EMP 219 - Computational Mathematics - Part 2 [1]

Prerequisites

$$\sin(2\theta) = 2\sin(\theta)\cos(\theta)$$

1 Jacobi Method

Given a linear system of equation and initial values for unknowns, assume zeros if there are no initial values.

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

solutions are

$$\begin{aligned} x_1 &= \frac{b_1 - a_{12}x_2 - a_{13}x_3}{a_{11}} \\ x_2 &= \frac{b_2 - a_{21}x_1 - a_{23}x_3}{a_{22}} \\ x_3 &= \frac{b_3 - a_{31}x_1 - a_{32}x_2}{a_{33}} \end{aligned} \tag{1}$$

Substitute with the initial values and repeat n times

To guarantee the convergence of Jacobi method, the coefficient matrix must be strictly diagonally dominant

$$|a_{ii}| > \sum_{i \neq j} |a_{ij}| \tag{2}$$

2 Bisection Method

To find a solution of the equation

$$f(x) = 0$$

We find the midpoint c of the interval $[a,\, b]$. Suppose that $f(c) \neq 0$ (otherwise we have found a solution). Either $f(a) \times f(c)$ is negative, so that the interval $[a,\, c]$ must contain a solution of the equation, or $f(c) \times f(b)$ is negative, so that the interval $[c,\, b]$ contains a solution of the equation.

Stopping criterion:

Repeat n times or until be in the range or $|x_{i+1} - x_i| < \epsilon$ where ϵ is the maximum error bound.

Relative percentage error:

$$\text{RPE} = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \tag{3}$$

note that tolerance = | exact solution − approximate solution |

Maximum error bound :

$$\epsilon = \frac{b - a}{2^n} \tag{4}$$

number of iterations [2] :

$$n = \left\lceil \log_2 \left(\frac{b - a}{\epsilon} \right) \right\rceil \tag{5}$$

To ensure the presence of at least one root, we choose the interval $[a,\, b]$ such that $f(a) \times f(b) < 0$

3 Newton's Method

Starting from an initial guess x_0, the process is the repeating of :

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{6}$$

4 Linear Regression

Given a set of data points, the best fit straight line equation is

$$y = a_0 + a_1 x$$

where a_0 and a_1 are obtained by solving the equations:

$$\begin{aligned} n\, a_0 + (\Sigma x_i)\, a_1 &= \Sigma y_i \\ (\Sigma x_i)\, a_0 + \left(\Sigma x_i^2\right) a_1 &= \Sigma\, x_i y_i \end{aligned} \tag{7}$$

where n = number of data points.

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[2] Usually, in mathematical notation we express rounding down with the floor function so $\lfloor a \rfloor$ is the largest integer less than or equal to a. Similarly, for rounding up, we use the ceiling function, so $\lceil a \rceil$ is the smallest integer greater than or equal to a.

4.1 Correlation Coefficient

How do we know how good the fit is? By correlation coefficient

S_r : Square differences between the data points and the straight line

$$S_r = \sum_{i=1}^{n}(y_i - a_0 - a_1 x_i)^2 \tag{8}$$

S_t : Square differences between the data points and the mean

$$S_t = \sum_{i=1}^{n}(y_i - \overline{y})^2 \tag{9}$$

where

$$\overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i \tag{10}$$

Coefficient of determination

$$r^2 = \frac{S_t - S_r}{S_t} \tag{11}$$

Correlation coefficient

$$r = \sqrt{r^2} \tag{12}$$

The more r is closer to 1, the better the linear regression is.

4.2 Linearized Model

4.2.1 Exponential Model

Given that $y = ae^{bx}$ and the linear fit equation is $Y = a_0 + a_1 X$, after simplifying we obtain that

$$\underbrace{\ln(y)}_{Y} = \underbrace{\ln(a)}_{a_0} + \underbrace{b}_{a_1}\underbrace{x}_{X}$$

Let:

$$\begin{aligned} Y &= \ln(y) \\ X &= x \\ a_0 &= \ln(a) \\ a_1 &= b \end{aligned} \tag{13}$$

To calculate S_t and S_r, use a_0 and a_1 not a and b

4.2.2 Power Model

Given that $y = ax^b$ and the linear fit equation is $Y = a_0 + a_1 X$, after simplifying we obtain that

$$\underbrace{\log(y)}_{Y} = \underbrace{\log(a)}_{a_0} + \underbrace{b}_{a_1}\underbrace{\log(x)}_{X}$$

Let:

$$\begin{aligned} Y &= \log(y) \\ X &= \log(x) \\ a_0 &= \log(a) \\ a_1 &= b \end{aligned} \tag{14}$$

