UNSW Mathematics Society presents

MATH2089 Revision Seminar

Numerical Methods & Statistics

Numerical Methods

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Presented by Janzen Choi

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Part I: Linear Systems

Matrix factorisation – LU factorisation

Given an $n \times n$ matrix A, if the leading principal sub-matrices A_k are non-singular for all $k = 1, \ldots, n$, then there exist $n \times n$ matrices L and U where L is unit lower triangular and U is upper triangular, such that

$$A = LU.$$

- If the factorisation exists, it is also *unique*.
- Obtain the LU factorisation by applying row operations of the form

$$R_i \leftarrow R_i - L_{ij} R_j.$$

Cost of factorisation

The cost of the LU factorisation is

$$\frac{2n^3}{3} + \mathcal{O}(n^2) \text{ flops.}$$

Effects of the permutation matrix

If A is non-singular, then there exist $n \times n$ matrices L, U and P with P being a **permutation** matrix such that

$$PA = LU.$$

- PA reorders the rows of A but does not change the solution to the linear system.
- AP reorders the columns of A and affects the solution to linear system.

Solving linear systems using LU factorisation

We note that

$$A\mathbf{x} = \mathbf{b} \implies (PA)\mathbf{x} = P\mathbf{b} \implies LU\mathbf{x} = P\mathbf{b}.$$

1. Forward substitution: Solve $L\mathbf{y} = P\mathbf{b} = \mathbf{z}$ for $\mathbf{y}$. Then

$$y_1 = z_1, \qquad y_i = z_i - \sum_{j=1}^{i-1} L_{ij} y_j, \qquad i = 2, \dots, n.$$

2. Back substitution: Solve $U\mathbf{x} = \mathbf{y}$ for $\mathbf{x}$. Then

$$x_n = \frac{y_n}{U_{nn}}, \qquad x_i = \frac{1}{U_{ii}} \left(y_i - \sum_{j=i+1}^{n} U_{ij} x_j \right), \qquad i = n-1, \dots, 1.$$

Solving linear systems using LU factorisation

Cost of solution

- LU factorisation: $\dfrac{2n^3}{3} + \mathcal{O}(n^2)$ flops.
- Forward substitution: $n^2 + \mathcal{O}(n)$ flops.
- Back substitution: $n^2 + \mathcal{O}(n)$ flops.
- **Total cost**: $\dfrac{2n^3}{3} + \mathcal{O}(n^2)$ flops.

Matrix factorisation – Cholesky factorisation

Given an $n \times n$ matrix A, if the Cholesky factorisation exists, then it is of the form

$$A = R^\intercal R$$

where R is an $n \times n$ upper triangular matrix, with $R_{ii} > 0$ for all $i = 1, \ldots, n$.

- A Cholesky factorisation is *unique* when it exists.
- The matrix A is positive definite and symmetric.
- All eigenvalues of A are positive.

Cost of factorisation

The cost of the Cholesky factorisation is

$$\frac{n^3}{3} + \mathcal{O}(n^2) \text{ flops.}$$

Solving linear systems using Cholesky factorisation

We note that

$$A\mathbf{x} = \mathbf{b} \implies (R^\top R)\,\mathbf{x} = \mathbf{b}.$$

1. Forward substitution: Solve $R^\top \mathbf{y} = \mathbf{b}$ for $\mathbf{y}$.

$$y_1 = \frac{b_1}{R_{11}}, \qquad y_i = \frac{1}{R_{ii}}\left(b_i - \sum_{j=1}^{i-1} R_{ji} y_j\right), \qquad i = 2, \ldots, n.$$

2. Back substitution: Solve $R\mathbf{x} = \mathbf{y}$ for $\mathbf{x}$.

$$x_n = \frac{y_n}{R_{nn}}, \qquad x_i = \frac{1}{R_{ii}}\left(y_i - \sum_{j=i+1}^{n} R_{ij} x_j\right), \qquad i = n-1, \ldots, 1.$$

Solving linear systems using Cholesky factorisation

Cost of solution

- Cholesky factorisation: $\dfrac{n^3}{3} + \mathcal{O}(n^2)$ flops.
- Forward substitution: $n^2 + \mathcal{O}(n)$ flops.
- Back substitution: $n^2 + \mathcal{O}(n)$ flops.
- **Total cost**: $\dfrac{n^3}{3} + \mathcal{O}(n^2)$ flops.

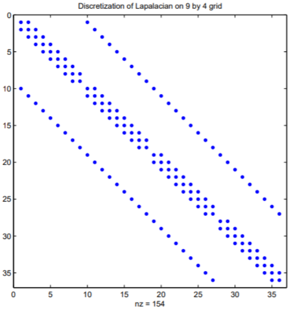
Sparsity of matrices

The **sparsity** of a matrix A is given by

$$\text{Sparsity} = \left(\frac{\text{non-zero elements of } A}{\text{total number of elements in } A}\right)\%.$$

Example: (MATH2089, 2010 Q3h)

You are given that using a row-ordering of the variables $c_{i,j}^{\ell}$ produces the coefficient matrix A whose non-zero entries are illustrated below.



Calculate the sparsity of A.

Recall that the sparsity of a matrix is given by

$$\text{Sparsity} = \left(\frac{\text{non-zero elements of } A}{\text{total number of elements in } A}\right)\%.$$

The number of nonzero entries in a spy plot is given by the variable `nz`. The dimension of the matrix is given by the grid size, which in this case is $9 \times 4 = 36$. Hence the sparsity is

$$\text{Sparsity} = \left(\frac{154}{36 \times 36}\right)\% \approx 11.9\%.$$

Vector norm

Properties of vector norms

A vector norm $\|\cdot\|$ is an operation on the vector with the following properties:

- $\|\mathbf{x}\| \geq 0$ with $\|\mathbf{x}\| = 0$ only if $\mathbf{x} = \mathbf{0}$.
- **Triangle inequality**: $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$.
- For any constant α, $\|\alpha\mathbf{x}\| = |\alpha| \, \|\mathbf{x}\|$.

