Numerical Methods for Differential Equations

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Outline

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1. Introduction
2. Euler formula
3. Runge-Kutta method
4. The stability and convergence of the one-step method
5. Linear multi-step method

In this course, we mainly consider about the numerical methods of the first order ODE

$$\begin{cases} y' = f(x,y), a \leq x \leq b \\ y(a) = n. \end{cases} \tag{1}$$

Which under the following assumption

(1).$f(x,y)$ and $\dfrac{\partial f(x,y)}{\partial y}$ are continues.

(2).The system 1 has a unique solution $y(x)$ and the solution is smooth on the region $\Omega = [a,b]$.

When we consider the numerical methods of this kind of systems. First we discrete the region Ω into n equal parts. We set space step $h = (b-a)/n$, $x_i = a + ih, (i = 0, 1, \ldots, n)$. The numerical solution is regarded as the approximation of the solution of the (1) on the discrete points $x_i, (i = 0, 1, \ldots, n)$.
In order to design the numerical schemes for the ODE problem, we have two concepts.
1) Design the scheme based on the differential form.
2) Design the scheme based on the integral form.

Also, we have two main computation ways to get the solution. If we just use the information of y_i to get the y_{i+1}, we call these methods the one-step methods. On the other hand, if we need the information of the previous r steps, we call these kind of methods the r-steps methods.

Numerical integration formula

This part will shows some popular integration formulas

- Left rectangle formula

$$\int_a^b g(x)dx = (b-a)g(a) + \frac{(b-a)^2}{2}g'(\xi), \quad \xi \in (a, b)$$

- Right rectangle formula

$$\int_a^b g(x)dx = (b-a)g(b) + \frac{(b-a)^2}{2}g'(\xi), \quad \xi \in (a, b)$$

- Middle rectangle formula

$$\int_a^b g(x)dx = (b-a)g(\frac{a+b}{2}) + \frac{(b-a)^3}{24}g''(\xi), \quad \xi \in (a, b)$$

- Trapezoid formula

$$\int_a^b g(x)dt = \frac{b-a}{2}[g(a)+g(b)] - \frac{(b-a)^3}{12}g''(\xi) \quad \xi \in (a, b)$$

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Euler formula

We integrate the function (1) on the region $[x_i, x_{i+1}]$

$$\int_{x_i}^{x_{i+1}} y'(x)dx = \int_{x_i}^{x_{i+1}} f(x, y(x))dx, \tag{2}$$

then, we can have

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y(x))dx. \tag{3}$$

After using the left rectangle formula to deal the integral operator, we can get

$$y(x_{i+1}) = y(x_i) + hf(x_i, y(x_i)) + R_{i+1}^{(1)}, \tag{4}$$

where

$$R_{i+1}^{(1)} = \frac{1}{2}\frac{df(x,y(x))}{dx}|_{x=\xi_i}h^2 = \frac{1}{2}y''(\xi_i)h^2, \xi_i \in (x_i, x_{i+1}). \quad (5)$$

If we ignore the $R_{i+1}^{(1)}$, we have

$$y(x_{i+1}) \approx y(x_i) + hf(x_i, y(x_i)), 0 \leq i \leq n-1. \quad (6)$$

Under the initial condition, we have

$$y(x_0) = \eta \equiv y_0. \quad (7)$$

Putting this into (6) we can get

$$y(x_1) \approx y(x_0) + hf(x_0, y(x_0)) = y_0 + hf(x_0, y_0). \quad (8)$$

Normally, if we already know the appromaximation y_i of the solution $y(x_i)$, we can get from (6)

$$y(x_{i+1}) \approx y(x_i) + hf(x_i, y(x_i)) \approx y_i + hf(x_i, y_i) \equiv y_{i+1}. \tag{9}$$

Then we can have

$$y_{i+1} = y_i + hf(x_i, y_i), i = 0, 1, ..., n-1. \tag{10}$$

We call the (10) the Euler formula and we can use this to get the approximation of $y(x_i)$

$$y_i, 0 \leq i \leq n.$$

Obviously, the Euler formula is a one-step explicit scheme.

