MULTISTEP METHODS

http://www.phys.uconn.edu/~rozman/Courses/m3510_19f/

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We are interested in the numerical solution of the initial value problem (IVP):

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f(t,y), \quad a \le t \le b, \quad y(a) = y_0. \tag{1}$$

We denote the time at the nth time step by t_n, the computed solution at the nth time step by y_n,

$$y_n \equiv y(t_n), \tag{2}$$

and the value of the right hand side of Eq. (1) at the nth time step by f_n,

$$f_n \equiv f(t_n, y_n). \tag{3}$$

The step size h (assumed to be constant for the sake of simplicity) is

$$h = t_n - t_{n-1}. \tag{4}$$

So far all of the numerical methods that we have developed for solving initial value problems are *one-step methods* — they only use the information about the solution at time t_n to approximate the solution at time t_{n+1} (possibly taking intermediate steps but then discarding this additional information). *Multistep methods* attempt to gain efficiency by keeping and using the information from the previous steps. A method is called *linear multistep method* if a linear combination of the values of the computed solution and possibly its derivative in the previous points are used.

An example of multistep method is the following expression

$$\begin{aligned} y_{n+1} &= y_n + h\left(\beta_0 f_{n+1} + \beta_1 f_n + \beta_2 f_{n-1} + \ldots + \beta_s f_{n-s+1}\right) && (5) \\ &= y_n + h\sum_{i=0}^{s} \beta_i f_{n+1-i}, && (6) \end{aligned}$$

where s is the number of steps in the method. If $\beta_0 = 0$, the multistep method is said to be *explicit*, because then y_{n+1} can be described using an explicit formula. If $\beta_0 \neq 0$, the method is said to be *implicit*, because then an equation, generally nonlinear, must be solved to compute y_{n+1}.

The constants β_i satisfy the constraint

$$\sum_{i=0}^{s} \beta_i = 1 \tag{7}$$

originating from the requirement that if $f(t,y) = \alpha = \text{const}$, the correct solution $y(t) = \alpha t + C$ is produced by the numerical scheme.

A broad category of multistep methods that are called *Adams methods* involve the integral form of Eq. (1):

$$y(t_{n+1}) = y(t_n) + \int_{t_n}^{t_{n+1}} f(\tau, y(\tau))\,\mathrm{d}\tau. \tag{8}$$

The general idea behind Adams methods is to approximate the above integral using polynomial interpolation of f at the points t_{n+1-s}, t_{n+2-s}, $\ldots$, t_n if the method is explicit, and t_{n+1} as well if the method is implicit.

Explicit Adams methods are called *Adams-Bashforth methods*. Implicit Adams methods are known as *Adams-Moulton methods*.

1 Adams-Bashforth methods

To derive the integration formula for Adams-Bashforth method, we interpolate f at the points t_{n+1-s}, t_{n+2-s}, $\ldots$, t_n with a polynomial of the degree $s-1$. We then integrate this polynomial exactly.

Let's derive the three-step Adams-Bashforth method with the local truncation error $O(h^3)$.

The interpolating polynomial for $f(\tau, y(\tau))$ passing through three points (t_{n-2}, f_{n-2}), (t_{n-1}, f_{n-1}), and (t_n, f_n) is as following:

$$P_3(\tau) = f_{n-2}L_{n-2}(\tau) + f_{n-1}L_{n-1}(\tau) + f_n L_n(\tau), \tag{9}$$

where the Lagrange polynomials are

$$\begin{aligned} L_{n-2}(\tau) &= \frac{(\tau - t_{n-1})(\tau - t_n)}{(t_{n-2} - t_{n-1})(t_{n-2} - t_n)} = \frac{1}{2h^2}(\tau - t_{n-1})(\tau - t_n), \\ L_{n-1}(\tau) &= \frac{(\tau - t_{n-2})(\tau - t_n)}{(t_{n-1} - t_{n-2})(t_{n-1} - t_n)} = -\frac{1}{h^2}(\tau - t_{n-2})(\tau - t_n), \\ L_n(\tau) &= \frac{(\tau - t_{n-2})(\tau - t_{n-1})}{(t_n - t_{n-2})(t_n - t_{n-1})} = \frac{1}{2h^2}(\tau - t_{n-2})(\tau - t_{n-1}). \end{aligned} \tag{10}$$