Vector p-norms

Vector p norms are special types of norms on $n \times 1$ vectors. By definition, for $p \geq 1$, the p-norm of an $n \times 1$ vector is given by

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^{n} \mathbf{x}^p \right)^{1/p}$$

Vector p norms

Examples of p-norms

- Vector 1-norm:

$$\|\mathbf{x}\|_1 = \sum_{i=1}^{n} |\mathbf{x}|.$$

- Vector 2-norm (Euclidean norm):

$$\|\mathbf{x}\|_2 = \left(\sum_{i=1}^{n} \mathbf{x}^2 \right)^{1/2} = \sqrt{\mathbf{x}^\intercal \mathbf{x}}.$$

- Vector ∞-norm (max norm):

$$\|\mathbf{x}\|_\infty = \max_{1 \le i \le n} |\mathbf{x}_i|.$$

Matrix norms

Properties of vector norms

A matrix norm $\|\cdot\|$ is an operation on a matrix with the following properties:

- $\|A\| \geq 0$ with $\|A\| = 0$ only if $A = 0$.
- **Triangle inequality**: $\|A + B\| \leq \|A\| + \|B\|$.
- For any constant α, $\|\alpha A\| = |\alpha| \, \|A\|$.

Consistent matrix norms

A matrix norm is said to be *consistent* if

$$\|AB\| \leq \|A\| \, \|B\|.$$

Matrix p-norms

For $p \geq 1$, the p-norm of an $m \times n$ matrix is given by

$$\|A\|_p = \max_{\mathbf{x} \neq 0} \frac{\|A\mathbf{x}\|_p}{\|\mathbf{x}\|_p}$$

Examples of matrix p-norms

- Matrix 1-norm (maximum column sum):

$$\|A\|_1 = \max_{1 \le j \le n} \left(\sum_{1 \le i \le m} |a_{ij}| \right).$$

- Matrix ∞-norm (maximum row sum):

$$\|A\|_\infty = \max_{1 \le j \le m} \left(\sum_{1 \le i \le n} |a_{ij}| \right).$$

- Matrix 2-norm (square root of the largest eigenvalue of $A^\intercal A$):

$$\|A\|_2 = \sqrt{\max_{1 \le j \le n} \lambda_j \left(A^\intercal A \right)}$$

Condition number

A square matrix A is *non-singular* if and only if

- $\det(A) \neq 0$ (invertible).
- All eigenvalues of A are non-zero.

Condition number

For a non-singular matrix A, the *condition number* is defined as

$$\kappa(A) = \|A\| \, \|A^{-1}\|.$$

Condition number

Properties of condition numbers

- $\kappa(A) \geq 1$ for consistent matrix norms.
- $\kappa(\alpha I) = 1$ for all $\alpha \neq 0$.
- For a real symmetric matrix, the 2-norm condition number is

$$\kappa_2(A) = \|A\|_2 \, \|A^{-1}\|_2 = \frac{\max_{1\leq i\leq n}|\lambda_i(A)|}{\min_{1\leq i\leq n}|\lambda_i(A)|}.$$

- A is said to be *ill-conditioned* if $\kappa(A) > \dfrac{1}{\varepsilon} \approx 10^{16}$.

Example: (MATH2089, S1 2010, Q1c)

The coefficient matrix A and the right-hand-side vector $\mathbf{b}$ are known to 8 significant figures, and

$$\|A\| = 1.9 \times 10^1, \qquad \|A^{-1}\| = 2.2 \times 10^3.$$

What is the condition number $\kappa(A)$?

By definition, for non-singular matrices,

$$\kappa(A) = \|A\|\|A^{-1}\|.$$

Hence,

$$\kappa(A) = \|A\|\|A^{-1}\| = \left(1.9 \times 10^1\right) \times \left(2.2 \times 10^3\right) = 4.18 \times 10^4.$$

Example

Let $A = \begin{bmatrix} 2 & -1 & 2 \\ -1 & 1 & -1 \\ 2 & -1 & 3 \end{bmatrix}$ and $A^{-1} = \begin{bmatrix} 2 & 1 & -1 \\ 1 & 2 & 0 \\ -1 & 0 & 1 \end{bmatrix}$.
Compute the condition numbers $\kappa_\infty(A)$ and $\kappa_1(A)$.

The condition number $\kappa_\infty(A)$ is simply just

$$\kappa_\infty(A) = \|A\|_\infty \|A^{-1}\|_\infty.$$

The sum of the magnitude of the rows of A are simply $|2| + |-1| + |2| = 5$, $|-1| + |1| + |-1| = 3$, and $|2| + |-1| + |3| = 6$. Hence $\|A\|_\infty$ is just 6. We repeat the same process for A^{-1} and get $\|A^{-1}\|_\infty = 4$. So

$$\kappa_\infty(A) = 6 \times 4 = 24.$$

Repeat the process for the columns to get $\kappa_1(A)$.

Sensitivity of a linear system

- Let $\bar{\mathbf{x}}$ be an *approximation* to $\mathbf{x}$. Then the absolute error of $\mathbf{x}$ is $\|\mathbf{x} - \bar{\mathbf{x}}\|$ and the relative error is

$$\rho_{\mathbf{x}} = \frac{\|\mathbf{x} - \bar{\mathbf{x}}\|}{\|\mathbf{x}\|}.$$

- Let $\bar{A}$ be an approximation to A. Then the absolute error is $\|A - \bar{A}\|$ and the relative error is

$$\rho_A = \frac{\|A - \bar{A}\|}{\|A\|}.$$

(Theorem) Sensitivity of a linear system

The sensitivity of a linear system $A\mathbf{x} = \mathbf{b}$ to the error in input data A and $\mathbf{b}$ is given by

$$\rho_{\mathbf{x}} \approx \kappa(A) \times (\rho_A + \rho_{\mathbf{b}}).$$

Sensitivity of a linear system

Properties of the errors

- If A or $\mathbf{b}$ are known **exactly**, then the errors ρ_A and $\rho_\mathbf{x}$ are 0. That is, there is no error in precision.
- If $\mathbf{x}$ is known to k significant figures, then

$$\rho_\mathbf{x} \leq 0.5 \times 10^{-k}.$$

Example: (MATH2089, 2009 Q1c)

