

# ODE SOLVERS: MULTI-STEP METHODS

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ABSTRACT.

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We consider numerical methods for solving the nonlinear ODE

$$(1) \quad y' = f(x, y), \quad y(a) = y_0,$$

where  $t \in \mathbb{R}$  is the independent variable,  $y = y(x) \in \mathbb{R}^d$  may be a vector-valued function, and the function  $f(x, y)$  is given. The independent variable is change back to  $x$  as the multi-step schemes is highly related to the interpolation of function  $f(x)$ .

## 1. MULTI-STEPS METHODS

1.1. **Notation.** It will be useful to introduce the following symbols representing indices, function value and derivative at various locations.

We use subscript to indicates the function evaluated at the corresponding grid points. For  $s = 0, 1, \dots, k$

$$x_{n+s} = x_n + ih, \quad y_{n+s} = y(x_{n+s}), \quad f_{n+s} = f(x_{n+s}, y(x_{n+s})).$$

To simply the notation and easy of analysis, we apply the change of variable

$$u(\hat{x}) = y(x_n + \hat{x}h), \quad \hat{x} \in [0, k] \rightarrow x = x_n + \hat{x}h \in [x_n, x_{n+k}].$$

Therefore

$$(2) \quad u_s = y_{n+s}, \quad dx = h d\hat{x}, \quad u'(\hat{x}) = hy'(x_n + \hat{x}h).$$

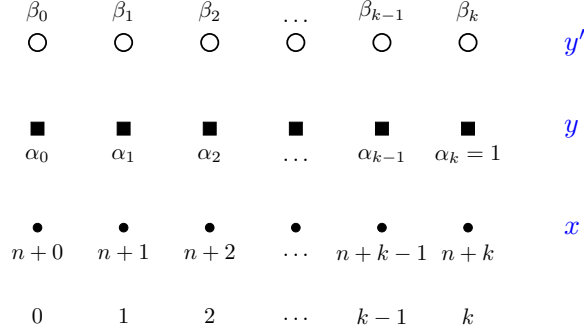


FIGURE 1. Notation for multi-step methods

1.2. **Schemes.** We can use more information on the previous steps to get a higher order methods. A general form is

$$(3) \quad \sum_{s=0}^k \alpha_s y_{n+s} = h \sum_{s=0}^k \beta_s f(x_{n+s}, y_{n+s}).$$

Without loss of generality, we can assume  $\alpha_k = 1$ .

1.  $\beta_k = 0$ : the scheme is explicit.
2.  $\beta_k \neq 0$ : the scheme is implicit. Need to solve a nonlinear equation

$$y_{n+k} = \dots h \beta_k f(x_{n+k}, y_{n+k}).$$

In total we have  $2(k+2)$  parameters, or equivalently, we know function value at  $k+1$  points and its derivative at  $k+1$  points, ideally we can fit a polynomial of degree  $p \leq 2k+3$ .

We define residual operators by

$$(4) \quad (Rv)(x) := v'(x) - f(x, v(x)), \quad v \in C^1[a, b],$$

$$(T_h)_n = (R_h v)_n := \frac{1}{h} \sum_{s=0}^k \alpha_s v_{n+s} - \sum_{s=0}^k \beta_s f(x_{n+s}, v_{n+s}), \quad v \in \Gamma_h[a, b].$$

To study the truncation error, we introduce the linear operator

$$Lu := \sum_{s=0}^k [\alpha_s u(s) - \beta_s u'(s)], \quad u \in C^1[\mathbb{R}].$$

Notice that the coordinate is changing to  $\hat{x} \in [0, k]$  and due to the relation (2), no  $h$  is in front of  $u'$ .

The scheme has degree  $p$  if  $Lu = 0$  for all  $u \in \mathbb{P}_p$ . By linearity, this is equivalent to

$$(5) \quad Lt^r = 0, \quad r = 0, 1, \dots, p$$

Indeed we can use (5) to determine the coefficients  $(\alpha_s, \beta_s)$ . For example, we obtain the relation

$$p = 0 : \quad \alpha_0 + \alpha_1 = 0,$$

$$p = 1 : \quad \alpha_0 + \alpha_1 = 0, \alpha_0 + \beta_0 + \beta_1 = 1.$$

Here we give several popular examples.

### 1.3. Adams-Bashforth and Adams-Moulton methods.

1.3.1. *Adams-Bashforth method.* We take  $\alpha_{k-1} = -1, \alpha_k = 1$  and write out the solution  $y' = f(x, y)$  as

$$(6) \quad y_{n+k} = y_{n+k-1} + \int_{x_{n+k-1}}^{x_{n+k}} y'(t) dt = y_{n+k-1} + \int_{x_{n+k-1}}^{x_{n+k}} f(x, y(x)) dx.$$

