Math 5620 Spring 2019

Notes of 1/18/19

Linear Multistep Methods

We consider the Initial Value Problem (IVP)

\[ y' = f(x, y), \quad y(a) = y_0, \quad x \in [a, b], \quad y(x), f(x, y) \in \mathbb{R}^m \]  

(1)

where we assume that there exists some Lipschitz Constant \( L \) such that

\[ \|f(x, y) - f(x, z)\| \leq L\|y - z\|, \quad \text{for all } (x, y), (x, z) \in [a, b] \times \mathbb{R}^m \]  

(2)

Assumption (2) implies that the initial value problem (1) possesses a unique solution.

We use the notation

\[ x_n = a + nh, \quad y_n \approx y(x_n), \quad f_n = f(x_n, y_n), \quad n = 0, 1, 2, \ldots \]

(3)

Our fundamental problem for the first few weeks of this semester is how to compute the \( y_n \). They may be defined by Linear Multistep Methods (LMMs):

\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \]  

(4)

Here, \( k \) is the step-number, \( h \) is the step-size (assumed constant for the moment), \( \alpha_k = 1 \), \( y_{n+1} = y_n + hf_n \)

\( E.M. \quad y_{n+1} - y_n = hf_n \)

(5)

EM:

\[ \begin{align*}
E = M; \quad y_{n+1} - y_n &= hf_n \\
\alpha_k &= 1 \\
\alpha_i &= 1 \\
\beta_i &= -1 \\
\beta_i &= 0 \\
\beta_i &= 1
\end{align*} \]
\begin{align*}
\kappa &= 2 \\
\omega &= 1 \\
\alpha &= 0 \\
\alpha_0 &= -1 \\
\beta_2 &= \frac{1}{3} \\
\beta_1 &= \frac{1}{3} \\
\beta_0 &= \frac{1}{3}
\end{align*}

|α₀| + |β₀| ≠ 0, the method is explicit if β₀ = 0, otherwise it is implicit.

- We also usually normalize the equation by requiring that

\[ α_k = 1. \]
Local Truncation Error

The **local truncation error** of a LMM is defined as follows.

1. Rewrite the method as

\[
\sum_{j=0}^{k} \alpha_j y_{n+j} - h \sum_{j=0}^{k} \beta_j f_{n+j} = 0 \quad (5)
\]

2. Substitute exact function values for the unknowns. Thus we replace \( y_n \) with \( y(x_n) \) and \( f_n \) with

\[
f(x_n y(x_n)) = y'(x_n). \quad (6)
\]

The resulting expression is the **local truncation error** given by

\[
\text{LTE} = \sum_{j=0}^{k} \alpha_j y_{n+j} - h \sum_{j=0}^{k} \beta_j f_{n+j} = 0 \quad (7)
\]

3. Expanding into a Taylor Series about \( h = 0 \) gives

\[
\text{LTE} = \sum_{j=0}^{\infty} C_j h^j y^{(j)}(x_n)
\]

\[
= C_{p+1} h^{p+1} y^{(p+1)}(x_n) + \text{HOT}
\]

where \( C_{p+1} \), called the **error constant** is the first non-zero coefficient in the expansion, and \( p \) is called the **order** of the method.
\[ \text{LTE} = \frac{1}{k} \sum_{j=0}^{k} \alpha_{j} y(k_{n+j}) - h \frac{1}{2} \sum_{j=0}^{k} \beta_{j} y'(k_{n+j}) \neq 0 \]

Example: \( \text{LTE} = y(k_{n+1}) - y(k_{n}) - h \frac{1}{2} \left( y'(k_{n+1}) + y'(k_{n}) \right) \)

\[ \text{LTE} = \sum_{j=0}^{k} \alpha_{j} \sum_{i=0}^{\infty} \frac{(i+h)!}{i!} y^{(i)}(k_{n}) + h \sum_{i=0}^{\infty} \frac{(i+h)!}{i!} y^{(i)}(k_{n}) \]

\[ = \sum_{i=0}^{\infty} C_{i} - h \sum_{i=0}^{\infty} y^{(i)}(k_{n}) \]

\[ C_{i} = \frac{1}{i!} \sum_{j=0}^{k} \alpha_{j} j^{i} - \frac{1}{(i-1)!} \sum_{j=0}^{k} \beta_{j} j^{i-1} \]

\[ C_{0} = \sum_{j=0}^{k} \alpha_{j} = g(1) \]

\[ C_{1} = \sum_{j=0}^{k} j \alpha_{j} - \sum_{j=0}^{k} \beta_{j} = g'(1) - g^{'(1)} \]

\[ \vdots \]

\[ C_{0} = C_{1} = \ldots \]

\[ C_{p} = 0 \quad C_{p+1} \neq 0 \]

p: order \quad C_{p+1}: \text{error constant}
Examples

This reference section lists some particularly important classes of LMMs. It contains some information (about convergence, order, and error constant) that will be defined only later in these notes.

