Multi Step Methods

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1 Adams Method

While solving an ODE in the form

$$y'(t) = f(t, y) \quad t > t_0, y(t_0) = y_0 \tag{1}$$

the exact solution only depends on the f and y_0. However, for numerical solutions, it is not necessarily the case. Fundamental iterative methods work like that we start with the y_0 to calculate the y_1, then we forget the y_0 and use the y_1 to calculate the y_2. It goes like that until we reach the wanted number of approximated points.

Yet, using the already calculated numbers may have a good impact on decreasing errors in the numerical estimations of the solution. To see that, let's derive an algorithm that intelligently benefits from past values.

Let y_n be the numerical solution for the $t_n = to + nh$. Let's assume that for a given integer $s \geq 1$, we have

$$y_m = y(t_m) + \mathcal{O}(h^{s+1}) \quad , m \in \{0, 1, 2, \cdots, n + s - 1\} \tag{2}$$

Now our focus is to improve the solution from t_{n+s-1} to t_{n+s}. Let's start with the identity

$$y(t_{n+s}) = y(t_{n+s-1}) + \int_{t_{n+s-1}}^{t_{n+s}} f(t, y(t))dt \tag{3}$$

Here, we want to do our best approximation. We use only the limits of the integral for the theta method. However, one should notice that we can use the whole interval $[t_{n+s-1}, t_{n+s}]$ for that approximation.

"The main idea of the Adams Method is to use the past values of the solution to approximate y', so does f in the interval of integration." This can be done by interpolation polynomials $P(t)$s that match with $f(t_m, y_m)$ for $m = n, n + 1, \cdots, n + s - 1$.

$$P(t) = \sum_{k=0}^{s-1} p_k(t) f(t_{n+k}, y_{n+k}) \tag{4}$$

where $p_k(t)$ is the Lagrange interpolation polynomials as

$$p_k(t) = \prod_{l=0 \ l \neq k}^{s-1} \frac{t - t_{n+l}}{t_{n+k} - t_{n+l}} = \frac{(-1)^{s-1-k}}{k!(s-1-k!} \prod_{l=0 \ l \neq k}^{s-1} \left(\frac{t - t_n}{h} - l \right) \tag{5}$$

[1] One should also notice that $f(t_m, y_m) = P(t_m)$. To show that, let's start with the (4)

$$P(t_{n+j}) = \sum_{k=0}^{s-1} p_k(t_{n+j}) f(t_{n+k}, y_{n+k})$$

where $l \in \{0, 1, 2, \cdots, s-1\}$. Then we have the following two cases.
if $j \neq k$

$$p_k(t_{n+j}) = \prod_{l=0 \ l \neq k}^{s-1} \frac{t_{n+j} - t_{n+l}}{t_{n+k} - t_{n+l}}$$

$$\frac{t_{n+j} - t_{n+j}}{t_{n+k} - t_{n+j}} \prod_{l=0 \ l \neq k \ l \neq j}^{s-1} \frac{t_{n+j} - t_{n+l}}{t_{n+k} - t_{n+l}} \tag{6}$$

The first term in the (6) vanishes, so we get

$$j \neq k \Rightarrow p_k(t_{n+j}) = 0 \tag{7}$$

If $j = k$

$$p_k(t_{n+j}) = \prod_{l=0 \ l \neq k}^{s-1} \frac{t_{n+k} - t_{n+l}}{t_{n+k} - t_{n+l}} = 1 \tag{8}$$

$$j = k \Rightarrow p_k(t_{n+j}) = 1 \tag{9}$$

As a result, we have the following

$$P(t_{n+j}) = \sum_{k=0}^{s-1} p_k(t_{n+j}) f(t_{n+k}, y_{n+k}) = f(t_{n+k}, y_{n+k}) \quad , k = j$$

$$\Rightarrow P(t_m) = f(t_m, y_m) \quad m \in \{n, n+1, \cdots, n+s-1\} \tag{10}$$

Now, we are at the point where we can develop s-step Adams-Bashford Method. We basically use the identity (3), calculate the integral by replacing f with the corresponding interpolation polynomial P, and replace $y(t_{n+s-1}) with y_{n+s-1}$ which will bring an error of order $\mathcal{O}(h^{s+1})$ by the relation (2).