The following MATLAB code generates the given output for a pre-defined real square array A.

```
chk1 = norm(A - A', 1)
chk1 = 1.4052e-015
ev = eig(A);
evlim = [min(ev) max(ev)]
evlim = 4.5107e-002 9.1213e+004
```

- Is A symmetric?
- Is A positive definite?
- Calculate the 2-norm condition number $\kappa_2(A)$ of A.
- When solving the linear system $A\mathbf{x} = \mathbf{b}$, the elements of A and $\mathbf{b}$ are known to 6 significant decimal digits. Estimate the relative error in the computed solution $\bar{\mathbf{x}}$.
- Given the Cholesky factorisation $A = R^\intercal R$, explain how to solve the linear system $A\mathbf{x} = \mathbf{b}$.

Example: (MATH2089, 2009 Q1c)

The following MATLAB code generates the given output for a pre-defined real square array A.

```
chk1 = norm(A - A', 1)
chk1 = 1.4052e-015
```

- Is A symmetric?

From the MATLAB command `chk1 = norm(A - A', 1)`, this implies that $\|A - A^\mathsf{T}\|_1 \approx 1.4 \times 10^{-15} \approx 7\varepsilon$ where $\varepsilon = 2.2 \times 10^{-16}$. Hence the value is small enough such that

$$\|A - A^\mathsf{T}\|_1 \approx 0 \implies A = A^\mathsf{T}.$$

Thus A is symmetric with rounding error.

Example: (MATH2089, 2009 Q1c)

The following MATLAB code generates the given output for a pre-defined real square array A.

```
ev = eig(A);
evlim = [min(ev) max(ev)]
evlim = 4.5107e-002 9.1213e+004
```

- Is A positive definite?

Because A is symmetric, then the following statements are equivalent.

- A is positive definite.
- All of the eigenvalues in A are positive.

From our MATLAB command, we see that the minimum eigenvalue, given by the command `min(ev)`, is $4.5 \times 10^{-2} > 0$. Hence all of the eigenvalues are positive and thus, A is positive definite.

Example: (MATH2089, 2009 Q1c)

The following MATLAB code generates the given output for a pre-defined real square array A.

```
ev = eig(A);
evlim = [min(ev) max(ev)]
evlim = 4.5107e-002 9.1213e+004
```

- Calculate the 2-norm condition number $\kappa_2(A)$ of A.

For a real symmetric matrix, the 2-norm condition number is

$$\kappa_2(A) = \|A\|_2 \|A^{-1}\|_2 = \frac{|\lambda_{\max}(A)|}{|\lambda_{\min}(A)|} = \frac{9.12 \times 10^4}{4.51 \times 10^{-2}} = 2.02 \times 10^6.$$

Example: (MATH2089, 2009 Q1c)

- When solving the linear system $A\mathbf{x} = \mathbf{b}$, the elements of A and $\mathbf{b}$ are known to 6 significant decimal digits. Estimate the relative error in the computed solution $\bar{\mathbf{x}}$.

Since A and $\mathbf{b}$ are known to 6 significant decimal digits, then we have

$$\rho_A \leq 0.5 \times 10^{-6}, \qquad \rho_{\mathbf{b}} \leq 0.5 \times 10^{-6}.$$

Then we have

$$\begin{aligned}\rho_{\mathbf{x}} &\approx \kappa_2(A)\left[\rho_A + \rho_{\mathbf{b}}\right] \\ &\leq \left(2 \times 10^6\right)\left[0.5 \times 10^{-6} + 0.5 \times 10^{-6}\right] \\ &= 2.\end{aligned}$$

Hence the relative error of $\mathbf{x}$ is 2.

Example: (MATH2089, 2009 Q1c)

- Given the Cholesky factorisation $A = R^\intercal R$, explain how to solve the linear system $A\mathbf{x} = \mathbf{b}$.

Apply forward substitution and back substitution. Let $A = R^\intercal R$ so that

$$A\mathbf{x} = \mathbf{b} \implies R^\intercal R\mathbf{x} = \mathbf{b} \implies R^\intercal \mathbf{y} = \mathbf{b},$$

where $R\mathbf{x} = \mathbf{y}$. Solve $R^\intercal \mathbf{y} = \mathbf{b}$ by forward substitution to get $R\mathbf{x} = \mathbf{y}$ and solve $R\mathbf{x} = \mathbf{y}$ by back substitution to get $\mathbf{x}$.

Part II: Least Squares & Polynomial Interpolation

Least squares

- Given a set of data points, determine the *line* or *curve* of best fit.

Methods to finding least squares

For a given $m \times n$ matrix A with $m > n$, we can apply two methods to finding least square solutions.

1. *Normal equation*: $A^\intercal A\mathbf{u} = A^\intercal \mathbf{y}$.
   - $\mathcal{O}(mn^2)$ flops.
2. *QR factorisation* and *back substitution*.
   - $\mathcal{O}(mn^2)$ flops.

Method 1: Normal equations

Assumptions.

- A is an $m \times n$ matrix (with $m > n$) and A has full rank.

$$A\mathbf{u} = \mathbf{y} \implies (A^\intercal A)\,\mathbf{u} = A^\intercal \mathbf{y}.$$

- Define a new matrix B to be the matrix $B = A^\intercal A$. B is symmetric and positive definite.
- Solve $B\mathbf{u} = A^\intercal \mathbf{y}$ by applying either Cholesky or LU factorisation with forward and backward substitutions.

Cost of method and issue

- Dominated by computing B: $\mathcal{O}(mn^2)$ flops.
- Issue: Condition number is squared!

$$\kappa_2(B) = \kappa_2(A^\intercal A) = [\kappa_2(A)]^2$$

Method 2: QR factorisation

We can try and write A as a product of two matrices

$$A = QR,$$

where Q is an orthogonal matrix and R is an upper triangular matrix.

