Computational Methods

CMSC/AMSC/MAPL 460

Ordinary differential equations

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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 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

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

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

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

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

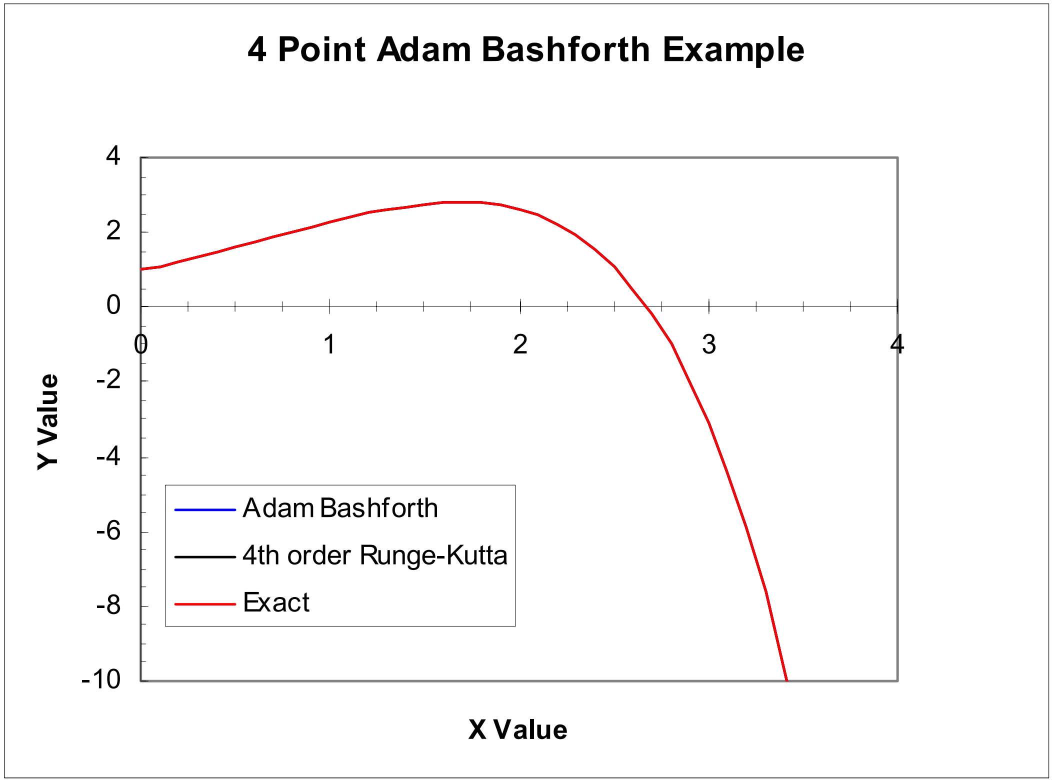
4 Point Adam Bashforth Method - Example

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.



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. 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

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

Four Point Adams-Moulton Method

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

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

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

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:

