

MA3105

# Numerical Analysis

Autumn 2021

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## 1 Time complexity

### 1.1 Runtime cost

When designing or implementing an algorithm, we care about its efficiency – both in terms of execution time, and the use of resources. This gives us a rough way of comparing two algorithms. However, such metrics are architecture and language dependent; different machines, or the same

program implemented in different programming languages, may consume different amounts of time or resources while executing the same algorithm. Thus, we seek a way of measuring the ‘cost’ in time for a given algorithm.

For example, we may look at each statement in a program, and associate a cost  $c_i$  with each of them. Consider the following statements.

```

one = 1;           // c_1
two = 2;          // c_2
three = 3;        // c_3

```

The total cost of running these statements can be calculated as  $T = c_1 + c_2 + c_3$ , simply by adding up the cost of each statement. Similarly, consider the following loop construct.

```

sum = 0;          // c_1
for (i = 0; i < n; i++) // c_2
    sum += a[i];  // c_3

```

The total cost can be shown to be  $T(n) = c_1 + c_2(n + 1) + c_3n$ ; this time, we must take into account the number of times a given statement is executed. Note that this is linear. Another example is as follows.

```

sum = 0;          // c_1
for (i = 0; i < n; i++) // c_2
    for (j = 0; j < n; j++) // c_2
        sum += a[i][j]; // c_4

```

The total cost can be shown to be  $T(n) = c_1 + c_2(n + 1) + c_3n(n + 1) + c_4n^2$ . Note that this is quadratic. Finally, consider the following recursive call.

```

int factorial (int n) {           // c_1
    if (n == 0)                   // c_2
        return 1;                 // c_3
    return n * factorial(n - 1); // c_4
}

f = factorial(n);                 // c_5

```

The cost can be shown to be  $T(n) = c_5 + (c_1 + c_2)(n + 1) + c_3 + c_4n$ . This turns out to be linear.

In all these cases, we care about our total cost as a function of the input size  $n$ . Moreover, we are interested mostly in the *growth* of our total cost; as our input size grows, the total cost can often be compared with some simple function of  $n$ . Thus, we can classify our cost functions in terms of their asymptotic growths.

## 1.2 Asymptotic growth

**Definition 1.1.** The set  $O(g(n))$  denotes the class of functions  $f$  which are asymptotically bounded above by  $g$ . In other words,  $f(n) \in O(g(n))$  if there exists  $M > 0$  and  $n_0 \in \mathbb{N}$  such that for all  $n \geq n_0$ ,

$$|f(n)| \leq Mg(n).$$

This amounts to writing

$$\limsup_{n \rightarrow \infty} \frac{|f(n)|}{g(n)} < \infty.$$

*Example.* Consider a function defined by  $f(n) = an + b$ , where  $a > 0$ . Then, we can write  $f(n) \in O(n)$ . To see why, note that for all  $n \geq 1$ , we have

$$|f(n)| = |an + b| \leq an + |b| \leq (a + |b|)n.$$

Thus, setting  $M = a + |b| > 0$  completes the proof.

*Example.* Consider a polynomial function defined by

$$f(n) = a_k n^k + a_{k-1} n^{k-1} + \cdots + a_1 n + a_0,$$

with some non-zero coefficient. Then, we can write  $f(n) \in O(n^k)$ . Like before, note that for all  $n \geq 1$ , we have

$$|f(n)| \leq \sum_{i=0}^k |a_i| n^i \leq \sum_{i=0}^k |a_i| n^k = (|a_k| + |a_{k-1}| + \cdots + |a_0|) n^k.$$

Thus, setting  $M = |a_k| + \cdots + |a_0| > 0$  completes the proof.