For the ordinary one-step formula, we have the following structure

$$y_{i+1} = y_i + h\varphi(x_i, y_i, h), \tag{11}$$

$$y_0 = \eta. \tag{12}$$

We call the $\varphi(x_i, y_i, h)$ increment function.
Next, we will show the definition of the local truncation error

Definition 1

We call

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + h\varphi(x_i, y(x_i), h)] \tag{13}$$

the local truncation error of the one-step formula (11) on the point x_{i+1}

From the definition we can see the local truncation error of the Euler formula can be written as

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + hf(x_i, y(x_i))] = \frac{h^2}{2} y''(\xi_i), \xi_i \in (x_i, x_{i+1}) \tag{14}$$

Backward Euler formula

If we use the right rectangle formula to deal with the integral operator of the (6), we can get

$$y(x_{i+1}) = y(x_i) + hf(x_{i+1}, y(x_{i+1})) + R_{i+1}^{(2)}, \tag{15}$$

where

$$R_{i+1} = -\frac{h^2}{2}\frac{df(x, y(x))}{dx}|_{x=\xi_i} = -\frac{h^2}{2}y''(\xi_i), \xi_i \in (x_i, x_{i+1}). \tag{16}$$

We can get

$$y(x_{i+1}) \approx y(x_i) + hf(x_{i+1}, y(x_{i+1})) \approx y_i + hf(x_{i+1}, y_{i+1}), \quad (17)$$

and the backward Euler formula is

$$y_{i+1} = y_i + hf(x_{i+1}, y_{i+1}), i = 0, 1, ..., n-1. \quad (18)$$

Obviously, the backward Euler formula is a one-step implicit scheme.

For the ordinary one-step implicit formula, we have the following structure

$$y_{i+1} = y_i + h\varphi(x_i, y_i, y_{i+1}, h), \tag{19}$$

$$y_0 = \eta. \tag{20}$$

We call the $\varphi(x_i, y_i, y_{i+1}, h)$ increment function.
Next, we will show the definition of the local truncation error

Definition 2

We call

$$R_{i+1} = y(x_{i+1}) - [y(x_i) + h\varphi(x_i, y(x_i), y(x_{i+1}), h)] \tag{21}$$

the local truncation error of the one-step implicit formula (19) on the point x_{i+1}

From the definition we can see the local truncation error of the backward Euler formula can be written as

$$\begin{aligned} R_{i+1} &= y(x_{i+1}) - y(x_i) - hf(x_{i+1}, y(x_{i+1})) \\ &= -\frac{h^2}{2} y''(\xi_i), \xi_i \in (x_i, x_{i+1}) \end{aligned} \tag{22}$$

Trapezoid formula

If we use the trapezoid formula to deal with the integral operator of the (6), we can get

$$y(x_{i+1}) = y(x_i) + \frac{h}{2}[f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1}))] + R^{(3)}_{i+1}, \quad (23)$$

where

$$\begin{aligned} R_{i+1} &= -\frac{h^3}{12}\frac{d^2 f(x, y(x))}{dx^2}\Big|_{x=\xi_i} \\ &= -\frac{1}{12}y'''(\xi_i)h^3, \xi_i \in (x_i, x_{i+1}). \end{aligned} \quad (24)$$

If we ignore the $R_{i+1}^{(3)}$, we can have

$$\begin{aligned} y(x_{i+1}) &\approx y(x_i) + \frac{h}{2}[f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1}))] \\ &\approx y_i + \frac{h}{2}[f(x_i, y_i) + f(x_{i+1}, y_{i+1})], \end{aligned} \tag{25}$$

then we can get the trapezoid scheme of the (6)

$$y_{i+1} = y_i + \frac{h}{2}[f(x_i, y_i) + f(x_{i+1}, y_{i+1})], i = 0, 1, ..., n-1. \tag{26}$$

It is a one-step implicit scheme, and the local truncation error is

$$\begin{aligned} R_{i+1} &= y(x_{i+1}) - \{y(x_i) + \frac{h}{2}[f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1}))]\} \\ &= -\frac{1}{12}y'''(\xi_i)h^3, \xi_i \in (x_i, x_{i+1}). \end{aligned} \tag{27}$$

Improved Euler formula

In this case, we use two steps to get the solution: the predicted step and the correction step.

$$\begin{cases} y_{i+1}^{(p)} = y_i + hf(x_i, y_i)(predicted \quad formula) \\ y_{i+1} = y_i + \frac{h}{2}[f(x_i, y_i) + f(x_{i+1}, y_{i+1}^{(p)})](correction \quad formula) \end{cases} \tag{28}$$

We call the above formula system the improved Euler formula. It is a one-step explicit formula and we can transform this into the following form