- $Q = \begin{bmatrix} Y & Z \end{bmatrix}$, where Y is an $m \times n$ matrix and Z is an $m \times (m-n)$ matrix.

Cost of method

- Cost: $\mathcal{O}(mn^2)$ flops.

Polynomial interpolation

- **Idea**: We want to make a new polynomial (interpolation) that passes through the data points.

Given data points (x_0, y_0) and (x_1, y_1), we solve the simultaneous equation

$$p(x) = a_0 + a_1 x \implies \begin{cases} y_0 = a_0 + a_1 x_0 \\ y_1 = a_0 + a_1 x_1 \end{cases}$$

Given n number of data points, an interpolating polynomial will have degree $(n-1)$.

Interpolating polynomials in Lagrange form

Given $(n+1)$ data points (x_j, y_j), construct Lagrange polynomials of degree n of the form

$$\ell_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \left(\frac{x - x_j}{x_i - y_j} \right) \qquad \text{for } i = 0, \ldots, n.$$

- Note that $\ell_i(x_j) = 1$ for $i = j$ and $\ell_i(x_j) = 0$ if $i \neq j$.
- The interpolating polynomial is then

$$p(x) = \sum_{i=0}^{n} y_i \ell_i(x).$$

Fora function f, the following data are known:

$$f(0) = 12.6, \quad f(1) = 6.7, \quad f(2) = 4.3, \quad f(3) = 2.7.$$

- What is the degree of the interpolating polynomial P for these data?
- Assume that we want to find P in the form

$$P(x) = a_0 + a_1 x + \cdots .$$

  - Write down the system of linear equations you need to solve to obtain $a_0, a_1, \ldots$.
  - Use `MATLAB` to set up and solve this linear system.
- Write down the Lagrange polynomials $\ell_j(x)$ for $j = 0, 1, 2, 3$.
- Write down the interpolating polynomial P using the Lagrange polynomials.

Fora function f, the following data are known:

$$f(0) = 12.6, \quad f(1) = 6.7, \quad f(2) = 4.3, \quad f(3) = 2.7.$$

- What is the degree of the interpolating polynomial P for these data?

As there are 4 data values and a polynomial of degree n has $n + 1$ coefficients, then the degree of the interpolating polynomial is $n = 4 - 1 = 3$.

- Assume that we want to find P in the form

$$P(x) = a_0 + a_1 x + \cdots .$$

  - Write down the system of linear equations you need to solve to obtain $a_0, a_1, \ldots$.
  - Use `MATLAB` to set up and solve this linear system.

- As the interpolating polynomial is of degree 3, then

$$P(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

We obtain the following system of linear equations

$$\begin{aligned}
f(0) = 12.6 &\implies P(0) = a_0 = 12.6 \\
f(1) = 6.7 &\implies a_0 + a_1 + a_2 + a_3 = 6.7 \\
f(2) = 4.3 &\implies P(2) = a_0 + 2a_1 + 4a_2 + 8a_3 = 4.3 \\
f(3) = 2.7 &\implies a_0 + 3a_1 + 9a_2 + 27a_3 = 2.7.
\end{aligned}$$

- Assume that we want to find P in the form

$$P(x) = a_0 + a_1 x + \cdots .$$

  - Write down the system of linear equations you need to solve to obtain $a_0, a_1, \ldots$.
  - Use `MATLAB` to set up and solve this linear system.

- Use the backslash command to solve for **a** to obtain the following solution

$$P(x) = 12.6 - 8.5x + 3.1x^2 - 0.45x^3.$$

- Write down the Lagrange polynomials $\ell_j(x)$ for $j = 0, 1, 2, 3$.

Recall that the Lagrange polynomials are the degree n polynomials

$$\ell_j(x) = \prod_{\substack{k=0 \\ k \neq j}}^{n} \frac{x - x_k}{x_j - x_k}.$$

For the given data $x_0 = 0, x_1 = 1, x_2 = 2, x_3 = 3$, this gives

$$\ell_0(x) = \frac{(x-1)(x-2)(x-3)}{(0-1)(0-2)(0-3)} = -\frac{1}{6}(x-1)(x-2)(x-3)$$

$$\ell_1(x) = \frac{(x-0)(x-2)(x-3)}{(1-0)(1-2)(1-3)} = \frac{1}{2}x(x-2)(x-3)$$

$$\ell_2(x) = \frac{(x-0)(x-1)(x-3)}{(2-0)(2-1)(2-3)} = -\frac{1}{2}x(x-1)(x-3)$$

$$\ell_3(x) = \frac{(x-0)(x-1)(x-2)}{(3-0)(3-1)(3-2)} = \frac{1}{6}x(x-1)(x-2)$$

Fora function f, the following data are known:

$$f(0) = 12.6, \quad f(1) = 6.7, \quad f(2) = 4.3, \quad f(3) = 2.7.$$

- Write down the interpolating polynomial P using the Lagrange polynomials.

The interpolating polynomial is simply

$$\begin{aligned}
P(x) &= \sum_{j=0}^{3} f_j \ell_j(x) \\
&= 12.6 \times \ell_0(x) + 6.7 \times \ell_1(x) + 4.3 \times \ell_2(x) + 2.7 \times \ell_3(x) \\
&= -\frac{12.6}{6}(x-1)(x-2)(x-3) + \frac{6.7}{2}x(x-2)(x-3) + \\
&- \frac{4.3}{2}x(x-1)(x-3) + \frac{2.7}{6}x(x-1)(x-2).
\end{aligned}$$

(Theorem) Interpolating polynomial error

If f is $(n+1)$ times continuously differentiable on the interval $[a, b]$, then the error in approximating $f(x)$ by $p(x)$ is

$$f(x) - p(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{j=0}^{n} (x - x_j)$$

for some unknown $\xi \in [a, b]$ depending on x.

