

Introduction

Numerical Analysis is concerned with the design and analysis of algorithms for solving mathematical problems that arise in many fields, especially science and engineering. *Scientific computing* could be regarded as a combination of modeling, visualization, and numerical analysis. In particular, *Numerical Methods*, the foundation of *Scientific computing* deals with quantities that are continuous, as opposed to discrete which occurred in most other parts of computer science.

- A Review of Calculus:

$$B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

Taylor's Theorem

Orders of Convergence: Big Oh and little oh

Truncation and Rounding

- Types of Errors

Absolute Error and Relative Error

Data Error and Computational Error

Truncation Error and Rounding Error

Sensitivity and Condition Number

Stability and Accuracy

- Computer Arithmetic

Floating-Point Numbers

Representation and Normalization

Machine Precision

Summing a series $\sum_{n=1}^{\infty} \frac{1}{n}$

Quadratic formula (Solving $ax^2 + bx + c = 0$)

- Mathematical Software and Environments

Reliability, Accuracy, Portability

Robustness, Efficiency, Maintainability

Usability, Applicability

Matlab, IMSL (PV-Wave), Netlib, NAG

- Historical Notes from Mathematicians

Newton (1642~1727), Euler (1707~1783), Lagrange (1736~1813)

Laplace (1749~1827), Legendre (1752~1833), Gauss (1777~1855)

Cauchy (1789~1857), Jacobi (1804~1851), Adams (1819~1892),

Chebyshev (1821~1894), Hermite (1822~1901), Laugerre (1834~1886)

A Review of Calculus

Show that

$$B(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}, \quad \forall a, b > 0$$

where

$$\Gamma(a) = \int_0^\infty e^{-x} x^{a-1} dx, \quad a > 0$$

$$B(a, b) = \int_0^1 x^{a-1} (1-x)^{b-1} dx, \quad a, b > 0$$

[Hint:] let $u = x/(x+y)$, $v = x+y$, then $x = uv$, $y = v - uv = (1-u)v$, then the Jacobian $J(x, y) = v$. Furthermore, show that $\Gamma(a)\Gamma(b) = \Gamma(a+b)B(a, b)$.

Taylor's Theorem: If $f \in C^n[a, b]$ and $f^{(n+1)}$ exists on the open interval (a, b) , then for any $c \in (a, b)$ and $x \in [a, b]$,

$$f(x) = \sum_{k=0}^n \frac{1}{k!} f^{(k)}(c)(x-c)^k + \frac{1}{(n+1)!} f^{(n+1)}(\xi)(x-c)^{n+1}$$

where ξ is between c and x . When $c = 0$, the above expansion is called a Maclaurin series for $f(x)$.

Examples

$$\sin x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!}, \quad -\infty < x < \infty$$

$$\cos x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!}, \quad -\infty < x < \infty$$

$$\ln(1+x) = \sum_{k=1}^{\infty} (-1)^{k-1} \frac{x^k}{k}, \quad -1 < x < 1$$

$$\frac{1}{1+x} = \sum_{k=0}^{\infty} (-1)^k x^k, \quad -1 < x < 1$$

$$e^{-x} = \sum_{k=0}^{\infty} \frac{(-1)^k x^k}{k!}, \quad x \in \mathbb{R}$$

$$\sqrt{1+2x} = 1 + x + \sum_{k=2}^{\infty} \alpha_k x^k, \quad -\frac{1}{2} < x < \frac{1}{2}$$

Orders of Convergence

Big Oh and little oh

$$\lim_{n \rightarrow \infty} \frac{n+1}{n} = 1$$

$$\lim_{n \rightarrow \infty} \left(1 + \frac{1}{n}\right)^n = e \approx 2.71828$$

Definition: Let $\{x_n\}$ and $\{\alpha_n\}$ be two different sequences, we write

$$x_n = O(\alpha_n)$$

if \exists constants C and n_0 such that $|x_n| \leq C|\alpha_n| \forall n \geq n_0$. Here we say that x_n is "big oh" of α_n . On the other hand,

$$x_n = o(\alpha_n)$$

if $\exists \epsilon_n \rightarrow 0$ such that $|x_n| \leq \epsilon_n |\alpha_n|$. Here we say that x_n is "little oh" of α_n .

