Computational Methods
CMSC/AMSC/MAPL 460

Ordinary differential equations

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Several slides adapted from Prof. ERIC SANDT, TAMU

ODE: Previous class

- Standard form
- Examples of converting equations to standard form
  - Volterra equation
- Euler Method (an explicit method)
- Backward Euler Method (an implicit/nonlinear method)
- A predictor corrector method

Today

- Explicit and Implicit methods
- Runge Kutta methods
- Matlab function RK45
- Solve volterra equation
- Multistep methods: Adams Bashforth
- Implicit methods: Adams Moulton

Runge-Kutta Methods

Explicit methods: Use known values

Derivation of the 2nd order RK method

Look for a formula of the type

$$y_{n+1} = y_n + ak_1 + bk_2$$

$$k_1 = hf\left(x_n, y_n\right)$$

$$k_2 = hf\left(x_n + \alpha\Delta h, y_n + \beta k_1\right)$$

Runge-Kutta Methods

The initial conditions are:

$$\frac{dy}{dx} = f(x, y) \qquad y(x_0) = y_0$$

The Taylor series expansion including 2nd order terms is

$$y(x_{n+1}) = y(x_n) + h\frac{dy(x_n, y_n)}{dx} + \frac{h^2}{2!}\frac{d^2y(x_n, y_n)}{dx^2}$$

Runge-Kutta Methods

Expand the derivatives:

$$\frac{d^2y}{dx^2} = \frac{d}{dx}\left[f(x,y)\right] = f_x + f_y\frac{dy}{dx} = f_x + f_y f$$

The Taylor series expansion becomes

$$y_{n+1} = y_n + hf + h^2\left[\frac{1}{2}\left(f_x + f_y f\right)\right]$$

Have expressed second derivative in terms of 1st derivatives of f

Runge-Kutta Methods

From the Runge-Kutta

$$y_{n+1} = y_n + ahf + bhf\left(x_n + \alpha h, y_n + \beta hf\right)$$

The definition of the function

$$f\left(x_n + \alpha h, y_n + \beta hf\right) = f + \alpha h f_x + \beta hf\, f_y$$

Expand the next step

$$y_{n+1} = y_n + ahf + bh\left(f + \alpha h f_x + \beta hf\, f_y\right)$$

$$= y_n + \left[a + b\right]hf + b\alpha h^2 f + b\beta h^2 f\, f_y$$

Runge-Kutta Methods

From the Runge-Kutta

$$y_{n+1} = y_n + \left[a + b\right] hf + b\alpha h^2 f + b\beta h^2 f\, f_y$$

Compare with the Taylor series

$$\left[a + b\right] = 1$$

$$\alpha b = \frac{1}{2}$$

$$\beta b = \frac{1}{2}$$

<u>4 Unknowns</u>

Runge-Kutta Methods

The Taylor series coefficients (3 equations/4 unknowns)

$$\left[a+b\right]=1,\ \alpha b=\frac{1}{2},\quad \beta b=\frac{1}{2}$$

If you select "a" as

$$a=\frac{2}{3},\ b=\frac{1}{3},\quad \alpha=\frac{3}{2},\quad \beta=\frac{3}{2}$$

If you select "a" as

$$a=\frac{1}{2}\ \ b=\frac{1}{2},\quad \alpha=\beta=1$$

Note: These coefficient would result in a modified Euler or Midpoint Method

Runge-Kutta Method (2nd Order) Example

Consider

$$\frac{dy}{dx} = -y^2$$

Exact Solution

$$y = \frac{1}{1+x}$$

The initial condition is: $y(0) = 1$

The step size is: $\Delta h = 0.1$

Use the coefficients $a = \frac{1}{2}\ b = \frac{1}{2},\ \ \alpha = \beta = 1$

Runge-Kutta Method (2^{nd} Order) Example

The values are

$$k_1 = hf\left(x_i, y_i\right)$$

$$k_2 = hf\left(x_i + h, y_i + k_1\right)$$

$$y_{i+1} = y_i + \frac{1}{2}\left[k_1 + k_2\right]$$

Runge-Kutta Method (2nd Order) Example

- The values are similar to that of the Modified Euler
  - also a second order method