Chebyshev points

- Choose x_j to minimise

$$\max_{x \in [-1,1]} \prod_{j=0}^{n} (x - x_j).$$

- On $[-1, 1]$, set $t_j = \cos\left[\left(\frac{2n+1-2j}{2n+2}\right)\pi\right]$ for $j = 0, \ldots, n$.
- On $[a, b]$, set $x_j = \frac{a+b}{2} + \left(\frac{b-a}{2}\right) t_j$ for $j = 0, \ldots, n$.
- Chebyshev nodes are the zeros of the Chebyshev polynomial $T_{n+1}(x)$.
    - Interpolation error is minimised by choosing Chebyshev nodes!

Part III: Nonlinear Equations

Nonlinear equation in standard form

$$f(x) = 0, \qquad x \in \mathbb{R}.$$

- We aim to solve for x (ie find the zeros of f)
- If necessary, rearrange the equation to have the equation in standard form.

Notation

Continuity and differentiability

- If $f \in C^n([a,b])$, then f is continuous on $[a,b]$ and n times differentiable on the interval (a,b).

Results of continuity

- (Intermediate Value Theorem)
  If $f \in C([a,b])$ and $f(a)f(b) < 0$, then there exists **at least one zero** of f in the interval on (a,b).
- (Strictly monotone)
  If $f'(x) > 0$ OR $f'(x) < 0$ for all $x \in (a,b)$, then f is strictly monotone on the interval $[a,b]$.
- (Uniqueness of root)
  If f is continuous AND strictly monotone on the interval $[a,b]$ and $f(a)f(b) < 0$, then f has a **unique root** on (a,b).

Iterative methods for solving equations

Iterations

- Have an initial guess or starting point x_1.
- Generate sequences of iterates x_k for $k = 2, 3, \ldots$ based on approximations of the problem.
- Determine whether the sequence generated converges to the true solution x^*.

Order of convergence

- Largest ν such that

$$\lim_{k\to\infty} \frac{e_{k+1}}{e_k^{\nu}} = \beta,$$

where β is the asymptotic constant and $e_k = |x_k - x^*|$.

Iterative method: Bisection

- Suppose that $f(a)f(b) < 0$ and we have $f \in C([a, b])$.
- Take the midpoint $x_{\text{mid}} = \dfrac{a+b}{2}$ as x_1.
- Choose a new interval depending on the result of $f(x_{\text{mid}}$.
  - If $f(a)f(x_{\text{mid}}) < 0$, then choose new interval to be $[a, x_{\text{mid}}]$.
  - If $f(x_{\text{mid}})f(b) > 0$, then choose $[x_{\text{mid}}, b]$.
- Iterate using the same process.

Order of convergence

- Linear convergence with asymptotic constant $\beta = \dfrac{1}{2}$.

Iterative method: Fixed point iteration

Given a starting point x_1, compute

$$x_{k+1} = g(x_k), \qquad \text{for } k = 1, 2, \ldots$$

Order of convergence

- If $g \in C^1([a, b])$ and there exists a $K \in (0, 1)$ such that $|g'(x)| \leq K$ for all $x \in (a, b)$, then the fixed point iteration converges linearly with asymptotic constant $\beta \leq K$, for any $x_1 \in [a, b]$.

Iterative method: Newton's method

Newton's approximation

- Approximate $f(x)$ by its tangent at the point $(x_k, f(x_k))$ to form

$$f(x) \approx f(x_k) + (x - x_k)f'(x_k).$$

- Choose $x = x_{k+1}$ and set $f(x) = 0$ to form

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, \qquad \text{assuming } f'(x_k) \neq 0.$$

Order of convergence

- If $f \in C^2([a, b])$ and x_1 is *sufficiently close* to a simple root $x^* \in (a, b)$, then Newton's method converges quadratically to x^*.

Example: (MATH2089, S1 2009)

To find the root of a real number, computers typically implement Newton's method. Let $a > 1$ and consider finding the cube root of a, that is $a^{1/3}$.

Show that Newton's method can be written as

$$x_{k+1} = \frac{1}{3}\left(2x_k + \frac{a}{x_k^2}\right).$$

We want to find $x = a^{1/3} \implies x^3 - a = 0$. So set $f(x) = x^3 - a$. We then have

$$f(x_k) = x_k^3 - a, \quad f'(x_k) = 3x_k^2.$$

By Newton's method, we obtain the result

$$\begin{aligned}
x_{k+1} &= x_k - \frac{f(x_k)}{f'(x_k)} \\
&= x_k - \frac{x_k^3 - a}{3x_k^2} \\
&= x_k - \frac{1}{3}x_k + \frac{a}{3x_k^2} \\
&= \frac{1}{3}\left[(3x_k - x_k) + \frac{a}{x_k^2}\right] \\
&= \frac{1}{3}\left(2x_k + \frac{a}{x_k^2}\right).
\end{aligned}$$

Example: (MATH2089, S1 2013, Q1d)

Consider the function $f(x) = e^x \sin(x) - 100$.

- You are given that $f(x)$ has a simple zero at $x^* \approx 6.443$. If you use a starting value x_1 near x^*, what is the expected order of convergence for Newton's method?

The function behaves well since e^x and $\sin(x)$ are continuous functions. So it passes the theorem! Hence the expected order of convergence is 2.

Iterative method: Secant method

- Approximate $f(x)$ by a line through the point $(x_k, f(x_k))$ and $(x_{k-1}, f(x_{k-1}))$ to form

$$f(x) \approx f(x_k) + (x - x_k)\frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}}.$$

- Choose $x = x_{k+1}$ and set $f(x) = 0$ to form

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})}.$$

Order of convergence

- If $f \in C^2([a, b])$ and x_1, x_2 are *sufficiently* close to x^*, then the secant method converges superlinearly with order $\nu = \dfrac{1+\sqrt{5}}{2}$.

Part IV: Numerical Differentiation and Integration

Taylor series

Taylor series

A **Taylor series** is an infinite polynomial series that approximates non-polynomial functions by taking higher order derivatives centred around a point x_0.

