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# CTMS-MAT-13: Numerical Methods

Summary from 5 February 2025

Notes for numerical methods course 2025. This can be downloaded from:
`https://djps.github.io/docs/numericalmethods/notes`

[5 February 2025 – Version 0.1.6]

## Contents

## Recommended Reading

- J. F. Epperson "*An Introduction to Numerical Methods and Analysis*", Wiley 2nd Edition (2013).
- R. L. Burden and J. D. Faires "*Numerical Analysis*", Brooks/Cole 9th Edition (2011).

# 1 Taylor Series

The Taylor series, or the Taylor expansion of a function, is defined as

**Definition 1.1** (Taylor Series). For a function $f : \mathbb{R} \mapsto \mathbb{R}$ which is infinitely differentiable at a point $c$, the Taylor series of $f(c)$ is given by

$$\sum_{k=0}^{\infty} \frac{f^{(k)}(c)}{k!} (x-c)^k$$

where $f^{(k)} = \dfrac{\mathrm{d}^k f}{\mathrm{d}x^k}$ is the $k^{\text{th}}$ derivative.

This is a power series, which is convergent for some radius.

**Theorem 1 (Taylor's Theorem).** For a function $f \in C^{n+1}([a,b])$, i.e. $f$ is $(n+1)$-times continuously differentiable in the interval $[a,b]$, then for some $c$ in the interval, the function can be written as

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

for some value $\xi \in [a,b]$ where

$$\lim_{\xi \to c} \frac{f^{(n+1)}(\xi)}{(n+1)!} (x-c)^{n+1} = 0.$$

# 2 Errors

**Definition 2.1** (Absolute and Relative Errors)**.** Let $\tilde{a}$ be an approximation to $a$, then the **absolute error** is given by

$$|\tilde{a} - a|\,.$$

If $|a| \neq 0$, the **relative error** may be given by

$$\left|\frac{\tilde{a} - a}{a}\right|.$$

The error bound is the magnitude of the admissible error.

**Theorem 2.** For both addition and subtraction the bounds for the *absolute errors* are added. In division and multiplication the bounds for the *relative errors* are added.

**Definition 2.2** (Linear Sensitivity to Uncertainties)**.** If $y(x)$ is a smooth function, i.e. is differentiable, then $|y'|$ can be interpreted as the **linear sensitivity** of $y(x)$ to uncertainties in $x$.

For functions of several variables, i.e. $f : \mathbb{R}^n \to \mathbb{R}$, then

$$|\Delta y| \leq \sum_{i=1}^{n} \left|\frac{\partial y}{\partial x_i}\right| |\Delta x_i|$$

where $|\Delta x_i| = |\tilde{x}_i - x_i|$ for an approximation $\tilde{x}_i$.

# 3 Number Representations

**Definition 3.1** (Base Representation)**.** Every number $x \in \mathbb{N}_0$ can be written as a unique expansion with respect to base $b \in \mathbb{N}\backslash\{1\}$ as

$$(x)_b = a_0 b^0 + a_1 b^1 + \ldots + a_n b^n = \sum_{i=0}^{n} a_i b^i.$$

A number can be written in a nested form:

$$\begin{aligned}(x)_b &= a_0 b^0 + a_1 b^1 + \ldots a_n b^n \\ &= a_0 + b\,(a_1 + b\,(a_2 + b\,(a_3 + \ldots + b a_n)\,\ldots)\end{aligned}$$

with $a_i < \mathbb{N}_0$ and $a_i < b$, i.e. $a_i \in \{0, \ldots, b-1\}$.
For a real number, $x \in \mathbb{R}$, write

$$\begin{aligned}x &= \sum_{i=0}^{n} a_i b^i + \sum_{i=1}^{\infty} \alpha_i b^{-i} \\ &= a_n \ldots a_0 \cdot \alpha_1 \alpha_2 \ldots\end{aligned}$$

**Algorithm** (Euclid)**.**
Euclid's algorithm can convert an integer $x$ in base 10, i.e. $(x)_{10}$ into another base, $b$, i.e. $(x)_b$.

1. Input $(x)_{10}$
2. Determine the smallest integer $n$ such that $x < b^{n+1}$
3. Let $y = x$. Then for $i = n, \ldots, 0$

$$\begin{aligned}a_i &= y \text{ div } b^i \\ y &= y \text{ mod } b^i\end{aligned}$$

   which at each steps provides an $a_i$ and updates $y$.

4. Output as $(x)_b = a_n a_{n-1} \cdots a_0$

where div is integer division, and mod is the remainder operator.

There are two issues: finding $n$ maybe difficult and for large values of $b^i$ division maybe computationally costly. Horner's algorithm seeks to overcome these issues.

**Algorithm** (Horner)**.**
Horner's algorithm is:

1. Input $(x)_{10}$
2. Set $i = 0$
3. Let $y = x$. Then while $y > 0$

$$\begin{aligned} a_i &= y \bmod b \\ y &= y \operatorname{div} b \\ i &= i + 1 \end{aligned}$$

   which at each steps provides an $a_i$ and updates $y$.

4. Output as $(x)_b = a_n a_{n-1} \cdots a_0$

**Definition 3.2** (Normalized Floating Point Representations)**.**
*Normalized* floating point representations with respect to some base $b$, store a number $x$ as

$$x = 0 \cdot a_1 \dots a_k \times b^n$$

where the $a_i \in \{0, 1, \dots b-1\}$ are called the **digits**, $k$ is the **precision** and $n$ is the **exponent**. The set $a_1, \dots, a_k$ is called the **mantissa**. Impose that $a_1 \neq 0$, it makes the representation unique.

**Theorem 3.** Let $x$ and $y$ be two normalized floating point numbers with $x > y > 0$ and base $b = 2$. If there exists integers $p$ and $q \in \mathbb{N}_0$ such that

$$2^{-p} \leq 1 - \frac{y}{x} \leq 2^{-q}$$

then, at most $p$ and at least $q$ significant bits (i.e. significant figures written in base 2) are lost during subtraction.

# 4 Linear Systems

**Definition 4.1** (Systems of Linear Equations)**.** A system of linear equations (or a linear system) is a collection of one or more linear equations involving the same variables. If there are $m$ equations with $n$ unknown variables to solve for, i.e.

$$\begin{aligned} a_{1,1}x_1 + a_{1,2}x_2 + \ldots + a_{1,n}x_n &= b_1 \\ a_{2,1}x_1 + a_{2,2}x_2 + \cdots + a_{2,n}x_n &= b_2 \\ &\vdots \\ a_{m,1}x_1 + a_{m,2}x_2 + \cdots + a_{m,n}x_n &= b_m \end{aligned}$$

then the system of linear equations can be written in matrix form $A\boldsymbol{x} = \boldsymbol{b}$, where

$$A = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{pmatrix}, \quad x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad \text{and} \quad b = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix},$$

with $A \in \mathbb{R}^{m \times n}$, $\boldsymbol{x} \in \mathbb{R}^n$ and $\boldsymbol{b} \in \mathbb{R}^m$.

