ESS101- Modeling and Simulation Lecture 15

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Today (Chapters 4, 5)

- Linear Multistep Methods
 - Trapezoidal rule
 - The Adams-Bashforth method
- Two-step methods
 - Consistency
- **☞** Convergence and Zero-stability

Basics on simulation (IVP)

We assume the mathematical model is in the form

$$\dot{x}(t) = f(t, x(t), u(t))$$

By assuming that u(t) is a known function of the time

$$\dot{x}(t) = f(t, x(t))$$

The problem of simulating the model $\dot{x} = f(t,x(t))$ can be formulated as follows

Given the initial condition x(0), finding a sequence of points $x_1, x_2, ... x_{tf}$ approximating the solution x at the time instants $0 < t_1 < t_2 < ... < t_f$, i.e., the $x(t_1), x(t_2), ..., x(t_f)$

FE and TS(p) methods

For FE

$$x_{n+1} = x_n + h\dot{x}_n$$
$$E_n = O(h)$$

For TS(p)

$$X_{n+1} = X_n + \sum_{i=1}^{p} \frac{1}{i!} h^i X_n^{(i)}$$

$$E_n = O(h^p)$$

But, TS(p) methods require high order derivative of the rhs

Impratical for larger ODE and when an analytical expression of \dot{x} is not available

Idea. Achieve accuracy of TS(p) methods by exploiting previous solutions rather than higher order derivatives

Trapezoidal rule

Idea. Achieve accuracy of TS(p) methods by exploiting previous solutions rather than higher order derivatives

Calculate the Taylor expansion

$$\dot{x}(t+h) = \dot{x}(t) + h\ddot{x}(t) + O(h^2)$$

Substitute
$$h\ddot{x}(t) = \dot{x}(t+h) - \dot{x}(t) + O(h^2)$$
 in
$$x(t+h) = x(t) + h\dot{x}(t) + \frac{1}{2!}h^2\ddot{x}(t) + O(h^3)$$

$$\underline{x_{n+1}} = x_n + h\dot{x}_n + \frac{1}{2}h(\dot{x}_{n+1} - \dot{x}_n)$$

$$= x_n + \frac{1}{2}h(f_{n+1} + f_n)$$

Trapezoidal rule

Note that in
$$x_{n+1} = x_n + \frac{1}{2}h(f_{n+1} + f_n)$$

We need to calculate $f_{n+1} = f(t_{n+1}, x_{n+1})$

That is, x_{n+1} is on both left and right hand sides

We may not have an explicit expression of x_{n+1} as function of the previous samples (*implicit method*)

Implicit and explicit methods

In general, an algorithm for solving a differential equation (or ODE solver) can be expressed as

$$x_{n+1} = G(t, x_{n-k+1}, x_{n-k+2}, \dots, x_n, x_{n+1})$$

Implicit method

k-steps method

$$x_{n+1} = G(t, x_{n-k+2}, \dots, x_n, x_{n+1})$$

This equation needs to be solved to find x_{n+1}

Explicit method

$$X_{n+1} = G(t, X_{n-k+1}, X_{n-k+2}, \dots, X_n)$$

2-step Adam-Bashforth method (AB(2))

Instead of

$$\dot{x}(t+h) = \dot{x}(t) + h\ddot{x}(t) + O(h^2)$$

calculate the Taylor expansion as

$$\dot{x}(t-h) = \dot{x}(t) - h\ddot{x}(t) + O(h^2)$$

The resulting iteration is

$$\underline{x_{n+1}} = x_n + h\dot{x}_n + \frac{1}{2}h(\dot{x}_n - \dot{x}_{n-1})$$

$$= x_n + \frac{1}{2}h(3f_n - f_{n-1})$$

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Example. Comparison of AB(2) and TS(2)

Simulate the system

$$\dot{x}(t) = (1 - 2t)x(t), \quad x(0) = 1$$

over the time interval $0 \le t \le 0.9$

Recall the *exact solution* $x(t) = e^{\frac{1}{4} - \left(\frac{1}{2} - t\right)^2}$