			k_1	Estimate	Solution	k_2	Exact	Error
x_n	y_n	y'_n	hy'_n	y^*_{n+1}	$y^{*\prime}_{n+1}$	$h(y^{*\prime}_{n+1})$		
0	1.00000	-1.00000	-0.10000	0.90000	-0.81000	-0.08100	1.000000	0.000000
0.1	0.90950	-0.82719	-0.08272	0.82678	-0.68357	-0.06836	0.909091	-0.000409
0.2	0.83396	-0.69549	-0.06955	0.76441	-0.58433	-0.05843	0.833333	-0.000629
0.3	0.76997	-0.59286	-0.05929	0.71069	-0.50507	-0.05051	0.769231	-0.000740
0.4	0.71507	-0.51133	-0.05113	0.66394	-0.44082	-0.04408	0.714286	-0.000789
0.5	0.66747	-0.44551	-0.04455	0.62292	-0.38802	-0.03880	0.666667	-0.000801
0.6	0.62579	-0.39161	-0.03916	0.58663	-0.34413	-0.03441	0.625000	-0.000790
0.7	0.58900	-0.34692	-0.03469	0.55431	-0.30726	-0.03073	0.588235	-0.000768
0.8	0.55629	-0.30946	-0.03095	0.52535	-0.27599	-0.02760	0.555556	-0.000738
0.9	0.52702	-0.27775	-0.02778	0.49925	-0.24925	-0.02492	0.526316	-0.000705
1	0.50067	-0.25067	-0.02507	0.47560	-0.22620	-0.02262	0.500000	-0.000671

Runge-Kutta Method (2nd Order) Example [b]

The values are $a = \frac{2}{3},\ b = \frac{1}{3},\ \alpha = \frac{3}{2},\ \beta = \frac{3}{2}$

$$k_1 = hf\left(x_i, y_i\right)$$

$$k_2 = hf\left(x_i + \alpha h, y_i + \beta k_1\right)$$

$$y_{i+1} = y_i + ak_1 + bk_2$$

Runge-Kutta Method (2nd Order) Example [b]

The values are

			k_1	Estimate	Solution	k_2	Exact	Error
x_n	y_n	y'_n	hy'_n	y^*_{n+1}	$y^{*\prime}_{n+1}$	$h(y^{*\prime}_{n+1})$	Exact	
0	1.00000	-1.00000	-0.10000	0.85000	-0.72250	-0.07225	1.000000	0.000000
0.1	0.90925	-0.82674	-0.08267	0.78524	-0.61660	-0.06166	0.909091	-0.000159
0.2	0.83358	-0.69486	-0.06949	0.72935	-0.53195	-0.05320	0.833333	-0.000248
0.3	0.76953	-0.59217	-0.05922	0.68070	-0.46335	-0.04634	0.769231	-0.000295
0.4	0.71460	-0.51066	-0.05107	0.63800	-0.40705	-0.04070	0.714286	-0.000317
0.5	0.66699	-0.44488	-0.04449	0.60026	-0.36031	-0.03603	0.666667	-0.000324
0.6	0.62532	-0.39103	-0.03910	0.56667	-0.32111	-0.03211	0.625000	-0.000321
0.7	0.58855	-0.34639	-0.03464	0.53659	-0.28793	-0.02879	0.588235	-0.000314
0.8	0.55586	-0.30898	-0.03090	0.50951	-0.25960	-0.02596	0.555556	-0.000303
0.9	0.52661	-0.27731	-0.02773	0.48501	-0.23523	-0.02352	0.526316	-0.000291
1	0.50028	-0.25028	-0.02503	0.46274	-0.21412	-0.02141	0.500000	-0.000278