**Definition 4.2** (Banded Systems)**.** A **banded** matrix is a matrix whose non-zero entries are confined to a diagonal band, comprising the main diagonal and zero or more diagonals on either side.

**Definition 4.3** (Symmetric & Hermitian Systems)**.** A square matrix $A$ is **symmetric** if $A = A^T$, that is, $a_{i,j} = a_{j,i}$ for all indices $i$ and $j$.

A square matrix is said to be **Hermitian** if the matrix is equal to its conjugate transpose, i.e. $a_{i,j} = \overline{a_{j,i}}$ for all indices $i$ and $j$. A Hermitian matrix is written as $A^H$.

**Definition 4.4** (Positive Definite Matrices)**.** A matrix, $M$, is said to be **positive definite** if it is symmetric (or Hermitian) and all its eigenvalues are real and positive.

An equivalent definition is that for any non-zero real column vector $\boldsymbol{z}$, then $\boldsymbol{z}^T M \boldsymbol{z}$ is always positive.

**Definition 4.5** (Nonsingular Matrices)**.** A matrix is **non-singular** or **invertible** if there exists a matrix $A^{-1}$ such that $A^{-1}A = AA^{-1} = I$, where $I$ is the identity matrix.

**Remarks** (Properties of Nonsingular Matrices)**.** For a nonsingular matrix, the following all hold:

- Nonsingular matrix has full rank
- A square matrix is nonsingular if and only if the determinant of the matrix is non-zero.
- If a matrix is singular, both versions of Gaussian elimination (i.e. with and without pivoting) will fail due to division by zero, yielding a floating exception error.

**Definition 4.6** (The Residual)**.** If $\tilde{\boldsymbol{x}}$ is an approximate solution to the linear problem $A\boldsymbol{x} = \boldsymbol{b}$, then the **residual vector** is defined as $\boldsymbol{r} = A\tilde{\boldsymbol{x}} - \boldsymbol{b}$.

## 4.1 Direct Methods

**Algorithm** (Gaussian Elimination)**.**
Gaussian elimination is a method to solve systems of linear equations based on forward elimination (a series of row-wise operations) to convert the matrix, $A$, to upper triangular form (echelon form), and then back-substitution to solve the system. The row operations are:

- row swapping
- row scaling, i.e. multiplying by a non-zero scalar
- row addition, i.e. adding a multiple of one row to another

1: **procedure Forward Elimination**
2: **for** $k = 1$ to $n - 1$ **do**
3: **for** $i = k + 1$ to $n$ **do**
4: **for** $j = k$ to $n$ **do**
5: $a_{i,j} = a_{i,j} - \frac{a_{i,k}}{a_{k,k}} a_{k,j}$
6: **end for**
7: $b_i = b_i - \frac{a_{i,k}}{a_{k,k}} b_k$
8: **end for**
9: **end for**
10: **end procedure**
11: **procedure Back Substitution**
12: $x_n = \frac{b_n}{a_{n,n}}$
13: **for** $i = n - 1$ to $1$ **do**
14: $y = b_i$
15: **for** $j = n$ to $i + 1$ **do**
16: $y = y - a_{i,j} x_j$
17: **end for**
18: $x_i = \frac{y}{a_{i,i}}$
19: **end for**
20: **end procedure**

**Algorithm** (Gaussian Elimination with Scaled Partial Pivoting)**.** A pivot element is the element of a matrix which is selected first to do certain calculations. Pivoting helps reduce errors due to rounding during forward elimination.
To use partial pivoting to produce a matrix in row-echelon form

1: Find maximal absolute values vector $s$ with entries $s_i = \max j = 1, \ldots, n \, |a_{i,j}|$
2: **for** $k = 1$ to $n - 1$ **do**
3: **for** $i = k$ to $n$ **do**
4: Compute $\left| \frac{a_{i,k}}{s_i} \right|$
5: **end for**
6: Find row with largest relative pivot element, denote this as row $j$
7: Swap rows $k$ and $j$ in the matrix $A$
8: Swap entries $k$ and $j$ in the vector $s$
9: Do forward elimination on row $k$
10: **end for**

**Definition 4.7** (Upper and Lower Triangular Matrices)**.** A square matrix is said to be a **lower triangular matrix** if all the elements above the main diagonal are zero and an **upper triangular** if all the entries below the main diagonal are zero.

**Theorem 4 (**$LU$**-Decomposition).** Let $A \in \mathbb{R}^{n\times n}$ be invertible. Then there exists a decomposition of $A$ such that $A = LU$, where $L$ is a lower triangular matrix and $U$ is an upper triangular matrix, and

$$L = U_1^{-1}U_2^{-1}\cdots U_{n-1}^{-1}$$

where each matrix $U_i$ is a matrix which describes the $i^{\text{th}}$ step in forward elimination part of Gaussian elimination.
The upper triangular matrix $U$ is given by

$$U = U_{n-1}\cdots U_2U_1A.$$

**Definition 4.8** (Cholesky-Decomposition)**.** A symmetric, positive definite matrix can be decomposed as $A = \tilde{L}\tilde{L}^T$, where $\tilde{L} = LD^{1/2}$, where $D$ is a diagonal matrix whose elements $d_i$ are all positive, so that $D^{1/2}$ has elements $\sqrt{d_i}$.

**Algorithm** (Cholesky-Decomposition)**.** Given a matrix $A$, the lower triangular matrix $\tilde{L}$ can be constructed via

**for** $i$=1 to $n$ **do**
  **for** $j = 1$ to $i-1$ **do**
    $y = a_{i,j}$
    **for** $k = 1$ to $j$-1 **do**
      $y = y - l_{i,k}l_{j,k}$
    **end for**
    $l_{i,j} = y/l_{j,j}$
  **end for**
  $y = a_{i,i}$
  **for** $k$= 1 to $i-1$ **do**
    $y = y - l_{i,k}l_{i,k}$
  **end for**
  **if** $y \leq 0$ **then**
    there is no solution
  **else**
    $l_{i,i} = \sqrt{y}$
  **end if**
**end for**

## 4.2 Indirect Methods

For a non-singular matrix $A$, consider an iterative scheme of the form

$$Qx_{k+1} = (Q - A)\, x_k + b.$$

This is equivalent to

$$x_{k+1} = \left(I - Q^{-1}A\right) x_k + Q^{-1}b.$$

**Definition 4.9** (Convergent Methods)**.** A numerical method is said to be **convergent** if $x_k \to x^*$ as $k \to \infty$ where $x^*$ is the exact solution.

**Definition 4.10** (Spectral Radius of a Matrix)**.** The **spectral radius** of a square matrix $A$ is defined as

$$\rho(A) = \max\left\{|\lambda_1|, |\lambda_2|, \ldots |\lambda_n|\right\}$$

where the $\lambda_i$ are the eigenvalues of the matrix.

**Theorem 5 (Convergence).** The iterative scheme converges if and only if the spectral radius of the matrix $I - Q^{-1}A$ is less than one, i.e.

$$\rho\left(I - Q^{-1}A\right) < 1.$$

**Corollary 4.11.** A sequence of vectors $e_k = M^k e_0$ convergences to the zero vector if and only if the spectral radius of the matrix $M$ is less than one.