The iteration is

$$x_{n+2} = x_{n+1} + \frac{1}{2}h(3f_{n+1} - f_n)$$

$$= x_{n+1} + \frac{1}{2}h[3(1 - 2t_{n+1})x_{n+1} - (1 - 2t_n)x_n]$$

Example. Comparison of AB(2) and TS(2)

For
$$n=0$$

$$x_2 = \left[1 + \frac{3}{2}h(1-2h)\right]x_1 - \frac{1}{2}h$$

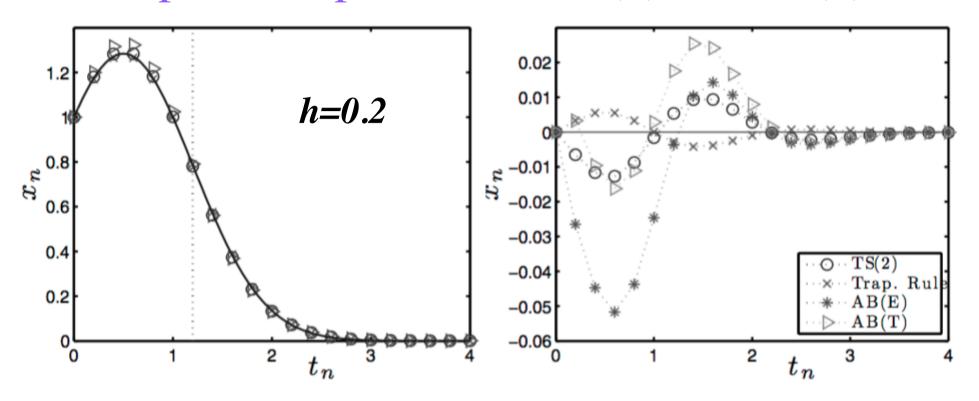
How do we calculate x_1 ?

1.
$$x_1 = (1+h)x_0$$
 Euler (ABE)

2.
$$x_1 = x_0 + \frac{1}{2}h[(1-2t_1)x_1 + (1-2t_0)x_0] \Rightarrow$$

$$\Rightarrow x_1 = \frac{1 + \frac{1}{2}(1 - 2t_0)}{1 - \frac{1}{2}(1 - 2t_1)} x_0$$
 Trapezoidal rule (ABT)

Example. Comparison of AB(2) and TS(2)



 $10^{3}GE@ t=1.2$

h	TS(2)	Trap.	ABE	ABT
0.2	5.4	-2.8	-3.6	17.6
0.1	1.4	-0.71	-0.66	4.0
Ratio	3.90	4.00	5.49	4.40

$$E_n \propto h^2$$

Two-step methods. Consistency

k	p	Method	Name
1	1	$x_{n+1} - x_n = hf_n$	Euler
1	1	$\mid x_{n+1} - x_n = h f_{n+1}$	Backward Euler
1	2	$x_{n+1} - x_n = \frac{1}{2}h(f_{n+1} + f_n)$	${ m trapezoidal}$
2	2	$x_{n+2} - x_{n+1} = \frac{1}{2}h(3f_{n+1} - f_n)$	two-step Adams–Bashforth
2	2	$x_{n+2} - x_{n+1} = \frac{1}{12}h(5f_{n+2} + 8f_{n+1} - f_n)$	two-step Adams-Moulton
2	4	$x_{n+2} - x_n = \frac{1}{3}h(f_{n+2} + 4f_{n+1} + f_n)$	Simpson's rule
2	3	$x_{n+2} + 4x_{n+1} - 5x_n = h(4f_{n+1} + 2f_n)$ D	ahlquist (see Example 4.11)