Substituting Eq. (9) into Eq. (8), we obtain:

$$\begin{aligned} y_{n+1} &= y_n + \int_{t_n}^{t_{n+1}} P_3(\tau)\,\mathrm{d}\tau = \\ &= y_n + f_{n-2}\int_{t_n}^{t_{n+1}} L_{n-2}(\tau)\,\mathrm{d}\tau + f_{n-1}\int_{t_n}^{t_{n+1}} L_{n-1}(\tau)\,\mathrm{d}\tau + f_n \int_{t_n}^{t_{n+1}} L_n(\tau)\,\mathrm{d}\tau. \end{aligned}$$

The integrals in Eq. (11) can be evaluated by introducing a new integration variable

$$u = \frac{\tau - t_n}{h}, \quad 0 \le u \le 1, \tag{11}$$

such that

$$\tau = t_n + hu, \quad \mathrm{d}\tau = h\,\mathrm{d}u, \tag{12}$$

$$\tau - t_{n+1} = -h + hu \quad \tau - t_n = hu, \quad \tau - t_{n-1} = h + hu, \quad \tau - t_{n-2} = 2h + hu. \tag{13}$$

Lagrange polynomials as the functions of u are,

$$\begin{aligned} L_{n-2}(u) &= \frac{1}{2}u(u+1), \\ L_{n-1}(u) &= -u(u+2), \\ L_n(u) &= \frac{1}{2}(u+1)(u+2). \end{aligned} \tag{14}$$

Integrating, we obtain

$$
\begin{aligned}
\int_{t_n}^{t_{n+1}} L_{n-2}(\tau)\,\mathrm{d}\tau &= h\int_0^1 L_{n-2}(u)\,\mathrm{d}u = \frac{h}{2}\int_0^1 u(u+1)\,\mathrm{d}u = \frac{5}{12}h,\\
\int_{t_n}^{t_{n+1}} L_{n-1}(\tau)\,\mathrm{d}\tau &= h\int_0^1 L_{n-1}(u)\,\mathrm{d}u = -h\int_0^1 u(u+2)\,\mathrm{d}u = -\frac{4}{3}h,\\
\int_{t_n}^{t_{n+1}} L_{n}(\tau)\,\mathrm{d}\tau &= h\int_0^1 L_{n}(u)\,\mathrm{d}u = \frac{h}{2}\int_0^1 (u+1)(u+2)\,\mathrm{d}u = \frac{23}{12}h.
\end{aligned} \tag{15}
$$

We conclude that the three-step Adams-Bashforth method is

$$
y_{n+1} = y_n + \frac{h}{12}\left(5f_{n-2} - 16f_{n-1} + 23f_n\right). \tag{16}
$$

Note that the coefficients in Eq. (22) satisfy the constraint Eq. (7).

2 Adams-Moulton methods

The same approach can be used to derive the integration formulas for *implicit Adams-Moulton methods*. The resulting interpolating polynomial is of degree one greater than in the explicit case, so the error in an s-step Adams-Moulton method is $O(h^{s+1})$, as opposed to $O(h^s)$ for an s-step Adams-Bashforth method.

The interpolating polynomial through (t_{n-2}, f_{n-2}), (t_{n-1}, f_{n-1}), (t_n, f_n), and (t_{n+1}, f_{n+1}) is as following:

$$
P_4(\tau) = f_{n-2}L_{n-2}(\tau) + f_{n-1}L_{n-1}(\tau) + f_nL_n(\tau) + f_{n+1}L_{n+1}(\tau), \tag{17}
$$

where the Lagrange polynomials are

$$
\begin{aligned}
L_{n-2}(\tau) &= \frac{(\tau-t_{n-1})(\tau-t_n)(\tau-t_{n+1})}{(t_{n-2}-t_{n-1})(t_{n-2}-t_n)(t_{n-2}-t_{n+1})} = -\frac{1}{6h^3}(\tau-t_{n-1})(\tau-t_n)(\tau-t_{n+1}),\\
L_{n-1}(\tau) &= \frac{(\tau-t_{n-2})(\tau-t_n)(\tau-t_{n+1})}{(t_{n-1}-t_{n-2})(t_{n-1}-t_n)(t_{n-1}-t_{n+1})} = \frac{1}{2h^3}(\tau-t_{n-2})(\tau-t_n)(\tau-t_{n+1}),\\
L_{n}(\tau) &= \frac{(\tau-t_{n-2})(\tau-t_{n-1})(\tau-t_{n+1})}{(t_{n}-t_{n-2})(t_{n}-t_{n-1})(t_{n}-t_{n+1})} = -\frac{1}{2h^3}(\tau-t_{n-2})(\tau-t_{n-1})(\tau-t_{n+1}),\\
L_{n+1}(\tau) &= \frac{(\tau-t_{n-2})(\tau-t_{n-1})(\tau-t_{n})}{(t_{n+1}-t_{n-2})(t_{n+1}-t_{n-1})(t_{n+1}-t_{n})} = \frac{1}{6h^3}(\tau-t_{n-2})(\tau-t_{n-1})(\tau-t_{n}).
\end{aligned} \tag{18}
$$