**Definition 4.12** (Order of Convergence)**.** If a sequence $x_n$ converges to $r$ as $n \to \infty$, then it is said to **converge linearly** if there exists a $\mu \in (0, 1)$ such that

$$\lim_{n\to\infty} \frac{|x_{n+1} - r|}{|x_n - r|} = \mu.$$

The sequences converges **super-linearly** if

$$\lim_{n\to\infty} \frac{|x_{n+1} - r|}{|x_n - r|} = 0$$

and **sub-linearly** if

$$\lim_{n\to\infty} \frac{|x_{n+1} - r|}{|x_n - r|} = 1.$$

More generally, a sequence converges with order $q$ if there exists a $\mu > 0$

such that

$$\lim_{n\to\infty} \frac{|x_{n+1} - r|}{|x_n - r|^q} = \mu.$$

Thus a sequence is said to converge quadratically when $q = 2$ and exhibit cubic convergence when $q = 3$.

**Definition 4.13** (Richardson Iteration)**.** Let $Q = I$. Then **Richardson iteration** computes the sequence of vectors

$$x_{k+1} = (I - A)\, x_k + b.$$

This may converge, depending on $A$.

The **modified Richardson iteration** scales $Q = \omega I$, so that

$$x_{k+1} = x_k + \omega\left(b - Ax_k\right).$$

**Definition 4.14** (Jacobi Iteration)**.** The **Jacobi iteration** has $Q = D$, where $D$ is the diagonal matrix of $A$, so

$$x_{k+1} = \left(I - D^{-1}A\right) x_k + D^{-1}b.$$

**Definition 4.15** (Diagonally Dominant Matrices)**.** A matrix $A \in \mathbb{R}^{n\times n}$ is said to be **diagonally dominant** if, for every row, the absolute value of the diagonal element is greater or equal to the sum of the magnitudes of all other elements, i.e.

$$|a_{i,i}| \geq \sum_{j=1, j\neq i}^{n} |a_{i,j}| \quad \text{for all } i \in (1, n).$$

**Theorem 6 (Convergence of Jacobi Scheme).** If a matrix $A$ is diagonally dominant, then the Jacobi scheme converges for any initial guess $x_0$.

**Definition 4.16** (Gauss-Seidel Scheme)**.** Let $Q = L + D$, where $L$ is the lower triangular matrix of $A$ and $D$ is the diagonal matrix of $A$, then the **Gauss-Seidel** scheme is given by

$$(D + L)x_{k+1} = -Ux_k + b.$$

**Theorem 7 (Convergence of Gauss-Seidel).** If a matrix $A$ is diagonally dominant, then the Gauss-Seidel scheme converges for any initial guess $x_0$.

**Definition 4.17** (Successive Over Relaxation)**.** The scheme uses $Q = L + \frac{1}{\omega}D$, where $L$ is the lower triangular matrix of $A$ and $D$ is the diagonal matrix of $A$, thus

$$(D + \omega L)x_{k+1} = -\left((\omega - 1)\, D + \omega U\right) x_k + \omega b.$$

**Theorem 8 (Convergence of Successive Over Relaxation).**
Let $A$ be a symmetric matrix with positive entries on the diagonal and let $\omega \in (0, 2)$. Then, if and only if $A$ is positive definite will the method of successive over relaxation converge.

## 4.3 Fundamental Theorem of Numerical Analysis

**Definition 4.18** (Stability)**.** A numerical method is said to be **stable** if and only if any initial error $e_0$ is damped during the iterations, i.e. $\|e_k\| < \|e_0\|$.

Note that $\|x\|$ is a *norm* of a vector, such as $\|x\|_2 = \sqrt{x_0^2 + x_1^2 + \ldots x_n^2}$.

**Definition 4.19** (Consistency)**.** A numerical method is said to be **consistent** if any fixed point $x^*$ of the iteration is a solution to the problem being solved.

For a linear system, a fixed point, $x^*$, fulfils

$$x^* = \left(I - Q^{-1}A\right) x^* + Q^{-1}b \Leftrightarrow Ax^* = b.$$

Thus, a fixed point of the iterative scheme is a solution of the linear system.

If the method is stable then

$$e_k = \left(I - Q^{-1}A\right)^k e_0,$$

so then $\left\|I - Q^{-1}A\right\| < 1$ for $\|e_k\| < \|e_0\|$. Note that $\left\|I - Q^{-1}A\right\|$ is the norm of a matrix, which is induced by a vector norm.

**Theorem 9 (Fundamental Theorem of Numerical Analysis).** A numerical method is convergent if and only if it is consistent and stable.

# 5 Nonlinear Solvers

## 5.1 Bisection Method

**Definition 5.1** (Bisection Method)**.**
The bisection method, when applied in the interval $[a, b]$ to a function $f \in C^0([a, b])$ with $f(a)f(b) < 0$

Bisect the interval into two subintervals $[a, c]$ and $[c, b]$ such that $a < c < b$.

- If $f(c) = 0$ or is sufficiently close, then $c$ is a root,
- else, if $f(c)f(a) < 0$ continue in the interval $[a, c]$,
- else, if $f(c)f(b) < 0$ continue in the interval $[c, b]$.

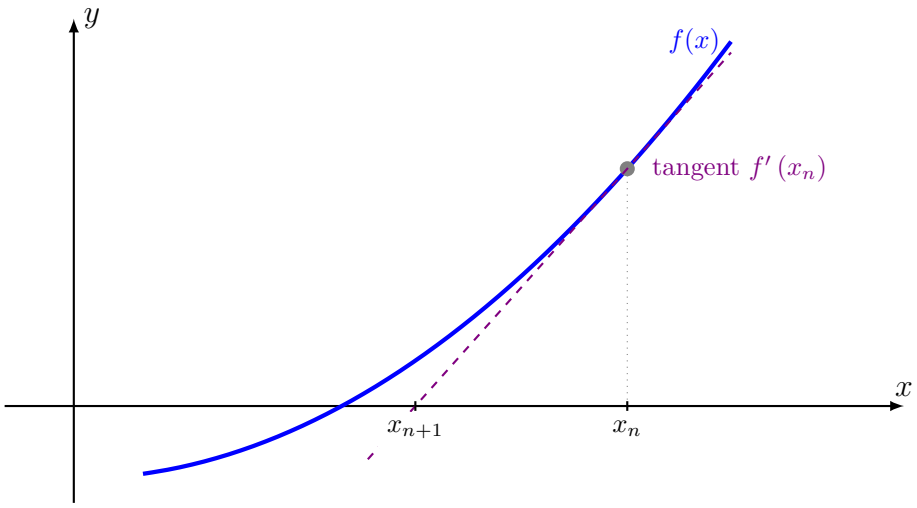
**Theorem 10.**
The bisection method, when applied in the interval $[a, b]$ to a function $f \in C^0([a, b])$ with $f(a)f(b) < 0$ will compute, after $n$ steps, an approximation $c_n$ of the root $r$ with error

$$|r - c_n| < \frac{b - a}{2n}.$$

## 5.2 Newton's Method

**Definition 5.2** (Newton's Method)**.**
Let a function $f \in C^1([a, b])$, then for an initial guess $x_0$, Newton's method is

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




**Theorem 11.**
When Newton's method converges, it converges to a root, $r$, of $f(x)$, i.e. $f(r) = 0$.

**Theorem 12.**
Let $f \in C^1([a,b])$, with

1. $f(a)f(b) < 0$,
2. $f'(x) \neq 0$ for all $x \in (a,b)$,
3. $f''(x)$ exists, is continuous and either $f''(x) > 0$ or $f''(x) < 0$ for all $x \in (a,b)$.

