Lecture 21: Numerical Solutions to IVPs for ODEs (Multistep Methods)

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Multistep Methods

One-step methods (Taylor's series method, Euler's method, Runge-Kutta method) use the information on the solution of the previous step (nth) to compute the solution at the next ($(n+1)$th) step. Whereas Multistep methods make use of information about the solution at more than one point. Consider the IVP of the form

$$y' = f(x, y), \quad y(x_0) = y_0, \tag{1}$$

Let us assume that we have already obtained approximations to y' and y at a number of equally spaced points, say x_0, $x_1, \ldots, x_n$. Integrate the differential equation (1) from x_n to x_{n+1}, to have

$$\int_{x_n}^{x_{n+1}} y' \, dx = \int_{x_n}^{x_{n+1}} f(x, y(x)) \, dx$$

$$\implies \qquad y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} f(x, y(x)) \, dx. \tag{2}$$

we now approximate $f(x, y(x))$ by a polynomial $p_m(x)$ which interpolates $f(x, y(x))$ at the $(m+1)$ points $x_n, x_{n-1}, x_{n-2}, \ldots, x_{n-m}$. Set

$$f(x_k, y(x_k)) = f_k.$$

Using Newton backward formula of degree m for this purpose, we write

$$p_m(x) = \sum_{k=0}^{m} \begin{pmatrix} -s \\ k \end{pmatrix} \Delta^k f_{n-k}, \quad s = \frac{x - x_n}{h},$$

where $\Delta f_i = f_{i+1} - f_i$. Inserting this into (2) and noting that $dx = hds$, we obtain

$$\begin{aligned} y_{n+1} &= y_n + h \int_0^1 \sum_{k=0}^{m} \begin{pmatrix} -s \\ k \end{pmatrix} \Delta^k f_{n-k}\, ds \\ &= y_n + h \left\{ \gamma_0 f_n + \gamma_1 \Delta f_{n-1} + \cdots + \gamma_m \Delta^m f_{n-m} \right\}, \end{aligned} \tag{3}$$

where

$$\gamma_k = (-1)^k \int_0^1 \begin{pmatrix} -s \\ k \end{pmatrix} ds.$$

The formula (3) is known as the Adams-Bashforth method. The first few values of γ_k are:

$$\gamma_0 = 1, \;\; \gamma_1 = 1/2, \;\; \gamma_2 = 5/12, \;\; \gamma_3 = 3/8, \;\; \gamma_4 = 251/720.$$

The simplest case, obtained by setting $m = 0$ in (3), again leads to Eulers method. For m = 3, we have from (3)

$$y_{n+1} = y_n + h\big(f_n + \frac{1}{2}\Delta f_{n-1} + \frac{5}{12}\Delta^2 f_{n-2} + \frac{3}{8}\Delta^3 f_{n-3}\big). \tag{4}$$

From the definition of forward-difference operator Δ we find that

$$\begin{aligned}
\Delta f_{n-1} &= f_n - f_{n-1} \\
\Delta^2 f_{n-2} &= \Delta(\Delta f_{n-2}) = \Delta(f_{n-1} - f_{n-2}) = f_n - 2f_{n-1} + f_{n-2} \\
\Delta^3 f_{n-3} &= f_n - 3f_{n-1} + 3f_{n-2} - f_{n-3}.
\end{aligned}$$

Substituting in (4) and regrouping, we obtain

$$y_{n+1} = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}).$$

The local discretization error in (4) is given by

$$E_{AB} = h^5 y^{(v)}(\xi)\frac{251}{720} = O(h^5).$$

Remarks.

- A major disadvantage of multistep formulas is that they are not self-starting. These starting values must be obtained by some independent method (e.g., Euler's method, Second-order Runge-Kutta method, Fourth-order Runge-Kutta method).
- A second disadvantage of the Adams-Bashforth method is that, although the local discretization error is $O(h^5)$, the coefficient in the error term is somewhat larger than for formulas of the Runge-Kutta type of the same order.
- On the other hand, the multistep formula require only one derivative evaluation per step, compared with four evaluations per step with Runge-Kutta methods, and is therefore considerably faster and require less computational work.