$$y(0.3) = 1.218597 + 0.121541 = 1.340138$$

$$f(0.3, 1.340184) = 1.250138$$

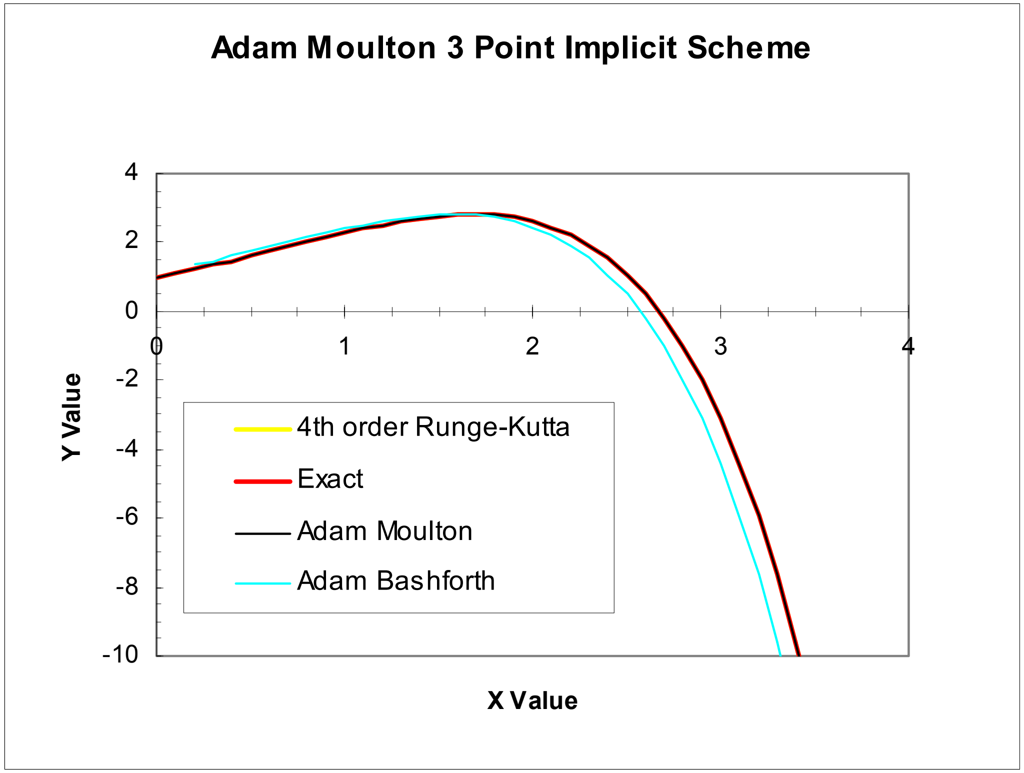
3 Point Adam Moulton Predictor-Corrector Method

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.



Nonlinearity

- In general the quantity on the right hand side, *f*, in the standard form can be a nonlinear function of *t* and *y*.
- Nonlinearity implies multiple solutions and “chaos”
- Also has a bearing on how well a numerical solver can integrate the ODE

Linearized Diff Eq.

- Standard form $\frac{dy}{dt} = f(t, y)$ $\quad y(t_0) = y_0$
- Local behavior of the solution to a differential equation near any point (t_c, y_c) can be analyzed by expanding $f(t,y)$ in a two-dimensional Taylor series.

$$f(t, y) = f(t_c, y_c) + \alpha(t - t_c) + J(y - yc) + \dots$$

- where $\alpha = \partial f/\partial t\ (t_c, y_c)$

$$J = \partial f/\partial y\ (t_c, y_c)$$

  - (We already used such expansions for deriving the RK method)
- These equations are linear and can consider the three terms on the rhs separately
- Behavior of differential equation governed by the structure of the Jacobian matrix *J*

Linearized differential equations

For a system of differential equations with n components,

$$\frac{d}{dt}\begin{bmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_n(t) \end{bmatrix} = \begin{bmatrix} f_1(t, y_1, \ldots, y_n) \\ f_2(t, y_1, \ldots, y_n) \\ \vdots \\ f_n(t, y_1, \ldots, y_n) \end{bmatrix}$$

the Jacobian is an n-by-n matrix of partial derivatives

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} & \cdots & \frac{\partial f_1}{\partial y_n} \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} & \cdots & \frac{\partial f_2}{\partial y_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial y_1} & \frac{\partial f_n}{\partial y_2} & \cdots & \frac{\partial f_n}{\partial y_n} \end{bmatrix}$$

Jacobian properties

- Interesting equation $$\frac{dy}{dt} = Jy$$
- In one dimension it can be integrated to obtain the local solution

$$y=C \exp(J\ t)$$

- Express solution similarly for a system.
- Use the eigendecomposition of the Jacobian matrix

$$J=V\Lambda\ V^{-1}$$

  - V matrix with columns as eigenvectors
  - Λ eigenvalues arranged as a diagonal matrix
- Why? It removes the coupling of terms in the right hand side by diagonalizing the matrix
- $y'=Jy.$ So $V^{-1}y'=V^{-1}JVV^{-1}y$
- Let $V x = y$ *so* $x=V^{-1}y$
- transforms the local system of equations to
- $dx_k/dt = \lambda_k x_k$ $x_k(t) = e^{\lambda_k(t-t_c)}\, x(t_c)$