Then $f(x) = 0$ has exactly one root, $r$, in the interval $(a,b)$ and the sequence generated by Newton iterations converges to the root when the initial guess is chosen according to

- if $f(a) < 0$ and $f''(a) < 0$ or $f(a) > 0$ and $f''(a) > 0$ then $x \in [a,r]$

or

- if $f(a) < 0$ and $f''(a) > 0$ or $f(a) > 0$ and $f''(a) < 0$ then $x \in [r,b]$.

The iterates in the sequence will satisfy

$$|x_n - r| < \frac{f(x_n)}{\min\limits_{x\in[a,b]} |f'(x)|}.$$

**Theorem 13.**
Let $f \in C^1([a,b])$, with

1. $f(a)f(b) < 0$,
2. $f'(x) \neq 0$ for all $x \in (a,b)$,
3. $f''(x)$ exists and is continuous, i.e. $f(x) \in C^2([a,b])$.

If $x_0$ is close enough to the root $r$, then Newton's method converges quadratically.

## 5.3 Secant Method

**Definition 5.3** (Secant Method)**.**
The secant method is defined as

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

where the derivative of $f$ is approximated via a Taylor expansion.

**Theorem 14.**
Let $f \in C^2([a,b])$, and $r \in (a,b)$ such that $f(r) = 0$ and $f'(r) \neq 0$. Furthermore, let

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

then there exists a $\delta > 0$ such that when $|r - x_0| < \delta$ and $|r - x_1| < \delta$, then the following holds:

1. $\lim_{n\to\infty} |r - x_n| = 0 \Leftrightarrow \lim_{n\to\infty} x_n = r$,
2. $|r - x_{n+1}| \leq \mu |r - x_n|^\alpha$ with $\alpha = \dfrac{1+\sqrt{5}}{2}$.

The properties of the three nonlinear solvers can be summarised as follows:

| Method | Regularity | Proximity to $r$ | Init. points | Func. calls | Convergence |
|---|---|---|---|---|---|
| Bisection | $\mathcal{C}^0$ | No | 2 | 1 | Linear |
| Newton | $\mathcal{C}^2$ | Yes | 1 | 2 | Quadratic |
| Secant | $\mathcal{C}^2$ | Yes | 2 | 1 | Superlinear |

## 5.4 Systems of Nonlinear Equation

**Definition 5.4** (Multi-Dimensional Newton Method)**.** For a vector-valued function $f : \mathbb{R}^n \to \mathbb{R}^n$, which takes as an argument the vector

$$x = (x_1, x_2 \dots x_n) \in \mathbb{R}^n,$$

the **Jacobian** matrix is defined as

$$J = \begin{pmatrix} \dfrac{\partial f_1}{\partial x_1} & \dfrac{\partial f_1}{\partial x_2} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \dfrac{\partial f_2}{\partial x_1} & & & \vdots \\ \vdots & & & \vdots \\ \dfrac{\partial f_n}{\partial x_1} & \dfrac{\partial f_n}{\partial x_2} & \cdots & \dfrac{\partial f_n}{\partial x_n} \end{pmatrix} \in \mathbb{R}^{n \times n}$$

where $f_1$ is the first component of the vector-valued function $f$.

If the derivatives are evaluated at the vector $x$, the Jacobian matrix can be parameterised as $J(x)$. Newton's method can then be written as a vector equation,

$$x_{m+1} = x_m - J^{-1}(x_m) f(x_m)$$

where $J^{-1}(x_m)$ is the inverse of the Jacobian matrix evaluated at the $m$-iterate of the approximation vector which is denoted by $x_m$.

In practice, as matrix inversion can be computationally expensive, the system

$$J(x_m)(x_{m+1} - x_m) = -f(x_m)$$

is solved for the unknown vector $x_{m+1} - x_m$, and then $x_{m+1}$ is found.

# 6 Interpolation

**Definition 6.1** (Interpolating Functions)**.** Given a set of points $p_0, \ldots, p_n$ and corresponding nodes $u_0, \ldots, u_n$, a function $f : \mathbb{R} \to \mathbb{R}$ with $f(u_i) = p_i$, i.e. maps the nodes to the points, is an called an **interpolating function**.

**Definition 6.2** (Collocation)**.** If the interpolating function is a polynomial, it can be written as

$$p(u) = \sum_{i=0}^{n} \alpha_i \varphi_i(u)$$

where $\varphi_i(u)$ are polynomials. Thus for every nodal value $j$, the polynomial exactly satisfies

$$p(u_j) = \sum_{i=0}^{n} \alpha_i \varphi_i(u_j),$$

for the weights $\alpha_i$. Thus, solving for all the values of $\alpha$ which fit the interpolating function to the data leads to a linear system of the form

$$\Phi\alpha = p$$

where $p$ is the vector defined the polynomial evaluated at the node points, i.e. $p = p(u_j)$ and $\Phi$ is the **collocation matrix**. If there are $n$ data points, the collocation matrix is given by

$$\Phi = \begin{pmatrix} \varphi_0(u_0) & \varphi_1(u_0) & \cdots & \varphi_n(u_0) \\ \vdots & & & \vdots \\ \varphi_0(u_n) & \cdots & \cdots & \varphi_n(u_n) \end{pmatrix}.$$

Thus the weights which define the interpolating polynomial are found as $\alpha = \Phi^{-1}p$.

The collocation matrix is invertible if and only if the set of functions $\varphi$ are linearly independent.

When the polynomials are given by $\varphi_i(u) = u^i$, then $\Phi$ is called the **Vandermonde matrix**.

**Definition 6.3** (Lagrange Polynomials)**.** The **Lagrange form of an interpolating polynomial** is given by

$$p(x) = \sum_{i=0}^{n} \alpha_i l_i(x)$$

where $l_i \in \mathbb{P}_n$ are such that $l_i(x_j) = \delta_{ij}$. The polynomials $l_i(x) \in \mathbb{P}_n$ for

$i = 0, \ldots, n$, are called **characteristic polynomials** and are given by

$$l_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}.$$

**Definition 6.4** (Newton Interpolation)**.** Newton interpolation interpolates a set of points $(x_i, y_i)$ as

$$p(x) = \sum_{i=0}^{n} \alpha_i n_i(x)$$

using a linear combination of Newton basis polynomials, which are defined as

$$\begin{aligned} n_0(x) = 1, \quad n_i(x) &= (x - x_0)(x - x_1)\cdots(x - x_{i-1}) \\ &= \prod_{j=0}^{j-1} (x - x_j). \end{aligned}$$