Examples of well-known Taylor series

- $e^x = \displaystyle\sum_{k=0}^{\infty} \frac{x^k}{k!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \ldots$
- $\ln(1+x) = \displaystyle\sum_{k=1}^{\infty} \frac{(-1)^{k+1} x^k}{k} = x - \frac{x^2}{2} + \frac{x^3}{3} - \ldots$ for $|x| < 1$.

(Theorem)

Let $f \in C^{n+1}([a,b])$. In other words, let f be continuous on $[a,b]$ and $n+1$ times differentiable on (a,b). Then

$$\begin{aligned} f(x+h) &= \sum_{k=0}^{n} \frac{f^{(k)}(x)}{k!} h^k + \frac{f^{(n+1)}(\xi)}{(n+1)!} h^{n+1} \\ &= f(x) + f'(x)h + \frac{f''(x)}{2!} h^2 + \cdots + \frac{f^{(n)}(x)}{n!} h^n + \mathcal{O}(h^{n+1}) \end{aligned}$$

for some unknown $\xi \in (a,b)$

Finite difference methods

Forward difference approximation

Let $f \in C^2([a, b])$. That is, let f be twice differentiable in the interval $[a, b]$. Then

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h).$$

- The *roundoff* error is

$$\mathcal{O}\left(\frac{\varepsilon}{h}\right) = \varepsilon \left| \frac{f(x+h) - f(x)}{h} \right|.$$

- The *truncation* error is $\mathcal{O}(h)$ and the total error is $\mathcal{O}\left(\frac{\varepsilon}{h}\right) + \mathcal{O}(h)$.

Finite difference methods

Central difference approximation

Let $f \in C^4([a,b]|)$. That is, let f be four times differentiable on the interval $[a,b]$. Then

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

- The *roundoff* error is $\mathcal{O}\left(\frac{\varepsilon}{h^2}\right)$ and the *truncation* error is $\mathcal{O}(h^2)$.
- The total error is $\mathcal{O}\left(\frac{\varepsilon}{h^2}\right) + \mathcal{O}(h^2)$.

Quadrature rules

- We are approximating integrals using weighted sums of functions values. That is,

$$\text{Quadrature rule: } Q_N(f) = \sum_{j=0 \text{ or } 1}^{N} w_j f(x_j),$$

where $\sum_j w_j = b - a$.

- Quadrature error:

$$E_N = I(f) - Q_N(f) = \int_a^b f(x)\,\mathrm{d}x - Q_N(f)$$

  - We want $E_N \to 0$ as $N \to \infty$ for convergence.

Quadrature rules

We look at three quadrature rules:

- Trapezoidal rule
- Simpson's rule
- Gauss-Legendre rule

Quadrature rule – Trapezoidal rule

$$Q_N(f) = h\left(\frac{f_0}{2} + f_1 + f_2 + \cdots + f_{N-1} + \frac{f_N}{2}\right).$$

- Approximate an integral using a bunch of trapeziums and sum up the area under $f(x)$ using the area of each trapezium.
- The height h is fixed: $h = \dfrac{b-a}{N}$.
- Function values are $f_j = f(x_j)$ for all $j = 0, \ldots, N$.
- Weights are $w_0 = w_N = \dfrac{h}{2}$ and $w_j = h$ for all $h = 1, \ldots, N-1$.

Quadrature rule – Trapezoidal rule

(Theorem) Error of trapezoidal rule

Let $f \in C^2([a,b])$. Then

$$E_N(f) = -\frac{b-a}{12} h^2 f''(\xi),$$

for some unknown $\xi \in [a,b]$.

- Rate of convergence: $E_N(f) = \mathcal{O}(h^2)$ or $E_N(f) = \mathcal{O}(N^{-2})$.

Quadrature rule – Simpson's rule

$$Q_N(f) = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 2f_{N-2} + 4f_{N-1} + f_N\right).$$

- Approximate an integral using a bunch of parabolas and sum up the area under $f(x)$ using the area of each parabola through integration.
- The height is fixed: $h = \dfrac{b-a}{N}$, with N **being even**.
- Function values are $f_j = f(x_j)$ for all $j = 0, \ldots, N$.
- Weights are $w_0 = w_N = \dfrac{h}{3}$ and $w_j = \begin{cases} \frac{4h}{3} & \text{for odd } j \\ \frac{2h}{3} & \text{for even } j \end{cases}$.

Quadrature rule – Simpson's rule

(Theorem) Error of Simpson's rule

Let $f \in C^4([a, b])$. Then

$$E_N(f) = -\frac{b-a}{180} h^4 f^{(4)}(\xi),$$

for some unknown $\xi \in [a, b]$.

- Rate of convergence: $E_N(f) = \mathcal{O}(h^4)$ or $E_N(f) = \mathcal{O}(N^{-4})$.

Quadrature rule – Gauss-Legendre rule

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \approx Q_N(f) = \sum_{j=1}^{N} w_j f(x_j).$$

- Nodes x_j are the zeros of the **Legendre polynomial** of degree N on $[-1, 1]$.
- Weights w_j are given in terms of the Legendre polynomials.

Quadrature rule – Gauss-Legendre rule

(Theorem) Error of Gauss-Legendre rule

Let $f \in C^{2N}([-1,1])$. Then

$$E_N(f) = -\frac{e_N}{(2N)!} f^{(2N)}(\xi),$$

where $\xi \in [-1,1]$ and e_N is some number that depends on N.

Quadrature properties

- Quadratures assume integrand f is sufficiently smooth on $[a, b]$.
    - Assume that $f \in C^2([a, b])$ for trapezoidal rule.
    - Assume that $f \in C^4([a, b])$ for Simpson's rule.
    - Assume that $f \in C^{2N}([a, b])$ for Gauss-Legendre rule.

