AM213B Numerical Methods for the Solution of Differential Equations

Lecture 04

List of topics in this lecture

- All Runge-Kutta methods are stable. All consistent RK methods are convergent.
- Linear multi-step methods (LMM), general design, general form
- Polynomial interpolation, order of accuracy of interpolation
- Construction of Adams methods
- Orders of accuracy of Adams-Bashforth methods and Adams-Moulton methods

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Stability of Runge-Kutta methods

Consider an explicit Runge-Kutta method:

$$k_i = hf\left(u_n + \sum_{j=1}^{i-1} a_{ij} k_j, t_n + c_i h\right), \qquad i = 1, \ldots, p$$

$$u_{n+1} = u_n + \sum_{i=1}^{p} b_i k_i$$

We write it in terms of numerical operator.

$$u_{n+1} = L_{num}(u_n), \qquad \text{where } L_{num}(u_n) = u_n + h\psi(u_n, t_n)$$

In general, $\psi(u, t)$ is Lipschitz continuous when $f(u, t)$ is Lipschitz continuous.

$$\left|\psi(u,t) - \psi(v,t)\right| \le C_L \left|u - v\right|$$

It follows that the Runge-Kutta method is stable.

$$\begin{aligned}\left|L_{num}(u_n) - L_{num}(v_n)\right| &\le \left|u_n - v_n\right| + \left|h\psi(u_n,t_n) - h\psi(v_n,t_n)\right| \\ &\le (1 + C_L h)\left|u_n - v_n\right|\end{aligned}$$

<u>Example:</u>

<u>Euler method:</u>

$$u_{n+1} = u_n + hf(u_n, t_n) \equiv u_n + h\psi(u_n, t_n)$$

==> $\psi(u,t) = f(u,t)$

Therefore, ψ and f have the same Lipschitz continuity.

Heun's method:

$$u_{n+1} = u_n + \frac{h}{2}\Big[f(u_n,t_n) + f\Big(u_n + hf(u_n,t_n),\ t_n + h\Big)\Big] \equiv u_n + h\psi(u_n,t_n)$$

==> $\psi(u,t) = \frac{1}{2} f(u,t) + \frac{1}{2} f\Big(u + hf(u,t),\ t+h\Big)$

Suppose f is Lipschitz continuous.

$$\begin{aligned}
&\left|\psi(u,t) - \psi(v,t)\right| \\
&\quad \le \frac{1}{2}\left| f(u,t) - f(v,t)\right| + \frac{1}{2}\left| f\Big(u + hf(u,t), t+h\Big) - f\Big(v + hf(v,t), t+h\Big)\right| \\
&\quad \le \frac{1}{2} C_L \left|u - v\right| + \frac{1}{2} C_L \left|(u - v) + h\Big(f(u,t) - f(v,t)\Big)\right| \\
&\quad \le C_L \left|u - v\right| + \frac{h}{2} C_L \left| f(u,t) - f(v,t)\right| \\
&\quad \le C_L \left|u - v\right| + \frac{h}{2} C_L^{\,2} \left|u - v\right| = \left(C_L + \frac{h}{2} C_L^{\,2} \right)\left|u - v\right|
\end{aligned}$$

==> ψ is Lipschitz continuous.

Conclusion: All explicit Runge-Kutta methods are stable.

We will see that implicit Runge-Kutta methods have even better stability.

Therefore, all consistent Runge-Kutta methods are convergent!

Advantage and disadvantage of Runge-Kutta methods

Advantage:

It is single-step. Given u_0, it requires no additional condition to get started.

We can change time step at any step.

Disadvantage:

"p-stage" means each time step requires p evaluations of function $f(u, t)$. If this function evaluation is computationally expensive, the method is slow.

Next we study multi-step methods, which require only 1 function evaluation per time step.

Linear Multi-step Methods (LMM)

The general picture:

Start with given $u(t)$ at r time levels $\{t_n, t_{n+1}, \ldots, t_{n+r-1}\}$.