Runge-Kutta Methods

- Fourth order Runge-Kutta method

$$y_{n+1}=y_n+1/6(k_1+2k_2+2k_3+k_4)$$

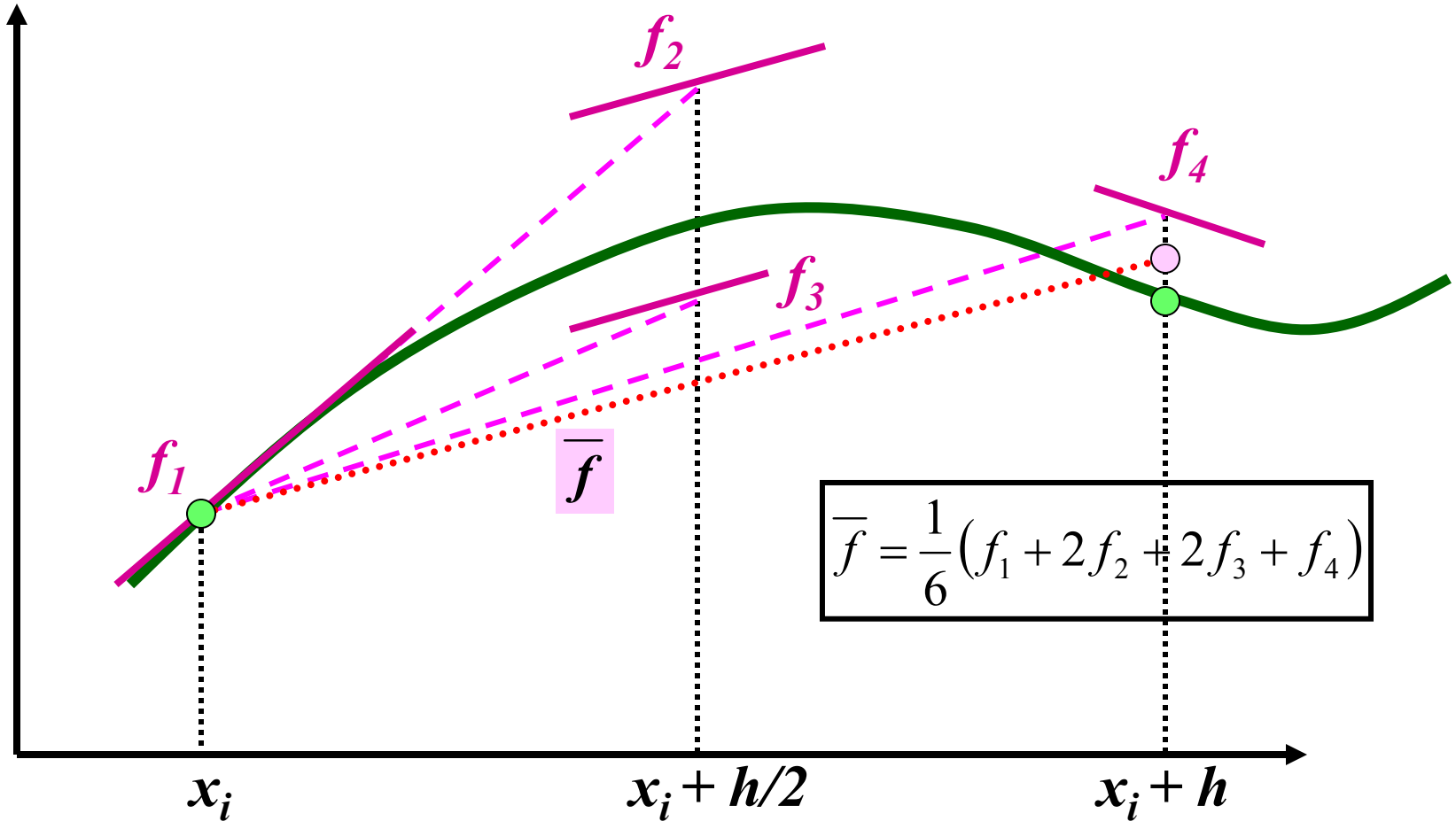
$$k_1=hf(x,y)$$

$$k_2=h(f(x+h/2,\ y+1/2\ k_1)$$

$$k_3=h(f(x+h/2,\ y+1/2\ k_2)$$

$$k_4=h(f(x+h,y+k_3))$$

4^{th}-order Runge-Kutta Method



Volterra example

- Write a function in standard form

```
function f = rabfox(t,y)
% Computes y' for the Volterra model.
% y(1) is the number of rabbits at time t.
% y(2) is the number of foxes at time t.
global alpha % interaction constant
t % a print statement, just so we can see how
  fast
% the progress is, and what stepsize is being
  used
f(1,1) = 2*y(1) - alpha*y(1)*y(2);
f(2,1) = -y(2) + alpha*y(1)*y(2);
```