By construction, $\alpha_0 = y_0$, and subsequent terms must be solved by evaluating the interpolating polynomial at increasing orders, leading to the formula

$$\alpha_{i+1} = \frac{y_{i+1} - p_i(x_{i+1})}{n_i(x_{i+1})}.$$

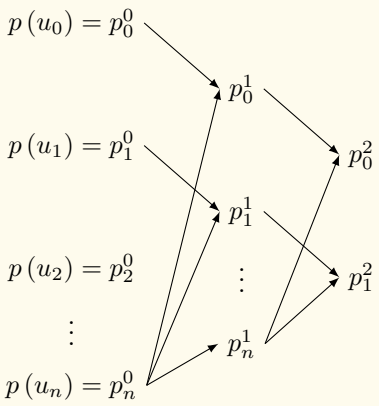
**Algorithm** (Aitken's Algorithm)**.**
**Aitken's algorithm** is an iterative process for evaluating Lagrange interpolation polynomials at an arbitrary point, $u^*$, without explicitly constructing them. If the interpolating polynomial is given by $p$, and is derived from $n$ data points $(u_i, y_i)$ for $i = 0, \ldots, n$

$$p(u) = \sum_{i=0}^{n} p_i^n l_i^n(u).$$

The interpolation is achieved by constructing a series of polynomials, evaluated at the $u = u^*$, where $p_i^k(u)$ is given by

$$p_i^{k+1}(u) = p_i^k(u)\left(\frac{u - u_{n-k}}{u_i - u_{n-k}}\right) + p_{n-k}^k(u)\left(1 - \frac{u - u_{n-k}}{u_i - u_{n-k}}\right)$$

with initial values $p_i^0 = y_i$, i.e.




where the coefficients are evaluated from left to right, until $p_0^n$ is evaluated.

## 6.1 Piecewise Polynomial Interpolation

**Definition 6.5** (Spline Functions)**.** A function $s(u)$ is called a **spline** of degree $k$ on the domain $[a,b]$ if $s \in C^{k-1}([a,b])$ and there exists nodes $a = u_0 < u_1 < \ldots < u_m = b$ such that $s$ is a polynomial of degree $k$ for $i = 0, \ldots m-1$.

**Definition 6.6** (B-Splines)**.** A spline is said to be a **b-spline** if it is of the form

$$s(u) = \sum_{i=0}^{m} \alpha_i \mathcal{N}_i^n(u)$$

where $\mathcal{N}^n$ are the **basis spline functions** of degree $n$ with minimal support. (That is they are positive in the domain and zero outside). The functions are defined recursively. Let $u_i$ be the set of nodes $u_0, u_1, \ldots, u_m$, then

$$\mathcal{N}_i^0(u) = \begin{cases} 1 & \text{for} \quad u_i \le u \le u_{i+1} \\ 0 & \text{else.} \end{cases}$$

and

$$\mathcal{N}_i^n(u) = \alpha_i^{n-1}(u)\mathcal{N}_i^{n-1}(u) + \left(1 - \alpha_{i+1}^{n-1}(u)\right)\mathcal{N}_{i+1}^{n-1}(u)$$

where

$$\alpha_i^{n-1}(u) = \frac{u - u_i}{u_{i+n} - u_i}$$

is a local parameter.

Given data with nodes $u_i$ and values $p_i$, to interpolate with splines, of order $n$, requires solving

$$\text{Find} \quad s = \sum_{i=0}^{m} \alpha_i \mathcal{N}_i^n(u) \quad \text{such that} \quad s(u_i) = p_i \quad \text{for} \quad i = 0, \ldots, m$$

which is matrix form is $\Phi\alpha = p$, where the collocation matrix, $\Phi \in \mathbb{R}^{(m+1)\times(m+1)}$ is given by

$$\Phi = \begin{pmatrix} \mathcal{N}_0^n(u_0) & \cdots & \mathcal{N}_m^n(u_0) \\ \vdots & & \vdots \\ \mathcal{N}_0^n(u_m) & \cdots & \mathcal{N}_m^n(u_m) \end{pmatrix}.$$

## 6.2 Least-Squares Approximation

**Definition 6.7** (Least-Squares Approximation)**.** Given a set of points $y = (y_0, y_1, \ldots y_n)$ at nodes $x_i$, seek a continuous function of $x$, with a given form characterized by $m$ parameters $\beta = (\beta_0, \beta_1, \ldots, \beta_m)$, i.e. $f(x, \beta)$, which approximates the points while minimizing the error, defined by the sum of the squares

$$E = \sum_{i=0}^{n} (y - f(x_i, \beta))^2.$$

The minimum is found when

$$\frac{\partial E}{\partial \beta_j} = 0 \quad \text{for all} \quad j = 1, \ldots m$$

i.e.

$$-2\sum_{i=0}^{n} (y_i - f(x_i, \beta_j)) \frac{\partial f(x_i, \beta)}{\partial \beta_j} = 0 \quad \text{for all} \quad j = 1, \ldots m.$$

**Definition 6.8** (Linear Least-Squares Approximation)**.** If the function $f$ is a function of the form

$$y = \sum_{j=1}^{m} \beta_j \varphi_j(x)$$

then the least squares problem can be expressed as

$$\frac{\partial E}{\partial \beta_j} = \sum_{j=1}^{m} \left( \sum_{i=1}^{n} \varphi_j(x_i) \varphi_k(x_i) \right).$$

Thus, the weights $\beta$ can be determined by solving the linear system,

$$\Phi\Phi^T \beta = \Phi y,$$

i.e. $\beta = \left(\Phi\Phi^T\right)^{-1} \Phi y$, where $\Phi$ is the collocation matrix.

# 7 Numerical Differentiation

**Definition 7.1** (Finite-Difference Quotients)**.** Consider the approximations to the first-order derivative:

1. **Forward Difference Quotient:**

$$D_j^+ u = \frac{u_{j+1} - u_j}{h}$$

2. **Backwards Difference Quotient:**

$$D_j^- u = \frac{u_j - u_{j-1}}{h}$$

3. **Central Difference Quotient:**

$$D_j^0 u = \frac{u_{j+1} - u_{j-1}}{2h}$$

The forward and backwards difference schemes are first order approximations to the derivative. The central difference scheme is a second order accurate approximation.

**Definition 7.2** (Richardson Extrapolation)**.** This is a method for deriving higher order approximations for derivatives from lower order approximations. Consider a first-order approximation to the derivative, $\varphi(h)$, such as backwards or forwards differencing, then

$$f'(x) = \varphi(h) + a_2 h^2 + a_3 h^3 + \dots$$

Now evaluate the derivative at $h = h/2$, so that

$$f'(x) = \varphi\left(\frac{h}{2}\right) + a_2\left(\frac{h}{2}\right)^2 + a_3\left(\frac{h}{2}\right)^3 + \dots$$

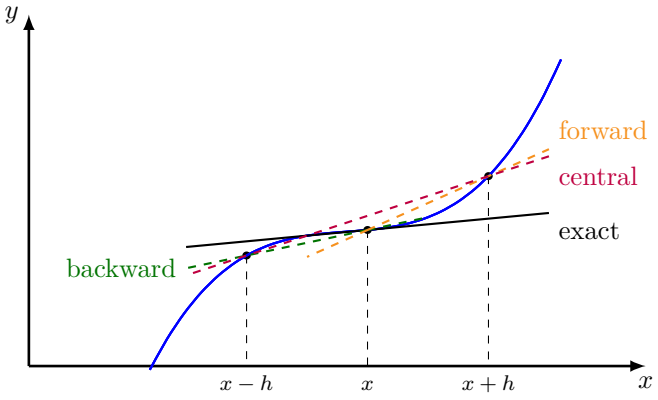
Combining the two terms so that the low order term cancel, i.e. via $f'(x) - 4f'(x)$, then a better approximation can be found as

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

The process can also be applied to second order accurate schemes, such as central differencing, to produce more accurate approximations, as well as to higher order derivatives.