- $$\begin{cases} y_{i+1}^{(p)} = y_i + hf(x_i, y_i) \\ y_{i+1}^{(c)} = y_i + hf(x_{i+1}, y_{i+1}^{(p)}) \\ y_{i+1} = \dfrac{1}{2}(y_{i+1}^{(p)} + y_{i+1}^{(c)}) \end{cases} \tag{29}$$

- $$y_{i+1} = y_i + \frac{1}{2}[f(x_i, y_i) + f(x_{i+1}, y_i + hf(x_i, y_i))]. \tag{30}$$

The local truncation error can be written as

$$R_{i+1} = y(x_{i+1}) - y(x_i) - \frac{h}{2}[f(x_i, y(x_i)) + f(x_{i+1}, y(x_i) + f(x_i, y(x_i)))]. \tag{31}$$

We have two ways to get the local truncation error of the improved Euler formula.
METHOD 1:

$$
\begin{aligned}
&R_{i+1} \\
&= y(x_{i+1}) - y(x_i) - \frac{h}{2}[f(x_i, y(x_i)) + f(x_{i+1}, y(x_{i+1}))] \\
&+ \frac{h}{2}[f(x_{i+1}, y(x_{i+1})) - f(x_{i+1}, y(x_i) + hf(x_i, y(x_i)))] \\
&= -\frac{1}{2}y'''(\xi_i)h^3 + \frac{h}{2}\frac{\partial f(x_{i+1}, \eta_{i+1})}{\partial y}[y(x_{i+1}) - y(x_i) - hf(x_i, y(x_i))] \\
&= -\frac{1}{12}y'''(\xi_i)h^3 + \frac{h}{4}\frac{\partial f(x_{i+1}, \eta_{i+1})}{\partial y}y''(\tilde{\xi}_i)h^2 \\
&= [-\frac{1}{12}y'''(\xi_i) + \frac{1}{4}\frac{\partial f(x_{i+1}, \eta_{i+1})}{\partial y}y''(\tilde{\xi}_i)]h^3.
\end{aligned}
$$

METHOD 2:

We make the Taylor expansion of $y(x_i)$ on the point x_i and make the Taylor expansion of $f(x_{i+1}, y(x_i) + hf(x_i, y(x_i)))$ on the point $(x_i, y(x_i))$.

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{1}{2!}h^2 y''(x_i) + \frac{1}{3!}h^3 y'''(x_i) + O(h^4),$$

$$f(x_{i+1}, y(x_i) + hf(x_i, y(x_i))) = f(x_i + h, y(x_i) + hf(x_i, y(x_i)))$$

$$= f(x_i, y(x_i)) + h\frac{\partial f}{\partial x}(x_i, y(x_i)) + hf(x_i, y(x_i))\frac{\partial f}{\partial y}(x_i, y(x_i))$$

$$+ \frac{1}{2!}[h^2\frac{\partial^2 f}{\partial x^2}(x_i, y(x_i)) + 2h^2 f(x_i, y(x_i))\frac{\partial^2 f}{\partial x \partial y}(x_i, y(x_i))$$

$$+ h^2(f(x_i, y(x_i))^2\frac{\partial^2 f}{\partial y^2}(x_i, y(x_i))] + O(h^3)$$

$$= y'(x_i) + hy''(x_i) + \frac{1}{2}h^2(y'''(x_i) - y''(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))) + O(h^3)$$

Then we can have the local truncation error

$$\begin{aligned}
R_{i+1} = {} & y(x_i) + hy'(x_i) + \frac{1}{2!}h^2y''(x_i) + \frac{1}{3!}y'''(x_i) + O(h^4) \\
& - y(x_i) - \frac{1}{2}hy'(x_i) \\
& - \frac{1}{2}h[y'(x_i) + hy''(x_i) + \frac{1}{2}h^2(y'''(x_i) - y''(x_i\frac{\partial f}{\partial y}(x_i, y(x_i))))+ \\
& O(h^3)] \\
& = [-\frac{1}{12}y'''(x_i) + \frac{1}{4}y''(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))]h^3 + O(h^4).
\end{aligned}$$

Definition 3

If the local truncation error of the scheme is $R_{i+1} = O(h^{p+1})$, then we call this scheme the p-th order scheme.

According to this definition, we can see that the Euler formula and the backward Euler formula are first-order schemes, the trapezoid formula and the improved Euler formula are second-order schemes.