Study its solution for various values of encounter

```
% Run the rabbit-fox model for various values of
% the encounter parameter alpha, plotting each
% solution.
global alpha
for i=2:-1:0,
alpha = 10^(-i)
[t,y] = ode45('rabfox',[0:.1:2], [20,10]);
plot(t,y(:,1),'r',t,y(:,2),'b');
legend('rabbits','foxes')
title(sprintf('alpha = %f',alpha));
pause
end
```

Runge-Kutta Method (4^{th} Order) Example

Consider

$$\frac{dy}{dx} = y - x^2$$

Exact Solution

$$y = 2 + 2x + x^2 - e^x$$

The initial condition is: $y(0) = 1$

The step size is: $\Delta h = 0.1$

The 4th Order Runge-Kutta

The example of a single step:

$$k_1 = \Delta h\left[f\left(x, y\right)\right] = 0.1 f\left(0,1\right) = 0.1\left(1 - 0^2\right) = 0.1$$

$$k_2 = \Delta h\left[f\left(x + \frac{1}{2}\Delta h, y + \frac{1}{2}k_1\right)\right] = 0.1 f\left(0.05,1.05\right) = 0.10475$$

$$k_3 = \Delta h\left[f\left(x + \frac{1}{2}\Delta h, y + \frac{1}{2}k_2\right)\right] = 0.1 f\left(0.05,1. + k_2/2\right) = 0.104988$$

$$k_4 = \Delta h\left[f\left(x + \Delta h, y + k_3\right)\right] = 0.1 f\left(0.1,1.104988\right) = 0.109499$$

$$y_{n+1} = y_n + \frac{1}{6}\left[k_1 + 2k_2 + 2k_3 + k_4\right] = 1.104829$$

Runge-Kutta Method (4^{th} Order) Example

The values for the 4^{th} order Runge-Kutta method

x	y	f(x,y)	k_1	f_2	k_2	f_3	k_3	f_4	k_4	Change	Exact
0	1	1	0.1	1.0475	0.10475	1.049875	0.104988	1.094988	0.109499	0.628974	1
0.1	1.104829	1.094829	0.109483	1.13707	0.113707	1.139182	0.113918	1.178747	0.117875	0.682608	1.104829
0.2	1.218597	1.178597	0.11786	1.215027	0.121503	1.216848	0.121685	1.250282	0.125028	0.729263	1.218597
0.3	1.340141	1.250141	0.125014	1.280148	0.128015	1.281648	0.128165	1.308306	0.130831	0.768204	1.340141
0.4	1.468175	1.308175	0.130817	1.331084	0.133108	1.332229	0.133223	1.351398	0.13514	0.79862	1.468175
0.5	1.601278	1.351278	0.135128	1.366342	0.136634	1.367095	0.13671	1.377988	0.137799	0.819614	1.601279
0.6	1.73788	1.37788	0.137788	1.384274	0.138427	1.384594	0.138459	1.38634	0.138634	0.830196	1.737881
0.7	1.876246	1.386246	0.138625	1.383059	0.138306	1.382899	0.13829	1.374536	0.137454	0.82927	1.876247
0.8	2.014458	1.374458	0.137446	1.360681	0.136068	1.359992	0.135999	1.340457	0.134046	0.815626	2.014459
0.9	2.150396	1.340396	0.13404	1.314915	0.131492	1.313641	0.131364	1.28176	0.128176	0.787927	2.150397
1	2.281717	1.281717	0.128172	1.243303	0.12433	1.241382	0.124138	1.195855	0.119586	0.744694	2.281718

The 4th Order Runge-Kutta

The step sizes are:

$$\Delta y = \frac{1}{3}\left[k_1 + k_2 + k_3\right]$$

$$\Delta y' = \frac{1}{3\Delta h}\left[k_1 + 2k_2 + 2k_3 + k_4\right]$$

The next step would be:

$$y(x + \Delta h) = y(x) + \Delta h\, y'(x) + \Delta y$$
$$y'(x + \Delta h) = y'(x) + \Delta y'$$

Explicit Methods

Up until this point we have dealt with:

- Euler Method
- Modified Euler/Midpoint
- Runge-Kutta Methods

These methods are called explicit methods, because they use only the information from previous steps.

Moreover these are one-step methods

One Step Method

The techniques are defined as:

- These methods allow us to vary the step size.
- Use only one initial value.
- After each step is completed the past step is "forgotten: We do not use this information.