To calculate $u(t)$ at t_{n+r}, we use

- a linear combination of $u(t)$ at time levels $\{t_n, t_{n+1}, \ldots, t_{n+r-1}\}$,
- a linear combination of $f(u(t), t)$ at time levels $\{t_n, t_{n+1}, \ldots, t_{n+r-1}\}$, and
- possibly $f(u(t), t)$ at time level t_{n+r}

If $f(u(t), t)$ at t_{n+r} is used, the method is implicit.

Repeat the process with $u(t)$ at a new set of r time levels, $\{t_{n+1}, \ldots, t_{n+r-1}, t_{n+r}\}$ …

The general form:

An r-step linear multi-step method has the form

$$\sum_{j=0}^{r} \alpha_j u_{n+j} = h \sum_{j=0}^{r} \beta_j f(u_{n+j}, t_{n+j}), \qquad \alpha_r = 1$$

By convention, we set $\alpha_r = 1$.

Remarks:

- Here "linear" means "the RHS of the method is a linear combination of f". It does not mean "function f is linear in u". In particular, a linear multi-step method can be used to solve a non-linear ODE.
- A linear multi-step method is completely specified by coefficients $\{\alpha_j\}$ and $\{\beta_j\}$.
- It is explicit if and only if $\beta_r = 0$.
- It is a multi-step method if and only if $r > 1$.
- For numerical implementation, we use

$$u_{n+r} = \sum_{j=0}^{r-1} (-\alpha_j) u_{n+j} + h \sum_{j=0}^{r} \beta_j f(u_{n+j}, t_{n+j})$$

- At each time step, it requires ONLY 1 evaluation of function f.

The Adams methods:

$$u_{n+r} = u_{n+r-1} + h\sum_{j=0}^{r} \beta_j f(u_{n+j}, t_{n+j})$$

Coefficients $\{\alpha_j\}$ of Adams methods are given by

$$\alpha_j = \begin{cases} 1, & j = r \\ -1, & j = r-1 \\ 0, & j < (r-1) \end{cases}$$

There are two types of Adams methods: <u>explicit</u> and <u>implicit</u>.

<u>Adams-Bashforth</u> methods are characterized by

$\beta_r = 0$ ==> explicit

<u>Adams-Moulton</u> methods are characterized by

$\beta_r \neq 0$ ==> implicit

Now we look at how to construct these Adams methods.

<u>Basic idea of Adams methods:</u>

- Find a polynomial approximation for $f(u(t), t)$, based on values of f at $(s+1)$ time levels, $\{t_n, t_{n+1}, \ldots, t_{n+s}\}$. Let $p(t)$ denote the polynomial approximation.
- Integrate the ODE from t_{n+r-1} to t_{n+r} and use the polynomial $p(t)$ to replace $f(u(t), t)$. The relation between r and s will be discussed below.

$$u(t_{n+r}) = u(t_{n+r-1}) + \int_{t_{n+r-1}}^{t_{n+r}} u'(t)dt = u(t_{n+r-1}) + \int_{t_{n+r-1}}^{t_{n+r}} f\big(u(t), t\big)dt$$

$$\approx u(t_{n+r-1}) + \int_{t_{n+r-1}}^{t_{n+r}} p(t)dt$$

The Adams methods have the form

$$\boxed{u_{n+r} = u_{n+r-1} + \int_{t_{n+r-1}}^{t_{n+r}} p(t)dt}$$

For explicit Adams methods, we set $r = s + 1$ so that t_{n+r} is not one of the time levels used in polynomial interpolation, $\{t_n, t_{n+1}, \ldots, t_{n+s}\}$.

For implicit Adams methods, we set $r = s$. Time level $t_{n+r} = t_{n+s}$ is used in interpolation. As a result, the unknown u_{n+r} also appears on the RHS of the method.

We study the key component in this construction: polynomial interpolation.

Polynomial interpolation:

Given m data points of function $g(x)$:

$$\{x_j,\ y_j\}, \qquad j=1,2,...,m$$

where $y_j = g(x_j)$.

Goal: Find a polynomial of degree (m-1) or less, $p(x)$, such that

$$p(x_j)=y_j, \qquad j=1,2,...,m$$

That is, the fitting polynomial goes through all m data points exactly.

Solution: We can write out the polynomial $p(x)$ directly.

We introduce a sequence of m special polynomials, each of degree (m-1).