Suppose we know function values  $y_{n+s}$  for  $s = 0, \dots, k-1$ , we can evaluate to get  $f_{n+s}$  and fit the data  $(x_{n+s}, f_{n+s})$  with a polynomial of degree  $k-1$ . For example, the Lagrange interpolant  $p_n(f)$  to  $f$  can be written as

$$p_{k-1}(f; [x_n, x_{n+1}, \dots, x_{n+k-1}]; x) = \sum_{s=0}^{k-1} \ell_s(x) f_{n+s},$$

where  $\ell_s(x) \in \mathbb{P}_{k-1}$  and  $\ell_s(x_{n+j}) = \delta_{sj}$ . An explicit form of Lagrange basis is

$$\ell_s(x) = \prod_{j \neq i, j=0}^{k-1} \frac{(x - x_{n+j})}{(x_{n+s} - x_{n+j})}.$$

In the notation,  $p_n(f; [x_n, x_{n+1}, \dots, x_{n+k-1}]; x)$  we put grid points to emphasize the dependence. Usually we can simply write it as  $p_n(f; \cdot)$ .

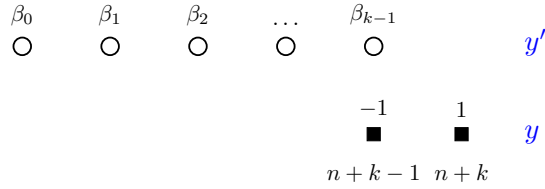


FIGURE 2. Adams-Bashforth method

Approximate  $f$  by  $p_n(f)$  and let

$$\beta_s = \frac{1}{h} \int_{x_{n+k-1}}^{x_{n+k}} \ell_s(x) dx = \int_{k-1}^k \prod_{j \neq i, j=0}^{k-1} \frac{(\hat{x} - j)}{(s - j)} d\hat{x}, \quad \text{for } s = 0, 1, \dots, k-1,$$

we then obtain the Adams-Bashforth method

$$(7) \quad y_{n+k} = y_{n+k-1} + h \sum_{s=0}^{k-1} \beta_s f_{n+s}.$$

1.3.2. *Adams-Moulton method.* The only difference is the point  $(x_{n+k}, f_{n+k})$  is included to fit the polynomial but  $(x_n, f_n)$  is not. Namely we are using

$$p_{k-1}(f; [x_{n+1}, \dots, x_{n+k}]; x) = \sum_{s=1}^k \ell_s^*(x) f_{n+s},$$

The superscript  $*$  is introduced to distinguish the same quantity used in A-B method.

Approximate  $f$  by  $p_{k-1}(f)$  and let

$$\beta_s^* = \frac{1}{h} \int_{x_{n+k-1}}^{x_{n+k}} \ell_s^*(x) dx = \int_{k-1}^k \prod_{j \neq i, j=1}^k \frac{(\hat{x} - j)}{(s - j)} d\hat{x}, \quad \text{for } s = 1, 2, \dots, k,$$

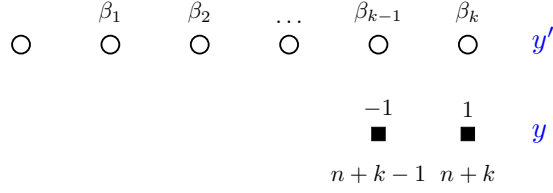


FIGURE 3. Adams-Moulton method

we then obtain the Adams-Moulton method

$$(8) \quad y_{n+k} = y_{n+k-1} + h \sum_{s=1}^{k-1} \beta_s^* f_{n+s} + h \beta_k^* f(x_{n+k}, y_{n+k}).$$

Here we single out the last term to emphasize A-M method is an implicit method and an iteration is needed to solve the nonlinear equation (8).

## 2. TRUNCATION ERROR ANALYSIS

**2.1. Truncation error.** For  $u \in C^{p+1}[0, k]$ , we expand  $u$  by its Taylor series at  $\hat{x} = 0$  using the Peano kernel

$$(9) \quad u(\hat{x}) = \sum_{i=0}^p \frac{1}{i!} u^{(i)}(0) \hat{x}^i + \frac{1}{p!} \int_0^{\hat{x}} (\hat{x} - \sigma)^p u^{(p+1)}(\sigma) d\sigma.$$

By the order condition (5), apply  $L$  to the Taylor expansion (9), we get

$$Lu = \frac{1}{p!} \int_0^k \lambda_p(\sigma) u^{(p+1)}(\sigma) d\sigma, \quad \lambda_p(\sigma) = L(t - \sigma)_+^p.$$

Using the mean value theorem (or Lagrange remainder), we also have

$$Lu = \ell_{p+1} u^{(p+1)}(\bar{\sigma}), \quad 0 < \bar{\sigma} < k; \quad \ell_{p+1} = \frac{1}{(p+1)!} L t^{p+1}.$$

By change of variable, we get the order of the convergence.