**Theorem 1.1.** If  $f_1(n) \in O(g_1(n))$  and  $f_2(n) \in O(g_2(n))$ , then

$$f_1(n) + f_2(n) \in O(\max\{g_1(n), g_2(n)\}).$$

**Definition 1.2.** The set  $\Omega(g(n))$  denotes the class of functions  $f$  are asymptotically bounded below by  $g$ . In other words,  $f(n) \in \Omega(g(n))$  if there exists  $M > 0$  and  $n_0 \in \mathbb{N}$  such that for all  $n \geq n_0$ ,

$$|f(n)| \geq Mg(n).$$

This amounts to writing

$$\liminf_{n \rightarrow \infty} \frac{f(n)}{g(n)} > 0.$$

**Definition 1.3.** The set  $\Theta(g(n))$  denotes the class of functions  $f$  which are asymptotically bounded both above and below by  $g$ . In other words,  $f(n) \in \Theta(g(n))$  if there exist  $M_1, M_2 > 0$  and  $n_0 \in \mathbb{N}$  such that for all  $n \geq n_0$ ,

$$M_1g(n) \leq |f(n)| \leq M_2g(n).$$

This amounts to writing  $f(n) \in O(g(n))$  and  $f(n) \in \Omega(g(n))$ .

Another class of notation uses the idea of dominated growth.

**Definition 1.4.** The set  $o(g(n))$  denotes the class of functions  $f$  which are asymptotically dominated by  $g$ . In other words,  $f(n) \in o(g(n))$  if for all  $M > 0$ , there exists  $n_0 \in \mathbb{N}$  such that for all  $n \geq n_0$ ,

$$|f(n)| < Mg(n).$$

This amounts to writing

$$\lim_{n \rightarrow \infty} \frac{|f(n)|}{g(n)} = 0.$$

**Definition 1.5.** The set  $\omega(g(n))$  denotes the class of functions  $f$  which asymptotically dominate  $g$ . In other words,  $f(n) \in \omega(g(n))$  if for all  $M > 0$ , there exists  $n_0 \in \mathbb{N}$  such that for all  $n \geq n_0$ ,

$$|f(n)| > Mg(n).$$

This amounts to writing

$$\lim_{n \rightarrow \infty} \frac{|f(n)|}{g(n)} = \infty.$$

**Definition 1.6.** We say that  $f(n) \sim g(n)$  if  $f$  is asymptotically equal to  $g$ . In other words,  $f(n) \sim g(n)$  if for all  $\epsilon > 0$ , there exists  $n_0 \in \mathbb{N}$  such that for all  $n \geq n_0$ ,

$$\left| \frac{f(n)}{g(n)} - 1 \right| < \epsilon.$$

This amounts to writing

$$\lim_{n \rightarrow \infty} \frac{f(n)}{g(n)} = 1.$$

We often abuse notation and treat the following as equivalent.

$$T(n) \in O(g(n)), \quad T(n) = O(g(n)).$$

## 2 Root finding methods

Consider an equation of the form  $f(x) = 0$ , where  $f: [a, b] \rightarrow \mathbb{R}$  is given. We wish to solve this equation, i.e. find the roots of  $f$ .

Note that for *arbitrary* functions, this task is impossible. To see this, consider a function  $f$  which assumes the value 1 on  $[0, 1] \setminus \{\alpha\}$  and  $f(\alpha) = 0$ , for some  $\alpha \in [0, 1]$ . There is no way of pinpointing  $\alpha$  without checking  $f$  at every point in  $[0, 1]$ . Besides, a computer cannot reasonably store real numbers with arbitrary precision.

Thus, we direct our attention towards *continuous* functions  $f$ . We only seek sufficiently accurate approximations of its root  $\alpha \in (a, b)$ .

**Theorem 2.1** (Intermediate Value Theorem). *Let  $f: [a, b] \rightarrow \mathbb{R}$  be continuous. If  $f(a)f(b) < 0$ , then there exists  $\alpha \in (a, b)$  such that  $f(\alpha) = 0$ .*

## 2.1 Tabulation method

To identify the location of a root of  $f$  on an interval  $I = [a, b]$ , we subdivide  $I$  into  $n$  subintervals  $[x_i, x_{i+1}]$  where  $x_i = a + (b - a)i/n$ . Now, we simply apply the Intermediate Value Theorem to  $f$  on each of these intervals. If  $f(x_i)f(x_{i+1}) < 0$ , then  $f$  has a root somewhere in  $(x_i, x_{i+1})$ . Note that the error in our approximation is on the order of  $|b - a|/n$ . The precision of this method can be improved by increasing  $n$ .