Outline

The construction idea of Runge-Kutta method

Using the

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y(x))dx,$$

we can have

$$y(x_{i+1}) = y(x_i) + hf(x_i + \theta h, y(x_i + \theta h)).$$

The term $f(x_i + \theta h, y(x_i + \theta h))$ is called the average gradient of $y(x)$ on $[x_i, x_{i+1}]$ and we use k^* as the notation.
We set

$$k_1 = f(x_i, y_i),$$

$$k_2 = f(x_{i+1}, y_i + hk_1),$$

if we use k_1 to approximate the k^*, we will have the first-order Euler formula. If we use $\frac{k_1+k_2}{2}$ to approximate the k^*, we will have the second-order improved second-order Euler formula.

Generally, the r-level Runge-Kutta method have the following form

$$
\begin{cases}
y_{i+1} = y_i + h\sum_{j=1}^{r}\alpha_j k_j \\
k_1 = f(x_i, y_i) \\
k_j = f(x_i + \lambda_j h, y_i + h\sum_{l=1}^{j-1}\mu_{jl}k_l), j = 2, 3, ..., r
\end{cases}
\tag{32}
$$

After choosing appropriate coefficients $\alpha_j, \lambda_j, \mu_{jl}$, we can get any order scheme.

Specifically, we consider the local truncation of the r-level Runge-Kutta method

$$R_{i+1} = y(x_{i+1}) - y(x_i) - h\sum_{j=1}^{r} \alpha_j K_j,$$

where

$$K_1 = f(x_i, y(x_i)),$$

$$K_j = f(x_i + \lambda_j h, y(x_i) + h\sum_{l=1}^{j-1} \mu_{jl} K_l), j = 2, 3, .., r,$$

We then expand it into a power series of h

$$R_{i+1} = c_0 + c_1 h + ... + c_p h^p + c_{p+1} h^{p+1} + ...$$

Then we let the $c_0 = c_1 = ... = c_p$ and $c_{p+1} \neq 0$ by choosing appropriate coefficients $\alpha_j, \lambda_j, \mu_{jl}$. Then we get a p_{th}-order Runge-Kutta method.

Second-order Runge-Kutta method

The ordinary form of the second-order Runge-Kutta method can be written as

$$\begin{cases} y_{i+1} = y_i + h(\alpha_1 k_1 + \alpha_2 k_2) \\ k_1 = f(x_i, y_i) \\ k_2 = f(x_i + \lambda_2 h, y_i + h\mu_{21} k_1) \end{cases} \tag{33}$$

The local truncation error is

$$\begin{cases} R_{i+1} = y(x_{i+1}) - y(x_i) - h(\alpha_1 K_1 + \alpha_2 K_2) \\ K_1 = f(x_i, y(x_i)) \\ K_2 = f(x_i + \lambda_2 h, y(x_i) + h\mu_{21} K_1) \end{cases} \tag{34}$$

We also have

$$\begin{aligned}
y(x_{i+1}) &= y(x_i) + hy'(x_i) + \frac{1}{2}h^2y''(x_i) + \frac{1}{3!}h^3y'''(x_i) + O(h^4)\\
&= y(x_i) + hy'(x_i) + \frac{1}{2}h^2[\frac{\partial f}{\partial x}(x_i, y(x_i))\\
&+ y'(x_i)\frac{\partial f}{\partial y}(x_i, y(x_i))] + O(h^4),
\end{aligned}$$

$$\begin{aligned}
K_1 &= y'(x_i),\\
K_2 &= f(x_i, y(x_i)) + \lambda_2 h\frac{\partial f}{\partial x}(x_i, y(x_i)) + h\mu_{21}y'(x_i)\frac{\partial f}{\partial x}(x_i, y(x_i))\\
&+ \frac{1}{2}[(\lambda_2 h)\frac{\partial^2 f}{\partial x^2}(x_i, y(x_i)) + 2\lambda_2\mu_{21}h^2y'(x_i)\frac{\partial^2 f}{\partial y^2}(x_i, y(x_i))\\
&+ (\mu_{21}hy'(x_i))^2\frac{\partial^2 f}{\partial y^2}(x_i, y(x_i))] + O(h^3).
\end{aligned}$$

