Chapter 6

Differential Equations-O.D.E

Consider an initial value problem

$$\begin{cases} y' = f(x,y) \\ y(x_0) = y_0. \end{cases} \quad (6.1)$$

Theorem 6.0.1 (Existence and uniqueness)**.** *Let $f, \frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$ be continuous on the region $R = [0,M] \times [a,b]$. Then there is some interval $[0,M_1]$ in which there exists a unique solution to (6.1).*

6.1 Numerical Differentiation

Given a differentiable function f we let

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}.$$

This is called a **forward difference**. The approximation

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}$$

is called a **backward difference**.

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f''(\xi_1), \quad \xi_1 \in (x, x+h) \\ \therefore \frac{f(x+h)-f(x)}{h} &= f'(x) + \frac{h}{2}f''(x) + \frac{h^2}{6}f''(\xi_1). \end{aligned}$$

Similarly,

$$\begin{aligned} f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f''(\xi_2), \quad \xi_2 \in (x-h, x) \\ \therefore \frac{f(x)-f(x-h)}{h} &= f'(x) - \frac{h}{2}f''(x) + \frac{h^3}{6}f''(\xi_2). \end{aligned}$$

Take the average

$$f'(x) = \frac{f(x+h)-f(x-h)}{2h} - \frac{h^2}{6}\frac{f'''(\xi_1)+f'''(\xi_2)}{2}.$$

By MVT the average $\frac{f'''(\xi_1)+f'''(\xi_2)}{2}$ is achieved by $f'''(\gamma)$ for some γ. Thus we obtain a second order approximation to $f'(x)$. This is a **central difference**.

$$\frac{f_{i+1}-f_{i-1}}{2h_i} - f'(x_i) = O(\frac{h_i^2}{6}) \quad \text{if } h_i = h_{i+1}.$$

Treating the end points

It is sometimes necessary to have a $O(h^2)$ method at end points. But we cannot use the central difference at end points. Can we derive $O(h^2)$ method at end points without using the central difference? Consider

$$\begin{aligned} f(x) &= f(x) \\ f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f''(\gamma_1), \\ f(x+2h) &= f(x) + 2hf'(x) + 2h^2 f''(x) + \frac{4h^3}{3}f''(\gamma_2). \end{aligned}$$

By taking a linear combination of these terms, we want to get an approximation to $f'(x)$. Assume

$$f'(x) = af(x) + bf(x+h) + cf(x+2h) + O(h^2)$$

and use the Taylor expansion to find a, b, c. From

$$\begin{aligned} f'(x) &= af(x) + b(f(x) + hf'(x) + \frac{h^2}{2}f''(x)) \\ &\quad + c(f(x) + 2hf'(x) + 2h^2 f''(x)) + O(h^3) \end{aligned}$$

we obtain

$$a+b+c=0,\ b+2c=\frac{1}{h},\ \frac{b}{2}+2c=0.$$

The solution is

$$a=-\frac{3}{2h},\ b=\frac{2}{h},\ c=-\frac{1}{2h}.$$

So

$$f'(x) = \frac{-3f(x)+4f(x+h)-f(x+2h)}{2h}+O(h^2).$$

Second derivative

Second derivative can be approximated by taking the difference of forward and backward approximation for $f'(x)$. With the notation $f_i = f(x_i)$, we see

$$f''(x_i) \approx \frac{f'(x_i)-f'(x_{i-1})}{h}.$$

We approximate both $f'(x_i)$ and $f'(x_{i-1})$ by forward difference:

$$f'(x_i) \approx \frac{f(x+h)-f(x)}{h}, \quad f'(x_{i-1}) \approx \frac{f(x)-f(x-h)}{h}$$

$$f''(x_i) \approx \frac{f'(x_i)-f'(x_{i-1})}{h} \approx \frac{(f_{i+1}-2f_i+f_{i-1})}{h^2}$$

Now we check the error.

$$\begin{aligned}
\frac{f_{i+1}-2f_i+f_{i-1}}{h^2} - f''(x_i) &= \frac{1}{h^2}\left(f_i + hf_i' + \frac{h^2}{2}f_i'' + \frac{h^3}{6}f^{(3)} + \frac{h^4}{24}f^{(4)}(\theta_1) - 2f_i\right) \\
&\quad + \frac{1}{h^2}\left(f_i - hf_i' + \frac{h^2}{2}f_i'' - \frac{h^3}{6}f^{(3)} + \frac{h^4}{24}f^{(4)}(\theta_2)\right) - f''(x_i) \\
&= \frac{h^2}{24}(f^{(4)}(\theta_1)+f^{(4)}(\theta_2)) + \text{ truncation error} \\
&= O(h^2).
\end{aligned}$$

6.2 Euler's methods

Consider the following I.V.P.

$$\begin{cases} y' &= f(x,y) \\ y(x_0) &= y_0. \end{cases} \tag{6.2}$$

Example 6.2.1.

$$\begin{cases} y' &= \sin(x^2) \\ y(0) &= 0. \end{cases}$$

$$y(x) = y(0) + \int_0^x \sin(t^2)\,dt.$$

One can use for example a trapezoidal rule to approximate the integral.