Let

$$p_j(x)\equiv\prod_{\substack{k=1\\k\neq j}}^{m}\left(\frac{x-x_k}{x_j-x_k}\right), \qquad j=1,2,...,m$$

Polynomial $p_j(x)$ is of degree (m-1) and satisfies

$$p_j(x_i)=\begin{cases}1, & i=j\\ 0, & \text{otherwise}\end{cases}$$

Claim: the polynomial interpolation, $p(x)$, is given by

$$\boxed{p(x)=\sum_{j=1}^{m}y_j\,p_j(x), \qquad p_j(x)\equiv\prod_{\substack{k=1\\k\neq j}}^{m}\left(\frac{x-x_k}{x_j-x_k}\right)}$$

Verifying the claim:

- $p(x)$ is a polynomial of degree (m–1) or less;
- $p(x)$ goes through all m data points exactly:

$$p(x_i)=\sum_{j=1}^{m}y_j\,p_j(x_i)=y_i$$

Example:

Consider 3 data points of function $g(x)$ at $\{x_1 = -2, x_2 = -1, x_3 = 0\}$.

$$\{\ y_j = g(x_j),\ \ j = 1, 2, 3\ \}$$

The 3 special polynomials have the general expression

$$p_j(x) \equiv \prod_{\substack{k=1 \\ k \neq j}}^{m} \left(\frac{x - x_k}{x_j - x_k} \right), \qquad j = 1, 2, 3$$

Notice that in $p_j(x)$,

Numerator = product of $(x - x_k)$ over index k, excluding $k = j$.

Denominator = (Numerator | $x = x_j$).

For our specific data set, we write out the 3 special polynomials

$$p_1(x) \equiv \frac{(x+1)x}{(x+1)x\big|_{x=-2}} = \frac{(x+1)x}{(-1)(-2)} = \frac{1}{2}(x^2 + x)$$

$$p_2(x) \equiv \frac{(x+2)x}{(x+2)x\big|_{x=-1}} = \frac{(x+2)x}{(1)(-1)} = -(x^2 + 2x)$$

$$p_3(x) \equiv \frac{(x+2)(x+1)}{(x+2)(x+1)\big|_{x=0}} = \frac{(x+2)(x+1)}{(2)(1)} = \frac{1}{2}(x^2 + 3x + 2)$$

The polynomial interpolation of the 3 data points is

$$p(x) = y_1 p_1(x) + y_2 p_2(x) + y_3 p_3(x)$$

Construction of Adams methods

We first calculate the interpolation of $f(u(t), t)$ at <u>3 time levels</u>, $\{t_n, t_{n+1}, t_{n+2}\}$. <u>Here $s = 2$</u>.

Then we use the interpolation to construct the Adams methods (explicit and implicit). The value of r depends on whether the method is explicit ($r = 3$) or implicit ($r = 2$).

We transform t by a shifting and a scaling to utilize the polynomial interpolation obtained above for $\{x_1 = -2, x_2 = -1, x_3 = 0\}$.

Let $\quad x = \dfrac{t - t_{n+2}}{h}$

$$\left\{ t_n, t_{n+1}, t_{n+2} \right\} \longrightarrow \left\{ x_1 = -2,\ x_2 = -1,\ x_3 = 0 \right\}$$

Let $p^{\{x\}}(x)$ denote the polynomial interpolation in variable x.

Let $p^{\{t\}}(t)$ denote the polynomial interpolation in variable t.

$p^{\{t\}}(t)$ is related to $p^{\{x\}}(x)$ as

$$p^{\{t\}}(t)=p^{\{x\}}\left(\frac{t-t_{n+2}}{h}\right)$$

Below we will denote $p^{\{x\}}(x)$ simply as $p(x)$ when there is no confusion.

<u>Adams-Bashforth method</u> (explicit, s = 2):

Explicit method ==> r = s + 1 = 3 (when s = 2)

It uses values of $f(u(t), t)$ at 3 time levels, $\{t_n, t_{n+1}, t_{n+2}\}$, to calculate u_{n+3}.