- A single component $x_k(t)$ has the following behaviors according to $\lambda_k = \mu_k + i\ \nu_k$
- If μ_k is positive it grows
- It decays if μ_k is negative,
- and oscillates if ν_k is nonzero.
- Example: harmonic oscillator $d^2 y / d t^2 = -y$
- s a linear system. The Jacobian is simply the matrix
- $J = [\ 0\ \ 1\ ]$

  $[\ -1\ 0\ ]$
- has purely imaginary eigenvalues

Eigenvalues of examples considered

Another example from the book

$$\ddot{u}(t) = -u(t)/r(t)^3$$
$$\ddot{v}(t) = -v(t)/r(t)^3$$

where

$$r(t) = \sqrt{u(t)^2 + v(t)^2}$$

$$J = \frac{1}{r^5}\begin{bmatrix} 0 & 0 & r^5 & 0 \\ 0 & 0 & 0 & r^5 \\ 2y_1^2 - y_2^2 & 3y_1y_2 & 0 & 0 \\ 3y_1y_2 & 2y_2^2 - y_1^2 & 0 & 0 \end{bmatrix}$$

- one eigenvalue is real and positive, so that component is growing.
- One eigenvalue is real and negative, corresponding to a decaying component.
- Two eigenvalues are purely imaginary, corresponding to oscillatory components.

The vector $y(t)$ has four components,

$$y(t) = \begin{bmatrix} u(t) \\ v(t) \\ \dot{u}(t) \\ \dot{v}(t) \end{bmatrix}$$

The differential equation is

$$\dot{y}(t) = \begin{bmatrix} \dot{u}(t) \\ \dot{v}(t) \\ -u(t)/r(t)^3 \\ -v(t)/r(t)^3 \end{bmatrix}$$

$$\lambda = \frac{1}{r^{3/2}}\begin{bmatrix} \sqrt{2} \\ i \\ -\sqrt{2} \\ -i \end{bmatrix}$$

Jacobian and ode behavior

- $J = \partial f / \partial y$
- Then a **single** ODE is
  - **stable** at a point (t_c, y_c) if $J(t_c, y_c) < 0$.
  - **unstable** at a point (t_c, y_c) if $J(t_c, y_c) > 0$.
  - **stiff** at a point (t_c, y_c) if $J(t_c, y_c) << 0$.
- A **system** of ODEs is
  - **stable** at a point (t_c, y_c) if the **real part** of all the **eigenvalues** of the matrix $J(t_c, y_c)$ are negative (converse if some are positive)
  - **stiff** at a point (t_c, y_c) if the **real parts** of more than one eigenvalue of $J(t_c, y_c)$ are negative and wildly different.

Stiffness

- Stiffness
  - *A problem is stiff if the solution being sought is varying slowly, but there are nearby solutions that vary rapidly, so the numerical method must take small steps to obtain satisfactory results.*
- Example problem: A match is lit and the fire grows as a ball of flame. until it reaches a critical size. It then remains at that size because the amount of oxygen being consumed by the combustion in the interior of the ball balances the amount available through the surface.
- Let *y(t)* represent the ball radius. y^2 is proportional to the surface area while y^3 to the volume
  - $y' = y^2 - y^3$
  - $y(0) = \eta$
  - $0 \leq t \leq 2/\eta$

Solution using regular and stiff-solver

- choose η=0.01 and 0.0001
- Solve with RK45
- Observe
- Solve with ode23s
- Observe

Error control

- Get estimate of the error at current step
  - change step size
  - change the order
- then use the difference in results to get an estimate of the error
- **Suppose error estimate is much too large:**
  - reduce the stepsize (usually by a factor of 2) and try again.
- **Suppose error estimate is much smaller than needed:**
  - Then we can increase the stepsize (usually doubling it) and save ourselves some work when we take the **next** step.

Chaos: The Lorenz attractor

- Expressed in standard form
- Seven of Nine coefficients are numerical
- Two are non-linear
- Solution keeps flipping between two basins of attraction

$$\dot{y} = Ay$$

$$y(t) = \begin{pmatrix} y_1(t) \\ y_2(t) \\ y_3(t) \end{pmatrix}$$

$$A = \begin{bmatrix} -\beta & 0 & y_2 \\ 0 & -\sigma & \sigma \\ -y_2 & \rho & -1 \end{bmatrix}$$