AN OVERVIEW

Numerical Methods for ODE Initial Value Problems

1. One-step methods (Taylor series, Runge-Kutta)

2. Multistep methods (Predictor-Corrector, Adams methods)

Both of these types of methods are widely used, with the multistep methods probably being more widely used. We will first study multistep methods, returning in §6.10 to the single step methods.

PLAN OF STUDY

§6.3 Simplified general theory
§6.4, 6.5, 6.6 Low order examples
§6.7 Modern higher order methods
§6.8 General theory
§6.9 Stiff equations & Method of Lines
§6.10 Single step methods
§6.11 Boundary value problems

WHAT IS A MULTISTEP METHOD?

As before let the node points be given by

$$x_n = x_0 + nh, \quad n = 0, 1, 2, \ldots$$

with corresponding numerical solutions $y_{0,} y_1, y_2, \ldots.$

General form of <u>multistep method</u>:

$$y_{n+1} = \sum_{j=0}^{p} a_j y_{n-j} + h \sum_{j=-1}^{p} b_j f(x_{n-j}, y_{n-j}), \quad n \geq p$$

In this, $p \geq 0$ is a given integer, and $\left\{a_j\right\}$ and $\left\{b_j\right\}$ are given coefficients.
This is called a $(p+1)$-step method.

EXAMPLES

(1) The *midpoint rule*:

$$y_{n+1} = y_{n-1} + 2hf(x_n, y_n), \quad n = 1, 2, 3, ...$$

This is a two-step method. Note that $y_0 = Y_0$ in general; but y_1 must be obtained by some other means. y_2 is obtained from y_0 and y_1; and similarly for y_3, etc.
In this case, $p = 1$.

(2) The *trapezoidal rule*:

$$y_{n+1} = y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_{n+1}, y_{n+1})\right], \quad n \geq 0$$

This is a single step method. It is also our first example of an *implicit method*; and many of the most desirable formulas are of this type. In this case, $p = 0$.

PROBLEMS

- How do we derive multistep methods?
- What is the truncation error?
- Does the method converge? If so, how fast?
- Is the method stable?
- Is there an asymptotic error formula?

TRUNCATION ERROR

For any differentiable function $Y(x)$, define the truncation error in going from x_n to x_{n+1} by

$$T_n(Y) = Y(x_{n+1}) - \left[\sum_{j=0}^{p} a_j Y(x_{n-j}) + h \sum_{j=-1}^{p} b_j Y'(x_{n-j})\right], \quad n \geq p$$

By how much, does the numerical formula fail to predict $Y(x_{n+1})$ from the preceding values?
For the trapezoidal rule, we can show

$$T_n(Y) = -\frac{h^3}{12} Y'''(\xi_n), \quad x_n \leq \xi_n \leq x_{n+1}$$

For the midpoint rule, we can show

$$T_n(Y) = \frac{h^3}{3} Y'''(\xi_n), \quad x_{n-1} \leq \xi_n \leq x_{n+1}$$

CONSISTENCY

Introduce

$$\tau_n(Y) = \frac{1}{h} T_n(Y), \quad n \geq p$$

$$\tau(h; Y) = \max_{p \leq n \leq N-1} |\tau_n(Y)|$$

where the node points in $[x_0, b]$ are

$$x_0 < x_1 < \cdots < x_N \leq b$$

We say the multistep method is consistent if for every function $Y(x)$ that is continuously differentiable on $[x_0, b]$,

$$\tau(h; Y) \to 0 \quad \text{as} \quad h \to 0$$

The method has order m if

$$\tau(h; Y) = O(h^m)$$

for all such functions $Y(x)$.

When is a method consistent? When is it of order m?

