

# MAT 2384: Numerical Methods Lecture Notes

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# Chapter 1

## Iterative Methods to Solve The Equation $f(x) = 0$

Given a continuous function  $f$ , the goal of this chapter is to estimate the solution of the equation  $f(x) = 0$  in a certain interval  $I$  numerically.

**Theorem 1.0.1** (Intermediate Value Theorem). *Let  $f : [a, b] \rightarrow \mathbb{R}$  be a continuous function. Let  $y \in \mathbb{R}$  be any value between  $f(a)$  and  $f(b)$ . Then there exists  $z \in [a, b]$  such that  $f(z) = y$ .*

Bolzano's Theorem is a special case of the Intermediate Value Theorem, which states

**Theorem 1.0.2** (Bolzano's Theorem). *If a continuous function defined on an interval  $I$  is sometimes positive and sometimes negative, then it must be 0 at some point. So there exists  $x_0 \in I$  such that  $f(x_0) = 0$ .*

*Proof.* Without loss of generality, assume  $f(a) \leq f(b)$ . Let  $y \in [f(a), f(b)]$ . Set

$$S := \{x \in [a, b] : f(x) \leq y_0\}$$

$S$  is a subset of  $[a, b]$  so it is bounded,  $a \in S$  since  $f(a) \leq y_0$ . Therefore  $S \neq \emptyset$ . Thus by completeness, there exists  $x_0 := \sup S \in [a, b]$ . We want  $f(x_0) = y_0$ . Consider the cases where  $f(x_0) = y_0$ ,  $f(x_0) < y_0$ , and  $f(x_0) > y_0$ .

- **Case 1:**  $f(x_0) = y_0$  This case is trivial since this is the result we want.
- **Case 2:**  $f(x_0) < y_0$  Set  $\epsilon := y_0 - f(x_0)$ . Since  $f$  is continuous at  $x_0$ ,  $\exists \delta > 0$  such that

$$|x - x_0| < \delta \implies |f(x) - f(x_0)| < \epsilon$$

Since  $f(x_0) < y_0 \leq f(b)$ , we can find  $x > x_0$  such that  $x \in [a, b]$  and  $|x - x_0| < \delta$ . Then  $f(x) < f(x_0) + \epsilon = y_0$ . So  $x \in S$  by the definition of  $S$ , but  $x > x_0$  which contradicts the fact that  $x_0 = \sup S$ .

- **Case 3:**  $f(x_0) > y_0$  Set  $\epsilon := f(x_0) - y_0$ . Since  $f$  is continuous at  $x_0$ ,  $\exists \delta > 0$  such that if  $x \in [a, b]$  and  $|x - x_0| < \delta$ , then  $|f(x) - f(x_0)| < \epsilon$ . So  $f(x) > f(x_0) - \epsilon = y_0$  and  $x_0 > a$ . We can assume that  $x - \delta > a$  since  $\delta$  can be arbitrarily small, and we claim  $x_0 - \delta$  is an upper bound for  $S$ . To prove this, if  $x > x_0 - \delta$ , then either  $|x - x_0| < \delta$ , in which case  $f(x) > f(x_0) - \epsilon = y_0$ , or  $x > x_0$  then  $x \neq S$  since  $x_0$  is an upper bound for  $S$ . Therefore, if  $x > x_0 - \delta$ , then  $x \neq S$ , thus proving the claim. This contradicts that  $x_0$  is the supremum of  $S$ .

□

**Example.** Prove that the equation

$$2x^3 + 2x - 4 = 0$$

has a unique root in  $[0, 1]$ .

*Proof.* Set  $f(x) := 3x^2 + 2x - 4$ , this function is continuous since it is a polynomial. We have  $f(0) = -4 < 0$  and  $f(1) = 1 > 0$ , so by the intermediate value theorem, there exists  $c \in [0, 1]$  such that  $f(c) = 0$ . It follows that  $c$  is unique since the polynomial is injective by virtue of  $x^3$  and  $x$  being injective. □

## 1.1 Fixed-Point Iteration

**Definition 1.1.1.** We say that the value  $x = r$  is a fixed point for a function  $g(x)$  if  $g(r) = r$ .

**Example.**  $g(x) = \frac{5-x^2}{4}$ .  $r = 1$  is a fixed-point for  $g$  since  $g(1) = 1$ .

Graphically, fixed-point of  $g(x)$  correspond to the intersection of the graph of  $g(x)$  and the line  $y = x$ . Given an equation  $f(x) = 0$ , we can write it under the form

$$g(x) = x$$

by isolating one  $x$  in the equation.