Examples

$$\frac{n}{n^2 + 1} = O\left(\frac{1}{n}\right)$$

$$\frac{1}{n \ln(n)} = o\left(\frac{1}{n}\right)$$

$$\frac{1}{n} = o\left(\frac{1}{\ln(n)}\right)$$

$$\frac{5}{n} + e^{-n} = O\left(\frac{1}{n}\right)$$

$$e^{-n} = o\left(\frac{1}{n^2}\right)$$

$$\sin(x) = x - \frac{x^3}{6} + O(x^5)$$

$$\cos(x) = 1 - \frac{x^2}{2} + O(x^4)$$

Types of Errors

Let y be the true value, and let \hat{y} be the approximate value, then

$$\text{Absolute error} = \hat{y} - y$$

$$\text{Relative error} = \frac{\hat{y} - y}{y}$$

Let $f : R \rightarrow R$. Suppose that we must work with inexact input \hat{x} and we can compute only an approximation to the function \hat{f} . Then, we have

$$\text{Total error} = \hat{f}(\hat{x}) - f(x) = [\hat{f}(\hat{x}) - f(\hat{x})] + [f(\hat{x}) - f(x)]$$

$$\text{Computation error} = \hat{f}(\hat{x}) - f(\hat{x})$$

$$\text{Propagated data error} = f(\hat{x}) - f(x)$$

♣ Computing $\sin(\pi/8)$

Use $\hat{f}(x) = x$ instead of $f(x) = \sin(x)$ and use $\hat{x} = 3/8$ to approximate $x = \pi/8$. By calculator, we have

$$f(\pi/8) = \sin(\pi/8) \approx 0.3827 \quad \text{and} \quad f(3/8) \approx 0.3663$$

On the other hand,

$$\hat{f}(\hat{x}) - f(\hat{x}) = \hat{x} - \sin(3/8) = 0.3750 - 0.3663 = 0.0087$$

$$f(\hat{x}) - f(x) = 0.3663 - 0.3827 = -0.0164$$

So the total error is

$$\hat{f}(\hat{x}) - f(x) = [\hat{f}(\hat{x}) - f(\hat{x})] + [f(\hat{x}) - f(x)] = 0.0087 + (-0.0164) = -0.0077$$

♣ $3.14159 \approx 3.1415$ by truncation, $3.14159 \approx 3.1416$ by round-off.

♣ $f(x+h) = f(x) + f'(x)h + f''(\theta)h^2/2$ for some $\theta \in [x, x+h]$

Condition Number

Suppose that we want to compute $y = f(x)$, where $f : R \rightarrow R$, but we obtain instead an approximate value \hat{y} . The discrepancy $\Delta y = \hat{y} - y$ is called the *forward error*. On the other hand, how much data error in the initial input would be required to explain all of the error in the final computed result? The quantity $\Delta x = \hat{x} - x$, where $f(\hat{x}) = \hat{y}$, is called *backward error*.

♣ Consider $f(x) = \sqrt{x}$, as an approximation to $y = \sqrt{2}$, $\hat{y} = 1.4$ has an absolute forward error $|\Delta y| = |1.4 - 1.4142\dots|$. The backward error $|\Delta x| = |\hat{x} - x| = |(1.4)^2 - 2| = 0.04$. So, $|\Delta y|/y \approx 1\%$ and $|\Delta x|/x \approx 2\%$.

A problem is said to be insensitive, or *well-conditioned*, if a given relative change in the input data causes a reasonably commensurate relative change in the solution. Otherwise, it is called sensitive, or *ill-conditioned*.

$$\text{Condition number} = \frac{|\Delta y/y|}{|\Delta x/x|} = \frac{|[f(\hat{x}) - f(x)]/f(x)|}{|[\hat{x} - x]/x|}$$

If f is continuously differentiable around x , then

$$\text{Condition number} = \left| \frac{x f'(x)}{f(x)} \right|$$

□ Implement and discuss the following problems.

- (1) $\sum_{n=1}^{\infty} \frac{1}{n}$ (Prob. 1.8 on p.45, Heath)
- (2) Solve $x^3 + ax^2 + bx + c = 0$ (Prob. 1.11 on p.46, Heath)
- (3) Evaluate $\|\mathbf{x}\|_2 = (\sum_{i=1}^n x_i^2)^{1/2}$ (Prob. 1.15 on p.47, Heath)

Miscellaneous Examples

(1) $A = \int_0^\infty e^{-x^2/2} dx = \frac{\sqrt{\pi}}{2}$

(2) $\Gamma(\frac{1}{2}) = \int_0^\infty e^{-x} x^{-1/2} dx = \sqrt{\pi}$

(3) If $x_{n+2} = x_{n+1} + x_n$, for $n \geq 0$, $x_0 = 1$, $x_1 = 1$, then $x_n = \frac{1}{\sqrt{5}} \left[\frac{1+\sqrt{5}}{2} \right]^{n+1} - \frac{1}{\sqrt{5}} \left[\frac{1-\sqrt{5}}{2} \right]^{n+1}$, for $n \geq 0$.

(4) $x = (-1)^s q \times 2^m$, where $q = (1.f)_2$, $m = e - 127$, and $e = 0$, or 255 are reserved for ± 0 , $\pm \infty$.