More in general

$$x_{n+2} + \alpha_1 x_{n+1} + \alpha_0 x_n = h \left(\beta_2 f_{n+2} + \beta_1 f_{n+1} + \beta_0 f_n \right)$$

that is *consistent* and of *order p* if

$$x(t+2h) + \alpha_1 x(t+h) + \alpha_0 x(t) - h \left[\beta_2 \dot{x}(t+2h) + \beta_1 \dot{x}(t+h) + \beta_0 \dot{x}(t) \right] = O(h^{p+1})$$

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Two-step methods. Consistency

Definition (Consistency). A two-step LMM method is consistent if a p>0 exists such that

$$x(t+2h) + \alpha_1 x(t+h) + \alpha_0 x(t) - h \left[\beta_2 \dot{x}(t+2h) + \beta_1 \dot{x}(t+h) + \beta_0 \dot{x}(t) \right] = O(h^{p+1})$$

Otherwise, it is *inconsistent*.

Example. The Euler method

The *n*-th iteration $x_{n+1} = x_n + hf_n$ stems from

$$x(t+h) = x(t) + h\dot{x}(t) + O(h^2) \Longrightarrow$$

$$\Rightarrow x(t+h) - x(t) - h\dot{x}(t) = O(h^2)$$

Hence, the method is consistent of order p=1

Example. Consistency

Determine the consistency order of the integration method (last in the table)

$$x_{n+2} + 4x_{n+1} - 5x_n = h(4f_{n+1} + 2f_n)$$

We have to find the *p* in

$$x(t+2h) + 4x(t+h) - 5x(t) - h[4\dot{x}(t+h) + 2\dot{x}(t)] = O(h^p)$$

Let's expand in Taylor series the terms on the lhs

$$x(t+2h) = x(t) + 2h\dot{x} + 2h^{2}\ddot{x}(t) + \frac{4}{3}h^{3}\ddot{x}(t) + \frac{2}{3}h^{4}x^{(4)}(t) + O(h^{5})$$

$$x(t+h) = x(t) + h\dot{x} + \frac{1}{2}h^{2}\ddot{x}(t) + \frac{1}{6}h^{3}\ddot{x}(t) + \frac{1}{24}h^{4}x^{(4)}(t) + O(h^{5})$$

Example. Consistency

$$\dot{x}(t+h) = \dot{x}(t) + h\ddot{x}(t) + \frac{1}{2}h^2\ddot{x}(t) + \frac{1}{6}h^3x^{(4)}(t) + O(h^4)$$

By summing up the and collecting the terms

$$x(t+2h) + 4x(t+h) - 5x(t) - h\left[4\dot{x}(t+h) + 2\dot{x}(t)\right] =$$

$$(1+4-5)x(t) + h\left[2+4-(4+2)\right]\dot{x}(t)$$

$$+h^{2}\left[2+2-4\right]\ddot{x}(t) + h^{3}\left[\frac{4}{3}+4\times\frac{1}{6}-4\times\frac{1}{2}\right]\ddot{x}(t)$$

$$+h^{4}\left[\frac{2}{3}+4\times\frac{1}{24}-4\times\frac{1}{6}\right]x^{(4)}(t)$$

Example. Consistency

After simplification

$$x(t+2h) + 4x(t+h) - 5x(t) - h[4\dot{x}(t+h) + 2\dot{x}(t)] = \frac{1}{6}h^4x^{(4)}(t) + O(h^5)$$

$$\frac{1}{6}h^4x^{(4)}(t)$$
 is dominating and $O(h^5)$ can be neglected

$$\frac{1}{6}h^4x^{(4)}(t) = O(h^4)$$
 and the method is of order 3

Two-step methods. Consistency conditions

Theorem (consistency conditions for two-step LMMs). Given the two-step LMM

$$x_{n+2} + \alpha_1 x_{n+1} + \alpha_0 x_n = h \left(\beta_2 f_{n+2} + \beta_1 f_{n+1} + \beta_0 f_n \right)$$

define the two polynomials

$$\rho(r) = r^2 + \alpha_1 r + \alpha_0$$

$$\sigma(r) = \beta_2 r^2 + \beta_1 r + \beta_0$$

The method is consistent if and only if

$$\rho(1) = 0$$
, $\rho'(1) = \sigma(1)$

Two-step methods. Necessary condition for convergence

Theorem (necessary condition for convergence). A convergent LMM is consistent.