$$\begin{aligned} y_{n+1} &= y_n + \int\limits_{t_n}^{t_{n+1}} P_4(\tau)\,\mathrm{d}\tau = \qquad (19)\\ &= y_n + f_{n-2}\int\limits_{t_n}^{t_{n+1}} L_{n-2}(\tau)\,\mathrm{d}\tau + f_{n-1}\int\limits_{t_n}^{t_{n+1}} L_{n-1}(\tau)\,\mathrm{d}\tau + f_n\int\limits_{t_n}^{t_{n+1}} L_n(\tau)\,\mathrm{d}\tau + f_{n+1}\int\limits_{t_n}^{t_{n+1}} L_{n+1}(\tau)\,\mathrm{d}\tau. \end{aligned}$$

Lagrange polynomials as the functions of the variable u Eq. (11) are,

$$\begin{aligned} L_{n-2}(u) &= \frac{1}{6}u(1-u^2),\\ L_{n-1}(u) &= -\frac{1}{2}u(u+2)(1-u),\\ L_n(u) &= \frac{1}{2}(u+2)(1-u^2),\\ L_{n+1}(u) &= \frac{1}{6}u(u+1)(u+2). \end{aligned} \qquad (20)$$

Integrating, we obtain

$$\begin{aligned} \int\limits_{t_n}^{t_{n+1}} L_{n-2}(\tau)\,\mathrm{d}\tau &= h\int\limits_0^1 L_{n-2}(u)\,\mathrm{d}u = \frac{h}{6}\int\limits_0^1 u(1-u^2)\,\mathrm{d}u = \frac{1}{24}h,\\ \int\limits_{t_n}^{t_{n+1}} L_{n-1}(\tau)\,\mathrm{d}\tau &= h\int\limits_0^1 L_{n-1}(u)\,\mathrm{d}u = -\frac{h}{2}\int\limits_0^1 u(u+2)(1-u)\,\mathrm{d}u = -\frac{5}{24}h, \qquad (21)\\ \int\limits_{t_n}^{t_{n+1}} L_n(\tau)\,\mathrm{d}\tau. &= h\int\limits_0^1 L_n(u)\,\mathrm{d}u = \frac{h}{2}\int\limits_0^1 (u+2)(1-u^2)\,\mathrm{d}u = \frac{19}{24}h.\\ \int\limits_{t_n}^{t_{n+1}} L_{n+1}(\tau)\,\mathrm{d}\tau. &= h\int\limits_0^1 L_{n+1}(u)\,\mathrm{d}u = \frac{h}{6}\int\limits_0^1 u(u+1)(u+2)\,\mathrm{d}u = \frac{3}{8}h. \end{aligned}$$

We conclude that the three-step Adams-Moulton method is

$$y_{n+1} = y_n + \frac{h}{24}\left(f_{n-2} - 5f_{n-1} + 19f_n + 9f_{n+1}\right). \qquad (22)$$

Note that the coefficients in Eq. (22) satisfy the constraint Eq. (7).

3 Predictor-corrector method

An Adams-Moulton method can be impractical because, being implicit, it requires solving nonlinear equations during every time step. An alternative is to pair an Adams-Bashforth method with an Adams-Moulton method to obtain an Adams-Moulton *predictor-corrector method*. Such a method proceeds as follows:

Predict: use the Adams-Bashforth method to compute a first approximation to y_{n+1}, which we denote by $\hat{y}_{n+1}$.

Evaluate: evaluate $f(t_{n+1}, \hat{y}_{n+1})$.

Correct: use the Adams-Moulton method to compute y_{n+1}, but instead of solving an equation, use $f(t_{n+1}, \hat{y}_{n+1})$ in place of $f(t_{n+1}, y_{n+1})$ so that the Adams-Moulton method can be used as if it was an explicit method.

Evaluate: evaluate $f(t_{n+1}, y_{n+1})$ to use during the next time step.

4 Conclusions

A drawback of multistep methods is that because they rely on values of the solution from previous time steps, they cannot be used during the first time steps. Therefore, it is necessary to use a one-step method, with the same order of accuracy, to compute enough starting values of the solution to be able to use the multistep method. For example, to use the three-step Adams-Bashforth method, it is necessary to first use a one-step method such as the fourth-order Runge-Kutta method to compute y_1 and y_2, and then the Adams-Bashforth method can be used to compute y_3 using y_2, y_1 and y_0.