Computational Methods
CMSC/AMSC/MAPL 460

Ordinary differential equations

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Explicit and One-Step 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 one-step techniques

- 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.

- Represent f(x,y) as a polynomial in x using known values over the past few steps.
- E.g., using Lagrangian form and equal steps, we have for 3 steps
- $(-2h, f_{-2})$ $(-h, f_{-1})$, $(0,f_0)$
- So the polynomial is
- $f(x)=f_{-2}(x+h)x/(2h^2)$ $-f_{-1}(x+2h)x/h^2+f_0(x+h)$ $(x+2h)$ $/(2h^2)$ $=(x^2(f_{-2}+2f_{-1}+f_0)+hx(f_{-2}+4f_{-1}+3f_0)+2h^2f_0)/2h^2$
- Integrate from (x_i,x_{i+1})

$$y_{n+1} = y_n + h\left(\frac{23}{12}f(t_n, y_n) - \frac{16}{12}f(t_{n-1}, y_{n-1}) + \frac{5}{12}f(t_{n-2}, y_{n-2})\right)$$

Multi-Step Methods

These methods are 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 of the same order to start the initial value problem solution.

Adam Bashforth Method (4 Point) 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: $h = 0.1$

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:

$$\Delta y = \frac{0.1}{24}\begin{bmatrix} 55(1.250141) - 59(1.178597) \\ +37(1.094829) - 9(1) \end{bmatrix}$$

$$= 0.128038$$

Upgrade the values

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

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

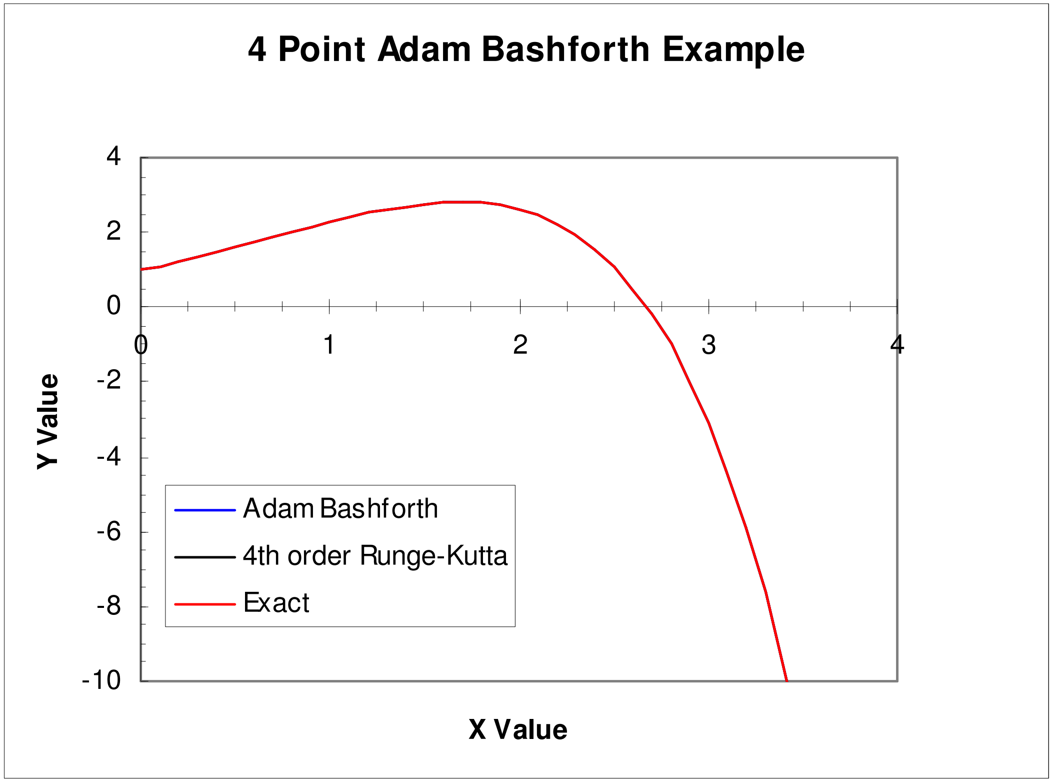
4 Point Adam Bashforth Method - Example

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.



