Math 5620 Spring 2022

Announcement

• Home work 1 is now available on our Canvas home page. You’ll notice that there is some overlap with the quadrature work we did in 5610. The home work is due February 4.

Notes of 1/21/22

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), $\alpha_k = 1$, $|\alpha_0| + |\beta_0| \neq 0$, the method is **explicit** if $\beta_k = 0$, otherwise it is **implicit**.

- We also usually normalize the equation by requiring that
  $$\alpha_k = 1.$$  

- With the linear multistep method we associate its first and second characteristic polynomial:

$$\rho(r) = \sum_{j=0}^{k} \alpha_j r^j$$

and

$$\sigma(r) = \sum_{j=0}^{k} \beta_j r^j$$
Local Truncation Error

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

1. Rewrite the method as

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

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

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

The resulting expression is the local truncation error given by

\[ \text{LTE} = \sum_{j=0}^{k} \alpha_j y(x_{n+j}) - h \sum_{j=0}^{k} \beta_j y'(x_{n+j}) \] (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.
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. $p = k = 1$, $C_2 = \frac{1}{2}$:
   \[
   y_{n+1} - y_n = hf_n \tag{8}
   \]

2. The Midpoint Rule. $p = k = 2$, $C_3 = \frac{1}{3}$:
   \[
   y_{n+2} - y_n = 2hf_{n+1} \tag{9}
   \]

3. Adams-Bashforth Methods. $p = k$, $k = 1, 2, 3, \ldots$:
   \[
   y_{n+k} - y_{n+k-1} = h \sum_{j=0}^{k-1} \beta^*_j f_{n+j} \tag{10}
   \]

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

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

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

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

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

8. **Backward Differentiation Methods.**  
\[ p = k, \quad k = 1, 2, 3, 4, 5, 6: \]
\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = h\beta_k f_{n+k} \quad (15) \]
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?
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. $k = 2, p = 3, C_4 = \frac{1}{6}$:

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

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

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

**Implicit LMMs**

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

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

\[ \lim_{h \to 0, nh = x-a} y_n = y(x) \]  \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
\[ y' = 0, \quad y(0) = y_0. \tag{22} \]
Clearly, the solution is
\[ y(x) = y_0. \tag{23} \]

Now let’s compute the general solution of the difference method
\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = 0. \tag{24} \]

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
\[ \rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j, \quad \text{and} \quad \sigma(\xi) = \sum_{j=0}^{k} \beta_j \xi^j. \tag{25} \]

It is obvious that if
\[ \rho(r) = 0 \tag{26} \]
then
\[ y_n = r^n \] (27)
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
\[ \rho(r) = \rho'(r) = \ldots = \rho^{(q)}(r) = 0 \] (28)
then \( q + 1 \) corresponding linearly independent solutions of (24) are given by
\[ y_n = n^j r^n \quad \text{where} \quad j = 0, 1, \ldots, q. \] (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
\[ y_n = \sum_{\mu=1}^{k} \gamma_\mu r_\mu^n. \] (30)
The coefficients \( \gamma_\mu \) 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 \( \rho \).

\[ \text{— Verifying this is a good exercise.} \]
— 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

a. $\rho(1) = 0$

b. $\rho(r) = 0 \implies |r| \leq 1$

c. $\rho(r) = 0$ and $|r| = 1 \implies \rho'(r) \neq 0$

(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

$$y' = 1, \quad y(0) = 0$$

(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

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

$$= \gamma h \sum_{j=0}^{k} \alpha_j j$$

$$= h \sum_{j=0}^{k} \beta_j$$

(36)

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

$$\gamma = 1. \quad (38)$$

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:

d. $\sigma(1) = \rho'(1). \quad (39)$

**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**

**Local Truncation Error**

Associated with the LMM is its **Local Trun-**
cation Error LTE$^{-3}$ defined by

$$LTE = \sum_{j=0}^{k} \alpha_j y(x_{n+j}) - h \sum_{j=0}^{k} \beta_j y'(x_{n+j}) \quad (42)$$

where $y(x)$ is the true solution of the IVP (1). Assuming that the solution can be expanded into a power series about $x_n$ it turns out that

$$LTE = \sum_{i=0}^{\infty} C_i h^i y^{(i)}(x_n) \quad (43)$$

There is also an ‘‘error under the localizing assumption’’

$$y_{n+j} = y(x_{n+j}), \quad j = 0, 1, \ldots, k - 1. \quad (40)$$

It follows by a simple application of the Mean Value Theorem that under that assumption

$$y(x_{n+k}) - y_{n+k} = LTE + O(h^{p+1}). \quad (41)$$

Thus, at least asymptotically, the local truncation error, and the error under the localizing assumption, are equivalent.
where

\[ C_0 = \sum_{j=0}^{k} \alpha_j \quad \left( = \rho(1) \right) \]

\[ C_1 = \sum_{j=1}^{k} j \alpha_j - \sum_{j=0}^{k} \beta_j \quad \left( = \rho'(1) - \sigma(1) \right) \]

\[ C_q = \frac{1}{q!} \sum_{j=1}^{k} j^q \alpha_j - \frac{1}{(q-1)!} \sum_{j=1}^{k} j^{q-1} \beta_j, \quad q = 2, 3, \ldots \]

The LMM is of order \( p \) if

\[ C_0 = C_1 = \ldots = C_p = 0, \quad C_{p+1} \neq 0. \]  \hspace{1cm} (44)

The number \( C_{p+1} \) is the **error constant of the LMM**.
**Note.** According to our earlier definition, a LMM is consistent if it is of order at least 1.

**Note.** We can now reinterpret the two requirements for convergence: Stability means that errors do not get unduly amplified, and consistency means that the error introduced at each step is not too large.

The following table gives the maximum order of convergent LMMs

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<tr>
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<th>explicit</th>
<th>implicit</th>
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<tbody>
<tr>
<td>$k$ even</td>
<td>$k$</td>
<td>$k + 2$</td>
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<tr>
<td>$k$ odd</td>
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