EXAMPLE

Consider the midpoint method

$$y_{n+1} = y_{n-1} + 2hf\left(x_n, y_n\right), \quad n = 1, 2, 3, \ldots$$

In this case,

$$T_n(Y) = Y(x_{n+1}) - Y(x_{n-1}) - 2hY'(x_n)$$

$$\tau_n(Y) = 2\left[\frac{Y(x_{n+1}) - Y(x_{n-1})}{2h} - Y'(x_n)\right]$$

Thus consistency in this case says that

$$\frac{Y(x_{n+1}) - Y(x_{n-1})}{2h} \approx Y'(x_n)$$

which seems a reasonable request in solving a differential equation.

THEOREM

(a) In order that the method be consistent, it is necessary and sufficient that

$$\sum_{j=0}^{p} a_j = 1$$

$$\sum_{j=-1}^{p} b_j - \sum_{j=0}^{p} j a_j = 1$$

(b) In order that $\tau(h; Y) = O(h^m)$ for some $m \geq 1$, it is necessary and sufficient that the method be consistent and that

$$\sum_{j=0}^{p} (-j)^i a_j + i \sum_{j=-1}^{p} (-j)^{i-1} b_j = 1$$

for $i = 2, ..., m$.

In this case that $\tau(h;Y) = O(h^m)$,

$$T_n(Y) = \frac{c_{m+1}}{(m+1)!} h^{m+1} Y^{(m+1)}(x_n) + O\left(h^{m+2}\right)$$

with

$$c_{m+1} = 1 - \left[\sum_{j=0}^{p} (-j)^{m+1}\, a_j + (m+1) \sum_{j=-1}^{p} (-j)^m\, b_j\right]$$

In addition,

$$\tau(h;Y) \le \frac{c_{m+1}}{(m+1)!} h^m \left\| Y^{(m+1)} \right\|_\infty + O\left(h^{m+1}\right)$$

DERIVATION OF TRUNCATION ERROR

Recall the formula

$$T_n(Y) = Y(x_{n+1}) - \left[\sum_{j=0}^{p} a_j Y(x_{n-j}) + h \sum_{j=-1}^{p} b_j Y'(x_{n-j})\right], \quad n \geq p$$

We expand $Y(x)$ and $Y'(x)$ about x_n with $x = x_{n+1}$, x_{n-1}, ..., x_{n-p}.

$$\begin{aligned} Y(x) &= Y(x_n) + (x - x_n)Y'(x_n) + \cdots \\ &\quad + \frac{(x - x_n)^m}{m!} Y^{(m)}(x_n) \\ &\quad + \frac{(x - x_n)^{m+1}}{(m+1)!} Y^{(m+1)}(x_n) + \cdots \end{aligned}$$

$$\begin{aligned} Y'(x) &= Y'(x_n) + (x - x_n)Y''(x_n) + \cdots \\ &\quad + \frac{(x - x_n)^{m-1}}{(m-1)!} Y^{(m)}(x_n) \\ &\quad + \frac{(x - x_n)^{m}}{m!} Y^{(m+1)}(x_n) + \cdots \end{aligned}$$

We substitute these into the formula for the truncation error, rearrange the terms, and obtain the formula

$$T_n(Y) = \sum_{i=0}^{m+1} \frac{c_i}{i!} h^i Y^{(i)}(x_n) + O(h^{m+2})$$

$$c_0 = 1 - \sum_{j=0}^{p} a_j$$

$$c_1 = 1 - \left[-\sum_{j=0}^{p} j a_j + \sum_{j=-1}^{p} b_j \right]$$

$$c_i = 1 - \left[\sum_{j=0}^{p} (-j)^i a_j + i \sum_{j=-1}^{p} (-j)^{i-1} b_j \right]$$

for $i \geq 2$.

For the consistency, we want to look at

$$\tau_n(Y) = \frac{1}{h} T_n(Y)$$

$$\tau_n(Y) = \frac{c_0}{h} Y(x_n) + c_1 Y'(x_n) + \frac{c_2}{2} h Y''(x_n) + \cdots$$

and we want it to go to zero as h goes to zero. This requires $c_0 = 0$ and $c_1 = 0$. These are exactly the equations asserted earlier. Consistency makes the error exactly zero whenever $Y(x)$ is a linear function.

