$$\begin{aligned}
&|F(t_i, h, w_{i+1}, w_i, w_{i-1}, w_{i-2},)\ -\ F(t_i, h, v_{i+1}, v_i, v_{i-1}, v_{i-2},)| \\
&\quad =\ \frac{h}{24}\ |[\ 9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) -\ 5f(t_{i-1}, w_{i-1}) +\ f(t_{i-2}, w_{i-2})] \\
&\quad -\ [\ 9f(t_{i+1}, v_{i+1}) + 19f(t_i, v_i) -\ 5f(t_{i-1}, v_{i-1}) +\ f(t_{i-2}, v_{i-2})]| \\
&\quad \leq \frac{9h}{24}L_1|w_{i+1} + v_{i+1}|\frac{19h}{24}L_2|w_i - v_i| + \frac{5h}{24}L_3|w_{i-1} - v_{i-1}| + \frac{h}{24}L_4|w_{i-2} - v_{i-2}| +
\end{aligned}$$

Take C as below:

$$C = \max\left(\frac{9h}{24}L_1, \frac{19h}{24}L_2\ , \frac{h}{24}L_3, \frac{h}{24}L_4\right)$$

Then:

$$|F(t_i, h, w_{i+1}, w_i, w_{i-1}, w_{i-2},) - F(t_i, h, v_{i+1}, v_i, v_{i-1}, v_{i-2},)| \le C\sum_{j=0}^{3}|w_{i+1-j} - v_{i+1-j}|$$

7

7. Investigate stability for the difference method

$$w_{i+1} = -4w_i + 5w_{i-1} + 2h[f(t_i, w_i) + 2hf(t_{i-1}, w_{i-1})],$$

for $i = 1, 2, \ldots, N-1$, with starting values w_0, w_1.

Using below theorems:

Definition 5.22 Let $\lambda_1, \lambda_2, \ldots, \lambda_m$ denote the (not necessarily distinct) roots of the characteristic equation

$$P(\lambda) = \lambda^m - a_{m-1}\lambda^{m-1} - \cdots - a_1\lambda - a_0 = 0$$

associated with the multistep difference method

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad \ldots, \quad w_{m-1} = \alpha_{m-1}$$

$$w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} + hF(t_i, h, w_{i+1}, w_i, \ldots, w_{i+1-m}).$$

If $|\lambda_i| \le 1$, for each $i = 1, 2, \ldots, m$, and all roots with absolute value 1 are simple roots, then the difference method is said to satisfy the **root condition**. ■

Definition 5.23

(i) Methods that satisfy the root condition and have $\lambda = 1$ as the only root of the characteristic equation with magnitude one are called **strongly stable**.

(ii) Methods that satisfy the root condition and have more than one distinct root with magnitude one are called **weakly stable**.

(iii) Methods that do not satisfy the root condition are called **unstable**. ■

Theorem 5.24 A multistep method of the form

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad \ldots, \quad w_{m-1} = \alpha_{m-1},$$

$$w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} + hF(t_i, h, w_{i+1}, w_i, \ldots, w_{i+1-m})$$

is stable if and only if it satisfies the root condition. Moreover, if the difference method is consistent with the differential equation, then the method is stable if and only if it is convergent. ■

The characteristics polynomial of this method is:

$$P(\lambda) = -5 + 4\lambda + \lambda^2 \rightarrow \lambda_1 = 1, \lambda_2 = -5 \rightarrow |\lambda_2| > 1 \rightarrow unstable$$

Discussion Question 1

1. Discuss the difference between local truncation error, local error, global truncation error, and global error.

- Roundoff Error

The roundoff error is the error which arises from the fact that numerical methods are implemented on digital computers which only calculate results to a fixed precision which is dependent on the computer system used. Note that since roundoff errors depend only on the number and type of arithmetic operations per step and is thus independent of the integration step size h.

If exact mathematical formula is replaced by some simple approximation to represent that formula; this error is called truncation error.

Assume here that we can carry out all computations with complete accuracy. That is, we can retain an infinite number of decimal places with no round-off error.

- Global Truncation Error (GTE):

At each step in a numerical method, the solution value (A_{t_n}) approximated by the value y_n.

The global truncation error is defined as

$$E_n = w_n - Y_n$$

This error arises from two causes:

1. At each step we use an approximate formula to determine y_{n+1}.

2. The input data at each step are only approximately correct, since A_{t_n}in general does not equal y_n.

In short at time point t_{k+1}, we assume only the initial condition is correct, the difference between the approximated solution and the exact solution is called global truncation error. GTE indicates stability.

- Local Truncation Error (LTE):

If we assume that $y_n = A_{t_n}$ at step n, then the only error at step n +1 is due to the use of an approximate formula. This error is known as the local truncation error e_n.

In short at time point t_{k+1} assume all the before answers were exact. the difference between the approximated solution and exact solution is called local truncation error. LTE indicates consistency.

For global error the difference between the exact and discrete solution is called global error. The difference of some step assuming the previous step was correct is local error.