Multi-Step Methods

The principle behind a multi-step method is to use past values, y and/or dy/dx to construct a polynomial that approximate the derivative function.

Multi-Step Methods

Similar to quadrature

$$\frac{dy}{dx} = f(x) \qquad \Rightarrow y_{i+1} = y_i + \int_{x_i}^{x_{i+1}} f(x)dx$$

$$dy = f(x)dx$$

$$\int dy = y_{i+1} - y_i = \int_{x_i}^{x_{i+1}} f(x)dx$$

Multi-Step Methods

The integral can be represented.

$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}\left[3f_i - f_{i-1}\right] \qquad \text{Two Point}$$

Three Point Adam Bashforth

$$= \frac{h}{12}\left[23f_i - 16f_{i-1} + 5f_{i-2}\right]$$

Multi-Step Methods

The integral can be represented.

$$\int_{x_i}^{x_{i+1}} f(x)dx$$

Four Point Adam Bashforth

$$= \frac{h}{24}\left[55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}\right]$$

Multi-Step Methods

These methods are known as explicit schemes because the use of current and past values are used to obtain the future step.

The method is initiated by using either a set of known results or from the results of a Runge-Kutta to start the initial value problem.

Adam Bashforth Method (4 Point) Example

Consider

$$\frac{dy}{dx} = y - x^2$$

Exact Solution

$$y = 2 + 2x + x^2 - e^{\mathrm{x}}$$

The initial condition is: $y(0) = 1$

The step size is: $h = 0.1$

4 Point Adam Bashforth

From the 4th order Runge Kutta

$$f(0,1) = 1.0000$$
$$f(0.1,1.104829) = 1.094829$$
$$f(0.2,1.218597) = 1.178597$$
$$f(0.3,1.340141) = 1.250141$$

The 4 Point Adam Bashforth is:

$$\Delta y = \frac{0.1}{24}\left[55 f_{0.3} - 59 f_{0.2} + 37 f_{0.1} - 9 f_0\right]$$

4 Point Adam Bashforth

The results are:

$$\Delta y = \frac{0.1}{24}\left[\begin{array}{c} 55(1.250141) - 59(1.178597) \\ +37(1.094829) - 9(1) \end{array}\right]$$