To have $\tau_n(Y) = O(h^m)$, we must also have

$$c_2 = ... = c_m = 0$$

Then

$$T_n(Y) = \frac{c_{m+1}}{(m+1)!} h^{m+1} Y^{(m+1)}(x_n) + O\left(h^{m+2}\right)$$

CONVERGENCE

The general multistep method for solving

$$y' = f(x, y), \quad x \geq x_0, \quad y(x_0) = Y_0$$

is given by

$$y_{n+1} = \sum_{j=0}^{p} a_j y_{n-j} + h \sum_{j=-1}^{p} b_j f(x_{n-j}, y_{n-j}), \quad n \geq p \tag{1}$$

with $y_0 \doteq Y_0$. The values $y_1, ..., y_p$ must be calculated by other means, sometimes by using a single step method. To talk about the accuracy of the method (1), we must also consider the accuracy in the initial values $y_1, ..., y_p$; and these will depend on the stepsize h, since

$$y_i = y_h(x_i) \approx Y(x_0 + ih), \quad i = 0, 1, ..., p$$

Introduce the maximum of the initial errors,

$$\eta(h; Y) = \max_{j=0,1,\ldots,p} |Y(x_0 + ih) - y_h(x_0 + ih)|$$

Also recall the quantity

$$\tau(h; Y) = \frac{1}{h} \max_{p \le n \le N-1} |T_n(Y)|$$

where $x_0, ..., x_N$ are the node points on $[x_0, b]$.

THEOREM

Assume: (a) The multistep method is consistent;
(b) All $a_j \ge 0$.
Then for all sufficiently small values of h, say $0 < h \le h_0$ for some choice of h_0, the multistep method has a solution $y_{n+1} \equiv y_h(x_{n+1})$ at each node point. In addition, we have

$$\max_{x_0 \le x_j \le b} \left| Y(x_j) - y_h(x_j) \right| \le c_1 \eta(h; Y) + c_2 \tau(h; Y)$$

with suitably chosen constants c_1, c_2 which depend on the function $f(x, y)$, but not on the stepsize h.

$\mathbb{EXAMPLE}$. Recall the *midpoint rule*

$$y_{n+1} = y_{n-1} + 2hf\left(x_n, y_n\right), \quad n = 1, 2, 3, ...$$

in which $p = 1$, $a_0 = 0$, $a_1 = 1$. In this case,

$$\eta(h; Y) = \max\left\{\left|Y(x_0) - y_h(x_0)\right|, \left|Y(x_1) - y_h(x_1)\right|\right\}$$

From earlier, I said

$$T_n(Y) = \frac{h^3}{3} Y'''(\xi_n), \quad x_{n-1} \leq \xi_n \leq x_{n+1}$$

Then

$$\tau(h; Y) \leq \frac{h^2}{3} \left\| Y''' \right\|_\infty$$

For the error,

$$\max_{x_0 \leq x_j \leq b} \left| Y(x_j) - y_h(x_j) \right| \leq c_1 \eta(h; Y) + c_2 \frac{h^2}{3} \left\| Y''' \right\|_\infty$$

We usually have $y_0 = Y_0$; and therefore, we should choose y_1 with an accuracy of

$$Y(x_1) - y_h(x_1) = O(h^2)$$

THE PROOF

Recall that

$$T_n(Y) = Y(x_{n+1}) - \left[\sum_{j=0}^{p} a_j Y(x_{n-j}) \right.$$
$$\left. + h \sum_{j=-1}^{p} b_j Y'(x_{n-j}) \right], \quad n \geq p$$

$$\tau_n(Y) = \frac{1}{h} T_n(Y), \quad n \geq p$$

$$Y'(x) = f(x, Y(x))$$

Then we can write

$$\begin{aligned} Y(x_{n+1}) &= \sum_{j=0}^{p} a_j Y(x_{n-j}) \\ &\quad + h \sum_{j=-1}^{p} b_j f(x_{n-j}, Y(x_{n-j})) \\ &\quad + h\tau_n(Y), \quad n \geq p \end{aligned}$$