4.3 Growth Rate Model

Given that $y = \dfrac{ax}{b+x}$ and the linear fit equation is $Y = a_0 + a_1 X$, after simplifying we obtain that

$$\underbrace{\frac{1}{y}}_{Y} = \underbrace{\frac{1}{a}}_{a_0} + \underbrace{\frac{b}{a}}_{a_1}\underbrace{\frac{1}{x}}_{X}$$

Let:

$$\begin{aligned} Y &= \frac{1}{y} \\ X &= \frac{1}{x} \\ a_0 &= \frac{1}{a} \\ a_1 &= \frac{b}{a} \end{aligned} \tag{15}$$

5 Numerical Differentiation

5.1 1st Derivative

Forward :

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \tag{16}$$

Backward :

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h) \tag{17}$$

Central :

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \tag{18}$$

5.2 2nd Derivative

Central :

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2) \tag{19}$$

where h is the step size.

When h decreases, error decreases and accuracy increases

6 The Trapezoidal Rule

Trapezoidal Rule is a rule that evaluates the area under the curves by dividing the total area into smaller trapezoids rather than using rectangles. This integration works by approximating the region under the graph of a function as a trapezoid, and it calculates the area.

$$I = \int_a^b f(x)dx$$

$$I \approx \frac{h}{2}\left(f(a) + f(b) + 2\sum_{k=1}^{n-1} f(a+kh)\right)$$

$$I \approx \frac{h}{2}\left(y_0 + y_n + 2\sum_{k=1}^{n-1} y_k\right) \tag{20}$$

$$h = \frac{b-a}{n}$$

where

$n :$ number of segments.

$h :$ step size.

7 Simpson's 1/3 Rule

Simpson's rules are several approximations for calculating definite integrals

$$\int_a^b f(x)\,dx \approx \frac{h}{6}\left[y_0 + y_n + 4\sum_{\text{k : odd}} y_k + 2\sum_{\text{k : even}} y_k\right].$$

$$h = \frac{b-a}{n}$$

$n :$ number of segments, must be **even**.

$h :$ step size.

8 Euler's Method

The Euler method is a first-order numerical procedure for solving ordinary differential equations (ODEs) with a given initial value.

Given the differential equation $y' = \frac{\mathrm{d}y}{\mathrm{d}x} = F(x, y)$ and initial condition (x_0, y_0) or $y_0 = f(x_0)$

$$\text{new value} = \text{old value} + \text{step size} \times \text{slope}$$

$$y_{i+1} = y_i + hF(x_i, y_i) \tag{21}$$

9 Heun's Method

Heun's method is also known as improved Euler's method. The idea is ti replace the slope from Euler's method by the average value of two slopes.

Results of Heun's Method are more accurate than results of Euler's method.

$$\text{New slope} = \frac{F(x_n, y_n) + F(x_{n+1}, y^*_{n+1})}{2}$$

$$y^*_{n+1} = y_n + hF(x_n, y_n) \qquad \text{(predictor)}$$

$$y_{n+1} = y_n + \frac{h}{2}\left(F(x_n, y_n) + F(x_{n+1}, y^*_{n+1})\right) \qquad \text{(corrector)} \tag{22}$$

10 The Gamma Function

$$\Gamma(n) = \int_0^\infty x^{n-1}e^{-x}\,\mathrm{d}x \tag{23}$$

or

$$\Gamma(n) = 2\int_0^\infty x^{2n-1}e^{-x^2}\,\mathrm{d}x \tag{24}$$

$$\Gamma(n) = (n-1)\Gamma(n-1) \tag{25}$$

When $n \in \mathbb{Z}^+$:

$$\Gamma(n) = (n-1)! \tag{26}$$

when $n = \frac{1}{2}$:

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi} \tag{27}$$

11 Beta Function

$$\mathrm{B}(n,\, m) = \int_0^1 x^{n-1}(1-x)^{m-1}\,\mathrm{d}x \tag{28}$$

note that $(n > 0,\ m > 0)$

Property 1:

$$\mathrm{B}(n,\, m) = \mathrm{B}(m,\, n) \tag{29}$$

Property 2 : The polar form

$$\mathrm{B}(n,\, m) = 2\int_0^{\pi/2} (\cos\theta)^{2n-1}(\sin\theta)^{2m-1}\,\mathrm{d}\theta \tag{30}$$

note that $(n > 0,\ m > 0)$

Relation between Γ-function and B-function :

$$\mathrm{B}(n,\, m) = \frac{\Gamma(n)\Gamma(m)}{\Gamma(n+m)} \tag{31}$$

12 Bessel Function

12.1 Bessel Differential Equation

$$x^2y'' + xy' + (x^2 - n^2)y = 0 \tag{32}$$

Solution:

$$y = c_1 J_n(x) + c_2 J_{-n}(x) \qquad (n \notin \mathbb{Z}^+)$$

$$y = c_1 J_n(x) + c_2 Y_n(x) \qquad (n \in \mathbb{Z}^+)$$

12.2 Bessel Function of the 1st Kind

$$J_n(x) = \sum_{k=0}^{\infty} \frac{(-1)^k (x/2)^{n+2k}}{k!\,\Gamma(n+k+1)} \qquad \text{(Given)} \tag{33}$$