Predictor-Corrector Methods

Integrating from x_n to x_{n+1} we have

$$\int_{x_n}^{x_{n+1}} y'\,dx = \int_{x_n}^{x_{n+1}} f(x, y(x))\,dx$$

$$\implies \qquad y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} f(x, y(x))\,dx. \tag{5}$$

Approximating the integral by the trapezoidal rule we obtain

$$y_{n+1} = y_n + \frac{h}{2}\,[f(x_n, y_n) + f(x_{n+1}, y_{n+1})], \quad n = 0, 1, 2, \ldots, \tag{6}$$

The error of this formula is $E = -(h^3/12)y'''$. The formula (6) is known as improved Euler method. Note that (6) is an implicit equation for y_{n+1}.

If $f(x, y)$ is a nonlinear function, then it is difficult to solve (6) for y_{n+1} exactly. However, one can attempt to obtain y_{n+1} by means of iteration. Thus, keeping x_n fixed, we obtain a first approximation to y_{n+1} by means of Eulers formula

$$y_{n+1}^{(0)} = y_n + hf(x_n, y_n).$$

Then, compute $f(x_{n+1}, y_{n+1}^{(0)})$ and obtain the approximation

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

Next, evaluate $f(x_{n+1}, y_{n+1}^{(1)})$ and obtain $y_{n+1}^{(2)}$ as

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

In general, the iteration is given by

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

Algorithm(A second-order predictor-corrector method) For the differential equation $y' = f(x, y),\ y(x_0) = y_0$ with h given and $x_n = x_0 + nh$, for each fixed $n = 0, 1, \ldots,$

- Compute $y_{n+1}^{(0)}$ using $y_{n+1}^{(0)} = y_n + hf(x_n, y_n)$.
- Compute $y_{n+1}^{(k)}$ $(k = 1, 2, \ldots)$, using

  $$y_{n+1}^{(k)} = y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(k-1)})\right],$$

  iterating on k until
  $$\frac{|y_{n+1}^{(k)} - y_{n+1}^{(k-1)}|}{|y_{n+1}^{(k)}|} < \epsilon$$

  for a prescribed ϵ (tolerance).

Remarks.

- It is customary to call an explicit formula such as Euler's formula an open-type formula, while an implicit formula such as (6) is said to be of closed type.
- When they are used as a pair of formulas, the open-type formula is also called a predictor, while the closed-type formula is called a corrector.

Q. Under what conditions will the inner iteration on k converge?

Theorem. Let $f(x,y), \frac{\partial f}{\partial y} \in C(R)$, where R is a closed rectangle with $(x_0, y_0) \in R$. Then, the inner iteration defined by

$$y_{n+1}^{(k)} = y_n + \frac{h}{2}\left[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(k-1)})\right], \quad k = 1, 2, \dots \tag{7}$$

will converge, provided h is chosen small enough so that, for $x = x_n$, and for all y with $|y - y_{n+1}| < |y_{n+1}^{(0)} - y_{n+1}|$,

$$\left|\frac{\partial f}{\partial y}\right| h < 2.$$

Proof. Observe that with x_n is fixed and setting $y_{n+1}^{(k)} = Y^{(k)}$, we can write the iteration (7) in the form

$$Y^{(k)} = F(Y^{(k-1)}), \tag{8}$$

where $F(Y) = \frac{h}{2} f(x_{n+1}, Y) + C$. Here C depends on n not on Y. Consider (8) as a fixed point iteration with iteration function $F(Y)$. The iteration will converge provided

$$|F'(Y)| < 1, \;\; \forall Y \text{ with } |Y - y_{n+1}| < |Y^{(0)} - y_{n+1}|,$$

where y_{n+1} is the fixed point of $F(Y)$.

The iteration will converge if

$$|F'(Y)| = \left|\frac{h}{2}\frac{\partial f}{\partial y}\right| < 1 \implies h < \frac{2}{|\partial f/\partial y|},$$

and this proves the theorem.