**Definition 7.3** (Higher Order Derivatives)**.** From the Taylor expansion of $f(x+h)$ and $f(x-h)$, the second order derivative can be expressed as

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



# 8 Numerical Integration

**Definition 8.1** (Riemann Sum)**.** Create a partition, $p$, of the domain of integration: define $n+1$ nodes $a = x_0 < x_1 < \ldots < x_n = b$, so that there are $n$ sub-intervals $[x_i, x_{i+1}]$. Then approximate the area under the curve by summing the areas in each subinterval defined as

$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_{i=0}^{n-1} (x_{i+1} - x_i)\, f(x^*)\,, \quad x^* \in [x_i, x_{i+1}]\,.$$

If $f$ is continuous, the value of $x_i^*$ may be chosen arbitrarily in the interval $[x_i, x_{i+1}]$. Then the **lower** and **upper Riemann sums** are given by

$$L(f,p) = \sum_{i=0}^{n-1} (x_{i+1} - x_i)\, m_i \quad \text{where} \quad m_i = \min_{x \in [x_i, x_{i+1}]} f(x)$$
$$U(f,p) = \sum_{i=0}^{n-1} (x_{i+1} - x_i)\, M_i \quad \text{where} \quad M_i = \max_{x \in [x_i, x_{i+1}]} f(x)$$

so that bounds for the value of the quadrature can be made

$$L(f,p) \le \int_a^b f(x)\ \mathrm{d}x \le U(f,p)\,.$$

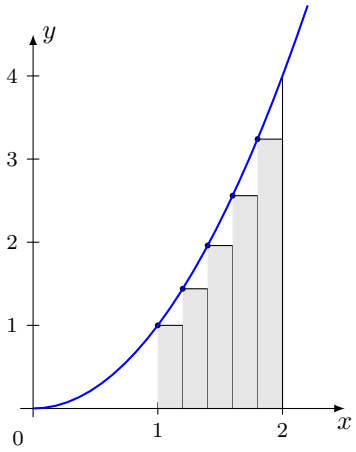
Additionally, the **left** and **right Riemann sums** are given by

$$\sum_{i=0}^{n-1} (x_{i+1} - x_i)\, f(x_{i-1})\,,$$
$$\sum_{i=0}^{n-1} (x_{i+1} - x_i)\, f(x_i)\,.$$

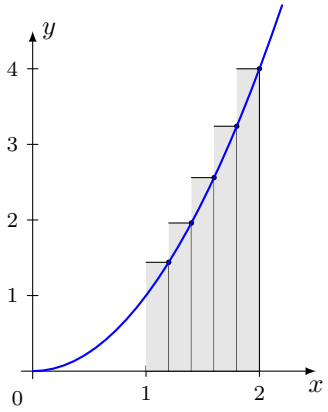
**Definition 8.2** (Trapezoidal Rule)**.** Rather than rectangles, use trapezoids to approximate the integral in a sub domain

$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_{i=0}^{n-1} (x_{i+1} - x_i)\, \frac{f(x_i) + f(x_{i+1})}{2}.$$

If the nodes of the partition are equally spaced, so that $h = x_{i+1} - x_i$, then




(a) Lower Riemann Sum




(b) Upper Riemann Sum

the formula can be given by

$$T(f,p) = \frac{h}{2}\left(f\left(x_0\right) + f\left(x_n\right)\right) + h\sum_{i=1}^{n-2} f\left(x_i\right).$$

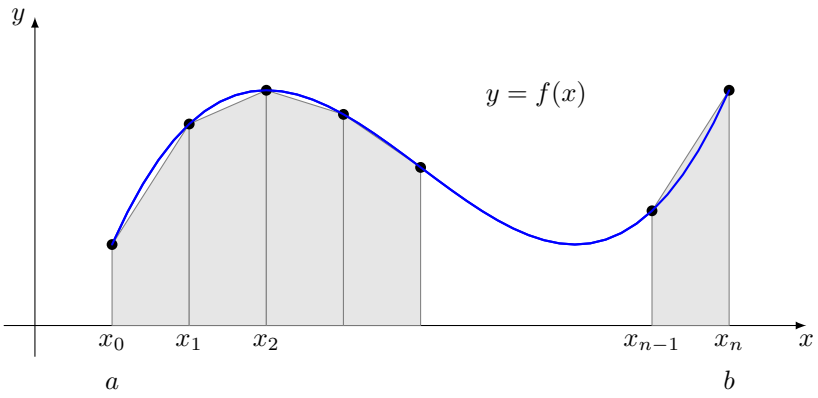
**Theorem 15 (Error for Trapezoidal Rule).** Let $f \in C^2\left([a,b]\right)$ and $p$ be equidistant partition of $[a,b]$, with $h = x_{i+1} - x_i$. The error can be shown to have the form:

$$\left|\int_a^b f\left(x\right)\,\mathrm{d}x - T\left(f,p\right)\right| = a_2h^2 + a_4h^4 + \dots$$

that is, the error terms are even powers of the discretization. The error for the trapezium rule is

$$\left|\int_a^b f\left(x\right)\,\mathrm{d}x - T\left(f,p\right)\right| = \frac{1}{12}\left|\left(b-a\right)h^2 f''\left(\xi\right)\right|$$

for a $\xi \in (a,b)$.



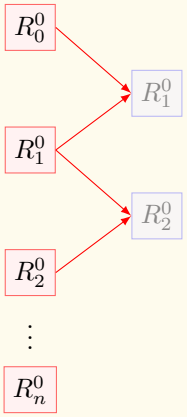

**Definition 8.3** (Simpson's Rule)**.** The integral is approximated as

$$\int_a^b f(x)\,\mathrm{d}x \approx \frac{b-a}{6}\left(f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right).$$

Simpson's rule uses interpolation with quadratic polynomials. It can be applied in a composite manner, i.e. on many subdomains. It has an asymptotic error of $\mathcal{O}\left(h^4\right)$.

**Algorithm** (Romberg Algorithm)**.** Romberg's method uses the Trapezoidal Rule and then Richardson Extrapolation to estimate integrals.

First consider a sequence of partitions, $p_i$, of equal spacing given by $h_i = \dfrac{b-a}{2^i}$ for $i = 0, \ldots, n$, which yield a sequence of integrals $R_i^0 = T_i\left(f, p_i\right)$. Refinements of the integrals can then be produced by Richardson Extrapolation.