Change of variables

Transform integral

$$\int_a^b f(x)\,\mathrm{d}x \to \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{a+b}{2}+\frac{b-a}{2}y\right)\,\mathrm{d}y$$

by substituting

$$x = \frac{a+b}{2}+\frac{b-a}{2}y.$$

Tips for estimating difficult integrals

- Unbounded derivatives: apply a change of variables.
- Discontinuity on derivative: split the integral and remove the discontinuous derivative.
- High oscillatory: requires a special analytic method.
- Narrow spike: either underestimate or overestimate the spikes.

Part V: Ordinary Differential Equations

First order Initial Value Problems (IVP)

First order ODE

Ordinary differential equations are equations that involve its derivative. A first order differential equation is one such equation where the highest order of derivative is 1. A first order initial value problem is simply a first order ODE with initial conditions.

- First order ODE: $\dfrac{\mathrm{d}y}{\mathrm{d}x} = y$.
- First order IVP: $\dfrac{\mathrm{d}y}{\mathrm{d}x} = y$ with $y(0) = 1$.

Existence and uniqueness of solutions

(Theorem)

If $f(t, y)$ and $\dfrac{\partial f(t, y)}{\partial y}$ are continuous and bounded for all $t \in [t_0, t_{\max}]$ and $y \in \mathbb{R}$, then the IVP has a unique solution in the time interval $[t_0, t_{\max}]$.

Euler's method

Solve a first order IVP $y' = f(t, y), \quad t \in [t_0, t_{\max}], \quad y(t_0) = y_0$ by

$$y_{n+1} = y_n + h \cdot f(t_n, y_n), \qquad n = 0, 1, \ldots, N-1.$$

System of first order ODEs

- Often times, we may have a system of many equations involving derivatives.
- We can write it in the form

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(t, \mathbf{x}).$$

Example: (MATH2089, 2010 Q2b)

Consider the initial value problem (IVP)

$$y''' + 2y' - (\pi^2 + 1)y = \pi(\pi^2 + 1)e^{-t}\sin(\pi t)$$
$$y(0) = 1, \quad y'(0) = -1, \quad y''(0) = 1 - \pi^2.$$

Reformulate the IVP as a system of first-order differential equations

$$\mathbf{x}'(t) = \mathbf{f}(t, \mathbf{x})$$

with the appropriate initial condition.

Begin by observing that the degree of derivative is 3. Hence, we use

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y \\ y' \\ y'' \end{bmatrix}.$$

Then we see that

$$\mathbf{x}' = \begin{bmatrix} x_1' \\ x_2' \\ x_3' \end{bmatrix} = \begin{bmatrix} y' \\ y'' \\ y''' \end{bmatrix} = \begin{bmatrix} x_2 \\ x_3 \\ y''' \end{bmatrix},$$

where y''' is just

$$y''' = \pi(\pi^2 + 1)e^{-t}\sin(\pi t) - 2x_2 + (\pi^2 + 1)x_1.$$

So we obtain

$$\mathbf{x}' = \mathbf{f}(t, \mathbf{x}) = \begin{bmatrix} x_2 \\ x_3 \\ \pi(\pi^2 + 1)e^{-t}\sin(\pi t) - 2x_2 + (\pi^2 + 1)x_1 \end{bmatrix}.$$

To find the appropriate initial conditions, take $t = 0$ to get

$$\mathbf{x}(0) = \begin{bmatrix} y(0) \\ y'(0) \\ y''(0) \end{bmatrix} = \begin{bmatrix} 1 \\ -1 \\ 1 - \pi^2 \end{bmatrix}.$$

2-stage Runge Kutta method

$$k_1 = f(t_n, y_n), \qquad k_2 = f\left(t_n + \frac{2}{3}h, y_n + \frac{2}{3}hk_1\right)$$

$$y_{n+1} = y_n + \frac{h}{4}\left[k_1 + 3k_2\right]$$

4-stage Runge Kutta method

$$k_1 = f(t_n, y_n), \qquad k_2 = f\left(t_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1\right)$$

$$k_3 = f\left(t_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_2\right), \qquad k_4 = f\left(t_n + h, y_n + hk_3\right)$$

$$y_{n+1} = y_n + \frac{h}{6}\left[k_1 + 2k_2 + 2k_3 + k_4\right].$$

Example

Find the solution of the initial value problem

$$y' = 3y + 3t, \qquad y(0) = 1, t = 0.2$$

,

- Using Euler's method with $h = 0.2$.
- Using the fourth-order Runge Kutta method with $h = 0.2$.

- Using Euler's method:
  - We observe that, here, $f(t_n, y_n) = 3y + 3t$.
  - Next, using our initial value of $y(t_0) = y_0 \implies y(0) = 1$, we obtain $t_0 = 0$ and $y_0 = 1$.
  - Next, we want to find $y_{0.2}$ given $t = 0.2$.

$$\begin{aligned} y_{0.2} &= y_0 + h\left[f(t_0, y_0)\right] \\ &= 1 + 0.2\left[3y_0 + 3t_0\right] \\ &= 1 + 0.2\left[3 + 0\right] \\ &= 1.6. \end{aligned}$$

- Using the fourth-order Runge Kutta method:
  - Observe that

$$y_{0.2} = y_0 + \frac{h}{6}\left[k_1 + 2k_2 + 2k_3 + k_4\right].$$

  - Calculate the values of k_1, k_2, k_3 and k_4 respectively.

$$\begin{aligned}
k_1 &= f(t_0, y_0) = 3. \\
k_2 &= f\left(t_0 + \frac{1}{2}h, y_0 + \frac{1}{2}hk_1\right) = 4.2 \\
k_3 &= f\left(t_0 + \frac{1}{2}h, y_0 + \frac{1}{2}hk_2\right) = 4.56 \\
k_4 &= f\left(t_0 + h, y_0 + hk_3\right) = 6.336.
\end{aligned}$$

- Then,

$$y_{0.2} = 1 + \frac{0.2}{6}\left[3 + 2 \times 4.2 + 2 \times 4.56 + 6.336\right] = 1.8952.$$

Other useful methods for solving IVPs

Taylor method of order 2

$$y_{n+1} = y_n + hf(t_n, y_n) + \frac{h^2}{2}\frac{\partial f(t,y)}{\partial t}\Big|_{t=t_n, y=t_n}$$

Implicit Euler's method

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

Trapezoidal method

$$y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_{n+1}\right]$$

Heun's method

$$y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_n + hf(t_n, y_n))\right]$$

Part VI: Partial Differential Equations

Partial Differential Equations

- Partial Differential Equations (PDEs) are functions of *more than one variable* defined by equations involving their *partial derivatives*.
- Order of the PDE is the order of the highest derivative present!

