INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
DEPARTMENT OF MATHEMATICS

MA 322: SCIENTIFIC COMPUTING

Quiz - II (Answer Key), Semester II, Academic Year 2022-23

Full Marks: 15 **Duration: 1 hour**

1. Derive the Adams-Bashforth and Adams-Multon methods of order two. **[3]**

Answer: Adams methods are multi-step method. The general form of this method is given by

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

Adams-Bashforth (AB) method is an explicit method. Second order AB method is obtained by approximating the integral in (1) as

$$\int_{x_n}^{x_{n+1}} f(x, y(x))\,\mathrm{d}x = h[B_0 f_n + B_1 f_{n-1}]. \tag{2}$$

The coefficients B_0 and B_1 are obtained such that the integral in (2) be exact whenever the integrand is a polynomial of degree ≤ 1.

Without loss of generality, we assume $h = 1$ and $x_n = 0$; thus, $x_{n-j} = -j,\ j = 0, 1$. Using $f(x, y(x)) = 1$ in (2), we obtain

$$1 = B_0 + B_1. \tag{3}$$

Similarly, using $f(x, y(x)) = x$ in (2), we obtain

$$\frac{1}{2} = 0 \cdot B_0 + (-1) \cdot B_1. \tag{4}$$

Therefore, $B_0 = 3/2$ and $B_1 = -1/2$ and the required second-order AB method is

$$y_{n+1} = y_n + \frac{h}{2}[3f_n - f_{n-1}]. \tag{5}$$

Adams-Multon (AM) method is an implicit method. Second order AM method is obtained by approximating the integral in (1) as

$$\int_{x_n}^{x_{n+1}} f(x, y(x))\,\mathrm{d}x = h[B_0 f_n + B_{-1} f_{n+1}]. \tag{6}$$

The coefficients B_0 and B_{-1} are obtained such that the integral in (2) be exact whenever the integrand is a polynomial of degree ≤ 1.

As before, using $h = 1$ and $x_n = 0$; thus, $x_{n-j} = -j,\ j = -1, 0$. Using $f(x, y(x)) = 1$ in (2), we obtain

$$1 = B_0 + B_1. \tag{7}$$

Similarly, using $f(x, y(x)) = x$ in (2), we obtain

$$\frac{1}{2} = 0 \cdot B_0 + 1 \cdot B_1. \tag{8}$$

Therefore, $B_0 = 1/2$ and $B_{-1} = 1/2$ and the required second-order AB method is

$$y_{n+1} = y_n + \frac{h}{2}[f_n + f_{n+1}]. \tag{9}$$

2. Consider $f \in C^\infty(\mathbb{R})$ and equidistant points $x_0 < x_1 < \cdots < x_n$. Derive the central difference formula for f''' at the point x_i using $f_j,\ j = i-2, i-1, i, i+1, i+2$. Determine the order of the method.

   Suppose that the numerical values for f_j are available of n-digit rounded decimal arithmetic. Determine optimal grid-spacing $h(> 0)$ that minimizes the total error of numerical differentiation of f''' using the central difference formula derived above. Here, $x_i = x_0 + ih,\ i = 0, 1, 2, \ldots$ **[3+1+4]**

   Answer: Since $f \in C^\infty(\mathbb{R})$, we can expand $f(x_j \pm 2h)$ and $f(x_j \pm h)$ using Taylor series as follows:

$$\begin{aligned} f(x_j \pm 2h) &= f(x_j) \pm 2hf'(x_j) + \frac{2^2h^2}{2!}f''(x_j) \pm \frac{2^3h^3}{3!}f'''(x_j) + \frac{2^4h^4}{4!}f^{(iv)}(x_j) \\ &\qquad \pm \frac{2^5h^5}{5!}f^{(v)}(x_j) + \cdots, \qquad (10) \\ f(x_j \pm h) &= f(x_j) \pm hf'(x_j) + \frac{h^2}{2!}f''(x_j) \pm \frac{h^3}{3!}f'''(x_j) + \frac{h^4}{4!}f^{(iv)}(x_j) \\ &\qquad \pm \frac{h^5}{5!}f^{(v)}(x_j) + \cdots, \qquad (11) \end{aligned}$$

Combining these equations, we obtain

$$\begin{aligned} f_{j+2} - 2f_{j+1} + 2f_{j-1} - f_{j-2} &= \frac{12h^3}{3!}f_j''' + \frac{h^5}{2}f_j^{(v)} + \mathbf{O}(h^6) \\ \therefore \qquad f_j''' &= \frac{f_{j+2} - 2f_{j+1} + 2f_{j-1} - f_{j-2}}{2h^3} + \frac{h^2}{4}f_j^{(v)} + \mathbf{O}(h^3) \end{aligned}$$