Put all the above equation into (34), we can have

$$
\begin{aligned}
R_{i+1} = {} & h(1-\alpha_1-\alpha_2)y'(x_i) + h^2[(\frac{1}{2}-\alpha_2\lambda_2)\frac{\partial f}{\partial x}(x_i, y(x_i)) \\
& + (\frac{1}{2}-\alpha_2\mu_{21})y'(x_i)\frac{\partial f}{\partial x}(x_i, y(x_i))] \\
& + h^3[\frac{1}{6}y'''(x_i) - \frac{1}{2}\alpha_2((\lambda+2)^2\frac{\partial^2 f}{\partial x^2}(x_i, y(x_i)) \\
& + 2\lambda_2\mu_{21}y'(x_i)\frac{\partial^2 f}{\partial x \partial y}(x_i, y(x_i)) \\
& + (\mu_{21}y'(x_i))^2\frac{\partial^2 f}{\partial y^2}(x_i, y(x_i)))] + O(h^4).
\end{aligned}
$$

If we want to get a second-order Runge-Kutta scheme, we need to solve the following system

$$\begin{cases} 1 - \alpha_1 - \alpha_2 = 0 \\ \dfrac{1}{2} - \alpha_2 \lambda_2 = 0 \\ \dfrac{1}{2} - \alpha_2 \mu_{21} = 0 \end{cases}$$

Obviously, α_2 cannot be zero.

When $\alpha_2 \neq 0$, we can get

$$\begin{cases} \alpha_1 = 1 - \alpha_2 \\ \lambda_2 = \dfrac{1}{2\alpha_2} \\ \mu_{21} = \dfrac{1}{2\alpha_2}. \end{cases}$$

So we can get a series of second-order Runge-Kutta formulas

$$\begin{cases} y_{i+1} = y_i + h[(1-\alpha_2)k_1 + \alpha_2 k_2] \\ k_1 = f(x_i, y_i) \\ k_2 = f(x_i + \dfrac{1}{2\alpha_2}h, y_i + \dfrac{1}{2\alpha_2}hk_1). \end{cases}$$

When $\alpha_2 = \frac{1}{2}$, we can get the improved Euler formula. When $\alpha = 1$, we can get transformed Euler formula

$$\begin{cases} y_{i+1} = y_i + hk_2 \\ k_1 = f(x_i, y_i) \\ k_2 = f(x_i + \dfrac{1}{2}h, y_i + \dfrac{1}{2}hk_1). \end{cases}$$

If we choose $\alpha_2 = \dfrac{3}{4}$, we can have

$$\begin{cases} y_{i+1} = y_i + \dfrac{h}{4}(k_1 + 3k_2) \\ k_1 = f(x_i, y_i) \\ k_2 = f(x_i + \dfrac{2}{3}h, y_i + \dfrac{2}{3}hk_1). \end{cases}$$

We can also use the similar technic to build third-order, 4_{th}-order or even higher order Runge-Kutta schemes.

Outline

Convergence

Definition 4

If $\{y(x_i)\}_{i=1}^{n}$ is the solution of the (1), $\{y_i^{[h]}\}_{i=1}^{n}$ is the approximate solution resulted from some numerical scheme. We call

$$E(h) = max|y(x_i) - y_i^{[h]}|, \quad 1 \leq i \leq n$$

the global truncation error of the numerical scheme. If

$$lim_{h \to 0} E(h) = 0,$$

we call the scheme is convergent.

Now we consider the one-step formula

$$\begin{cases} y_{i+1} = y_i + h\varphi(x_i, y_i, h), \quad i = 0, 1, ..., n-1, \\ y_0 = \eta. \end{cases} \tag{35}$$

Theorem 5

Set $y(x)$ is the solution of the (1), $\{y_i\}_{i=0}^{n}$ is the solution of the (35). If

- *There exists a constant $c_0 > 0$,*

$$|R_{i+1}| \leq c_0 h^{p+1}, \quad i = 0, 1, ..., n-1,$$

- *There exists $h_0 > 0$, $L > 0$,*

$$max|\frac{\partial\varphi(x, y, h)}{\partial y}| \leq L.$$

Then, when $h \leq min\{h_0 \sqrt[p]{\frac{\delta}{c}}\}$, we have

$$E(h) \leq ch^p.$$

where

$$D_\delta = \{(x, y)|a \leq x \leq b, y(x) - \delta \leq y \leq y(x) + \delta\},$$

$$c = \frac{c_0}{L}[e^{L(b-a)} - 1].$$

Stability

Definition 6

To the problem (1), we assume that $\{y_i\}_{i=0}^{n}$ is the approximate solution of the (35), $\{z_i\}_{i=0}^{n}$ is the solution with a tiny perturbation of the (35). Which have

$$\begin{cases} z_{i+1} = z_i + h[\varphi(x_i, y_i, h) + \delta_{i+1}], \quad i = 0, 1, ..., n-1 \\ z_0 = \eta + \delta_0. \end{cases} \tag{36}$$

If we have positive constants C, ε_0, h_0, for all $\varepsilon \in (0, \varepsilon_0]$, $h \in (0, h_0]$. When $max|\delta_i| \le \varepsilon$, we have

$$max|y_i - z_i| \le C_\varepsilon.$$

We call the one-step scheme (35) stable.