Finite difference methods

- Treat them no differently to functions of one variable.
- The only difference is changing the variable in the derivative!

$$\frac{\partial u(x,t)}{\partial x} = \frac{u(x+h,t) - u(x-h,t)}{2h} + \mathcal{O}(h^2).$$

Types of PDEs

We will restrict ourselves to PDEs involving only two variables. A second order quasi-linear PDE is of the form

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} = F\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right).$$

- Elliptic if $B^2 - 4AC < 0$.
- Parabolic if $B^2 - 4AC = 0$.
- Hyperbolic if $B^2 - 4AC > 0$.

Elliptic PDEs

- Divide x interval $[0, L_x]$ into $m+1$ equal length subintervals such that
$$h_x = \frac{L_x}{m+1}.$$
- Divide y interval $[0, L_y]$ into $n+1$ equal length subintervals such that
$$h_y = \frac{L_y}{n+1}.$$
- Central difference approximation of $\mathcal{O}(h^2)$ at the grid points x_i

$$\frac{\partial^2 u}{\partial x^2}(x_i, y_j) \approx \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h_x^2}$$
$$\frac{\partial^2 u}{\partial y^2}(x_i, y_j) \approx \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{h_y^2}$$

Parabolic PDEs

Method 1 (Explicit method)

- Forward difference approximation to the time derivative

$$\frac{\partial u}{\partial t}(x_i, t_\ell) \approx \frac{u_i^{\ell+1} - u_i^\ell}{h_t}.$$

- Central difference approximation to the space derivative

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_\ell) \approx \frac{u_{i-1}^\ell - 2u_i^\ell + u_{i+1}^\ell}{h_x^2}.$$

- Substitute into PDE and multiply by h_t to obtain

$$u_i^{\ell+1} = su_{i-1}^\ell + (1-2s)u_i^\ell + su_{i+1}^\ell, \qquad s = \frac{Dh_t}{h_x^2}.$$

Parabolic PDEs

Method 2 (Implicit method)

- Backward difference approximation to the time derivative

$$\frac{\partial u}{\partial t}(x_i, t_{\ell+1}) \approx \frac{u_i^{\ell+1} - u_i^{\ell}}{h_t}.$$

- Central difference approximation to the space derivative

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_{\ell+1}) \approx \frac{u_{i-1}^{\ell+1} - 2u_i^{\ell+1} + u_{i+1}^{\ell+1}}{h_x^2}.$$

- Substitute into PDE and multiply by h_t to obtain

$$-su_{i-1}^{\ell+1} + (1-2s)u_i^{\ell+1} - su_{i+1}^{\ell+1} = u_i^{\ell}, \qquad s = \frac{Dh_t}{h_x^2}.$$

Parabolic PDEs

Method 3 (Crank-Nicolson method)

- Take the average between the explicit and implicit method to obtain

$$u_i^{\ell+1} = u_i^\ell + \frac{s}{2}\left[\left(u_{i-1}^\ell - 2u_i^\ell + u_{i+1}^\ell\right) + \left(u_{i-1}^{\ell+1} - 2u_i^{\ell+1} + u_{i+1}^{\ell+1}\right)\right]$$

Stability of methods

- Explicit method: Stable if and only if $s \leq \frac{1}{2}$.
- Implicit method: Unconditionally stable.
- Crank-Nicolson method: Unconditionally stable.

Hyperbolic PDEs

Method (Explicit method)

- Central difference approximation to the time derivative

$$\frac{\partial^2 u}{\partial t^2}(x_i, t_\ell) \approx \frac{u_i^{\ell-1} - 2u_i^\ell + u_i^{\ell+1}}{h_t^2}.$$

- Central difference approximation to the space derivative

$$\frac{\partial^2 u}{\partial x^2}(x_i, t_\ell) \approx \frac{u_{i-1}^{\ell} - 2u_i^\ell + u_{i+1}^{\ell}}{h_x^2}.$$

- Substitute into PDE and multiply through h_t^2 to obtain

$$u_i^{\ell+1} = ru_{i-1}^\ell + 2(1-r)u_i^\ell + ru_{i+1}^\ell - u_i^{\ell-1}, \qquad r = \frac{c^2 h_t^2}{h_x^2}.$$

A final problem

The heat conduction equation which models the temperature in an insulated rod with ends held at constant temperatures can be written in the dimensionless form as

$$\frac{\partial \Theta(x,t)}{\partial t} = \frac{\partial^2 \Theta(x,t)}{\partial x^2}$$

- Write a finite difference approximation of this equation using the Forward-Time, Central-Space scheme and rearrange it to be solved by an explicit method.

By applying the FTCS scheme, we get

$$\frac{\partial \Theta}{\partial t}(x_i, t_\ell) \approx \frac{\Theta_i^{\ell+1} - \Theta_i^\ell}{h_t} \frac{\partial^2 \Theta}{\partial t^2}(x_i, t_\ell) \quad \approx \frac{\Theta_{i-1}^\ell - 2\Theta_i^\ell + \Theta_{i+1}^\ell}{h_x^2}.$$

By rearranging to allow explicit solving, we get

$$\Theta_i^{\ell+1} = \left(\frac{\Delta t}{\Delta x^2}\right)\Theta_{i-1}^{\ell} + \left(1 - \frac{2\Delta t}{\Delta x^2}\right)\Theta_i^{\ell} + \left(\frac{\Delta t}{\Delta x^2}\right)\Theta_{i+1}^{\ell}.$$