A consistent LMM is not guaranteed to be convergent

Example

Solve the IVP $\dot{x}(t) = -x(t)$, x(0) = 1 with the LMM

$$x_{n+2} + 4x_{n+1} - 5x_n = h(4f_{n+1} + 2f_n)$$

with h=0.1, 0.01, 0.001

The LMM can be rewritten as

$$x_{n+2} + 4x_{n+1} - 5x_n = -h(4x_{n+1} + 2x_n)$$

and rearranged as

$$x_{n+2} = -4(1+h)x_{n+1} + (5-2h)x_n$$

Example

h = 0.1		h = 0.01		h = 0.001	
$x_7 =$	0.544	$x_{13} =$	0.938	$x_{19} =$	1.070
$x_8 =$	0.199	$x_{14} =$	0.567	$x_{20} =$	0.535
$x_9 =$	1.735	$x_{15} =$	2.384	$x_{21} =$	3.205
$x_{10} =$	-6.677	$x_{16} =$	-6.810	$x_{22} = -$	-10.159
$x_{11} =$	37.706	$x_{17} =$	39.382	$x_{23} =$	56.697
$x_{12} = -197.958$		$x_{18} = -193.017$		$x_{24} = -277.788$	

No matter how small is h, the solution oscillates

k-step methods

The two-step LMM

$$x_{n+2} + \alpha_1 x_{n+1} + \alpha_0 x_n = h \left(\beta_2 f_{n+2} + \beta_1 f_{n+1} + \beta_0 f_n \right)$$

can be generalized to k-step LMM

$$x_{n+k} + \alpha_{k-1} x_{n+k-1} + \dots + \alpha_0 x_n = h \left(\beta_k f_{n+k} + \beta_{k-1} f_{n+k-1} + \dots + \beta_0 f_n \right)$$

Given the starting values $x_0, x_1, ..., x_{k-1}$

Any method is required to *converge* as $h \rightarrow 0$

That is, the approximated solution should be equal to the actual as $h \rightarrow 0$

Convergence is required also for $x_1, ..., x_{k-1}$, since they are calculated with a numerical method as well

k-step methods. Consistency

In order to have convergence, we must have consistency

Define the polynomials

$$\rho(r) = \sum_{i=0}^{k} \alpha_i r^i, \ \alpha_k = 1 \text{ and } \sigma(r) = \sum_{i=0}^{k} \beta_i r^i$$

The consistency conditions become

$$\sum_{i=0}^{k} \alpha_i = 0, \ \alpha_k = 1, \text{ and } \sum_{i=0}^{k} i\alpha_i = \sum_{i=0}^{k} \beta_i$$

Example

Solve the IVP $\dot{x}(t) = 0$, x(0) = 1 with the LMM

$$x_{n+2} + 4x_{n+1} - 5x_n = h(4f_{n+1} + 2f_n)$$

Use $x_1 = 1 + h$

The LMM becomes $x_{n+2} + 4x_{n+1} - 5x_n = 0$

Note that the polynomial $\rho(r) = r^2 + 4r - 5$ has two roots r=1 and r=5

The solution of the equation is $x_n = A + B(-5)^n$ where A, B are determined from the initial condition and x_1

 x_n diverges while it should be constant and equal to 1

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Convergence and Zero-stability

Definition (**Zero-stability**). A LMM is zero stable if all the roots of

$$\rho(r) = \sum_{i=0}^{k} \alpha_i r^i, \ \alpha_k = 1$$

satisfy the condition $|r| \le 1$ (root condition) and the ones satisfying |r| = 1 have multiplicity 1

Theorem (necessary and sufficient condition for convergence). A LMM is convergent if and only if is consistent and zero-stable