

## JTMS-MAT-13: Numerical Methods

Summary from 17 April 2024

Notes for numerical methods course 2024. This can be downloaded from:  
<https://djps.github.io/courses/numericalmethods24/notes>

Note that proofs for theorems marked with \* were presented in class.

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## Recommended Reading

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

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

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

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

## 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 error 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.  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , 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  $\tilde{x}_i$ , thus  $|\Delta y_i| = |\tilde{y}_i - y_i| = |f(\tilde{x}_i) - f(x_i)|$ .

### 3 Number Representations

**Definition 3.1** (Base Representation).

Let  $b \in \mathbb{N} \setminus \{1\}$ . Every number  $x \in \mathbb{N}_0$  can be written as a unique expansion with respect to base  $b$  as

$$(x)_b = a_0b^0 + a_1b^1 + \dots + a_nb^n = \sum_{i=0}^n a_ib^i$$

A number can be written in a nested form:

$$\begin{aligned} (x)_b &= a_0b^0 + a_1b^1 + \dots + a_nb^n \\ &= a_0 + b(a_1 + b(a_2 + b(a_3 + \dots + ba_n) \dots)) \end{aligned}$$

with  $a_i < \mathbb{N}_0$  and  $a_i < b$ , i.e.  $a_i \in \{0, \dots, b-1\}$ .

For a real number,  $x \in \mathbb{R}$ , write

$$\begin{aligned} x &= \sum_{i=0}^n a_ib^i + \sum_{i=1}^{\infty} \alpha_ib^{-i} \\ &= a_n \dots a_0 \cdot \alpha_1 \alpha_2 \dots \end{aligned}$$

**Algorithm** (Euclid).

Euclid's algorithm can convert number  $x$  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  $i = n, \dots, 0$

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

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

4. Output as  $(x)_b = a_na_{n-1} \dots a_0$

**Algorithm** (Horner).

1. Input  $(x)_{10}$
2. Set  $i = 0$

3. Let  $y = x$ . Then while  $y > 0$

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

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

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

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.

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

then the system of linear equations can be written in matrix form  $Ax = b$ , where

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

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

**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.

**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 will fail due to division by zero, yielding a floating exception error.

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

If the magnitude of the residual,  $|r|$ , is large due to rounding, the matrix is said to be **ill-conditioned**.

## 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
    $s_i = \max_{j=1, \dots, n} |a_{i,j}|$ 
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

$$U = U_{n-1} \cdots U_2 U_1 A.$$

**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

```

1: for  $i=1$  to  $n$  do
2:   for  $j = 1$  to  $i - 1$  do
3:      $y = a_{i,j}$ 
4:     for  $k = 1$  to  $j-1$  do
5:        $y = y - l_{i,k}l_{j,k}$ 
6:     end for
7:      $l_{i,j} = y/l_{j,j}$ 
8:   end for
9:    $y = a_{i,i}$ 
10:  for  $k= 1$  to  $i - 1$  do
11:     $y = y - l_{i,k}l_{i,k}$ 
12:  end for
13:  if  $y \leq 0$  then
14:    there is no solution
15:  else
16:     $l_{i,i} = \sqrt{y}$ 
17:  end if
18: end for

```

## 4.2 Indirect Methods

For a non-singular matrix  $A$ , consider the iterative scheme  $Qx_{k+1} = (Q - A)x_k + b$ . This is equivalent to

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

**Definition 4.9** (Spectral Radius of a Matrix). The **spectral radius** of a matrix  $A$  is defined as

$$\rho(A) = \max\{|\lambda_1|, |\lambda_2|, \dots, |\lambda_n|\}$$

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

**Definition 4.10**. If a sequence  $x_n$  converges to  $r$  as  $n \rightarrow \infty$ , then it is said to **converge linearly** if there exists a  $\mu \in (0, 1)$  such that

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

The sequences converges **super-linearly** if

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

and **sub-linearly** if

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

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

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

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

**Definition 4.11** (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

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

**Definition 4.12** (Jacobi Iteration). The **Jacobi iteration** has  $Q = D$ , so

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

**Definition 4.13** (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 4.14** (Gauss-Seidel Scheme). Let  $Q = L + D$ , then the **Gauss-Seidel** scheme is given by

$$(D + L)x^{(n+1)} = -Ux^{(n)} + b.$$

**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 4.15** (Successive Over Relaxation). The scheme uses  $Q = L + \frac{1}{\omega}D$ , thus

