Math/CS 714: Initial value problems

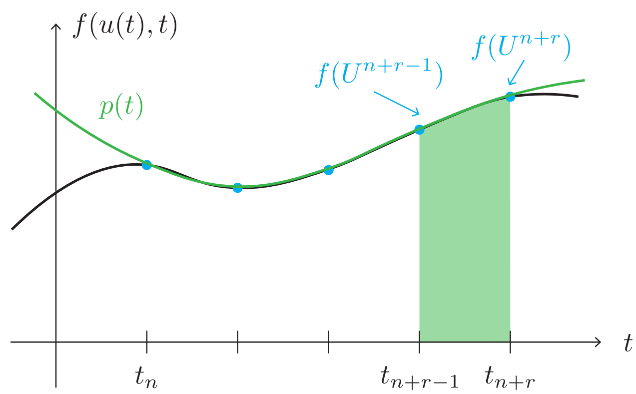
We start with the integral relation

$$u(t_{n+r}) = u(t_{n+r-1}) + \int_{t_{n+r-1}}^{t_{n+r}} f(u(t),t)\,dt,$$

then

$$U^{n+r} = U^{n+r-1} + \int_{t_{n+r-1}}^{t_{n+r}} p(t)\,dt$$

where $p(t)$ is a polynomial interpolant of $f(u(t),t)$ using several prior values of U^{n+j}. Our goal is to derivate parameters for an r-step method by first interpolating (finding $p(t)$) and then integrating the interpolant.



There are two families of multistep methods:

- Adams–Bashforth methods: explicit, use only previous values of f $(f_n, \ldots, f_{n+r-1})$.
- Adams–Moulton methods: implicit, use previous values of f and the current value $(f_n, \ldots, f_{n+r})$.

The derivation below considers two-step ($r = 2$) Adams–Bashforth and Adams–Moulton methods.

1 Derivation of Adams–Bashforth methods

A mathematical solution to the ODE $u'(t) = f(t,u)$ satisfies

$$u(t_{n+2}) = u(t_{n+1}) + \int_{t_{n+1}}^{t_{n+2}} f(t,u)\,dt. \tag{1.1}$$

We aim to approximate $f(t,u)$ over the interval $[t_{n+1}, t_{n+2}]$ using a polynomial interpolant $p(t)$ based on r previous values of f, $t_{n-r+1}, t_{n-r+2}, \ldots, t_n$. Function values at these points, $f_l = f(t_l, u(t_l))$, are known.

When $r = 2$, we have two values (f_n, f_{n+1}), and thus use linear interpolation to construct $p(t)$:

$$p(t) = f_{n+1} + s(f_{n+1} - f_n), \tag{1.2}$$

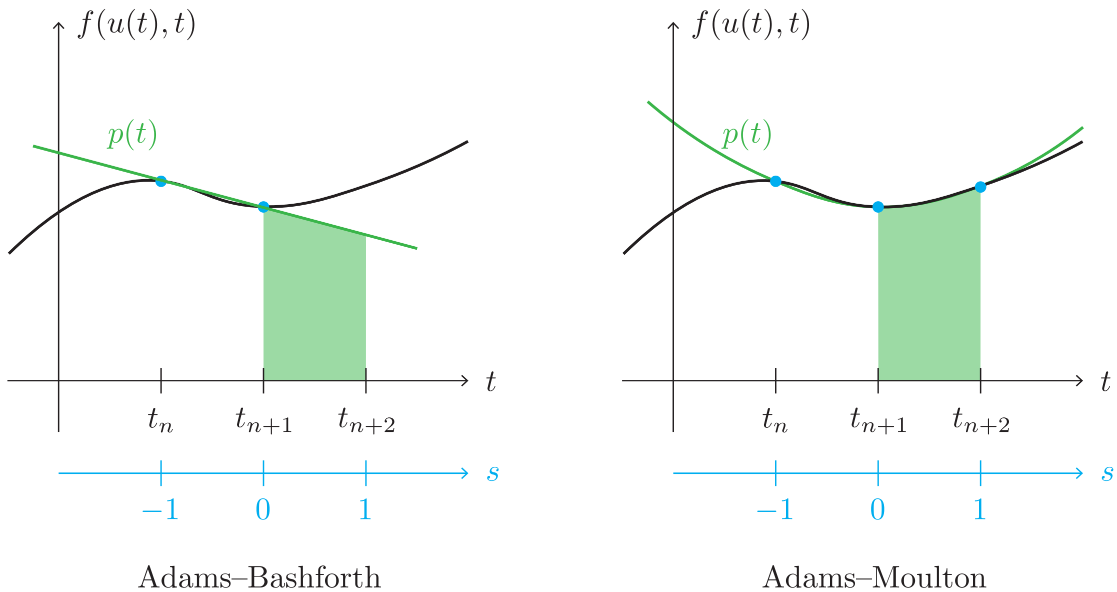
where s is a new variable that satisfies $t = t_{n+1} + sh$ and $h = t_{n+2} - t_{n+1}$. The variable s varies from 0 to 1 as t goes from t_{n+1} to t_{n+2}.