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For the ordinary linear multi-step method we have the following general form

$$y_{i+1} = \sum_{j=0}^{k-1} a_j y_{i-j} + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y_{i-j}), \tag{37}$$

where a_{k-1} and b_{k-1} can not be zero at the same time. When $b_{-1} = 0$, we have a explicit scheme; When $b_{-1} \neq 0$, we have a implicit scheme.

Definition 7

We call

$$R_{i+1} = y(x_{i+1}) - [\sum_{j=0}^{k-1} a_j y(x_{i-j}) + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y(x_{i-j}))]$$

the local truncation error of (37) at the point x_{i+1}. When $R_{i+1} = O(h^{p+1})$, we call the (37) is a p_{th} order scheme.

Scheme based on the integration-Adams formula

We integrate the equation $y'(x) = f(x, y(x))$ on the interval $[x_i, x_{i+1}]$, we have

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x_{i+1}} f(x, y(x))dx. \tag{38}$$

1) Adams explicit scheme

Using the $x_i, x_{i-1}, \ldots, x_{i-r}$ as the interpolation points, we get the Lagrange interpolation formula $L_r(x)$ from $f(x, y(x))$:

$$\begin{aligned} L_{i,r}(x) &= \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j}))l_{i-j}(x) \\ &= \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \prod_{l=0, l\neq j}^{r} \frac{x - x_{i-l}}{x_{i-j} - xi - l} \end{aligned}$$

We have

$$\begin{aligned} f(x,y(x)) &= L_{i,r}(x) + R_{i,r}(x) \\ &= L_{i,r}(x) + \frac{1}{(r+1)!}\frac{d^{r+1}f(x,y(x))}{dx^{r+1}}\Big|_{x=\eta_i}\prod_{j=0}^{r}(x-x_{i-j}) \\ &= L_{i,r}(x) + \frac{1}{(r+1)!}y^{(r+2)}(\eta_i)\prod_{j=0}^{r}(x-x_{i-j}). \end{aligned} \tag{39}$$

Put (39) into (38), we have

$$y(x_{i+1}) = y(x_i) + \int_{x_i}^{x^{i+1}} L_{i,r}(x)dx + \int_{x_i}^{x^{i+1}} R_{i,r}(x)dx$$

$$= y(x_i) + \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \int_{x_i}^{x_{i+1}} \prod_{l=0, l\neq j}^{r} \frac{x - x_{i-l}}{x_{i-j} - xi - l} dx$$

$$+ \frac{1}{(r+1)!} \int_{x_i}^{x_{i+1}} y^{(r+2)}(\eta_i) \prod_{j=0}^{r} (x - x_{i-j}) dx$$

$$= y(x_i) + h \sum_{j=0}^{r} f(x_{i-j}, y(x_{i-j})) \int_0^1 \prod_{l=0, l\neq j}^{r} \frac{l+t}{l-j} dt \quad (\text{set } x = x_i + th)$$

$$+ h^{r+2} y^{(r+2)}(\xi_i) \frac{1}{(r+1)!} \int_0^1 \prod_{j=0}^{r} (j+t) dt,$$

where $\xi_i \in (x_{i-r}, x_{i+1})$

$$\beta_{rj} = \int_0^1 \prod_{l=0,l\neq j}^{r} \frac{l+t}{l-j} dt, \quad j = 0, 1, ..., r,$$

$$\alpha_{r+1} = \frac{1}{(r+1)!} \int_0^1 \prod_{j=0}^{r} (j+t) dt,$$

then

$$y(x_{i+1}) = y(x_i) + h \sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y(x_{i-j})) + \alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i).$$

If we ignore the $\alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i)$ and replace the $y(x_{i-j})$ with y_{i-j}. We can get the r-steps Adams explicit formula:

$$y_{i+1} = y_i + h \sum \beta_{rj} f(x_{i-j}, y_{i-j}). \tag{40}$$

The local truncation error of the (40) is

$$
\begin{aligned}
R_{i+1} &= y(x_{i+1}) - [y(x_i) + h\sum_{j=0}^{r} \beta_{rj} f(x_{i-j}, y(x_{i-j}))] \\
&= \alpha_{r+1} h^{r+2} y^{(r+2)}(\xi_i)
\end{aligned}
$$

So, (40) is a (r+1) steps and (r+1) order Adams formula.