The multistep method is

$$y_{n+1} = \sum_{j=0}^{p} a_j y_{n-j} + h \sum_{j=-1}^{p} b_j f(x_{n-j}, y_{n-j}), \quad n \geq p$$

We subtract these to get

$$\begin{aligned} e_{n+1} &= \sum_{j=0}^{p} a_j e_{n-j} \\ &+ h \sum_{j=-1}^{p} b_j \left[f(x_{n-j}, Y(x_{n-j})) - f(x_{n-j}, y_{n-j}) \right] \\ &+ h\tau_n(Y), \quad n \geq p \end{aligned}$$

with $e_j \equiv Y(x_j) - y_h(x_j)$.
Recall the Lipschitz condition

$$|f(x, y) - f(x, z)| \leq K\,|y - z|$$

Then

$$\begin{aligned} |e_{n+1}| \;\leq\; & \sum_{j=0}^{p} a_j \left| e_{n-j} \right| \\ & + hK \sum_{j=-1}^{p} \left| b_j \right| \left| e_{n-j} \right| \\ & + h\tau_n(Y), \quad n \geq p \end{aligned}$$

Introduce

$$f_j = \max_{i=0,1,\ldots j} |e_i|$$

the maximum of the errors up thru x_j. Then

$$\begin{aligned} |e_{n+1}| \;\; &\leq \;\; f_n \sum_{j=0}^{p} a_j + hK f_{n+1} \sum_{j=-1}^{p} \left| b_j \right| \\ &\quad + h\tau(h;Y), \quad n \geq p \end{aligned}$$

Using consistency,

$$\sum_{j=0}^{p} a_j = 1$$

Introduce

$$c = K \sum_{j=-1}^{p} \left| b_j \right|$$

Then we can write

$$|e_{n+1}| \leq f_n + hc f_{n+1} + h\tau(h;Y), \quad n \geq p$$

Clearly, the right side also bounds f_n alone; and thus

$$f_{n+1} \leq f_n + hcf_{n+1} + h\tau(h;Y), \quad n \geq p$$

Also,

$$f_p = \eta(h;Y)$$

We can combine these results, together with the type of analysis used for Euler's method, to get

$$f_n \leq e^{2c(x_n - x_0)}\eta(h;Y) + \frac{e^{2c(x_n - x_0)} - 1}{c}\tau(h;Y)$$

for $n \geq p$. We also require $2hc \leq 1$; but this can be relaxed for multistep methods which are explicit.

Not all multistep methods can be analyzed as above, but this does include many of the most widely used method.

STABILITY

There is a similar result for stability of multistep solutions

$$y_{n+1} = \sum_{j=0}^{p} a_j y_{n-j} + h \sum_{j=-1}^{p} b_j f(x_{n-j}, y_{n-j}), \quad n \geq p$$

Suppose we perturb the initial values $y_0, ..., y_p$ to $z_0, ..., z_p$, with

$$|y_i - z_i| \leq \epsilon, \quad i = 0, 1, ..., p$$

Consider the numerical solution

$$z_{n+1} = \sum_{j=0}^{p} a_j z_{n-j} + h \sum_{j=-1}^{p} b_j f(x_{n-j}, z_{n-j}), \quad n \geq p$$

Then by methods similar to the above, we can show (with the same assumptions) that

$$|y_n - z_n| \leq \epsilon \, e^{2c(x_n - x_0)}$$

OTHER ANALYSES

We can also do asymptotic error analyses, rounding error analyses, and analyses involving systems of first order ODEs. Rather than doing a general theory, we do special cases in later sections.