$$(D + \omega L)x^{(n+1)} = -((\omega - 1)D + \omega U)x^{(n)} + \omega b.$$

**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.

## 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 9** (Bisection Method).

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

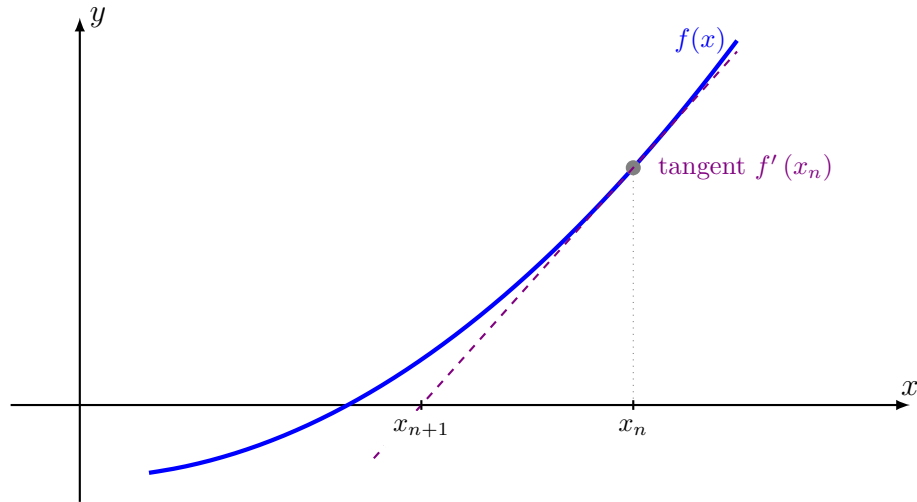
$$|r - c_n| < \frac{b - a}{2^n}.$$

### 5.2 Newton's Method

**Definition 5.2.**

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 10.**

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

**Theorem 11.**

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 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 iterate in the sequence satisfies

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

**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 and is continuous, i.e.  $f(x) \in C^2([a, b])$ .

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

**5.3 Secant Methods****Definition 5.3.**

The secant method is defined as

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

**Theorem 13.**

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

**5.4 Convergence**

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

## 5.5 Systems of Nonlinear Equation

**Definition 5.4** (Multi-Dimensional Newton Method). For a vector-valued function  $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ , 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

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

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

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

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



## 6 Interpolation

**Definition 6.1.** Given a set of points  $p_0, \dots, p_n \in \mathbb{R}$  and corresponding nodes  $u_0, \dots, u_n \in \mathbb{R}$ , a function  $f : \mathbb{R} \rightarrow \mathbb{R}$  with  $f(u_i) = p_i$  is an **interpolating function**.

This can be generalised to higher dimensions, i.e.  $f : \mathbb{R} \rightarrow \mathbb{R}^N$ .

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

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

So that for every  $j$ , the polynomial satisfies  $p(u_j) = \sum_{i=0}^n \alpha_i \varphi_i(u_j)$ , for weights  $\alpha_j$ . Thus, solving for 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**, given by

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

Thus  $\alpha = \Phi^{-1}p$ .

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

When the  $\varphi_i(u) = u^i$ , then  $\Phi$  is 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  $i = 0, \dots, n$ , are called **characteristic polynomials** and are given by

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

**Algorithm (Aitken's Algorithm).**

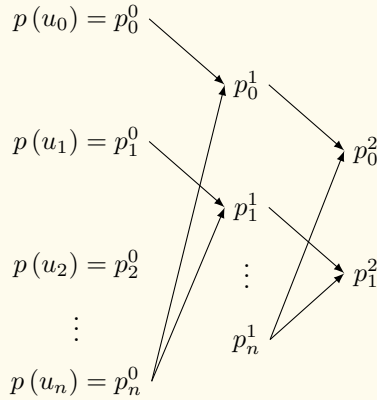
**Aitken's algorithm** is an iterative process for evaluating Lagrange interpolation polynomials at an arbitrary point,  $u^*$ , without explicitly constructing them. If the interpolating polynomial is given by  $p$ , and is derived from  $n$  data points  $(u_i, y_i)$  for  $i = 0, \dots, n$

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

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 6.4.** 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  $a = u_0 < u_1 < \dots < u_m = b$  such that  $s$  is a polynomial of degree  $k$  for  $i = 0, \dots, m-1$ .

**Definition 6.5 (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  $u_0, u_1, \dots, u_m$ , then

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

and

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

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

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

which in 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 6.6** (Least-Squares Approximation). Given a set of points  $y = (y_0, y_1, \dots, y_n)$  at nodes  $x_i$ , seek a continuous function of  $x$ , with a given form characterized by  $m$  parameters  $\beta = (\beta_0, \beta_1, \dots, \beta_m)$ , i.e.  $f(x, \beta)$ , which approximates the points while minimizing the error, defined by the sum of the squares

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

The minimum is found when

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

i.e.