To reach a degree of approximation  $\epsilon$ , we must iterate  $n$  times, where

$$n > \frac{b - a}{\epsilon}.$$

## 2.2 Bisection method

Here, we first verify that  $f(a)f(b) < 0$ , thus ensuring that  $f$  has a root within  $(a, b)$ . Now, set  $x_1 = a + (b - a)/2$  and apply the Intermediate Value Theorem on the subintervals  $[a, x_1]$  and  $[x_1, b]$ . One of these *must* contain a root of  $f$ . Note that if  $f(x_1) = 0$ , we are done; otherwise, let  $I_1 = [a_1, b_1]$  be the subinterval containing the root. Repeat the above process, obtaining successive subintervals  $I_n$  with lengths  $|b - a|/2^n$ . The error in our approximation is of this order, and can be controlled by stopping at appropriately large  $n$ .

The quantity  $x_{n+1} = (a_n + b_n)/2$  is a good approximation for the actual root  $\alpha$  since we know that  $x_{n+1}, \alpha \in [a_n, b_n]$ , so

$$|x_{n+1} - \alpha| \leq |b_n - a_n| = 2^{-n}|b - a| \rightarrow 0.$$

To reach a degree of approximation  $\epsilon$ , we must iterate  $n$  times, where

$$n > \log_2 \frac{b - a}{\epsilon}.$$

## 2.3 Newton-Raphson method

Assuming that  $f$  is twice differentiable, use Taylor's theorem to write

$$f(x) = f(x_0) + f'(x)(x - x_0) + \frac{1}{2}f''(c)(x - x_0)^2$$

for all  $x \in [a, b]$ , where  $c$  is between  $x$  and  $x_0$ . The first two terms represent the tangent line to  $f$ , drawn at  $(x_0, f(x_0))$ . Now, define

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}.$$

Note that this is the point at which the tangent line to  $f$  at  $x_0$  cuts the  $x$ -axis. We have implicitly assumed that  $f'(x_0) \neq 0$ . In this manner, create the sequence of points

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

We wish to show that  $x_n \rightarrow \alpha$ , under certain circumstances.

**Definition 2.1** (Order of convergence). Let  $x_n \rightarrow \alpha$ . We say that this convergence is of order  $p \geq 1$  if

$$\lim_{n \rightarrow \infty} \frac{|\alpha - x_{n+1}|}{|\alpha - x_n|^p} > 0.$$

**Theorem 2.2.** Let  $f$  be a real function on  $[\alpha - \delta, \alpha + \delta]$  such that

1.  $f(\alpha) = 0$ .
2.  $f$  is twice differentiable, with non-zero derivatives.
3.  $f''$  is continuous.
4.  $|f''(x)/f'(y)| \leq M$  for all  $x, y$ .

If  $x_0 \in [\alpha - h, \alpha + h]$  where  $h = \min\{\delta, 1/M\}$ , then the Newton-Raphson sequence generated by  $x_0$  converges to the root  $\alpha$  quadratically.

*Proof.* Pick  $x_n \in [\alpha - h, \alpha + h]$ . Using Taylor's theorem,

$$f(\alpha) = f(x_n) + f'(x_n)(\alpha - x_n) + \frac{1}{2}f''(c)(\alpha - x_n)^2.$$

Also note that  $f(\alpha) = 0$ , and  $x_n - x_{n+1} = f(x_n)/f'(x_n)$ . Thus, dividing by  $f'(x_n)$  and substituting gives

$$\alpha - x_{n+1} = -\frac{1}{2} \frac{f''(c)}{f'(x_n)} (\alpha - x_n)^2.$$

Using our estimates on  $f''(c)/f'(x_n)$  and  $x_n$  along with  $h \leq 1/M$ , we see that

$$|\alpha - x_{n+1}| \leq \frac{1}{2} M h |\alpha - x_n| \leq \frac{1}{2} |\alpha - x_n|.$$

Indeed, we have shown that

$$|\alpha - x_n| \leq \frac{1}{2^n} |\alpha - x_0|,$$

which directly gives the convergence  $x_n \rightarrow \alpha$ . Furthermore, we have

$$\frac{|\alpha - x_{n+1}|}{|\alpha - x_n|^2} = \frac{1}{2} \left| \frac{f''(c)}{f'(x_n)} \right| \leq \frac{1}{2} M,$$

hence taking the limit  $n \rightarrow \infty$  proves that the convergence is quadratic.  $\square$

**Corollary 2.2.1.** Suppose that  $f$  satisfies the conditions of the previous theorem, along with  $f' > 0$  and  $f'' > 0$  on some interval  $[\alpha, x]$ . Then, the Newton-Raphson sequence generated by  $x_0 \in [\alpha, x]$  converges to the root  $\alpha$  quadratically.