To obtain a numerical update formulate, we just need to substitute Eq. (1.2) into Eq. (1.1) and then evaluate the integral:

$$
\begin{aligned}
u(t_{n+2}) &= u(t_{n+1}) + \int_{t_{n+1}}^{t_{n+2}} p(t)\, dt \\
&= u(t_{n+1}) + \int_0^1 p(t_{n+1} + sh) h\, ds \\
&= u(t_{n+1}) + h \int_0^1 \left[f_{n+1} + s(f_{n+1} - f_n)\right] ds \\
&= u(t_{n+1}) + h \left[f_{n+1}s + (f_{n+1} - f_n)\frac{s^2}{2}\right]_0^1 \\
&= u(t_{n+1}) + h \left(\frac{3}{2} f_{n+1} - \frac{1}{2} f_n\right).
\end{aligned}
\tag{1.3}
$$

The two-step explicit Adams–Bashforth method is second-order accurate, and is thus given by

$$
U^{n+2} = U^{n+1} + \frac{h}{2}\left(-f(U^n) + 3f(U^{n+1})\right). \tag{1.4}
$$



2 Derivation of Adams–Moulton methods

We have the same mathematical solution to the ODE as in Eq. (1.1). The difference is that we now use r previous values of f and the current value to construct the polynomial interpolant $p(t)$—so we have $r+1$ values of f to interpolate.

When $r = 2$, we have three values (f_n, f_{n+1}, f_{n+2}), and thus use quadratic interpolation to construct $p(t)$. Suppose we use the same change of variable s as before, then we have

$$
u(t_{n+2}) = u(t_{n+1}) + h \int_0^1 p(s)\, ds \tag{2.1}
$$

where $p(s)$ is a quadratic polynomial that interpolates f_n, f_{n+1}, f_{n+2} at $s = -1, 0, 1$, respectively. Using Lagrange interpolation, we have

$$p(s) = f_n L_0(s) + f_{n+1} L_1(s) + f_{n+2} L_2(s) \tag{2.2}$$

where $L_i(s)$ are the Lagrange polynomials for $\{-1, 0, 1\}$:

$$L_0(s) = \frac{(s-1)s}{2}, \quad L_1(s) = 1 - s^2, \quad L_2(s) = \frac{s(s+1)}{2}.$$

Substituting Eq. (2.2) into the integral, we have

$$\begin{aligned} u(t_{n+2}) &= u(t_{n+1}) + h \int_0^1 \left[f_n \frac{(s-1)s}{2} - f_{n+1}(1-s^2) + f_{n+2} \frac{s(s+1)}{2} \right] ds \\ &= u(t_{n+1}) + h \left[f_n \left(\frac{s^3}{6} - \frac{s^2}{4} \right) + f_{n+1} \left(s - \frac{s^3}{3} \right) + f_{n+2} \left(\frac{s^3}{6} + \frac{s^2}{4} \right) \right]_0^1 \\ &= u(t_{n+1}) + h \left(f_n \left(\frac{1}{6} - \frac{1}{4} \right) + f_{n+1} \left(1 - \frac{1}{3} \right) + f_{n+2} \left(\frac{1}{6} + \frac{1}{4} \right) \right) \\ &= u(t_{n+1}) + \frac{h}{12} \left(5 f_{n+2} + 8 f_{n+1} - f_n \right). \end{aligned} \tag{2.3}$$

The two-step implicit Adams–Moulton method is third-order accurate, and is thus given by

$$U^{n+2} = U^{n+1} + \frac{h}{12} \left(-f(U^n) + 8 f(U^{n+1}) + 5 f(U^{n+2}) \right). \tag{2.4}$$