[1]The calculation of the very right-hand side of identity (5) is in the handwritten notes.

Let's start with the integral calculation.

$$\int_{t_{n+s-1}}^{t_{n+s}} f(t,y(t))dt = \int_{t_{n+s-1}}^{t_{n+s}} P(t)dt \tag{11}$$

$$= \int_{t_{n+s-1}}^{t_{n+s}} \left[\sum_{k=0}^{s-1} p_k(t) f(t_{n+k}, y_{n+k})\right] dt \tag{12}$$

$$= \sum_{k=0}^{s-1} \left[\int_{t_{n+s-1}}^{t_{n+s}} p_k(t)dt\right] f(t_{n+k}, y_{n+k}) \tag{13}$$

By the transformation $t = t_{n+s-1} + \tau$, we get

$$\int_{t_{n+s-1}}^{t_{n+s}} f(t,y(t))dt = \sum_{k=0}^{s-1} h \left[h^{-1} \int_0^h p_k(t_{n+s-1}+\tau)d\tau\right] f(t_{n+k}, y_{n+k}) \tag{14}$$

Let $h^{-1}\int_0^h p_k(t_{n+s-1}+\tau)d\tau = b_k$ where $k \in \{0, 1, \cdots, s-1\}$. Consequently,

$$y(t_{n+s}) = y_{n+s-1} + h\sum_{k=0}^{s-1} b_k f(t_{n+k}, y_{n+k}) + \mathcal{O}(h^{s+1}) \tag{15}$$

Finally, by using the relation (2) again, $y(t_{n+s}) = y_{n+s} + \mathcal{O}(h^{s+1})$, we reach the S-step Adams-Bashford method as

$$y_{n+s} = y_{n+s-1} + h\sum_{k=0}^{s-1} b_k f(t_{n+k}, y_{n+k}) \tag{16}$$

Another important point about the method is that if one calculates the coefficients b_k using the identity (5), they can see that these coefficients depend neither on n nor h. They are just s dependent.

2 Order and Convergence of the Multistep Methods

General form of the s-step method is

$$\sum_{m}^{s} a_m y_{n+m} = h\sum_{m}^{s} b_m f(t_{n+}, y_{n+m}) \tag{17}$$

where a_m and b_m are constants that independent from n,h, and the given differential equation.
If $a_s = 1$ and $b_s = 0$, we have the Adamas-Bashford Method which is the only explicit multistep method.
Determining the coefficients is the main problem of a multistep method. To do that one should be sure the method has a reasonable order. This is important

because if order is not enough, we cannot be sure that our method converges. We know that a method is order of $p \geq 1$ if and only if

$$\Psi(t, y) = \sum_{m}^{s} a_m y(t + mh) - h \sum_{m}^{s} b_m y'(t + mh) = \mathcal{O}(h^{p+1}), \quad h \to 0 \tag{18}$$

where y is sufficiently smooth, and there exist at least one y such that we cannot improve upon the decay $\mathcal{O}(h^{p+1})$ Before passing into the showing when a multistep method has order $p \geq 1$, one should note that we can characterize such a method in terms of polynomials

$$\rho(w) = \sum_{m=0}^{s} a_m w^m \quad , \quad \sigma(w) = \sum_{m=0}^{s} b_m w^m \tag{19}$$

Theorem 2.1. *The multistep method is of order $p \geq 1$ if and only if $c \neq 0$ such that*

$$\rho(w) - ln(w)\sigma(w) = c(w-1)^{p+1} + \mathcal{O}(|w-1|^{p+2})$$

as $w \to 1$

Proof. We first assume that y is analytic and the radius of converges is greater than sh. Then we start with taylor expanding the y and y' in the (17) around t.

$$\Psi(t, y) = \sum_{m=0}^{s} a_m \left[\sum_{k=0}^{\infty} \frac{1}{k!} y^{(k)}(t) m^k h^k \right] - h \sum_{m=0}^{s} b_m \left[\sum_{k=0}^{\infty} \frac{1}{k!} y^{(k+1)}(t) m^k h^k \right]$$

By some algebraic manipulations[2], we get

$$\sum_{m=0}^{s} y(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left[\sum_{m=0}^{s} a_m m^k - k \sum_{m=0}^{s} b_m m^{k-1} \right] h^k y^{(k)}(t) \tag{20}$$