*Remark.* The convexity of  $f$  means that the tangent drawn at  $x_n$  lies below the curve, and hence cuts the  $x$ -axis between  $\alpha$  and  $x_n$ .

**Theorem 2.3.** *If  $\alpha$  is a multiple root of  $f$  such that  $f(\alpha) = 0$ ,  $f'(\alpha) = 0$ ,  $f''(\alpha) \neq 0$ , then the Newton-Raphson sequence converges to  $\alpha$  linearly under suitable conditions.*

*Proof.* Use Rolle's Theorem to replace  $f'(x_n) = f'(x_n) - f'(\alpha) = f''(\alpha)(x_n - \alpha)$ . □

## 2.4 Secant method

The chief difference between this method as Newton's method is that we approximate the tangent with a secant, i.e. perform an approximation of the derivative,

$$f'(x)h \approx f(x+h) - f(x)$$

for small  $h$ . Thus, our iterations proceed as

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

**Theorem 2.4.** *Let  $f$  be a real function on  $[a, b]$  such that*

1.  $f(\alpha) = 0$  where  $\alpha \in (a, b)$ .
2.  $f$  is continuously differentiable, with non-zero derivatives.

*Then, there exists  $\delta > 0$  such that the sequence generated by the secant method converges to  $\alpha$  when  $x_0, x_1 \in (\alpha - \delta, \alpha + \delta)$ .*

*Proof.* Consider

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

Now, use the Mean Value Theorem to write  $f(x_n) = f(x_n) - f(\alpha) = f'(\xi)(x_n - \alpha)$  for some  $\xi$  between  $\alpha$  and  $x_n$ . Similarly, write  $f(x_n) - f(x_{n-1}) = f'(\zeta)(x_n - x_{n-1})$  for some  $\zeta$  between  $x_n$  and  $x_{n-1}$ . Thus,

$$\alpha - x_{n+1} = \alpha - x_n + \frac{f'(\xi)(x_n - \alpha)}{f'(\zeta)} = (\alpha - x_n) \left( 1 - \frac{f'(\xi)}{f'(\zeta)} \right).$$

We want  $|1 - f'(\xi)/f'(\zeta)| < 1$ . Since  $f'(\alpha) \neq 0$ , there is a  $\delta$ -neighbourhood of  $\alpha$  where  $3f'(\alpha)/4 < f'(x) < 5f'(\alpha)/4$  (without loss of generality) using the continuity of  $f'$ . Thus, whenever  $x_0, x_1 \in (\alpha - \delta, \alpha + \delta)$ , we have  $\xi, \zeta$  belonging to the same neighbourhood. This gives  $3/5 < f'(\zeta)/f'(\xi) < 5/3$ . This gives

$$-\frac{2}{3} < 1 - \frac{f'(\xi)}{f'(\zeta)} < \frac{2}{5}.$$

In other words,  $|1 - f'(\xi)/f'(\zeta)| < 2/3$ , so

$$|\alpha - x_{n+1}| < \frac{2}{3} |\alpha - x_n|,$$

which directly gives  $x_n \rightarrow \alpha$ .

The order of convergence turns out to be  $\varphi = (1 + \sqrt{5})/2$ . To show this, we want

$$\lim_{n \rightarrow \infty} \frac{|\alpha - x_{n+1}|}{|\alpha - x_n|^\varphi} > 0.$$

Assume that  $f'(\alpha) > 0$ ,  $f''(\alpha) > 0$ . First, we will show that

$$\lim_{n \rightarrow \infty} \frac{|\alpha - x_{n+1}|}{|\alpha - x_n||\alpha - x_{n-1}|} = \frac{f''(\alpha)}{2f'(\alpha)}.$$

Denote the quantity in the limit as  $\psi(x_n, x_{n-1})$ . We examine the equivalent limit

$$\lim_{x_{n-1} \rightarrow \alpha} \lim_{x_n \rightarrow \alpha} \psi(x_n, x_{n-1}).$$