(5) Write a program to solve the quadratic equation and test the values of coefficients as listed in Table 1 (*Heath*).

$$ax^2 + bx + c = 0$$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad \text{or} \quad x = \frac{2c}{-b \mp \sqrt{b^2 - 4ac}}$$

Problem	a	b	c
(A)	6	5	-4
(B)	0	1	1
(C)	1	-10^5	1
(D)	1	-4	3.999999
(E)	10^{-155}	-10^{155}	10^{155}
(F)	6×10^{154}	5×10^{154}	-4×10^{154}

Table 1: Miscellaneous Coefficients of Quadratic Equations.

Vector Norms

Definition: A vector norm on R^n is a function

$$\tau : R^n \rightarrow R^+ = \{x \geq 0 \mid x \in R\}$$

that satisfies

- (1) $\tau(\mathbf{x}) > 0 \quad \forall \mathbf{x} \neq \mathbf{0}, \tau(\mathbf{0}) = 0$
- (2) $\tau(c\mathbf{x}) = |c|\tau(\mathbf{x}) \quad \forall c \in R, \mathbf{x} \in R^n$
- (3) $\tau(\mathbf{x} + \mathbf{y}) \leq \tau(\mathbf{x}) + \tau(\mathbf{y}) \quad \forall \mathbf{x}, \mathbf{y} \in R^n$

Hölder norm (p-norm) $\|\mathbf{x}\|_p = (\sum_{i=1}^n |x_i|^p)^{1/p}$ for $p \geq 1$.

(p=1) $\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i|$ (Mahattan or City-block distance)

(p=2) $\|\mathbf{x}\|_2 = (\sum_{i=1}^n |x_i|^2)^{1/2}$ (Euclidean distance)

(p= ∞) $\|\mathbf{x}\|_\infty = \max_{1 \leq i \leq n} \{|x_i|\}$ (∞ -norm)

Matrix Norms

Definition: A matrix norm on $R^{m \times n}$ is a function

$$\tau : R^{m \times n} \rightarrow R^+ = \{x \geq 0 \mid x \in R\}$$

that satisfies

- (1) $\tau(A) > 0 \quad \forall A \neq O, \tau(O) = 0$
- (2) $\tau(cA) = |c|\tau(A) \quad \forall c \in R, A \in R^{m \times n}$
- (3) $\tau(A + B) \leq \tau(A) + \tau(B) \quad \forall A, B \in R^{m \times n}$

Consistency Property: $\tau(AB) \leq \tau(A)\tau(B) \quad \forall A, B$

- (a) $\tau(A) = \max\{|a_{ij}| \mid 1 \leq i \leq m, 1 \leq j \leq n\}$
- (b) $\|A\|_F = \left[\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2 \right]^{1/2}$ (Fröbenius norm)

Subordinate Matrix Norm: $\|A\| = \max_{\|\mathbf{x}\| \neq 0} \{\|A\mathbf{x}\| / \|\mathbf{x}\|\}$

- (1) If $A \in R^{m \times n}$, then $\|A\|_1 = \max_{1 \leq j \leq n} (\sum_{i=1}^m |a_{ij}|)$
- (2) If $A \in R^{m \times n}$, then $\|A\|_\infty = \max_{1 \leq i \leq m} (\sum_{j=1}^n |a_{ij}|)$
- (3) Let $A \in R^{n \times n}$ be real symmetric, then $\|A\|_2 = \max_{1 \leq i \leq n} |\lambda_i|$, where $\lambda_i \in \lambda(A)$

Problems Solved by Matlab

Let $A, B, H, \mathbf{x}, \mathbf{y}, \mathbf{u}, \mathbf{b}$ be matrices and vectors defined below, and $H = I - 2\mathbf{u}\mathbf{u}^t$

$$A = \begin{bmatrix} 2 & 1 & 1 \\ 4 & 6 & 0 \\ -2 & 7 & 2 \end{bmatrix}, \quad B = \begin{bmatrix} -3 & 1 & 0 \\ 1 & -3 & 0 \\ 0 & 0 & 3 \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 6 \\ 2 \\ -5 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}$$

1. Let $A=LU=QR$, find $L, U; Q, R$.
2. Find determinants and inverses of matrices A, B , and H .
3. Solve $A\mathbf{x} = \mathbf{b}$, how to find the number of floating-point operations are required?
4. Find the ranks of matrices A, B , and H .
5. Find the characteristic polynomials of matrices A and B .
6. Find 1-norm, 2-norm, and ∞ -norm of matrices A, B , and H .
7. Find the eigenvalues/eigenvectors of matrices A and B .
8. Find matrices U and V such that $U^{-1}AU$ and $V^{-1}BV$ are diagonal matrices.
9. Find the singular values and singular vectors of matrices A and B .
10. Randomly generate a 4×4 matrix C with $0 \leq C(i, j) \leq 9$.