The Adams-Bashforth method is constructed as

$$u_{n+3}=u_{n+2}+\int_{t_{n+2}}^{t_{n+3}} p\left(\frac{t-t_{n+2}}{h}\right)dt=u_{n+2}+h\int_0^1 p(x)dx\ , \qquad x=\frac{t-t_{n+2}}{h}$$

Let us calculate $\int_0^1 p_j(x)dx$ for j = 0, 1, 2.

$$\int_0^1 p_1(x)dx=\int_0^1 \frac{1}{2}(x^2+x)dx=\frac{1}{2}\cdot\frac{1}{3}+\frac{1}{2}\cdot\frac{1}{2}=\frac{5}{12}$$

$$\int_0^1 p_2(x)dx=\int_0^1 -(x^2+2x)dx=\frac{-16}{12}$$

$$\int_0^1 p_3(x)dx=\int_0^1 \frac{(x^2+3x+2)}{2}dx=\frac{23}{12}$$

$$\Longrightarrow \qquad \int_0^1 p(x)dx=\int_0^1\Big(y_1p_1(x)+y_2p_2(x)+y_3p_3(x)\Big)dx$$

$$=\frac{1}{12}\Big(5y_1-16y_2+23y_3\Big)$$

Based on the correspondence between $\{x_1, x_2, x_3\}$ and $\{t_n, t_{n+1}, t_{n+2}\}$, we have

$$y_1=g(x_1) \ \longleftrightarrow\ f\Big(u(t_n),t_n\Big)$$
$$y_2=g(x_2) \ \longleftrightarrow\ f\Big(u(t_{n+1}),t_{n+1}\Big)$$
$$y_3=g(x_3) \ \longleftrightarrow\ f\Big(u(t_{n+2}),t_{n+2}\Big)$$

<u>The 3-step Adams-Bashforth method</u> is

$$\boxed{u_{n+3}=u_{n+2}+\frac{h}{12}\Big[5f(u_n,t_n)-16f(u_{n+1},t_{n+1})+23f(u_{n+2},t_{n+2})\Big]}$$

Adams-Moulton method (implicit, s = 2):

Implicit method ==> $r = s = 2$ (when s = 2).

It uses values of $f(u(t), t)$ at 3 time levels, $\{t_n, t_{n+1}, t_{n+2}\}$, to calculate u_{n+2}.

The unknown u_{n+2} is used in interpolation so the method is implicit.

The Adams-Moulton method is constructed as

$$u_{n+2} = u_{n+1} + \int_{t_{n+1}}^{t_{n+2}} p\left(\frac{t-t_{n+2}}{h}\right)dt = u_{n+1} + h\int_{-1}^{0} p(x)dx\,, \qquad x = \frac{t-t_{n+2}}{h}$$

Let us calculate $\int_{-1}^{0} p_j(x)dx$ for j = 0, 1, 2.

$$\int_{-1}^{0} p_1(x)dx = \int_{-1}^{0} \frac{1}{2}(x^2+x)dx = \frac{-1}{12}$$

$$\int_{-1}^{0} p_2(x)dx = \int_{-1}^{0} -(x^2+2x)dx = \frac{8}{12}$$

$$\int_{-1}^{0} p_3(x)dx = \int_{-1}^{0} \frac{(x^2+3x+2)}{2}dx = \frac{5}{12}$$

$$\Longrightarrow \quad \int_{-1}^{0} p(x)dx = \int_{-1}^{0}\Big(y_1 p_1(x) + y_2 p_2(x) + y_3 p_3(x)\Big)dx$$

$$= \frac{1}{12}\Big(-y_1 + 8y_2 + 5y_3\Big)$$

The 2-step Adams-Moulton method is

$$\boxed{u_{n+2} = u_{n+1} + \frac{h}{12}\Big[-f(u_n,t_n) + 8f(u_{n+1},t_{n+1}) + 5f(u_{n+2},t_{n+2})\Big]}$$

A list of Adams-Bashforth methods:

1-step Adams-Bashforth:

$$u_{n+1} = u_n + hf(u_n,t_n)$$ This is the same as the forward Euler.