$$= 0.128038$$

Upgrade the values

$$y(0.4) = 1.340141 + 0.128038 = 1.468179$$

$$f(0.4, 1.468179) = 1.308179$$

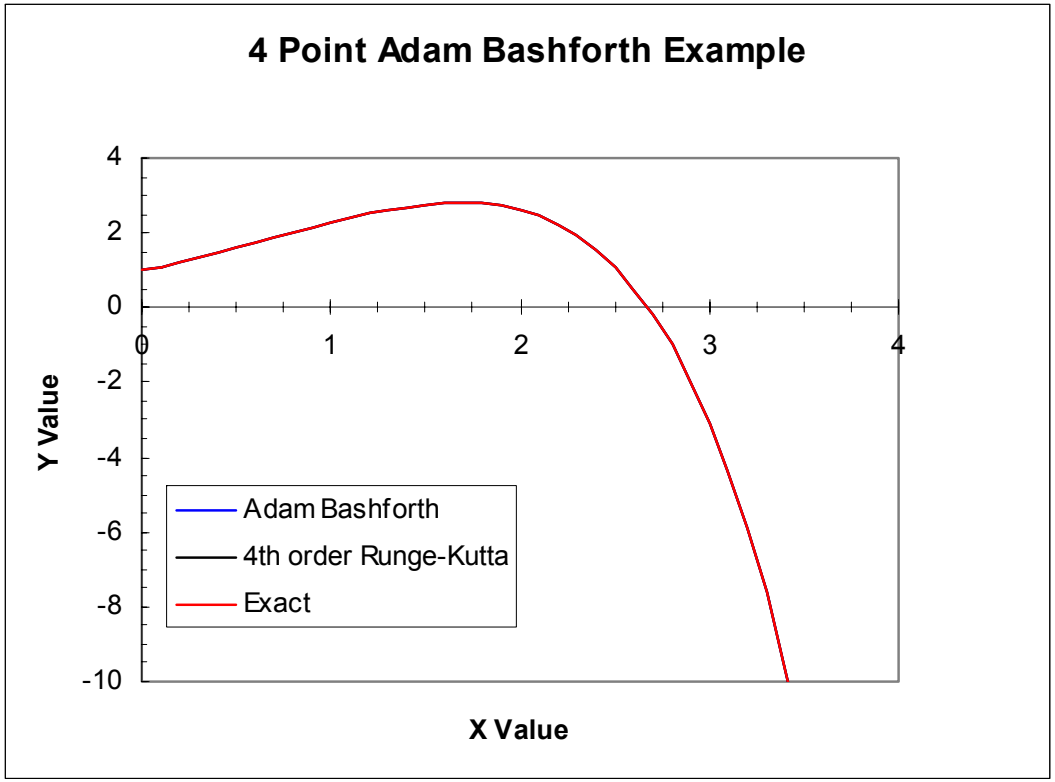
4 Point Adam Bashforth Method - Example

The values for the Adam Bashforth

x	Adam Bashforth	f(x,y)	sum	4th order Runge-Kutta	Exact
0	1	1		1	1
0.1	1.104828958	1.094829		1.104828958	1.104829
0.2	1.218596991	1.178597		1.218596991	1.218597
0.3	1.34014081	1.250141	30.72919	1.34014081	1.340141
0.4	1.468179116	1.308179	31.94617	1.468174786	1.468175
0.5	1.601288165	1.351288	32.78612	1.601278076	1.601279
0.6	1.737896991	1.377897	33.20969	1.737880409	1.737881
0.7	1.876270711	1.386271	33.17302	1.876246365	1.876247
0.8	2.014491614	1.374492	32.62766	2.014458009	2.014459
0.9	2.150440205	1.34044	31.52015	2.150395695	2.150397
1	2.281774162	1.281774	29.79136	2.281716852	2.281718

4 Point Adam Bashforth Method - Example

The explicit Adam Bashforth method gave solution gives good results without having to go through large number of calculations.



Implicit Methods

There are second set of multi-step methods, which are known as implicit methods. The implicit methods use the future steps to modify the future steps.

Since future data is used an iterative method must be used
iterate an initial guess until convergence

Could use Runge-Kutta or Adams Bashforth to start the initial value problem.

Implicit Multi-Step Methods

The main method is Adams Moulton Method

Three Point Adams-Moulton Method

$$\Delta y = \frac{h}{12}\left[5f_{i+1} + 8f_i - f_{i-1}\right]$$

Four Point Adams-Moulton Method

$$\Delta y = \frac{h}{24}\left[9f_{i+1} + 19f_i - 5f_{i-1} + f_{i-2}\right]$$

Implicit Multi-Step Methods

- The method uses what is known as a Predictor-Corrector technique.
- explicit scheme to estimate the initial guess
- uses the value to guess the future y^* and $dy/dx = f^*(x,y^*)$
- Using these results, apply Adam Moulton method

Implicit Multi-Step Methods

Adams third order Predictor-Corrector scheme.

Use the Adam Bashforth three point explicit scheme for the initial guess.

$$y^*_{i+1} = y_i + \frac{\Delta h}{12}\left[23 f_i - 16 f_{i-1} + 5 f_{i-2}\right]$$

Use the Adam Moulton three point implicit scheme to take a second step.

$$y_{i+1} = y_i + \frac{\Delta h}{12}\left[5 f^*_{i+1} + 8 f_i - f_{i-1}\right]$$

Adam Moulton Method (3 point)
Example

Consider

$$\frac{dy}{dx} = y - x^2$$

Exact Solution

$$y = 2 + 2x + x^2 - e^{\mathrm{x}}$$

The initial condition is: $y(0) = 1$

The step size is: $\Delta h = 0.1$

4 Point Adam Bashforth

From the 4th order Runge Kutta

$$f(0,1) = 1.0000$$
$$f(0.1,1.104829) = 1.094829$$
$$f(0.2,1.218597) = 1.178597$$

The 3 Point Adam Bashforth is:

$$\Delta y = \frac{0.1}{12}\left[23 f_{0.2} - 16 f_{0.1} + 5 f_{0.0}\right]$$

3 Point Adam Moulton Predictor-Corrector Method

The results of explicit scheme is:

$$\Delta y = \frac{0.1}{12}\left[23(1.178597) - 16(1.094829) + 5(1)\right]$$
$$= 0.121587$$