The Adams-Moulton Method. Consider the IVP:

$$y' = f(x,y), \quad y(x_0) = y_0, \tag{9}$$

Integrate the differential equation (1) from x_n to x_{n+1}, to have

$$y_{n+1} = y_n + \int_{x_n}^{x_{n+1}} f(x, y(x))\, dx. \tag{10}$$

In this case, we approximate $f(x, y(x))$ by a polynomial which interpolates at $x_{n+1}, x_n, \ldots, x_{n-m}$ for an integer $m > 0$. Then, use of Newton's backward interplation formula which interpolates f at these $m+2$ points in terms of $s = (x - x_n)/h$ yields

$$p_{m+1}(s) = \sum_{k=0}^{m+1} (-1)^k \binom{1-s}{k} \Delta^k f_{n+1-k}.$$

These differences are based on the values $f_{n+1}, f_n, \ldots, f_{n-m}$. Replacing f by p_{m+1} in (10), we have

$$\begin{aligned} y_{n+1} &= y_n + h\int_0^1 \sum_{k=0}^{m+1} (-1)^k \begin{pmatrix} 1-s \\ k \end{pmatrix} \Delta^k f_{n+1-k}\, ds \\ &= y_n + h\left(\gamma_0' f_{n+1} + \gamma_1' \Delta f_n + \cdots + \gamma_{m+1}' \Delta^{m+1} f_{n-m}\right), \qquad (11) \end{aligned}$$

where

$$\gamma_k' = (-1)^k \int_0^1 \sum_{k=0}^{m+1} \begin{pmatrix} 1-s \\ k \end{pmatrix} ds, \quad k = 0, 1, \ldots, m+1.$$

The formula (11) is known as Adams-Mouton multistep formula.

With $m = 2$ and the values of $\gamma_0' = 1$, $\gamma_1' = -\frac{1}{2}$, $\gamma_2' = -\frac{1}{12}$ and $\gamma_3' = -\frac{1}{24}$, we obtain the formula

$$y_{n+1} = y_n + h\left(f_{n+1} - \frac{1}{2}\Delta f_n - \frac{1}{12}\Delta^2 f_{n-1} - \frac{1}{24}\Delta^3 f_{n-2}\right).$$

Since

$$\begin{aligned}\Delta f_n &= f_{n+1} - f_n \\ \Delta^2 f_{n-1} &= \Delta(\Delta f_{n-1}) = \Delta(f_n - f_{n-1}) = f_{n+1} - 2f_n + f_{n-1} \\ \Delta^3 f_{n-2} &= f_{n+1} - 3f_n + 3f_{n-1} - f_{n-2}\end{aligned}$$

we obtain

$$y_{n+1} = y_n + \frac{h}{24}(9f_{n+1} + 19f_n - 5f_{n-1} + f_{n-2}).$$

In this case, the error is

$$E_{AM} = -\frac{19}{270} h^5 y^v(\xi).$$

Algorithm (The Adams-Moulton predictor-corrector method): For the IVP: $y' = f(x, y)$, $y(x_0) = y_0$ with h fixed, $x_n = x_0 + nh$, and given (y_0, f_0), (y_1, f_1), (y_2, f_2), (y_3, f_3), where $f_i = f(x_i, y_i)$.

- Compute $y_{n+1}^{(0)}$ using the Adams-Bashforth formula

$$y_{n+1}^{(0)} = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}), \quad n = 3, 4, \ldots$$

- Compute $f_{n+1}^{(0)} = f(x_{n+1}, y_{n+1}^{(0)})$
- Improve the value of y_{n+1} using the Adams-Moulton formula

$$y_{n+1}^{(k)} = y_n + \frac{h}{24}\left(9f(x_{n+1}, y_{n+1}^{(k-1)}) + 19f_n - 5f_{n-1} + f_{n-2}\right), \quad k = 1, 2, \ldots$$

- Iterate on k until

$$\frac{|y_{n+1}^{(k)} - y_{n+1}^{(k-1)}|}{|y_{n+1}^{(k)}|} < \epsilon, \quad \text{for prescribed tolerance } \epsilon.$$

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