2-step Adams-Bashforth:

$$u_{n+2} = u_{n+1} + \frac{h}{2}\Big[-f(u_n,t_n) + 3f(u_{n+1},t_{n+1})\Big]$$

3-step Adams-Bashforth:

$$u_{n+3}=u_{n+2}+\frac{h}{12}\Big[5f(u_n,t_n)-16f(u_{n+1},t_{n+1})+23f(u_{n+2},t_{n+2})\Big]$$

<u>4-step Adams-Bashforth:</u>

$$u_{n+4}=u_{n+3}+\frac{h}{24}\Big[-9f(u_n,t_n)+37f(u_{n+1},t_{n+1})-59f(u_{n+2},t_{n+2})+55f(u_{n+3},t_{n+3})\Big]$$

A list of Adams-Moulton methods:

<u>1-step Adams-Moulton:</u>

$$u_{n+1}=u_n+\frac{h}{2}\Big[f(u_n,t_n)+f(u_{n+1},t_{n+1})\Big]$$ This is the same as the trapezoidal.

<u>2-step Adams-Moulton:</u>

$$u_{n+2}=u_{n+1}+\frac{h}{12}\Big[-f(u_n,t_n)+8f(u_{n+1},t_{n+1})+5f(u_{n+2},t_{n+2})\Big]$$

<u>3-step Adams-Moulton:</u>

$$u_{n+3}=u_{n+2}+\frac{h}{24}\Big[f(u_n,t_n)-5f(u_{n+1},t_{n+1})+19f(u_{n+2},t_{n+2})+9f(u_{n+3},t_{n+3})\Big]$$

<u>4-step Adams-Moulton:</u>

$$\begin{aligned}u_{n+4}=u_{n+3}+\frac{h}{720}\Big[&-19f(u_n,t_n)+106f(u_{n+1},t_{n+1})-264f(u_{n+2},t_{n+2})\\&+646f(u_{n+3},t_{n+3})+251f(u_{n+4},t_{n+4})\Big]\end{aligned}$$

Order of accuracy of Adams methods

First we study that of polynomial interpolation.

<u>Order of accuracy of polynomial interpolation</u>

Consider the polynomial interpolation of function $g(t)$ at $(s + 1)$ time levels,

$\{t_n, t_{n+1}, \ldots, t_{n+s}\}$. In our application, $g(t) = f(u(t), t)$.

Let "Intp" denote the interpolation operator.

Intp: $g(t) \longrightarrow p(t)$

<u>Remark:</u> Intp is a linear operator.

$$\text{Intp}\Big(c_1 g_1(t)+c_2 g_2(t)\Big)=c_1\cdot\text{Intp}\Big(g_1(t)\Big)+c_2\cdot\text{Intp}\Big(g_2(t)\Big)$$

Forecast of the result:

The error of the interpolation is

$$E(h) = g(t) - \text{Intp}\big(g(t)\big) = O(h^{s+1}) \quad \text{over } t \in \left[t_n, t_{n+s+1}\right]$$

That is, the error = $O(h^m)$ where m is # of points used in interpolation.

Derivation of the result:

To isolate the effect of h, we map t to x: $\qquad x = \dfrac{t - t_{n+s}}{h}$

$\{t_n, t_{n+1}, \ldots, t_{n+s}\}$ are mapped to $\{x_1, x_2, \ldots, x_{s+1}\}$

$$\begin{aligned} t_n &\longrightarrow x_1 = -s \\ t_{n+1} &\longrightarrow x_2 = -(s-1) \\ &\vdots \\ t_{n+s} &\longrightarrow x_{s+1} = 0 \end{aligned}$$

We write the interpolation mapping as

$$\text{Intp}\big(g(t)\big) = \sum_{j=1}^{s+1} g(t_{n+j-1}) p_j^{\{x\}}(x), \qquad x = \frac{t - t_{n+s}}{h}$$

We point out several properties of "Intp":

- Function $p_j^{\{x\}}(x)$ is independent of h.
- The range of x is also independent of h:

  $$t \in \left[t_n,\ t_{n+s+1}\right] \longrightarrow x \in \left[x_1,\ x_{s+2}\right] = \left[-s,\ 1\right].$$

- The range of $p_j^{\{x\}}(x)$ over $x \in [-s, 1]$ is independent of h, and, therefore, is bounded.
- The effect of h is solely contained in $g(t_{n+j-1})$.