Of particular importance among the following examples are the Adams Methods and the Backward Differentiation formulas. These are the ones used in the many versions of Gear’s package.

Here are some examples for explicit convergent LMMs:

1. Euler’s Method. \( p = k = 1, \quad C_2 = \frac{1}{2} \):

\[
y_{n+1} - y_n = hf_n
\]  

2. The Midpoint Rule. \( p = k = 2, \quad C_3 = \frac{1}{3} \):

\[
y_{n+2} - y_n = 2hf_{n+1}
\]  

3. Adams-Bashforth Methods. \( p = k, \quad k = 1, 2, 3, \ldots \):

\[
y_{n+k} - y_{n+k-1} = h \sum_{j=0}^{k-1} \beta_j^* f_{n+j}
\]  

(Note that the requirement \( p = k \) uniquely defines the \( \beta_j^* \).)

Here are some examples for implicit convergent LMMs:
4. Backward (or Implicit) Euler Method.  
\[ p = k = 1, \quad C_2 = -\frac{1}{2}: \]
\[ y_{n+1} - y_n = hf_{n+1} \quad (11) \]

5. The Trapezoidal Rule.  
\[ p = 2, \quad k = 1, \quad C_3 = -\frac{1}{12}: \]
\[ y_{n+1} - y_n = \frac{h}{2} (f_{n+1} + f_n) \quad (12) \]

\[ p = 4, \quad k = 2, \quad C_5 = -\frac{1}{90}: \]
\[ y_{n+2} - y_n = \frac{h}{3} (f_{n+2} + 4f_{n+1} + f_n) \quad (13) \]

In spite of being convergent, the performance of Simpson’s Rule is mediocre (due to the spurious root of the first characteristic polynomial being -1).

\[ p = k+1, \quad k = 1, 2, 3, \ldots: \]
\[ y_{n+k} - y_{n+k-1} = h \sum_{j=0}^{k} \beta_j f_{n+j} \quad (14) \]

Ex.: \( k = 1 \) Trapezoidal Rule
(Note that the requirement \( p = k+1 \) uniquely defines the \( \beta_j \).)

\[ p = k, \quad k = 1, 2, 3, 4, 5, 6: \]
\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_k f_{n+k} \quad (15) \]
These methods are not zero-stable if $k > 6$. Note that the requirement $p = k$ uniquely defines the $\alpha_j$. 
Non-Convergent Maximal Linear Multistep Methods

The coefficients of an LMM can be chosen so as to maximize the order. How high an order is possible?

\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \]

\[ c_0 = c_1 = \ldots = c_\rho = 0 \]

\# conditions = \rho + 1

\# parameters = 2k + 1

= when \( \rho = 2k \) implicit

2k - 1 explicit
Matching the number of parameters with the number of conditions suggests that an explicit method can have order $2k - 1$, and implicit one order $2k$. It turns out that the linear equations are always consistent, and that you don’t get a higher order for free. Thus these values are indeed attained. LMMs of maximum possible order are called maximal. Note that they may not be convergent. Examples of maximal methods listed above include: Euler’s Method, the Trapezoidal Rule, and Simpson’s Rule. Following are some additional maximal divergent methods:

**Explicit LMMs**

**9.** $k = 2, p = 3, C_4 = \frac{1}{6}$:

$$yn+2 + 4yn+1 - 5yn = h (4f_{n+1} + 2f_n) \quad (16)$$

**10.** $k = 3, p = 5, C_6 = \frac{1}{2}$.

$$yn+3 + 18yn+2 - 9yn+1 - 10yn = h (9f_{n+2} + 18f_{n+1} + 3f_n) \quad (17)$$

**Implicit LMMs**

**11.** $k = 3, p = 6, C_7 = \frac{-3}{140}$.

$$11yn+3 + 27yn+2 - 27yn+1 - 11yn = h (3f_{n+3} + 27f_{n+2} + 27f_{n+1} + 3f_n) \quad (18)$$
Convergence

We are concerned with the Global Truncation Error

\[ e_n = y(x_n) - y_n. \]  \hspace{1cm} (19)

The LMM (4) is said to be convergent if, for all IVPs (1) satisfying (2), all \( x \in [a, b] \), and all starting strategies \( y_\mu = \eta_\mu(h), \mu = 0, 1, \ldots, k-1 \) satisfying

\[ \lim_{h \to 0} \eta_\mu(h) = y_0 \]  \hspace{1cm} (20)

the following holds:

\[ \lim_{h \to 0, nh=x-a \text{ and } n \to \infty} y_n = y(x) \]  \hspace{1cm} (21)

(Note that the requirement on the starting values is rather weak, it is satisfied e.g. by the “strategy” \( y_\mu = y_0 \).)

An obvious minimum requirement for a LMM is that it be convergent.