**Example.**  $3x^3 + 2x - 5 = 0$ . We can write this as

$$x = \frac{5 - 3x^3}{2}$$

Set  $g(x) := \frac{5-3x^3}{2}$ . Then  $g(x) = x$ . Finding a root for  $f(x) = 0$  is equivalent to finding a fixed-point for  $g(x)$ .

### 1.1.1 Steps to Solving Using Fixed-Point Iteration

Start with a first estimation  $x_0$  (will be given) of the root, and form the following sequence (known as the *iteration sequence*)

$$x_0, x_1 = g(x_0), x_2 = g(x_1), \dots, x_n = g(x_{n-1})$$

If this sequence converges to a value  $a$ , then we can prove that  $a$  is a fixed-point for  $g$ , hence a root for  $f(x) = 0$ .

**Theorem 1.1.1.** Assume that the function  $g$  has a fixed-point  $s$  on an interval  $I$ , if

- (i)  $g(x)$  is continuous on  $I$
- (ii)  $g'(x)$  is continuous on  $I$
- (iii)  $|g'(x)| < 1$  for all  $x \in I$

Then the iteration sequence converges.

The steps for solving are as follows

1. Start with  $f(x) = 0$
2. Rewrite  $f(x) = 0$  under the form  $x = g(x)$
3. Verify that the sequence  $x_0, x_1 = g(x_0), x_2 = g(x_1), \dots, x_n = g(x_{n-1})$  converges using the above theorem (or otherwise)
4. Compute terms of the above sequence and stop when you reach the required accuracy

**Example.** Consider the equation

$$x^3 + 12x - 3 = 0$$

1. Prove that the equation has a unique root in  $[-1.9, 1.9]$
2. Use the Fixed-Point iteration method to estimate the value of the root to 6 decimal points starting with  $x_0 = 1.8$

**Solution:** Using the steps, we have

1. Set  $f(x) := x^3 + 12x - 3$ . Since  $f(x)$  is a polynomial, it is continuous, so by the intermediate value theorem, we have there exists  $c \in [-1.9, 1.9]$  such that  $f(c) = 0$ .  $f(x)$  is injective since  $x^3$  and  $x$  are injective, so  $c$  is unique.
2. Set  $g(x) := \frac{3-x^3}{12}$ .

3. Checking the conditions of the theorem,  $g(x)$  is continuous since it is a polynomial,  $g'(x) = -\frac{x^2}{4}$  is continuous since it is a polynomial. Then

$$|g'(x)| = \frac{x^2}{4} \leq \frac{1.9^2}{4} = 0.902 < 1$$

Therefore, the sequence converges.

4. We have to calculate the terms of the iteration sequence,

$$\begin{aligned}x_0 &= 1.8 \\x_1 &= g(x_0) = \frac{3 - 1.8^2}{12} = -0.236000 \\x_2 &= g(x_1) = \frac{3 - (0.236)^2}{12} = 0.251095 \\x_3 &= g(x_2) = \frac{3 - (0.251095)^2}{12} = 0.24861 \\x_4 &= g(x_3) = \frac{3 - (0.24861)^2}{12} = 0.248718 \\x_5 &= g(x_4) = \frac{3 - (0.248718)^2}{12} = 0.248718\end{aligned}$$

We stop when 2 consecutive terms agree on the first 6 decimal points. So the root is 0.248718 correct to 6 decimal points.

## 1.2 Newton's Method

Newton's method is a technique for solving equations of the form  $f(x) = 0$  by successive approximation. The idea is to pick an initial guess  $x_0$  such that  $f(x_0)$  is reasonably close to 0. We then find the equation of the line tangent to  $y = f(x)$  at  $x = x_0$ , and determine where this tangent line intersects the  $x$  axis at the new point  $x_1$ . So,

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

We then find the equation of the line tangent to  $y = f(x)$  at  $x = x_1$ , and repeat this process, so we have

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

**Example.** Using Newton's method, estimate the value of the root of the equation

$$x^3 + 12x - 3 = 0$$

on  $[0, 2]$ . Start by showing that the equation has a unique root on  $[0, 2]$ , then approximate (to 6 decimal places) with the starting point  $x_0 = 1.8$ .