Thus, consider the two integrals

$$\int_a^b f(x)\,\mathrm{d}x = R_{i-1}^0 + a_2 h^2 + a_4 h^4 + \dots$$

$$\int_a^b f(x)\,\mathrm{d}x = R_i^0 + a_2 \left(\frac{h}{2}\right)^2 + a_4 \left(\frac{h}{2}\right)^4 + \dots$$

Note that there no odd terms in the error. Then, define the next set of refinements as

$$R_i^1 = \frac{1}{3}\left(4R_i^0 - R_{i-1}^0\right).$$

which has an error $\mathcal{O}\left(h^4\right)$. The extrapolated values are equivalent to integrals approximated by Simpson's rule. The recurrence formula can be derived

$$R_i^m = \frac{1}{4^m - 1}\left(4^m R_i^{m-1} - R_{i-1}^{m-1}\right).$$

## 8.1 Gauss Quadrature

Generalise the quadrature formula so that an integral is approximated as

$$I_n[f] = \sum_{i=0}^{n} \alpha_i f(x_i)$$

The above equation is a weighted sum of the values of $f$ at the points $x_i$, for $i = 0, \dots, n$. These points are said to be the *nodes* of the quadrature formula, while the $\alpha_i \in \mathbb{R}$ are its *coefficients* or *weights*. Both weights and nodes depend in general on $n$.

- Can the weights be chosen such that the error in an integral is minimized?

- Furthermore, can the nodes be chosen such that the integral can be improved?

**Definition 8.4** (Orthogonal functions)**.** Two real-valued functions $f(x)$ and $g(x)$ are said to be **orthogonal** if

$$\langle f, g \rangle = \int_a^b f(x)g(x)\,\mathrm{d}x = 0.$$

**Theorem 16 (Gaussian Quadrature).** Let $q(x)$ be a non-trivial polynomial of degree $n+1$ such that

1. it has $n+1$ distinct roots, denoted as $x_i$, in $[a, b]$,
2. the polynomial satisfies

$$\int_a^b x^k q(x)\,\mathrm{d}x = 0 \quad \text{for} \quad k = 0, \ldots, n.$$

   i.e. is orthogonal to $x^k$.

Then, denote the integral as

$$I[f] = \int_a^b f(x)\,\mathrm{d}x = \sum_{i=0}^{n} A_i f(x_i)$$

with $A_i = \int_a^b L_i(x)\,\mathrm{d}x$ for all polynomials $f(x)$ of degree less than or equal to $2n+1$. The integral $I[f]$ integrates all polynomials of degree $2n+1$ *exactly.*
The degree of exactness of $I[f]$ is $2n+1$.

**Definition 8.5** (Gauss-Legendre Quadrature)**.** The Legendre polynomials are a set of orthogonal polynomials where

$$\int_{-1}^{1} P_m(x)P_n(x)\,\mathrm{d}x = 0 \quad \text{for} \quad n \neq m.$$

and $P_0 = 1$. Thus, $P_1 = x$, $P_2 = \left(3x^2 - 1\right)/2$ etc. The Legendre polynomials obey a recursive formula:

$$P_n = \frac{2n-1}{n} x P_{n-1}(x) - \frac{n-1}{n} P_{n-2}(x), \quad \text{for} \quad n \geq 2.$$

Gauss-Legendre quadrature uses the roots of the Legendre polynomials as the nodes for integration, and weights found by equating the quadrature expressions with the exact integrals for $f = 1, x, x^2$.

The domain of integration can be scaled via the invertible transformation $x = \dfrac{b-a}{2}t + \dfrac{a+b}{2}$, so that

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

# 9 Differential Equations

## 9.1 Finite Difference Methods for Differential Equations

Solutions to differential equations are functions.

**Definition 9.1** (Ordinary Differential Equations)**.** An **ordinary differential equation** (ODE) is an equation that involves one of more derivatives of a function of a single variable.

For example, with only the first derivative $y'(t) = f(y(t), t)$.

**Definition 9.2** (Initial Value Problems)**.** An **initial value problem** (IVP) is given by an ordinary differential equation of the form $y'(t) = f(y(t), t)$ and initial value $y(a) = y_a$ for the unknown function $y(t)$, with $t \geq a$.

Often $a = 0$, and the initial condition is denoted by $y(0) = y_0$.

**Definition 9.3** (One-step methods)**.** A numerical method for approximating the solution to a differential equation is called a **one-step method** if the solution at time step $t_{n+1}$, denoted by $u_{n+1}$, depends only on the previous one, $t_n$, where $t_{n+1} = t_n + h$, for some small increment $h = \Delta t$.

**Definition 9.4** (Forward Euler)**.** This approximates the derivative through a first-order forward difference approximation of the first-order derivative, i.e. for $u_n$, the solution $u$ at $t_n$, the computed solution to a differential equation $\dot{u} = f(u)$, evolves according to

$$u_{n+1} = u_n + hf_n$$

where $f_n = f(u_n, t_n)$ and $h = t_{n+1} - t_n$. The error is $\mathcal{O}\left(h^2\right)$.

**Definition 9.5** (Backward Euler Method)**.** This method uses the backward finite difference approximation of the first-order derivative, so that the solution is computed via

$$u_{n+1} = u_n + hf_{n+1}$$

where $f_{n+1} = f(u_{n+1}, t_{n+1})$.

**Definition 9.6** (Crank-Nicolson Method)**.** This method is given by

$$u_{n+1} = u_n + \frac{h}{2}\left(f_n + f_{n+1}\right).$$

**Definition 9.7** (Heun's Method)**.** This method is given by

$$u_{n+1} = u_n + \frac{h}{2}\left(f_n + f\left(u_n + hf_n, t_{n+1}\right)\right).$$

Alternatively, one-step methods can be considered to be integrators

$$y\left(t+h\right) = y\left(t\right) + \int_t^{t+h} f\left(y\left(\tau\right), \tau\right)\, \mathrm{d}\tau.$$

Thus, the forward Euler method is equivalent to the left Riemann sum, backward Euler is equivalent to the right right Riemann sum and the Crank-Nicolson is the trapezoidal rule.

**Definition 9.8** (Implicit and Explicit Schemes)**.** A numerical method is said to be **explicit** if an approximation $u_{n+1}$ can be calculated directly from already computed values $u_i$, $i < n$. Otherwise, the method is said to be **implicit**.

Often, implicit methods require, at each step, the solution of a nonlinear equation for computing $u_{n+1}$.

Both the Forward Euler and Heun's method are explicit, whereas the Backward Euler and Crank-Nicolson methods are implicit.

Huen's method can be interpreted as the Crank-Nicolson method with the approximation $u_{n+1} \approx u_n + hf_n$ replacing the explicit $f_{n+1}$ term, which depends on $u_{n+1}$.

## 9.2 Analysis of One-Step Methods

Any explicit one-step method has the form

$$u_{n+1} = u_n + h\Phi\left(t_n, u_n, f_n, h\right)$$

with $\Phi$ the increment function.