But in general, we are working with a problem of the form $y' = f(x,y)$, so

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f(t, y(t))\,dt. \tag{6.3}$$

We thus need to approximate the integral. A possible way is to the trapezoidal rule, which yields

$$y_{n+1} = y_n + \frac{h}{2}(f(x_n, y_n) + f(x_{n+1}, y_{n+1})). \tag{6.4}$$

However, this is an implicit scheme. To avoid an implicit scheme one may consider a one point quadrature

$$y_{n+1} = y_n + hf(x_n, y_n).$$

This is called **forward Euler method**.

Taylor series expansion

We note the Taylor formula:

$$y(x+h) \approx y(x) + hy'(x) + \frac{h^2}{2}y''(x) + \frac{h^3}{6}y^{(3)}(x) + \cdots,. \tag{6.5}$$

Since $y' = f(x,y)$, we obtain

$$y_{n+1} = y_n + h_n f(x_n, y_n) + \frac{h^2}{2}y''(x) + \cdots.$$

Dropping higher order term we obtain the **forward Euler method** based on tangent approximation. The error grows quickly.

If we replace $f(x_n, y(x_n)$ in (6.4) by $f(x_{n+1}, y(x_{n+1})$ we obtain

$$y(x_{n+1}) \approx y(x_n) + h_n f(x_{n+1}, y(x_{n+1})).$$

This is called the **Backward Euler method**. This is more stable but need to iterate to find the solution.

Errors

Several kinds of errors.

(1) local truncation error(LTE)

(2) global error(GE)

6.3 Improved Euler's Method

We try to improve the Euler's method. We consider the trapezoidal rule again:

$$y_{n+1} = y_n + \frac{h_n}{2}(f(x_n, y_n) + f(x_{n+1}, y_{n+1})).$$

We may apply some approximation to y_{n+1} such as the explicit Euler's method: This results in the **improved Euler's method, Modified Euler's method**

$$y_{n+1} = y_n + \frac{h_n}{2}(f(x_n, y_n) + f(x_{n+1}, y_n + h_n f(x_n, y_n))).$$

Predictor-corrector methods

We start from the integral form:

$$y(x_{n+1}) \quad = \quad y(x_n) + \int_{x_n}^{x_{n+1}} f(x, y(x))\, dx.$$

If we use trapezoidal rule to approximate the integral, we get

$$y_{n+1} \quad = \quad y_n + \frac{h}{2}[f(x_n, y_n) + f(x_{n+1}, y_{n+1})].$$

The result is a nonlinear equation in y_{n+1}. One way of solving it is to replace(Predict) the term y_{n+1} on the right by some approximation.

If we use Euler's method as a predictor,(i.e, replace y_{n+1} by $y_n + h(x_n, y_n)$) we obtain the Heun's method:

$$y_{n+1}^{(P)} = y_n + hf(x_n, y_n) \tag{6.6}$$

$$y_{n+1} = y_n + \frac{h}{2}[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(P)})]. \tag{6.7}$$

This is another interpretation of the Heun's method. We can go one step further: If we use the result of Heun's method as a corrector then the **corrected Heun's method** is obtained:

$$\begin{aligned} y_{n+1}^{(P)} &= y_n + hf(x_n, y_n) \\ y_{n+1}^{(C)} &= y_n + \frac{h}{2}[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(P)})] \\ y_{n+1} &= y_n + \frac{h}{2}[f(x_n, y_n) + f(x_{n+1}, y_{n+1}^{(C)})]. \end{aligned}$$

6.4 Analysis of One Step Methods

One Step vs Multi Step

So far, the approximation at $x(t_{n+1})$ depends on the value of f only at $x_n = x(t_n)$. The known values $x_{n-1}, x_{n-2}, \cdots$ are *not* used. More efficient methods can be derived if one utilizes these values.

Consider again (6.2). Integrating we get

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f(t, y(t))dt.$$

The integral on the right side can be approximated by a numerical quadrature using one or several points. If it is approximated by

$$y_{n+1} = y_n + h\Phi_f(x_n, y_n, h) \tag{6.8}$$

then we have an **explicit one step method**. Of if it is approximated by

$$y_{n+1} = y_n + h\Phi_f(x_n, x_{n+1}, y_n, y_{n+1}, h) \tag{6.9}$$

then we have an **implicit one step method**.