When $(n \in \mathbb{Z}^+)$, $J_n(x)$ and $J_{-n}(x)$ are linearly dependent

$$J_n(x) = (-1)^n J_{-n}(x) \tag{34}$$

$J_{1/2}(x)$ and $J_{-1/2}(x)$ are

$$J_{1/2}(x) = \sqrt{\frac{2}{\pi\, x}}\sin(x) \qquad \text{(Given)} \tag{35}$$

$$J_{-1/2}(x) = \sqrt{\frac{2}{\pi\, x}}\cos(x) \tag{36}$$

12.3 Bessel Function of the 2nd Kind

$$Y_n(x) = \frac{\cos(n\pi)J_n(x) - J_{-n}(x)}{\sin(n\pi)} \tag{37}$$

12.4 Bessel Recurrence Relations

$$J_{n+1}(x) + J_{n-1}(x) = \frac{2n}{x}J_n(x) \qquad \text{(Given)} \tag{38}$$

$$J_{n-1}(x) - J_{n+1}(x) = 2J_n'(x) \qquad \text{(Given)} \tag{39}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}(x^n J_n(x)) = x^n J_{n-1}(x) \rightarrow \qquad \text{(Given)}$$

$$\int x^n J_{n-1}(x)\,\mathrm{d}x = x^n J_n(x) + c \tag{40}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}(x^{-n} J_n(x)) = -x^{-n} J_{n+1}(x) \rightarrow \qquad \text{(Given)}$$

$$\int x^{-n} J_{n+1}(x)\,\mathrm{d}x = -x^{-n} J_n(x) + c$$

Note :

$$\int x^m J_n(x)\,\mathrm{d}x$$

if $m+n$ is odd and $m > n$, use:

$$\int x^n J_{n-1}(x)\,\mathrm{d}x = x^n J_n(x)$$

if $m+n$ is odd and $m < n$, use:

$$\int x^{-n} J_{n+1}(x)\,\mathrm{d}x = -x^{-n} J_n(x) + c$$

if $m+n$ is even, use any integral results in

$$\int J_0(x)\,\mathrm{d}x$$

13 Complex Analysis

if

$$z = x + iy$$

13.1 Polar Form

$$z = r(\cos\theta + i\sin\theta) \tag{41}$$

from cartesian to polar:

$$r = \sqrt{x^2 + y^2} \qquad \theta = \tan^{-1}\left(\frac{y}{x}\right) \tag{42}$$

from polar to cartesian:

$$x = r\cos(\theta) \qquad y = r\sin(\theta) \tag{43}$$

13.2 Euler's Formula

$$e^{i\theta} = \cos(\theta) + i\sin(\theta) \tag{44}$$

$$\therefore z = re^{i\theta}$$

13.3 Power of Complex Number(De Moivre's Theorem)

Case 1 : Integer power $(n \in \mathbb{Z})$

$$(\cos(\theta) + i\sin(\theta))^n = \cos(n\theta) + i\sin(n\theta) \tag{45}$$

Case 2 : Rational Power $\left(n = \frac{p}{q}\right)$

$$(\cos(\theta) + i\sin(\theta))^{p/q} = \cos(\varphi) + i\sin(\varphi) \tag{46}$$

$$\varphi = \frac{p\theta + 2\pi k}{q} \qquad k = 0,\, 1,\, 2,\, \ldots,\, (q-1)$$

14 Complex Differentiation

$$w = f(x) = u(x,\, y) + iv(x,\, y)$$

14.1 Cauchy-Riemann Equations

If this function is differentiable, then:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y} \qquad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \tag{47}$$

$$\frac{\mathrm{d}w}{\mathrm{d}z} = \frac{\partial u}{\partial x} + i\frac{\partial v}{\partial x} = \frac{\partial w}{\partial x} = \frac{1}{i}\frac{\partial w}{\partial y} \tag{48}$$

• If $f(z)$ is analytic at all points in a domain D, we call it an **analytic in D**

• If $f(z)$ is analytic at all points of the complex plane, we call it an **entire function**

• if $f(z)$ is not differentiable at $z = n$ (n is called singular point), then we call it **analytic except at** $z = n$

• If the Cauchy-Riemann equations are not satisfied, then $f(z)$ is not analytic in any domain, so we call it **no where analytic**