The functional values are:

$$y^*(0.3) = 1.218597 + 0.121587 = 1.340184$$
$$f^*(0.3, 1.340184) = 1.250184$$

3 Point Adam Moulton Predictor-Corrector Method

The results of implicit scheme is:

$$\Delta y = \frac{0.1}{12}\left[5(1.250184)+8(1.178597)-1(1.094829)\right]$$
$$= 0.121541$$

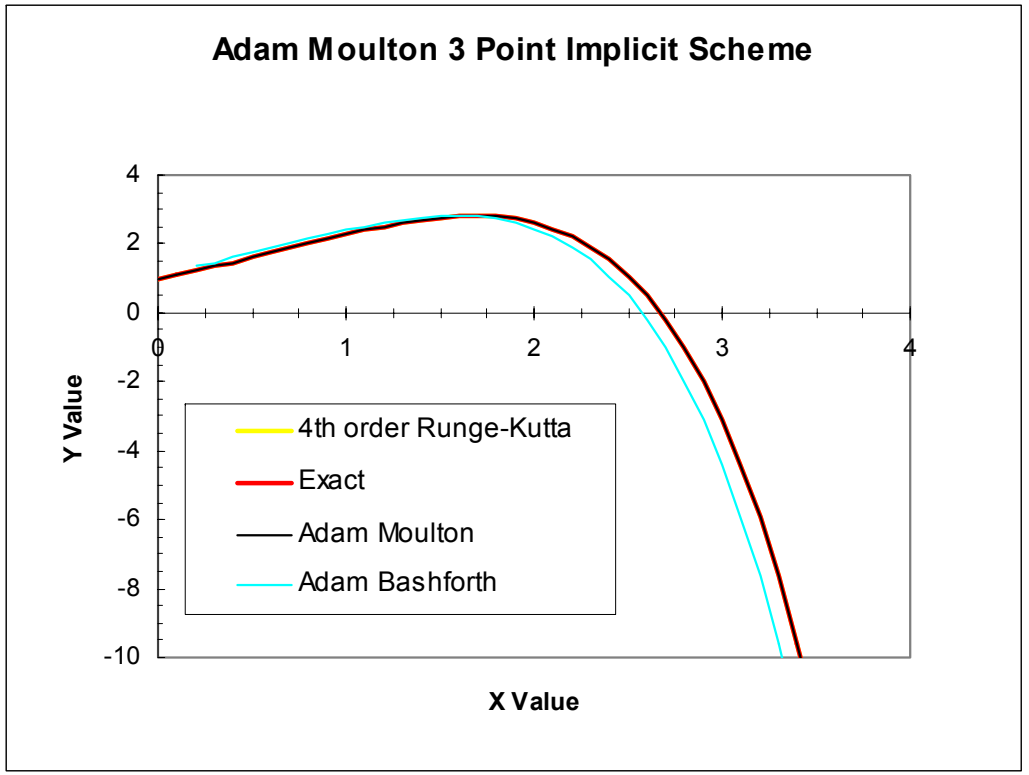
The functional values are:

$$y(0.3) = 1.218597 + 0.121541 = 1.340138$$
$$f(0.3,1.340184) = 1.250138$$

3 Point Adam Moulton Predictor-Corrector Method

The values for the Adam Moulton

	Adam Moulton Three Point Predictor-Corrector Scheme					
x	y	f	sum	y*	f*	sum
0	1	1				
0.1	1.104829	1.094829				
0.2	1.218597	1.178597	0.121587	1.340184	1.250184	0.121541
0.3	1.340138	1.250138	0.128081	1.468219	1.308219	0.12803
0.4	1.468168	1.308168	0.133155	1.601323	1.351323	0.133098
0.5	1.601266	1.351266	0.136659	1.737925	1.377925	0.136597
0.6	1.737863	1.377863	0.138429	1.876291	1.386291	0.138359
0.7	1.876222	1.386222	0.13828	2.014502	1.374502	0.138204
0.8	2.014425	1.374425	0.136013	2.150438	1.340438	0.135928
0.9	2.150353	1.340353	0.131404	2.281757	1.281757	0.13131
1	2.281663	1.281663	0.124206	2.405869	1.195869	0.124102

3 Point Adam Moulton Predictor-Corrector Method

The implicit Adam Moulton method gave solution gives good results without using more than a three points.