In general we can use several steps. We use the notation $f_n = f(x_n, y_n)$.

The explicit method

$$y_{n+1} = y_n + h \sum_{j=0}^{k-1} \alpha_j f_{n-j} \tag{6.10}$$

is an **explicit k- step method** and the implicit method

$$y_{n+1} = y_n + h \sum_{j=0}^{k} \alpha_j f_{n+1-j} \tag{6.11}$$

is an **implicit k- step method**.

Analysis of Euler's Method

We return to the one step methods. A general one step method has the form

$$y_{n+1} = y_n + h\Phi(x_n, y_n, h). \tag{6.12}$$

Define the **local truncation error(LTE)** by

$$LTE_{n+1} = y(x_{n+1}) - [y(x_n) + h\Phi(x_n, y(x_n), h)] \tag{6.13}$$

The error

$$GE_{n+1} = y(x_{n+1}) - y_{n+1} \tag{6.14}$$

is called the **global error(GE)**.

Definition 6.4.1. For numerical methods such as (6.12) or (6.10)

(1) we say the scheme is **consistent** if the local truncation error approaches 0 as $h \to 0$.

(2) we say a method is **stable** if for all sufficiently small h and ϵ, there is a $K > 0$ such that the numerical solution of $y' = f(x, y),\ y(x_0) = y_0 + \epsilon$ differs from the exact solution by at most ϵK.

(3) we say a method is **convergent** if the global error approaches 0 as h tends to zero.

For Euler's methods, we have

$$\begin{aligned}
LTE_{n+1} &= y(x_{n+1}) - [y(x_n) + hf(x_n, y(x_n))] \\
&= y_n + hy'(x_n) + \frac{h^2}{2}y''(\xi_n) - y(x_n) - hf(x_n, y(x_n)) \\
&= y_n + hf(x_n, y(x_n)) + \frac{h^2}{2}y''(\xi_n) - y(x_n) - hf(x_n, y(x_n)) \\
&= \frac{h^2}{2}y''(\xi_n).
\end{aligned}$$

What about the global error?

$$\begin{aligned}
y(x_{n+1}) &= y(x_n) + hf(x_n, y(x_n)) + LTE_{n+1} \\
y(x_{n+1}) - y_{n+1} &= y(x_n) + hf(x_n, y(x_n)) + LTE_{n+1} - y_{n+1} \\
&= y(x_n) + hf(x_n, y(x_n)) + LTE_{n+1} - [y_n + hf(x_n, y_n)] \\
&= y(x_n) - y_n + h[f(x_n, y(x_n)) - f(x_n, y_n)] + LTE_{n+1} \\
GE_{n+1} &= GE_n + h[f(x_n, y(x_n)) - f(x_n, y(x_n) - GE_n)] + LTE_{n+1}.
\end{aligned}$$

Let us write $e_{n+1} = |GE_{n+1}|$. Then

$$e_{n+1} \leq e_n + h|f(x_n, y(x_n)) - f(x_n, y(x_n) - GE_n)| + M$$

for some positive M which bounds LTE_{n+1}. Let f be a Lipschitz constant for f w.r.t y. Then

$$\begin{aligned}
|f(x_n, y(x_n)) - f(x_n, y(x_n) - GE_n)| &\leq L|GE_n| \\
&\leq Le_n
\end{aligned}$$

Hence

$$\begin{aligned}
e_{n+1} &\leq e_n + hLe_n + M = (1 + hL)e_n + M \\
&\leq (1 + hL)((1 + hL)e_{n-1} + M) + M \\
&\leq (1 + hL)^2 e_{n-1} + M(1 + hL) + M \\
&\leq (1 + hL)^{n+1} e_0 + M(1 + hL)^n + \cdots + M(1 + hL) + M \\
&\leq (1 + hL)^{n+1} e_0 + M\frac{(1 + hL)^{n+1} - 1}{hL}
\end{aligned}$$

Use $1+x \leq e^x$ to get

$$\begin{aligned}(1+hL)^n &\leq \exp(hL)^n \\ &= \exp(nhL).\end{aligned}$$

Since $M = O(h^2)$ and $\frac{\exp(nhL)-1}{hL} = O(n)$

$$\begin{aligned}e_n &\leq \frac{\exp(nhL)-1}{hL}M + \exp(nhL)e_0 \\ &\leq O(nh^2)(\text{consistency}) + O(1)e_0(\text{stability}).\end{aligned}$$

Since $e_0 = 0$ and $nh \approx O(1)$, we see the global error for the explicit Euler 's method is $O(h)$.