Like before, write

$$\alpha - x_{n+1} = (\alpha - x_n) \left( 1 - \frac{f'(\xi)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})} \right),$$

hence

$$\frac{\alpha - x_{n+1}}{(\alpha - x_n)(\alpha - x_{n-1})} = \frac{1}{\alpha - x_{n-1}} \left[ 1 - \frac{f'(\xi)(x_n - x_{n-1})}{f(x_n) - f(x_{n-1})} \right].$$

Thus,

$$\begin{aligned} \lim_{x_n \rightarrow \alpha} \psi(x_n, x_{n-1}) &= \frac{1}{\alpha - x_{n-1}} \left[ 1 + \frac{f'(\alpha)(\alpha - x_{n-1})}{f(x_{n-1})} \right] \\ &= \frac{f(x_{n-1}) + f'(\alpha)(\alpha - x_{n-1})}{f(x_{n-1})(\alpha - x_{n-1})}. \end{aligned}$$

Use Taylor's Theorem to approximate

$$f(x_{n-1}) = f(\alpha) + f'(\alpha)(x_{n-1} - \alpha) + \frac{1}{2}f''(\eta)(x_{n-1} - \alpha)^2,$$

giving

$$\lim_{x_n \rightarrow \alpha} \psi(x_n, x_{n-1}) = \frac{f''(\eta)(\alpha - x_{n-1})^2}{2f(x_{n-1})(\alpha - x_{n-1})},$$

and use the Mean Value Theorem to write  $f(x_{n-1}) = f'(\kappa)(x_{n-1} - \alpha)$  giving

$$\lim_{x_n \rightarrow \alpha} \psi(x_n, x_{n-1}) = -\frac{f''(\eta)}{2f'(\kappa)},$$

This gives

$$\lim_{x_{n-1} \rightarrow \alpha} \lim_{x_n \rightarrow \alpha} |\psi(x_n, x_{n-1})| = \frac{f''(\alpha)}{2f'(\alpha)} = C.$$

Now, suppose that

$$\lim_{n \rightarrow \infty} \frac{|\alpha - x_{n+1}|}{|\alpha - x_n|^q} = A > 0.$$

Dividing, we have

$$\lim_{n \rightarrow \infty} \frac{|\alpha - x_n|^{q-1}}{|\alpha - x_{n-1}|} = \frac{C}{A}, \quad \lim_{n \rightarrow \infty} \frac{|\alpha - x_n|}{|\alpha - x_{n-1}|^{1/(q-1)}} = \left( \frac{C}{A} \right)^{1/(q-1)} > 0.$$

For  $q$  to be minimal, we must have  $1/(q-1) = q$ , or  $q$  is the golden ratio  $\varphi$ . □



## 2.5 Fixed point method

Note that a root of  $f$  is simply a fixed point of  $f + x$ .

**Theorem 2.5.** *Let  $f: [a, b] \rightarrow [a, b]$  be continuous. Then,  $f$  has a fixed point  $\beta \in [a, b]$ ,  $f(\beta) = \beta$ .*

Thus, let  $f: [a, b] \rightarrow [a, b]$  be continuous. Define the fixed point sequence  $x_{n+1} = f(x_n)$ , seeded by some  $x_0 \in [a, b]$ . Note that if this sequence converges with  $x_n \rightarrow \beta$ , then  $\beta$  is a fixed point of  $f$ .

**Definition 2.2.** A function  $f: [a, b] \rightarrow \mathbb{R}$  is said to be a contraction if there exists  $L \in (0, 1)$  such that  $|f(x) - f(y)| \leq L|x - y|$  for all  $x, y \in [a, b]$ .

*Remark.* Note that  $f$  is Lipschitz continuous. If  $f$  is also differentiable, then  $|f'| < 1$ .

**Theorem 2.6.** *Let  $f: [a, b] \rightarrow [a, b]$  be a contraction map. Then, any fixed point sequence converges to the unique fixed point of  $f$ .*

*Proof.* First, we show that  $f$  has at most one fixed point. Let  $\beta_1, \beta_2$  be fixed points of  $f$ . Then,  $|f(\beta_1) - f(\beta_2)| \leq L|\beta_1 - \beta_2|$  where  $L \in (0, 1)$ . This forces  $\beta_1 = \beta_2$ . Thus,  $f$  has a unique fixed point in  $[a, b]$ .