Now, we will put some conditions[3] which will make our method order of $p \geq 1$.

$$\sum_{m=0}^{s} a_m = 0 \tag{21}$$

$$\sum_{m=0}^{s} a_m m^k = k \sum_{m=0}^{s} b_m m^{m-1}, \quad k = 0, 1, \cdots, p \tag{22}$$

$$\sum_{m=0}^{s} a_m m^k \neq k \sum_{m=0}^{s} b_m m^{m-1}, \quad k \geq p + 1 \tag{23}$$

[2] It can be checked in the handwritten notes.
[3] Derivation of the condition is **here**

The above conditions give

$$\sum_{k=p+1}^{\infty} \frac{1}{k!} \left[\sum_{m=0}^{s} a_m m^k - k \sum_{m=0}^{s} b_m m^{k-1} \right] h^k y^{(k)}(t) = \mathcal{O}(h^{p+1})$$

, so

$$\Psi(t, y) = \mathcal{O}(h^{p+1}) \tag{24}$$

Now, we have a method of order p. To end the proof, we should show that the equality in the theorem holds under the presence of the above conditions.
Let $w = e^z$, so $z \to 0$ as $w \to 1$. Then

$$\rho(e^z) ln(e^z) \sigma(e^z) = \sum_{m=0}^{s} a_m e^{zm} - z \sum_{m=0}^{s} b_m e^{zm} \tag{25}$$

By taylor expanding the e^{zm}, we get

$$\sum_{m=0}^{s} a_m \left[\sum_{k=0}^{\infty} \frac{1}{k!} m^k z^k \right] - z \sum_{m=0}^{s} b_m \left[\sum_{k=0}^{\infty} \frac{1}{k!} m^k z^k \right] \tag{26}$$

Shift the index of the infinite sum as

$$\sum_{m=0}^{s} a_m + \sum_{m=0}^{s} a_m \left[\sum_{k=1}^{\infty} \frac{1}{k!} m^k z^k \right] - \sum_{m=0}^{s} b_m \left[\sum_{k=1}^{\infty} \frac{1}{(k-1)!} m^{k-1} z^k \right]$$

Again, after some arrangements on the subtraction and imposing the above conditions, we get

$$\sum_{k=p+1}^{\infty} \frac{1}{k!} \left[\sum_{m=0}^{s} a_m m^k - k \sum_{m=0}^{s} b_m m^{k-1} \right] z^k \tag{27}$$

$$\frac{1}{p+1} \left[\sum_{m=0}^{s} a_m m^{p+1} - k \sum_{m=0}^{s} b_m m^p \right] z^{p+1} + \mathcal{O}(z^{p+2}) \tag{28}$$

Let $\frac{1}{p+1} \left[\sum_{m=0}^{s} a_m m^{p+1} - k \sum_{m=0}^{s} b_m m^p \right] = c$. Consequently, we get

$$\rho z - \sigma(z) ln(e^z) = c z^{p+1} + \mathcal{O}(z^{p+1}) \tag{29}$$

as $z \to 0$ $\square$

2.1 Failure to Converge

It is characteristic of non-convergent methods that decreasing step size makes things worse. As $h \to 0$, small perturbations grow at an increasing pace and result in meaningless solutions.

Theorem 2.2. *(The Dahlquist Equivalence Theorem) Suppose that the error in the starting values* $y_1, y_2, \cdots, y_{s-1}$ *tends to zero as* $h \to 0^+$*. The multistep method is convergent if and only if it is of order* $p \geq 1$ *and the polynomial* $\rho(w)$ *obeys the root condition*[4]

A multistep (s-step) method has $2s+1$ *parameters. An implicit s-step method is of order* $2s$*, and such a method is not convergent for* $s \geq 3$*. In general, we have the Dahlquist Barrier as the maximal order of a convergent s-step method is at most* $2\frac{s+2}{2}$ *if it is an implicit method, and* s *if it is an explicit method. The general practice for an s-step method is to employ order* $s+1$ *and* s *for implicit and explicit methods respectively.*

[4]"A polynomial obeys the root condition if all its zeros reside in the closed complex unit disc and all its zeros of unit modulus are simple."