Theorem 6.4.2. *A stable scheme is convergent iff it is consistent.*

Above argument shows that a consistent scheme is convergent. Conversely, a convergent scheme is clearly consistent because $LTE \leq GE$.

Taylor Series Method

Consider the Taylor series

$$y(x+h) = y(x) + hy'(x) + \frac{h^2}{2!}y''(x) + \frac{h^3}{3!}y^{(3)}(x) + \cdots \tag{6.15}$$

By taking derivatives, we see that

$$\begin{aligned}y'(x) &= f \\ y''(x) &= f_x + f_x y' = f_x + ff_y \\ y'''(x) &= f_{xx} + f_{xy}f + (f_x + f_y f)f_y + f(f_{yx} + f_{yy}f),\end{aligned}$$

where f, f_x, f_y etc are evaluated at (x, y). The first three terms in the Taylor series can be written as

$$\begin{aligned}y(x+h) &= y(x) + hf + \frac{1}{2}h^2(f_x + ff_y) + O(h^3) &(6.16)\\ &= y(x) + \frac{1}{2}hf + \frac{1}{2}h[f + hf_x + hff_y] + O(h^3). &(6.17)\end{aligned}$$

Runge -Kutta Method

One could define a numerical scheme using the formula (6.16). However, we have an efficient way of evaluating the value $y(x+h)$ without taking the derivative of f. The **Runge -Kutta Method** is a one step method that achieves this goal. Let

$$y_n = y_{n-1} + h(k_1 g_1 + k_2 g_2 + \cdots + k_N g_N)$$

where

$$\begin{aligned} g_1 &= f(x_{n-1} + c_1 h, y_{n-1}) \\ g_2 &= f(x_{n-1} + c_2 h, y_{n-1} + a_{2,1} h g_1) \\ g_3 &= f(x_{n-1} + c_3 h, y_{n-1} + a_{3,1} h g_1 + a_{3,2} h g_2) \\ &= \vdots \\ g_N &= f(x_{n-1} + c_N h, y_{n-1} + a_{N,1} h g_1 + \cdots + a_{N,N_1} h g_{N-1}) \end{aligned}$$

Example 6.4.3. With $c_1 = 0$(use the left end point of the interval)

$$\begin{aligned} y_{n+1} &= y_n + h(k_1 g_1 + k_2 g_2) && (6.18) \\ &= y_n + h k_1 f_n + h k_2 f(x_n + \alpha h, y_n + \beta h f_n) && (6.19) \end{aligned}$$

where k_1, k_2, α, β are parameters to be determined. Applying Taylor expansion to (6.19) ,

$$y(x+h) = y(x) + k_1 h f + k_2 h[f + \alpha h f_x + \beta h f f_y] + O(h^3).$$

Comparing this with the Taylor expansion of $y(x+h)$

$$y(x+h) = y(x) + hf + \frac{1}{2}h^2(f_x + f f_y) + O(h^3) \qquad (6.20)$$

we obtain

$$\begin{cases} k_1 + k_2 = 1 \\ k_2\alpha = \frac{1}{2} \\ k_2\beta = \frac{1}{2}. \end{cases}$$

One solution is $k_1 = k_2 = \frac{1}{2}, \alpha = \beta = 1$. Hence we get improved Euler's method

$$y_{n+1} = y_n + \frac{h_n}{2}(f(x_n, y_n) + f(x_{n+1}, y_n + h_n f(x_n, y_n))).$$

Other solution may exists, such as $k_1 = 0, k_2 = 1, \alpha = \beta = \frac{1}{2}$. The result is the mid point method

$$y_{n+1} = y_n + g_2,$$

where

$$\begin{cases} g_1 &= hf(x_n, y_n) \\ g_2 &= hf(x_n + \frac{1}{2}h, y_n + \frac{1}{2}g_1). \end{cases}$$

Another solution is $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}, \alpha = \beta = \frac{2}{3}$. Thus

$$y_{n+1} = y_n + \frac{h}{4}\left[f(x_n, y_n) + 3\left(f(x_{n+2/3}, y_n) + \frac{2h}{3}f(x_n, y_n)\right)\right].$$

Fourth order Runge-Kutta Method

Higher order Runge-Kutta method can be obtained by similar idea. The following is the fourth order Runge-Kutta method. See p 423.

