ODE SOLVERS: MULTI-STEP METHODS

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ABSTRACT.

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We consider numerical methods for solving the nonlinear ODE

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

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.

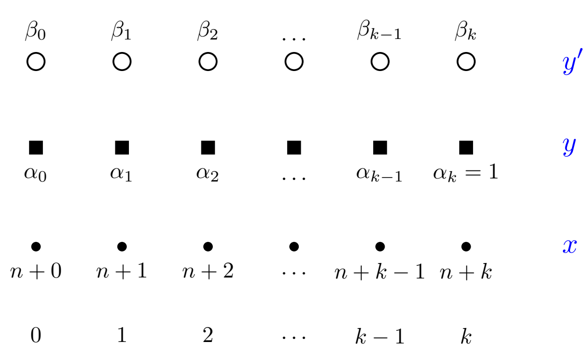

FIGURE 1. Notation for multi-step methods

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

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

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

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

Therefore

$$u_i = y_{n+i}, \quad \mathrm{d}x = h \,\mathrm{d}\hat{x}, \quad u'(\hat{x}) = hy'(x_n + \hat{x}h). \tag{2}$$

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

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f(x_{n+i}, y_{n+i}). \tag{3}$$

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

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

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

$$\begin{gathered}(Rv)(x) := v'(x) - f(x, v(x)), \quad v \in C^1[a, b], \\ (T_h)_n = (R_h \boldsymbol{v})_n := \frac{1}{h} \sum_{s=0}^{k} \alpha_s v_{n+s} - \sum_{s=0}^{k} \beta_s f\left(x_{n+s}, v_{n+s}\right), \boldsymbol{v} \in \Gamma_h[a, b].\end{gathered} \tag{4}$$

To study the truncation error, we introduce the linear operator

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

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

$$Lt^r = 0, \quad r = 0, 1, \ldots, p \tag{5}$$

Indeed we can use (5) to determine the coefficients (α_i, β_i). For example, we obtain the relation

$$\begin{aligned} p = 0: &\quad \alpha_0 + \alpha_1 = 0, \\ p = 1: &\quad \alpha_0 + \alpha_1 = 0, \alpha_0 + \beta_0 + \beta_1 = 1. \end{aligned}$$

Here we give several popular examples.

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

$$u(\hat{x}) = \sum_{i=0}^{p} \frac{1}{i!} u^{(i)}(0)\hat{x}^i + \frac{1}{p!}\int_0^{\hat{x}} (\hat{x}-\sigma)^p u^{(p+1)}(\sigma)\mathrm{d}\sigma. \tag{6}$$

By the order condition (5), apply L to the Taylor expansion (6), we get

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

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

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

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

Theorem 1.1. *A multistep method (3) of polynomial degree p has order p whenever the exact solution $\boldsymbol{y}(x)$ of (6.1) is in the smoothness class $C^{p+1}[a,b]$. If the associated functional L is definite, then*

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

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

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

1.4. **Adams-Bashforth and Adams-Moulton methods.**

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

$$y_{n+k} = y_{n+k-1} + \int_{x_{n+k-1}}^{x_{n+k}} y'(t)\,\mathrm{d}t = y_{n+k-1} + \int_{x_{n+k-1}}^{x_{n+k}} f(x,y(x))\,\mathrm{d}x. \tag{7}$$

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

$$p_n(f;[x_n,x_{n+1},\ldots,x_{n+k-1}];x) = \sum_{i=0}^{k-1}\ell_i(x) f_{n+i},$$

where $\ell_i(x)\in\mathbb{P}_{k-1}$ and $\ell_i(x_{n+j}) = \delta_{ij}$.

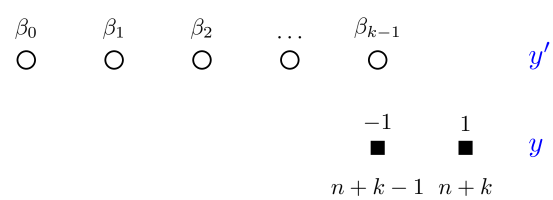

FIGURE 2. Adams-Bashforth method

Approximate f by f_I and let

$$\beta_i = \frac{1}{h}\int_{x_{n+k-1}}^{x_{n+k}} p_i(x)\,\mathrm{d}x,$$

we then obtain the Adams-Bashforth method

$$u_{n+k} = u_{n+k-1} + h\sum_{i=0}^{k-1}\beta_i f_{n+i}. \tag{8}$$

When studying the truncation error, we assume the function value y_{n+i} is known for $i = 0, 1, \ldots, k-1$. Then the truncation error

$$T_h^{\mathrm{AB}} := \frac{1}{h}(u_{n+k} - y_{n+k}) = \frac{1}{h}\int_{x_{n+k-1}}^{x_{n+k}} (f_I - f)\,\mathrm{d}x = \frac{1}{h}\int_{x_{n+k-1}}^{x_{n+k}} ((y')_I - y')\,\mathrm{d}x.$$

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

1.4.2. *Adams-Moulton method.* The only difference is the point (x_{n+k}, f_{n+k}) is included to fit the polynomial.

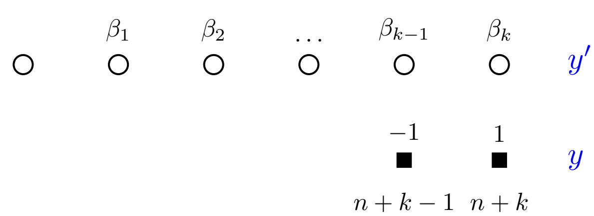

FIGURE 3. Adams-Moulton method

Now the Lagrange interpolant f_I to f will be

$$f_I(x) = \sum_{i=0}^{k} p_i^*(x) f_{n+i},$$

where $p_i^*(x) \in \mathbb{P}_k$ and $p_i^*(x_{n+j}) = \delta_{ij}$ for $i, j = 0, 1, \ldots, k$. The superscript * is introduced to distinguish the same quantity used in A-B method.

Approximate f by f_I and let

$$\beta_i^* = \frac{1}{h}\int_{x_{n+k-1}}^{x_{n+k}} p_i^*(x)\,\mathrm{d}x,$$

we then obtain the Adams-Moultion method

$$u_{n+k} = u_{n+k-1} + h\sum_{i=0}^{k-1}\beta_i^* f_{n+i} + h\beta_k^* f(x_{n+k}, u_{n+k}). \tag{9}$$

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 (9).