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

**Definition 6.7** (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.  $\beta = (\Phi \Phi^T)^{-1} \Phi y$ , 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

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

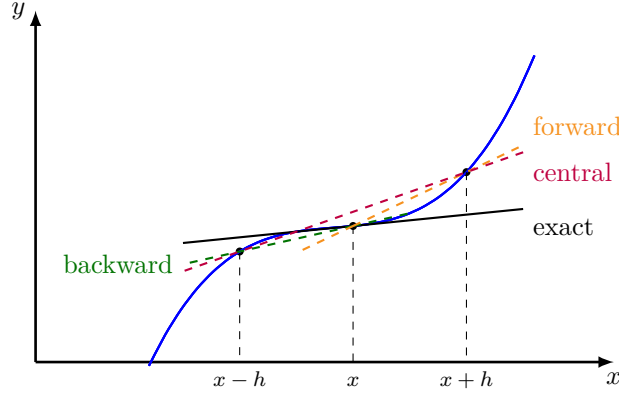
Combining the two terms so that the low order term cancel, i.e. via  $f'(x) - 4f'\left(\frac{h}{2}\right)$ , then a better approximation can be found as

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

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

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



## 8 Numerical Integration

**Definition 8.1** (Riemann Sum). Create a partition,  $p$ , of the domain of integration: define  $n+1$  nodes  $a = x_0 < x_1 < \dots < x_n = b$ , 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

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

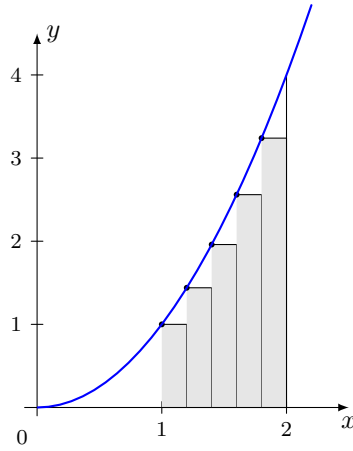
If  $f$  is continuous, the value of  $x_i^*$  may be chosen arbitrarily in the interval  $[x_i, x_{i+1}]$ . Then the **lower** and **upper Riemann sums** are given by

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

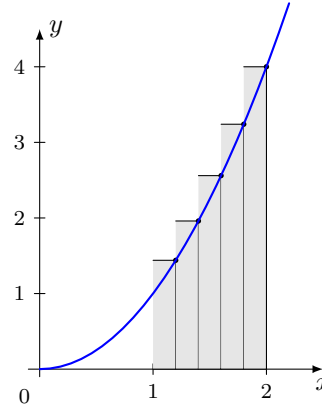
$$U(f, p) = \sum_{i=0}^{n-1} (x_{i+1} - x_i) M_i \quad \text{where} \quad M_i = \max_{x \in [x_i, x_{i+1}]} f(x)$$

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

$$L(f, p) \leq \int_a^b f(x) dx \leq U(f, p).$$



(a) Lower Riemann Sum



(b) Upper Riemann Sum

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

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

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

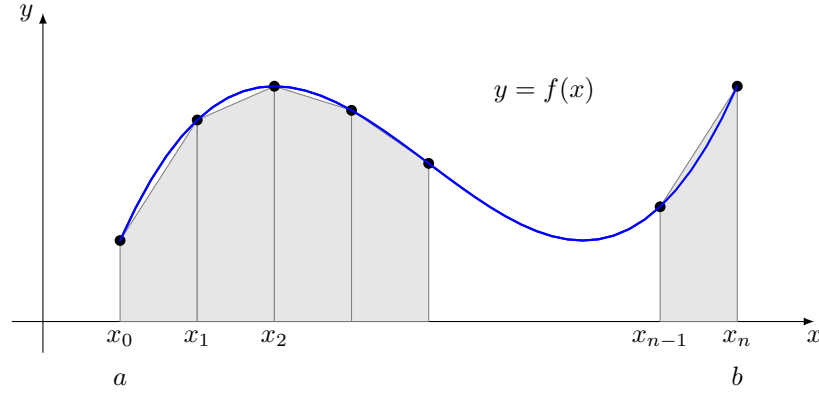
**Definition 8.2** (Trapezoidal Rule). Rather than rectangles, use trapezoids to approximate the integral in a sub domain