(a) r=0, we have the Euler formula

$$
\begin{aligned}
y_{i+1} &= y_i + hf(x_i, y_i), \\
R_{i+1} &= \frac{1}{2}h^2 y''(\xi_i), \quad \xi_i \in (x_i, x_{i+1}).
\end{aligned}
$$

(b) r=1, we have

$$
\begin{aligned}
y_{i+1} &= y_i + \frac{h}{2}[3f(x_i, y_i) - f(x_{i-1}, y_{i-1})], \\
R_{i+1} &= \frac{5}{12}h^3 y^{(3)}(\xi_i), \quad \xi_i \in (x_{i-1}, x_{i+1}).
\end{aligned}
$$

(c) r=2, we have

$$y_{i+1} = y_i + \frac{h}{12}[23f(x_i, y_i) - 16f(x_{i-1}, y_{i-1}) + 5f(x_{i-2}, y_{i-2})],$$
$$R_{i+1} = \frac{3}{8}h^4 y^{(4)}(\xi_i), \quad \xi_i \in (x_{i-2}, x_{i+1}).$$

(d) r=3, we have

$$y_{i+1} = y_i + \frac{h}{24}[55f(x_i, y_i) - 59f(x_{i-1}, y_{i-1})$$
$$+ 37f(x_{i-2}, y_{i-2}) - 9f(x_{i-3}, y_{i-3})],$$
$$R_{i+1} = \frac{251}{720}h^5 y^{(5)}(\xi_i), \quad \xi_i \in (x_{i-3}, x_{i+1}).$$

2) Adams implicit formula

Using the $x_{i+1}, x_i, x_{i-1}, \dots, x_{i-r+1}$ as the interpolation points, we get the Lagrange interpolation formula $L_r(x)$ from $f(x, y(x))$:

$$L_{i,r}(x) = \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) l_{i-j}(x)$$
$$= \sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j})) \prod_{l=-1, l\neq j}^{r-1} \frac{x - x_{i-l}}{x_{i-j} - xi - l}$$

We have

$$
\begin{aligned}
f(x,y(x)) &= L_{i,r}(x) + R_{i,r}(x) \\
&= L_{i,r}(x) + \frac{1}{(r+1)!}\frac{d^{r+1}f(x,y(x))}{dx^{r+1}}\Big|_{x=\eta_i}\prod_{j=-1}^{r-1}(x-x_{i-j}) \\
&= L_{i,r}(x) + \frac{1}{(r+1)!}y^{(r+2)}(\bar{\eta}_i)\prod_{j=-1}^{r-1}(x-x_{i-j}).
\end{aligned}
$$

We put the function above into (38), we can get

$$
\begin{aligned}
y(x_{i+1}) = y(x_i) + h\sum_{j=-1}^{r-1} f(x_{i-j}, y(x_{i-j}))\int_0^1 \prod_{l=-1, l\neq j}^{r-1}\frac{l+t}{l-j}dt \quad (x = x_i
\\
+ h^{r+2}y^{(r+2)}(\bar{\xi}_i)\frac{1}{(r+1)!}\int_0^1\prod_{j=-1}^{r-1}(j+t)dt.
\end{aligned}
$$

Where $\bar{\xi}_i \in (x_{i-r+1}, x_{i+1})$, and

$$\bar{\beta}_{rj} = \int_0^1 \prod_{l=-1,l\neq j}^{r-1} \frac{l+t}{l-j}.$$

$$\bar{\alpha}_{r+1} = \frac{1}{(r+1)!} \int_0^1 \prod_{j=-1}^{r-1} (j+t).$$

We can have

$$y(x_{i+1}) = y(x_i) + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y(x_{i-j})) + \bar{\alpha}_{r+1} h^{r+2} y^{(r+2)}(\bar{\xi}_i).$$

If we ignore $\bar{\alpha}_{r+1} h^{r+2} y^{(r+2)}(\bar{\xi}_i)$ and replace $y(x_{i-j})$ with y_{i-j}, we can get r steps Adams implicit formula:

$$y_{i+1} = y_i + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y_{i-j}). \tag{41}$$

Its local truncation error can be written as

$$\begin{aligned} R_{i+1} &= y(x_{i+1}) - [y(x_i) + h \sum_{j=-1}^{r-1} \bar{\beta}_{rj} f(x_{i-j}, y_{i-j})] \\ &= \bar{\alpha}_{r+1} h^{r+2} y^{(r+2)}(\bar{\xi}_i). \end{aligned}$$

So it is a r-steps, (r+1)-order implicit Adams formula.