Let  $\{x_n\}$  be a fixed point iteration. Then,

$$|x_{n+1} - \beta| = |f(x_n) - f(\beta)| \leq L|x_n - \beta|,$$

which directly gives  $x_n \rightarrow \beta$ . □

## 3 Interpolation

### 3.1 Lagrange interpolation

**Theorem 3.1.** *Let  $x_1, \dots, x_n \in \mathbb{R}$  be distinct, and let  $y_1, \dots, y_n \in \mathbb{R}$ . Then, the following polynomial of degree  $n - 1$  satisfies  $p(x_i) = y_i$ .*

$$p(x) = \sum_{i=1}^n \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} y_i.$$

*Furthermore, this choice of  $p$  is unique.*

*Proof.* The polynomials

$$p_i(x) = \prod_{j \neq i} \frac{x - x_j}{x_i - x_j}$$

satisfy  $p_i(x_j) = \delta_{ij}$ . These  $p_i$  form a basis of  $\mathcal{P}^{n-1}$ , the space of polynomials of degree at most  $n - 1$ . □

**Theorem 3.2.** Let  $f: [a, b] \rightarrow \mathbb{R}$  be  $n$  times differentiable, and let  $p$  be the Lagrange interpolating polynomial of  $f$  on the points  $x_1, \dots, x_n$ . Then, for any  $x \in [a, b]$ , there exists  $\xi \in (a, b)$  such that

$$f(x) - p(x) = \frac{f^{(n)}(\xi)}{n!} \prod_i (x - x_i)$$

*Proof.* This is clear when  $x = x_i$ . Suppose that  $x \neq x_i$  for any  $i$ . Define

$$g: [a, b] \rightarrow \mathbb{R}, \quad g(t) = f(t) - p(t) - (f(x) - p(x)) \prod_i \frac{t - x_i}{x - x_i}$$

We see that each  $g(x_i) = 0$ , as well as  $g(x) = 0$ , hence  $g$  has  $n + 1$  distinct roots. Hence,  $g'$  has exactly  $n$  distinct roots, and continuing in this fashion,  $g^{(n)}$  has one root. Set  $\xi$  such that  $g^{(n)}(\xi) = 0$ . On the other hand,

$$g^{(n)}(\xi) = f^{(n)}(\xi) - n!(f(x) - p(x)) \prod_i \frac{1}{x - x_i}. \quad \square$$

### 3.2 Newton's divided difference

**Theorem 3.3.** Let  $x_1, \dots, x_n \in \mathbb{R}$  be distinct, and let  $y_1, \dots, y_n \in \mathbb{R}$ . Define the divided difference recursively as

$$\Delta(x_i) = y_i, \quad \Delta(x_i, \dots, x_j) = \frac{\Delta(x_{i+1}, \dots, x_j) - \Delta(x_i, \dots, x_{j-1})}{x_j - x_i}.$$

Further denote

$$\Delta^k = \Delta(x_1, \dots, x_k).$$

Then, the following polynomial of degree  $n - 1$  interpolates the given data.

$$p(x) = \Delta^1 + (x - x_1)\Delta^2 + (x - x_1)(x - x_2)\Delta^3 + \dots + (x - x_1)\dots(x - x_{n-1})\Delta^n.$$

*Remark.* We already know that this must be identical to the Lagrange interpolating polynomial, hence all its properties carry over.

*Remark.* The divided difference  $\Delta(x_1, \dots, x_k)$  is independent of the order of  $x_1, \dots, x_k$ .

## 4 Numerical integration

Let  $f: [a, b] \rightarrow \mathbb{R}$  be continuously differentiable. We wish to approximate the value of the integral

$$\int_a^b f(x) dx.$$

The main way of doing this is to approximate the curve  $f$  using rectangles, trapeziums, parabolas, or even higher degree polynomials.