Deriving the Adams Weights

- Recall that

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_{n+1}} y'(t)\,dt$$

- The basic idea of an Adams method is to approximate $y'(t)$ in the above integral by a polynomial $P_k(t)$ of degree k.
- The coefficients of $P_k(t)$ are determined by using the $k+1$ previously calculated data points.
- For example, for $P_1(t) = At + B$, we use $(t_{n\text{-}1}, y_{n\text{-}1})$ and (t_n, y_n), with $P_1(t_{n\text{-}1}) = f(t_{n\text{-}1}, y_{n\text{-}1}) = f_{n\text{-}1}$ and $P_1(t_n) = f(t_n, y_n) = f_n$.
- Then

$$\left.\begin{array}{r} At_{n-1} + B = f_{n-1} \\ At_n + B = f_n \end{array}\right\} \Rightarrow A = \frac{1}{h}\left(f_n - f_{n-1}\right),\ B = \frac{1}{h}\left(f_{n-1}t_n - f_n t_{n-1}\right)$$

Second Order Adams-Bashforth Formula

- Substituting the polynomial in

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_{n+1}} y'(t)dt$$

gives

$$y(t_{n+1}) - y(t_n) = (A/2)\left(t_{n+1}^2 - t_n^2\right) + B\left(t_{n+1} - t_n\right)$$

- After substituting for *A* and *B* and simplifying, we obtain

$$y_{n+1} = y_n + (3/2)hf_n - (1/2)hf_{n-1}$$

- This equation is the **second order Adams-Bashforth** formula. It is an explicit formula for y_{n+1} in terms of y_n and y_{n-1}, and has local truncation error proportional to h^3.
- We note that when a constant polynomial $P_0(t) = A$ is used, the first order Adams-Bashforth formula is just Euler's formula

Fourth Order Adams-Bashforth Formula

- More accurate Adams formulas are obtained by using a higher degree polynomial $P_k(t)$ and more data points.
- For example, the coefficients of a 3rd degree polynomial $P_3(t)$ are found using (t_n, y_n), (t_{n-1}, y_{n-1}), (t_{n-2}, y_{n-2}), (t_{n-3}, y_{n-3}).
- As before, $P_3(t)$ then replaces $y'(t)$ in the integral equation

$$y(t_{n+1}) - y(t_n) = \int_{t_n}^{t_{n+1}} y'(t)\,dt$$

  to obtain the fourth order Adams-Bashforth formula

$$y_{n+1} = y_n + (h/24)\left(55 f_n - 59 f_{n-1} + 37 f_{n-2} - 9 f_{n-3}\right)$$

- The local truncation error of this method is proportional to h^5.

Stability

- It turns out that explicit methods are not very stable
- This means that the solution may oscillate if we use large time steps
- So, if we wish to integrate over a large interval, and we need to take many small steps to achieve accuracy, many function evaluations are needed.
- Implicit methods are usually more stable

Implicit Methods

- There are second set of multi-step methods, which are known as “implicit” methods.
  - “implicit” => not directly revealed
- Here it means that the value of the function at the later time is not provided in an “explicit” formula, but in an equation
- Since future data is used an iterative method must be used to iterate an initial guess to 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

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

Four Point Adams-Moulton Method

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

Deriving Adams-Moulton Weights

- A variation on the Adams-Bashforth formulas gives another set of formulas called the Adams-Moulton formulas.
- We begin with the second order case, and use a first degree polynomial $Q_1(t) = \alpha t + \beta$ to approximate $y'(t)$.
- To determine α and β, we now use (t_n, y_n) and (t_{n+1}, y_{n+1}):

$$\left.\begin{aligned} \alpha t_n + \beta &= f_n \\ \alpha t_{n+1} + \beta &= f_{n+1} \end{aligned}\right\} \Rightarrow \alpha = \frac{1}{h}\left(f_{n+1} - f_n\right),\ \beta = \frac{1}{h}\left(f_n t_{n+1} - f_{n+1} t_n\right)$$

- As before, $Q_1(t)$ replaces $y'(t)$ in the integral equation to obtain the second order Adams-Moulton formula

$$y_{n+1} = y_n + (h/2)\left(f_n + f_{n+1}(t_{n+1}, y_{n+1})\right) = y_n + (h/2)\left(f_n + f_{n+1}\right)$$

- Note that this equation implicitly defines y_{n+1}. The local truncation error of this method is proportional to h^3.

Fourth Order Adams-Moulton Formula

- When a constant polynomial $Q_0(t) = \alpha$ is used, the first order Adams-Moulton formula is just the backwards Euler formula.
- More accurate higher order formulas can be obtained using a polynomial of higher degree.
- For example, the fourth order Adams-Moulton formula is

$$y_{n+1} = y_n + (h/24)\left(9 f_{n+1} + 19 f_n - 5 f_{n-1} + f_{n-2}\right)$$

- The local truncation error of this method is proportional to h^5.

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

E.g., Adams third order Predictor-Corrector scheme.

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

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

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

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

Adam Moulton Method (3 point) 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: $\Delta h = 0.1$

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.