**Definition 9.9** (Hölder & Lipshitz Continuity)**.** A function $f$ is **Hölder continuous** if there exists real constants $C > 0$ and $\alpha \leq 0$ such that

$$|f\left(x\right) - f\left(y\right)| \leq C\|x - y\|^{\alpha}$$

for all $x$ and $y$. If $\alpha = 1$ the function is said to be **Lipshitz continuous**.

**Definition 9.10** (Consistent Schemes)**.** For the exact solution to the differential equation, $y\left(t_n\right) = y_n$, the solution can be written as

$$y_{n+1} = y_n + h\Phi\left(t_n, y(t_n), f_n, h\right) + \varepsilon_n$$

so that

$$\tau_n = \frac{y_{n+1} - y_n}{h} - \Phi\left(t_n, y(t_n), f_n, h\right)$$

where $\varepsilon_n = h\tau_n$ for a $\tau_n = \tau_n(h)$ is defined as the **local truncation error** at step $n$.

The **consistency error** is given by $\tau = \max_n |\tau_n|$.

A method is said to be **consistent** if

$$\lim_{h \to 0} \Phi = f.$$

This means the increment function is a good approximation to the differential equation as the step size tends to zero.

**Definition 9.11** (Order)**.** A one-step method is of order $p \in \mathbb{N}$, if for all $t \in [0, T]$, the solution satisfies the condition that $\tau(h) = \mathcal{O}(h^p)$ as $h \to 0$.

**Definition 9.12** (Zero Stable Methods)**.** A method of the form

$$u_{n+1} = u_n + h\Phi\left(t_n, u_n, f_n, h\right)$$

is called **zero-stable** if there exists both a maximal step size, $h_{\max}$ and a constant, $C$, such that for all $h \in [0, h_{\max}]$ and for $\varepsilon > 0$, then the following holds:
If, for all time-steps $0 \leq n \leq N$, there exists a $\delta_n \leq \varepsilon$ and

$$z_{n+1} = z_n + h\Phi\left(t_n, z_n, f_n\left(z_n, t_n\right), h\right) + \delta_{n+1}$$

and $z_0 = y_0 + \delta_0$, then

$$|z_n - u_n| \leq C\varepsilon \quad \text{for} \quad 0 \leq n \leq N.$$

Zero stability means that small perturbations in the computations lead to small perturbations in the approximations.

**Theorem 17.** If the increment function is Lipshitz continuous for $y_n$ for any $h$ and $t_n$, then the one-step method is zero-stable.

**Theorem 18.** If the increment function $\Phi$ is

(i) Lipshitz continuous for $u_n$ for any $h$ and $t_{n+1}$

and

(ii) the method is consistent

then

$$\lim_{h\to 0} |y_n - u_n| = 0.$$

Also, if the method is of order $p$ and if $|y_0 - u_0| = \mathcal{O}(h^p)$ as $h \to 0$, the convergence is of order $p$.

**Definition 9.13** (Absolute Stability)**.** A numerical scheme for approximating the solution to the linear differential equation $y'(t) = \lambda y(t)$ with $\lambda \in \mathbb{C}$ and initial condition $y_0 = 1$ is said to be **absolutely stable** if $|u_n| \to 0$ as $n \to \infty$, when $\mathrm{Re}(\lambda) < 0$, for a fixed value of $h$.

**Definition 9.14** (Well-posed)**.** A differential equation is said to be **well-posed** if

- a unique solution exists for any initial conditions and
- the solution's behaviour changes continuously with the initial conditions.

A differential equation which does not have these properties is said to be **ill-posed**.

**Theorem 19 (Lax Equivalence theorem).** The Lax Equivalence theorem or Lax–Richtmyer theorem is the equivalent form of the Fundamental Theorem of Numerical Analysis for differential equations, which states that for a *consistent* finite difference method for a well-posed linear initial value problem, the method is *convergent* if and only if it is *stable*.

**Runge-Kutta Schemes And Multi-Step Schemes**

**Definition 9.15** (Runge-Kutta Methods)**.** If an ordinary differential equation is given by $\dot{y} = f(y, t)$, then a Runge-Kutta scheme takes the form

$$u_{n+1} = u_n + hF(t_n, u_n, h; f)$$

where $F$ is an increment function given by

$$F(t_n, u_n, h; f) = \sum_{i=1}^{s} b_i k_i,$$

with $k_i$ defined as

$$k_i = f\left(u_n + h\sum_{j=1}^{s} a_{i,j}k_j, t_n + c_i h\right) \quad \text{for} \quad i = 1, \ldots, s$$

where $s$ is referred to as the number of stages of the method.

Thus, an $s$-stage scheme is characterised by coefficients $b_i$, $c_i$ and $a_{i,j}$. If the matrix defined by the elements $a_{i,j}$ is lower triangular, i.e. $a_{i,j} = 0$ for all $i \leq j$, then each $k_i$ can be computed explicitly in terms of the previous coefficients $k_1, \ldots, k_{i-1}$. Thus, such schemes are called **explicit**, otherwise they are said to be **implicit**.

The **local truncation error** is defined as

$$h\tau_{n+1}(h) = u(t_{n+1}) - u(t_n) - hF(t_n, u_n, h; f).$$

It can be shown that $\tau(h) = \max|\tau_{n+1}(h)| \to 0$ as $h \to 0$ if and only if $\sum_{i=1}^{s} b_i = 1$.

A Runge-Kutta method is of order $p \geq 1$ if $\tau(h) = \mathcal{O}(h^p)$ as $h \to 0$.

The components of a Runge-Kutta scheme are expressed in a **Butcher array**

$$\begin{array}{c|ccc} c_1 & a_{1,1} & \ldots & a_{1,s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s,1} & \ldots & a_{s,s} \\ \hline & b_1 & \ldots & b_s \end{array}$$

The order of an $s$-stage explicit Runge-Kutta method cannot be greater than $s$. Additionally, there does not exist a $s$-stage explicit Runge-Kutta method with order $s$ if $s \geq 5$.

The order of an $s$-stage implicit Runge-Kutta method cannot be greater than $2s$.

The most common form of the Runge-Kutta method is the fourth order Runge-Kutta method (RK4). It takes the form:

$$u_{n+1} = u_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

where

$$\begin{aligned} k_1 &= f(u_n, t_n), \\ k_2 &= f\left(u_n + \frac{h}{2}k_1, t_n + \frac{h}{2}\right), \\ k_3 &= f\left(u_n + \frac{h}{2}k_2, t_n + \frac{h}{2}\right), \\ k_4 &= f(u_n + hk_3, t_n + h). \end{aligned}$$

## 9.3 Partial Differential Equations

**Definition 9.16** (Partial Differential Equations)**.** A partial differential equation is a relation involving an unknown function of several free variables and partial derivatives with respect to these variables.

A partial differential equation is said to be linear if it only contains linear terms of the unknown and its derivatives. For example, a second-order linear partial differential equation for an unknown function $u(x,t)$ has the form

$$a_1 u_{xx} + a_2 u_{xt} + a_3 u_{tt} + a_3 u_x + a_4 u_t + a_5 u = f(x,t).$$

where $u_{xx} = \dfrac{\partial^2 u}{\partial x^2}$.

For finite-difference schemes, all partial derivatives must be approximated by discretized operators.