**Theorem 2.1.** *A multistep method (3) of polynomial degree  $p$  has order  $p$  whenever the exact solution  $y(x)$  of (6.1) is in the smoothness class  $C^{p+1}[a, b]$ . If the associated functional  $L$  is definite, then*

$$(Th)_n = \ell_{p+1} y^{(p+1)}(\bar{x}_n) h^p, \quad x_n < \bar{x}_n < x_{n+k}$$

where  $\ell_{p+1} = \frac{1}{(p+1)!} L t^{p+1}$ . Moreover, for the principal error function  $\tau$  of the method, whether definite or not, we have, if  $y \in C^{p+2}[a, b]$ ,

$$\tau(x) = \ell_{p+1} y^{(p+1)}(x).$$

**2.2. AB and AM methods.** When studying the truncation error, we assume the function value  $y_{n+s}$  is known for  $s = 0, 1, \dots, k-1$ . Then the truncation error

$$T_h^{\text{AB}} := \frac{1}{h} (u_{n+k} - y_{n+k}) = \frac{1}{h} \int_{x_{n+k-1}}^{x_{n+k}} (f_s - f) dx = \frac{1}{h} \int_{x_{n+k-1}}^{x_{n+k}} ((y')_s - y') dx.$$

We switch the integrand to  $y'$  since now the remainder can be written as derivative of exact solution  $y$ . As the Lagrange interpolant preserves polynomial

### 3. STABILITY ANALYSIS

Previously inside the index  $n + s$ , we consider  $n$  is fixed and let  $s = 0, 1, \dots, k$  to study the truncation error analysis. The stability is on the changing  $n$  and concern the uniform bound of  $|v_n|$  or in vector form  $\|v\|_\infty$ .

**3.1. Root condition.** Consider the homogenous difference equation

$$(10) \quad \sum_{s=0}^k \alpha_s v_{n+s} = 0 \quad n = 0, 1, \dots$$

with given initial condition  $v_0, v_1, \dots, v_{k-1}$ . Introduce the chacteristic function

$$\alpha(t) = \sum_{s=0}^k \alpha_s t^s.$$

For a root  $t_i$  of  $\alpha(t)$ , i.e.,  $\alpha(t_i) = 0$ ,  $v^n = t_i^n$  will be a solution of (10). If  $\alpha(t) = (t - t_i)^2 \dots$ , then  $\alpha'(t_i) = 0$ . On the other hand,  $\alpha'(t) = \sum_s s \alpha_s t^{s-1}$ . So  $v_n = n t_i^n$  is also a solution to (10).

If  $t_s, s = 1, 2, \dots, k' (k' \leq k)$ , denote the distinct roots of  $\alpha(t)$  and  $m_s$  their multiplicities, then the general solution of (10) is given by

$$v_n = \sum_{s=1}^{k'} \left( \sum_{r=0}^{m_s-1} c_{rs} r^r \right) t_s^n, \quad n = 0, 1, 2, \dots,$$

where  $c_{rs}$  are arbitrary (real or complex) constants and determined by the  $k$  starting values  $v_0, v_1, \dots, v_{k-1}$ .

**Theorem 3.1** (Root condition). *We have  $|v_n| \leq M$ , all  $n \geq 0$ , for every solution  $\{v_n\}$  of the homogeneous equation (10), with  $M$  depending only on the starting values  $v_0, v_1, \dots, v_{k-1}$  (but not on  $n$ ) if and only if*

$$\alpha(t_s) = 0 \text{ implies } \begin{cases} \text{either } |t_s| < 1 \\ \text{or } |t_s| = 1, m_s = 1 \end{cases}$$

Now consider the inhomogenous differenece equation

$$(11) \quad \sum_{s=0}^k \alpha_s v_{n+s} = \varphi_{n+k}, \quad n = 0, 1, \dots$$

Introduce another index  $m = n + k$ . For  $n = 0, 1, \dots, m = k, k+1, \dots$ . Define the discrete Green's function  $(g_{n,m})$  as the solution to the equation

$$(12) \quad \sum_{s=0}^k \alpha_s g_{n+s,m} = \delta_{n+k,m}, \quad n = 0, 1, \dots, m = k, k+1, \dots,$$

together with initial condition  $g_{0,m} = g_{1,m} = \dots = g_{k-1,m} = 0$ . For a fixed  $m$ , it is easy to see  $g_{n,m} = 0$  for all  $n < m$  since until  $n = m$ , there is a non-zero source is added.

**Lemma 3.2.** *The solution to (11) can be written as*

$$v_n = \sum_{m=k}^{\infty} g_{n,m} \varphi_m.$$

*Proof.*

$$\sum_{s=0}^k \alpha_s v_{n+s} = \sum_{s=0}^k \alpha_s \sum_{m=k}^{\infty} g_{n+s,m} \varphi_m = \sum_{m=k}^{\infty} \varphi_m \sum_{s=0}^k \alpha_s g_{n+s,m} = \varphi_{n+k}.$$

□

**Theorem 3.3.** *There exists a constant  $M > 0$ , independent of  $n$ , such that*

$$|v_n| \leq M \left\{ \max_{0 \leq s \leq k-1} |v_s| + \sum_{m=k}^n |\varphi_m| \right\}, n = 0, 1, 2, \dots,$$

*for every solution  $\{v_n\}$  of (6.73) and for every  $\{\varphi_{n+k}\}$ , if and only if the characteristic polynomial  $\alpha(t)$  of (6.73) satisfies the root condition (6.78).*