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

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

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

**Theorem 14 (Error for Trapezoidal Rule).** Let  $f \in C^2([a, b])$  and  $p$  be equidistant partition of  $[a, b]$ , with  $h = x_{i+1} - x_i$ . The error can be shown



to have the form:

$$\left| \int_a^b f(x) \, dx - T(f, p) \right| = a_2 h^2 + a_4 h^4 + \dots$$

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

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

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

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

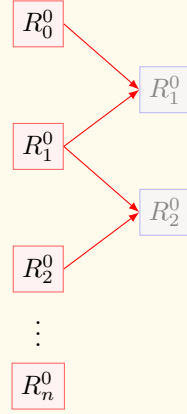
$$\int_a^b f(x) \, dx \approx \frac{b-a}{6} \left( f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right).$$

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

**Algorithm** (Romberg Algorithm). Romberg's method uses the Trapezoidal Rule 8.2 and then Richardson Extrapolation 7.2 to estimate integrals. First consider a sequence of partitions,  $p_i$ , of equal spacing given by  $h_i = \frac{b-a}{2^i}$  for  $i = 0, \dots, n$ , which yield a sequence of integrals  $R_i^0 = T_i(f, p_i)$ . Refinements



of the integrals can then be produced by Richardson Extrapolation



Thus, consider the two integrals

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

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

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

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

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

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

## 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

$$\langle f, g \rangle = \int_a^b f(x)g(x) \, dx = 0.$$

**Theorem 15 (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

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

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

Then, denote the integral as

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

with  $A_i = \int_a^b L_i(x) \, dx$  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

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

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

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

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  $x = \frac{b-a}{2}t + \frac{a+b}{2}$ , so that

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

## 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 or 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  $y(t)$ .

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  $i + 1$  depends only on the previous one. The time step is  $t_{i+1} = t_i + h$ , for some time step  $h = \Delta t$ .

#### Forward Euler Method

**Definition 9.4. Forward Euler** 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  $\mathcal{O}(h^2)$ .

#### Backward Euler Method

**Definition 9.5. Backward Euler** 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  $f_{n+1} = f(u_{n+1}, t_{n+1})$ .

#### Crank-Nicolson Method

**Definition 9.6.** The **Crank-Nicolson method** is given by

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

## Heun's Method

**Definition 9.7.** Heun's method is

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

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

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

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

## 9.2 Analysis of One-Step Methods

**Definition 9.8.** A numerical method is said to be **explicit** if an approximation  $y_{k+1}$  can be calculated directly from already computed values  $y_i$ ,  $i < k$ . Otherwise, the method is said to be **implicit**.

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

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

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

$$|f(x) - f(y)| \leq C \|x - y\|^\alpha$$

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

**Definition 9.10** (Stable). stable

**Definition 9.11** (Consistent). Let  $y(t)$  be the solution to an initial value problem and  $h_{\max} = \max_{x_k} h_k$ . A method is said to be **consistent** if the func-

tion  $f$  satisfies the Lipschitz condition, with respect to  $y$ , in an interval then

$$\lim_{h_{\max}} \left( \max_{x_k \in I_h} \|f(t_k, y(t_k)) - \Phi(t_k, y(t_k), h_k)\| \right) = 0.$$

**Definition 9.12 (Order).** A one-step method is of order  $p \in \mathbb{N}$ , if for all  $t \in [0, \tau]$ , the solution satisfies the condition that  $\tau(h) = \mathcal{O}(h^p)$  as  $h \rightarrow 0$ .

**Definition 9.13 (Zero Stable Methods).** A method of the form

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

is called **zero-stable** if there exists both a maximal step size,  $h_0$  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

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

and  $z_0 = y_0 + \delta_0$ , then

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

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

**Theorem 16.** If increment function is Lipschitz continuous for  $y_n$  for any  $h$  and  $t_n$ , then the one step method is zero-stable.

**Theorem 17.** If the increment function  $\Phi$  is

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

and

- (ii) the method is consistent

then

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

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

**Definition 9.14 (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  $|u_n| \rightarrow 0$  as  $n \rightarrow \infty$ , when  $\text{Re}(\lambda) < 0$ , for a fixed value of  $h$ .

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

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

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  $k_1, \dots, k_{i-1}$ . 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  $\tau(h) = \max |\tau_{n+1}(h)| \rightarrow 0$  as  $h \rightarrow 0$  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  $h \rightarrow 0$ .

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 9.15.** A partial differential equation is relation involving a 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 a unknown function  $u(x, t)$  has the form

$$a_1 u_{xx} + a_2 u_{xt} + a_3 u_{tt} + a_4 u_x + a_5 u_t + a_6 u = f(x, t).$$

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

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