Two simple Examples

To get an idea of what’s involved in convergence, let’s look at two extremely simple examples. This will illustrate a

Major Technique. Consider a test problem, compute the general solutions of the numerical
method and the analytical problem, and compare them.

What’s the simplest IVP imaginable? How about
\[ y' = 0, \quad y(0) = y_0. \]  
(22)
Clearly, the solution is
\[ y(x) = y_0. \]  
(23)

Now let’s compute the general solution of the difference method
\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = 0. \]  
(24)
This is a homogeneous linear difference equation whose solutions define a \( k \) dimensional linear space of sequences \( y_n, n = 0, 1, 2, 3, \ldots \).

To understand the space of solutions better we associate with the LMM (4) its first and second characteristic polynomial \( \rho \) and \( \sigma \), respectively by
\[ \rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j, \quad \text{and} \quad \sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j. \]  
(25)

It is obvious that if
\[ \rho(r) = 0 \]  
(26)
then
$$y_n = r^n$$

is a solution of the difference equation (24). Any linear combination of solutions of the form (27) also solves (24). If there are $k$ distinct roots of $\rho$ then all solutions are linear combinations of solutions of the form (27). If there is a multiple root $r$ satisfying
$$\rho(r) = \rho'(r) = \ldots = \rho^{(q)}(r) = 0$$

then $q + 1$ corresponding linearly independent solutions of (24) are given by
$$y_n = n^j r^n \quad \text{where} \quad j = 0, 1, \ldots, q. \quad (29)$$

In what follows let’s suppose for simplicity that all roots $r_1, r_2, \ldots, r_k$ of $\rho$ are distinct. The general solution of the difference equation is then given by
$$y_n = \sum_{\mu=1}^{k} \gamma_\mu r_\mu^n. \quad (30)$$

The coefficients $\gamma_j$ are defined by the starting values.

How can this solution converge to the true solution of the IVP (22)? Clearly we must have:

— 1 must be a root of $\rho$.

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Verifying this is a good exercise.
— No root of $\rho$ can exceed 1 in absolute value.
— In view of what was said above about multiple roots, any root of $\rho$ of absolute value equal to 1 must be simple.

Let’s note these properties formally

\begin{itemize}
  \item a. $\rho(1) = 0$
  \item b. $\rho(r) = 0 \implies |r| \leq 1$
  \item c. $\rho(r) = 0$ and $|r| = 1 \implies \rho'(r) \neq 0$
\end{itemize}

(31)

**Definition.** A method that satisfies properties b. and c. is said to be zero-stable.

To gain more insight, let’s look at a slightly more complicated IVP, say \( y' = 1, \ y(0) = 0 \)

(32)

which obviously has the solution

\( y(x) = x. \)

(33)

The difference equation now becomes:

\[
\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j
\]

(34)

This is an **inhomogeneous** linear difference equation and its **general** solution can be written as
any particular solution plus the general solution of the homogeneous equation (22). To find a particular solution we have to do some inspired guessing. Considering the analytical solution suggests to try a solution of the form

\[ y_n = \gamma x_n = \gamma nh \]  \hspace{1cm} (35)

where \( \gamma \) is as yet undetermined. Plugging this into the difference equation and using property a. above yields

\[
\gamma \sum_{j=0}^{k} \alpha_j (n + j)h = \gamma \left( nh \sum_{j=0}^{k} \alpha_j + h \sum_{j=0}^{k} \alpha_j j \right) \\
= \gamma h \sum_{j=0}^{k} \alpha_j j \\
= h \sum_{j=0}^{k} \beta_j 
\]

Clearly, the last equation requires

\[
\gamma = \frac{\sum_{j=0}^{k} \beta_j}{\sum_{j=0}^{k} \alpha_j j} = \frac{\sigma(1)}{\rho'(1)}. \hspace{1cm} (37)
\]

It is now almost obvious\(^{-2-}\) that for convergence

\(^{-2-}\) Work out the details! Also, what happens if \( \rho'(1) = 0 \)?
we have to have that

\[ \gamma = 1. \]  

(38)

Let’s summarize: For the LMM to converge just for the simple DEs \( y' = 0 \) and \( y' = 1 \) we have to have properties a.–c. above, and, in addition:

\[ a. \quad \sigma(1) = 0 \]

\[ d. \quad \sigma(1) = \rho'(1). \]  

(39)

**Definition.** A method that satisfies a. and d. is said to be **consistent**.

Why did we do all this? Most amazingly, it turns out that these properties are also sufficient for convergence in general! Thus

**the LMM will converge for all IVPs (1) if**

**it converges just for \( y' = 0 \) and \( y' = 1 \)!**

Marvel at that! A proof of this fact is given in Henrici’s book but is beyond the scope of this course.

Thus it turns out that

**LMM convergent \( \iff \)**

it is consistent and zero-stable

**Convergence \( \iff \) Consistency and Stability**