Therefore, the required central difference formula is

$$f_j''' \approx \frac{f_{j+2} - 2f_{j+1} + 2f_{j-1} - f_{j-2}}{2h^3} \tag{12}$$

and the method is second order accurate, (i.e., the method is $\mathbf{O}(h^2)$.)
We denote

$$D_h^{(3)}f(x_n) = \frac{f_{j+2} - 2f_{j+1} + 2f_{j-1} - f_{j-2}}{2h^3}. \tag{13}$$

If the computer representation of f_j is $\tilde{f}_j$ with error $\tilde{\epsilon}_j$, i.e.,

$$f_j = \tilde{f}_j + \tilde{\epsilon}_j \qquad j = 0, 1, 2, \cdots \tag{14}$$

Therefore,

$$\tilde{D}_h^{(3)} f(x_n) = \frac{\tilde{f}_{j+2} - 2\tilde{f}_{j+1} + 2\tilde{f}_{j-1} - \tilde{f}_{j-2}}{2h^3}. \tag{15}$$

Therefore, the total error is bounded above by

$$|f'''(x_n) - \tilde{D}_h^{(3)} f(x_n)| \leq \frac{h^2}{4} M + \frac{6E}{2h^3}, \tag{16}$$

where $|f^{(v)}(\xi)| \leq M$ for $x_{j-2} < \xi < x_{j+2}$ and $-E \leq \epsilon := \max_j\{\epsilon_j\} \leq E$. Define

$$\mathcal{E}(h) = \frac{h^2}{4} M + \frac{6E}{2h^3}. \tag{17}$$

Thus,

$$\frac{\mathrm{d}\mathcal{E}(h)}{\mathrm{d}h} = \frac{h}{2} M - \frac{9E}{h^4}. \tag{18}$$

Now,

$$\frac{\mathrm{d}\mathcal{E}(h)}{\mathrm{d}h} = 0 \Rightarrow h = \left(\frac{18E}{M}\right)^{1/5} := h_* \text{ (say)}. \tag{19}$$

We have

$$\left.\frac{\mathrm{d}^2\mathcal{E}(h)}{\mathrm{d}h^2}\right|_{h_*} = \left(\frac{M}{2} + \frac{36E}{h^5}\right)_{h_*} = M > 0. \tag{20}$$

For a n-digit rounded decimal arithmetic, $E = \frac{1}{2} \times 10^{-n}$. Therefore, the required step size is

$$h = \left(\frac{9}{M}\right)^{1/5} 10^{-n/5}. \tag{21}$$

3. The stability of a numerical integration method is an important concept and it is related to the stability region, which is described by $|r(\lambda h)| < 1$, where $r(\lambda h) = y_{n+1}/y_n$ is the stability function. For example, the stability region of the forward Euler method

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

is the region given by $|1+\lambda h| < 1$ in the complex λ-plane. Determine the stability region of trapezoidal rule. Draw the stability region in the complex λ-plane (or, complex λh-plane). **[4]**

Answer: Consider the ODE

$$y' = \lambda y \qquad \lambda \in \mathbb{C},\ \Re(\lambda) < 0. \tag{22}$$

Equation (22) exhibits a decaying solution. A numerical method is stable if the numerical method captures the decay.

Trapezoidal rule is given by

$$y_{n+1} = y_n + \frac{h}{2}[f_n + f_{n+1}]. \tag{23}$$

Using (22) in (23) we get

$$\begin{aligned}
y_{n+1} &= y_n + \frac{h}{2}[\lambda y_n + \lambda y_{n+1}], \\
&= \left(1 + \frac{\lambda h}{2}\right) y_n + \frac{\lambda h}{2} y_{n+1}, \\
\Rightarrow \left(1 - \frac{\lambda h}{2}\right) y_{n+1} &= \left(1 + \frac{\lambda h}{2}\right) y_n, \\
\Rightarrow y_{n+1} &= \frac{1 + \frac{\lambda h}{2}}{1 - \frac{\lambda h}{2}} y_n.
\end{aligned}$$

Therefore, the stability function is

$$r(\lambda h) := \frac{y_{n+1}}{y_n} = \frac{1 + \frac{\lambda h}{2}}{1 - \frac{\lambda h}{2}}. \tag{24}$$

For the stability of the trapezoidal rule, we require

$$\begin{aligned}
& |r(\lambda h)| < 1 \\
\Rightarrow \quad & |1 + \frac{\lambda h}{2}| < |1 - \frac{\lambda h}{2}| \\
\Rightarrow \quad & |2 + \lambda h| < |2 - \lambda h|.
\end{aligned}$$

The stability region of the trapezoidal rule is given by

$$R_h(\lambda) = \{\lambda \in \mathbb{C} : |2 + \lambda h| < |2 - \lambda h|\}, \tag{25}$$

which corresponds to the left-half plane in the complex λ-plane.