(a) r=1, we get the trapezoid formula

$$y_{i+1} = y_i + \frac{h}{2}[f(x_{i+1}, y_{i+1}) + f(x_i, y_i)]$$
$$R_{i+1} = -\frac{1}{12}h^3 y'''(\xi_i), \quad \xi_i \in (x_i, x_{i+1}).$$

(b) r=2, we get

$$y_{i+1} = y_i + \frac{h}{12}[5f(x_{i+1}, y_{i+1}) + 8f(x_i, y_i) - f(x_{i-1}, y_{i-1})]$$
$$R_{i+1} = -\frac{1}{24}h^4 y^(4)(\xi_i), \quad \xi_i \in (x_{i-1}, x_{i+1})$$

Adams predictor-corrector method

Combining the explicit Adams formula and the implicit Adams formula, we can get the Adams predictor-corrector method. For example, if we combine the second-order explicit Adams formula and the second-order implicit Adams formula, we can get the following predictor-corrector method

$$\begin{aligned} &\textit{step 1} \;\; y_{i+1}^{(p)} = y_i + \frac{h}{2}[3f(x_i, y_i) - f(x_{i-1}, y_{i-1})] \\ &\textit{step 2} \;\; y_{i+1} = y_i + \frac{h}{2}[f(x_{i+1}, y_{i+1}^{(p)}) + f(x_i, y_i)] \end{aligned}$$

Here, we first use the explicit formula to get the predict term $y_{i+1}^{(p)}$. Then we use the predict term to get the y_{i+1}.

Also, we can give a fourth order Adams predictor-corrector method:

$$\textit{step 1} \;\; y_{i+1}^{(p)} = y_i + \frac{h}{24}[55f(x_i, y_i) - 59f(x_{i-1}, y_{i-1}) + 37f(x_{i-2}, y_{i-2})] - 9f(x_{i-3}, y_{i-3})$$

$$\textit{step 2} \;\; y_{i+1} = y_i + \frac{h}{24}[9f(x_{i+1}, y_{i+1}^{(p)}) + 19f(x_i, y_i) - 5f(x_{i-1}, y_{i-1}) + f(x_{i-2}, y_{i-2})$$

The method of undetermined coefficients based on the Taylor expansion

If we want to create the linear k-steps scheme as follows

$$y_{i+1} = \sum_{j=0}^{k-1} a_j y_{i-j} + h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y_{i-j}), \tag{42}$$

it has the local truncation error

$$R_{i+1} = y(x_{i+1}) - [\sum_{j=0}^{k-1} a_j y(x_{i-j}) - h \sum_{j=-1}^{k-1} b_j f(x_{i-j}, y(x_{i-j}))]$$

Using the equation (1) and the Taylor expansion we can get

$$R_{i+1} = y(x_{i+1}) - \sum_{j=0}^{k-1} a_j y(x_{i-j}) - h \sum_{j=-1}^{k-1} b_j y'(x_{i-j})$$

$$= (1 - \sum_{j=0}^{k-1} a_j) y(x_i) + \sum_{l=1}^{p+1} \frac{1}{l!}[1 - \sum_{j=0}^{k-1}(-j)^l a_j - l \sum_{j=-1}^{k-1}(-j)^{l-1} b_j]$$

$$h^l y^{(l)}(x_i) + O(h^{p+2}).$$

If we want (42) to be a p_{th} order scheme, the coefficients a_j and b_j need to obey

$$1-\sum_{j=0}^{k-1} a_j = 0$$

$$1-\sum_{j=0}^{k-1}(-j)^l a_j - l\sum_{j=-1}^{k-1}(-j)^{l-1} b_j = 0. \quad l = 1, 2, ..., p$$

Now, the local truncation error is shown as follows

$$R_{i+1} = \frac{1}{(p+1)!}[1-\sum_{j=0}^{k-1}(-j)^{p+1} a_j$$

$$-(p+1)\sum_{j=-1}^{k-1}(-j)^p b_j]h^{p+1}y^{(p+1)}(x_i) + O(h^{p+2})$$