Using these properties of "Intp", we conclude that for any $q > 0$ we have

$$\text{Intp}\big(O(h^q)\big) = \sum_{j=1}^{s+1} O(h^q) p_j^{\{x\}}(x) = O(h^q) \qquad \text{over } t \in \left[t_n, t_{n+s+1}\right]$$

In other words, the interpolation of a small function is also small.

This result is <u>the key</u> for deriving the error of polynomial interpolation.

By definition, the error of interpolation is

$$E(t,h) = g(t) - \text{Intp}\big(g(t)\big)$$

We expand $g(t)$ around t_n.

$$g(t) = \underbrace{\sum_{m=0}^{s} g^{(m)}(t_n)(t-t_n)^m}_{\text{Polynomial of degree } s} + O(h^{s+1}) \qquad \text{over } t \in \left[t_n, t_{n+s+1}\right]$$

Recall that the polynomial interpolation based on (s + 1) points is exact for polynomials of degree s. It follows that

$$\text{Intp}\big(g(t)\big) = \text{Intp}\left(\sum_{m=0}^{s} g^{(m)}(t_n)(t-t_n)^m\right) + \text{Intp}\big(O(h^{s+1})\big)$$

$$= \sum_{m=0}^{s} g^{(m)}(t_n)(t-t_n)^m + O(h^{s+1}) \qquad \text{over } t \in \left[t_n, t_{n+s+1}\right]$$

==> $$E(t,h) = g(t) - \text{Intp}\big(g(t)\big) = O(h^{s+1}) \qquad \text{over } t \in \left[t_n, t_{n+s+1}\right]$$

We summarize this result into a theorem.

<u>Theorem:</u>

Consider the polynomial interpolation of a smooth function $g(t)$ at (s + 1) time levels {t_n, t_{n+1}, ..., t_{n+s}}. The error of the interpolation is

$$E(t,h) = g(t) - \text{Intp}\big(g(t)\big) = O(h^{s+1}) \qquad \text{over } t \in \left[t_n, t_{n+s+1}\right].$$

OR concisely,

on a grid of size h, error of Intp = O(h^m) where m is # of points used.

We now use this theorem to derive the order of accuracy of Adams methods.

The r-step Adams methods have the form

$$u_{n+r} = u_{n+r-1} + \int_{t_{n+r-1}}^{t_{n+r}} p^{\{t\}}(t)\,dt$$

<u>The local truncation error</u> is

$$e_n(h) = u(t_{n+r}) - u(t_{n+r-1}) - \int_{t_{n+r-1}}^{t_{n+r}} \text{Intp}\big(f(u(t),t)\big)\,dt$$

Since $u(t)$ is an exact solution, we have

$$u(t_{n+r}) - u(t_{n+r-1}) = \int_{t_{n+r-1}}^{t_{n+r}} u'(t)\,dt = \int_{t_{n+r-1}}^{t_{n+r}} f(u(t),t)\,dt\,.$$

We write local truncation error $e_n(h)$ as

$$e_n(h) = \int_{t_{n+r-1}}^{t_{n+r}} \Big[f(u(t),t) - \mathrm{Intp}\big(f(u(t),t)\big) \Big] dt$$

$$= \int_{t_{n+r-1}}^{t_{n+r}} O(h^{s+1})\,dt = h \cdot O(h^{s+1}) = O(h^{s+2})$$

where $(s + 1)$ is the number of points used in interpolation, which is based on time levels $\{t_n, t_{n+1}, \ldots, t_{n+s}\}$. Here s may be different from r.

The global error is

$$E_N(h) = O\left(\frac{e_n(h)}{h} \right) = O(h^{s+1})$$

Order of r-step Adams-Bashforth (explicit):

For Adams-Bashforth, $r = s + 1$

==> Order = $s + 1 = r$

Order of r-step Adams-Moulton (implicit):

For Adams-Moulton, $r = s$

==> Order = $s + 1 = r + 1$

Conclusion:

r-step Adams-Bashforth has order r.

r-step Adams-Moulton has order $(r + 1)$.