$$y_{n+1} = y_n + \frac{1}{6}(g_1 + 2g_2 + 2g_3 + g_4),$$

where

$$\begin{cases} g_1 &= hf(x, y_n) \\ g_2 &= hf(x + \frac{1}{2}h, y_n + \frac{1}{2}g_1) \\ g_3 &= hf(x + \frac{1}{2}h, y_n + \frac{1}{2}g_2) \\ g_4 &= hf(x + h, y_n + g_3). \end{cases}$$

6.5 System of Equations

Consider the second order D.E

$$\begin{aligned} y'' + by' + cy &= f(x, y) \\ y(x_0) &= y_0 \\ y'(x_0) &= y_1. \end{aligned} \tag{6.21}$$

Introduce new variables $y_0 = y(x)$, $y_(x) = y_0'(x)$ and set

$$\begin{aligned} y_0' &= y_1 \\ y_1' &= -cy_0 - by_1 + f(x, y_0) \\ y_0(x_0) &= y_0 \\ y_1(x_0) &= y_1. \end{aligned} \tag{6.22}$$

This is a system of first order equations in $\mathbf{y} = (y_0, y_1)$. It can be written as

$$\begin{aligned} \mathbf{y}' &= \mathbf{F}(x, \mathbf{y}) \\ \mathbf{y}(x_0) &= \mathbf{y}_0. \end{aligned} \tag{6.23}$$

One can develop similar numerical methods as before.

6.6 Multi-Step Methods

Integrating the ODE, we get

$$y(x_{n+1}) = y(x_n) + \int_{x_n}^{x_{n+1}} f(x, y(x))dx.$$

The integral on the right side can be approximated by a numerical quadrature using one or several points. Recall an explicit method

$$y_{n+1} = y_n + h \sum_{j=0}^{k-1} \alpha_j f(x_{n-j}, y_{n-j}) \tag{6.24}$$

and an implicit method

$$y_{n+1} = y_n + h \sum_{j=0}^{k} \alpha_j f(x_{n+1-j}, y_{n-j}) \tag{6.25}$$

To find the coefficients for the explicit method, we assume f is function of x only and let the formula

$$\int_{x_n}^{x_{n+1}} f(x)dx = h \sum_{j=0}^{k-1} \alpha_j f(x_{n-j})$$

be exact for polynomials of degree up to $k-1$. Then we have

$$\int_{x_n}^{x_{n+1}} \sum_{j=0}^{k-1} f(x_{n-j}) L_j(x)\, dx = h \sum_{j=0}^{k-1} \alpha_j f(x_{n-j})$$

Hence

$$\alpha_j = \frac{1}{h} \int_{x_n}^{x_{n+1}} L_j(x) dx.$$

Adams Bashforth formula-Explicit Methods

We assume $h_n = h$ for all n. Suppose the formula is of the following form:

$$y_{n+1} = y_n + a f_n + b f_{n-1} + \cdots .$$

Such a formula is called Adams Bashforth Formula. The Adams Bashforth Formula of order $2, 3, 4$(resp.) are as follows:

$$y_{n+1} = y_n + \frac{h}{2}[3f_n - f_{n-1}] \tag{6.26}$$

$$y_{n+1} = y_n + \frac{h}{12}[23f_n - 16f_{n-1} + 5f_{n-2}] \tag{6.27}$$

$$y_{n+1} = y_n + \frac{h}{24}[55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}].$$

Adams Moulton formula-Implicit Methods

First, Adams-Moulton Formula of order $2, 3, 4, 5$ are as follows:

$$y_{n+1} = y_n + \frac{h}{2}[f_{n+1} + f_n](\text{ backward Euler}) \tag{6.28}$$

$$y_{n+1} = y_n + \frac{h}{12}[5f_{n+1} + 8f_n - f_{n-1}] \tag{6.29}$$

$$y_{n+1} = y_n + \frac{h}{24}[9f_{n+1} + 19f_n - 5f_{n-1} + f_{n-2}] \tag{6.30}$$

$$y_{n+1} = y_n + \frac{h}{720}[251f_{n+1} + 646f_n - 264f_{n-1} + 106f_{n-2} - 19f_{n-3}].$$

Combining these with Adams-Bashforth formula (6.27),(6.28), we can derive Adams-Moulton predictor- corrector methods: For example Adams-Moulton method of order 4 is

$$\begin{cases} y_{n+1}^P = y_n + \frac{h}{24}[55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3}] \\ y_{n+1} = y_n + \frac{h}{24}[9f_{n+1}(x_{n+1}, y_{n+1}^P) + 19f_n - 5f_{n-1} + f_{n-2}] \end{cases}$$

Starting Values for Multi-Step Methods

To start a multi-step methods we need a few starter values to evaluate. It is important to use the same order method to generate starter values. Usually RK methods are preferred.