### 4.1 Newton-Cotes formula

Perform Lagrange interpolation of  $f$  on the points  $x_1, \dots, x_n$ , and write

$$\int_a^b f(x) dx \approx \sum_{i=1}^n f(x_i) \int_a^b p_i(x) dx.$$

## 4.2 Midpoint rule

Here, we use the midpoints  $m_i = (x_i + x_{i+1})/2$ , and write

$$\int_a^b f(x) dx \approx \Delta x [f(m_1) + \cdots + f(m_{n-1})].$$

## 4.3 Trapezoidal rule

Perform linear interpolations of  $f$  at equal intervals  $\Delta x$  and write

$$\int_a^b f(x) dx \approx \frac{1}{2} \Delta x [f(x_1) + 2f(x_2) + \cdots + 2f(x_{n-1}) + f(x_n)].$$

It can be shown that there exists  $\xi$  between  $a$  and  $b$  such that the error in this approximation is

$$-\frac{(b-a)^3}{12(n-1)^2} f''(\xi).$$

## 4.4 Simpson's rule

Perform quadratic interpolations of  $f$ , and write

$$\int_a^b f(x) dx \approx \frac{1}{3} \Delta x [f(x_1) + 4f(x_2) + 2f(x_3) + \cdots + 4f(x_{n-2}) + 2f(x_{n-1}) + f(x_n)].$$

Note that we need odd  $n$ . For each arc between  $a_i, b_i$ , we have used the area under the interpolating quadratic,

$$\int_{a_i}^{b_i} f(x) dx \approx \frac{1}{6} (b_i - a_i) \left[ f(a_i) + 4f\left(\frac{a_i + b_i}{2}\right) + f(b_i) \right].$$

It can be shown that there exists  $\xi$  between  $a$  and  $b$  such that the error in this approximation is

$$-\frac{(b-a)^5}{180(n-1)^4} f^{(4)}(\xi).$$

# 5 Ordinary differential equations

Consider the initial value problem

$$y'(x) = f(x, y), \quad y(x_0) = y_0,$$

where  $f$  is a continuous function on some open subset of  $\mathbb{R}^2$ . We are looking for a differentiable function  $y$  on an open neighbourhood of  $x_0$ , where each  $(x, y(x))$  is in the domain of  $f$ .

## 5.1 Picard iterates

Any solution must satisfy

$$y(x) = y_0 + \int_{x_0}^x f(t, y(t)) dt.$$

We may iterate  $y_0(x) = y_0$ , and

$$y_{n+1}(x) = y_0 + \int_{x_0}^x f(t, y_n(t)) dt.$$

It can be shown that the Picard iterates do indeed converge to a solution of the given ODE.

**Theorem 5.1** (Picard-Lindelöf theorem). *Let  $f$  be uniformly Lipschitz continuous in  $y$ . Then the initial value problem has a unique solution  $y$  on some neighbourhood of  $x_0$ .*

## 5.2 Euler's method

Assume that a solution  $y$  exists on  $[x_0, x_M]$ . Construct the  $n$  evenly spaced mesh points  $x_0, x_1, x_2, \dots, x_n$ , where  $x_n = x_M$ . Setting  $h = \Delta x$ , we can approximate

$$y(x_{k+1}) = y(x_k + h) \approx y(x_k) + hy'(x_k) = y(x_k) + hf(x_k, y(x_k)).$$

This gives an iterative scheme to approximate  $y(x)$  on these mesh points.

## 5.3 Trapezoidal method

Here, we use perform the iterations

$$y(x_{n+1}) \approx y(x_n) + \frac{1}{2}h(f(x_n, y(x_n)) + f(x_{n+1}, y(x_{n+1}))).$$

In order to use this implicit relation, we can use Newton's method or fixed point iteration.

## 5.4 Runge-Kutta methods

The second order Runge-Kutta method uses the following iterations.

$$y_{n+1} = y_n + h(ak_1 + bk_2), \quad k_1 = f(x_n, y_n), \quad k_2 = f(x_n + \alpha h, y_n + \beta hk_1).$$

Additionally, we choose  $\beta = \alpha$ ,  $a = 1 - 1/2\alpha$ ,  $b = 1 - a$ .

The fourth order Runge-Kutta method uses the iterations

$$\begin{aligned} y_{n+1} &= y_n + \frac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4), \\ k_1 &= f(x_n, y_n), \quad k_2 = f(x_{n+\frac{1}{2}}, y_n + \frac{1}{2}hk_1), \\ k_3 &= f(x_{n+\frac{1}{2}}, y_n + \frac{1}{2}hk_2), \quad k_4 = f(x_{n+1}, y_n + hk_2). \end{aligned}$$