**Solution.** We have  $f(x) = x^3 + 12x - 3$ , and

$$f(0) = -3 \text{ and } f(2) = 29$$

Therefore by the intermediate value theorem, there exists  $c \in [0, 2]$  such that  $f(c) = 0$ .  $f(x)$  is injective since  $f'(x) = 2x^2 + 12$  is strictly increasing on  $[0, 2]$ , so  $c$  is unique. Now using Newton's method,

$$x_0 = 1.8$$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 0.675138$$

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 0.270469$$

$$x_3 = x_2 - \frac{f(x_2)}{f'(x_2)} = 0.248748$$

$$x_4 = x_3 - \frac{f(x_3)}{f'(x_3)} = 0.248718$$

$$x_5 = x_4 - \frac{f(x_4)}{f'(x_4)} = 0.248718$$

Therefore, the our root is 0.248718 correct to 6 decimal places.

**Example.** Consider the equation

$$x^3 - 2x - 5 = 0$$

- (i) Prove that the equation has a unique root in  $[2, 3]$
- (ii) Starting with  $x_0 = 3$ , estimate the root of the equation to 6 decimal places using Newton's method.

**Solution.**

- (i) We have  $f(2) = -1$  and  $f(3) = 16$ , therefore by the intermediate value theorem there exists  $c \in [2, 3]$  such that  $f(c) = 0$ .  $f'(x) = 3x^2 - 2$  is injective since if  $f(x_1) = f(x_2)$ , then we have

$$f(x_1) = f(x_2)$$

$$\implies x_1^3 - 2x_1 - 5 = x_2^3 - 2x_2 - 5$$

$$\implies x_1^3 - 2x_1 = x_2^3 - 2x_2$$

Then  $x^3$  and  $x$  are injective functions, so we must have that  $x_1 = x_2$  and therefore the root is unique. Alternatively, we can look at the derivative on its interval,

$$\begin{aligned} 2 &\leq x \leq 3 \\ 4 &\leq x^2 \leq 9 \\ 12 &\leq 3x^2 \leq 27 \\ 10 &\leq 3x^2 - 2 \leq 25 \end{aligned}$$

Therefore the derivative is positive so the function is strictly increasing, and thus injective.

(ii) Starting with  $x_0 = 3$ , using Newton's method we get

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 3 - \frac{3^3 - 2(3) - 5}{3(3)^2 - 2} = 2.600000$$

$$x_2 = 2.6 - \frac{f(2.6)}{f'(2.6)} = 2.127197$$

$$x_3 = x_2 - \frac{f(2.127197)}{f'(2.127197)} = 2.0945136$$

$$x_4 = x_3 - \frac{f(2.094552)}{f'(2.094552)} = 2.094552$$

$$x_5 = x_4 - \frac{f(x_4)}{f'(x_4)} = 2.094551$$

$$x_6 = x_5 - \frac{f(x_5)}{f'(x_5)} = 2.094551$$

Therefore, we have  $x \approx 2.094551$  correct to 6 decimal places.

**Example.** Use Newton's Method with  $x_0 = 2$  to estimate the value of  $\sqrt[3]{7.9}$  correct to 6 decimal places.

**Solution.** We can set  $x := \sqrt[3]{7.9}$ , so we have  $x^3 - 7.9 = 0$ . Then this can be solved the same as the previous examples.

## 1.3 The Secant Method

The tangent line to the curve of  $y = f(x)$  with the point of tangency  $(x_0, f(x_0))$  was used in Newton's approach. The graph of the tangent line about  $x = \alpha$  is essentially the same as the graph of  $y = f(x)$  when  $x_0 \approx \alpha$ . The root of the tangent line was used to approximate  $\alpha$ . Consider employing an approximating



line based on interpolation. Given 2 root estimations  $x_0$  and  $x_1$ , then we have a linear function

$$q(x) = a_0 + a_1x$$

with  $q(x_0) = f(x_0)$ , and  $q(x_1) = f(x_1)$ . This line is also known as the secant line, with the formula

$$q(x) = \frac{(x_1 - x)f(x_0) + (x - x_0)f(x_1)}{x_1 - x_0}$$

The linear equation  $q(x) = 0$  with the root denoted by  $x_2$  is given by

$$x_2 = x_1 - f(x_1) \cdot \frac{x_1 - x_0}{f(x_1) - f(x_0)}$$

This equation can now be employed for every term in the sequence,

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

**Example.** Use the secant method with  $x_0 = 2$  and  $x_1 = 1.9$  to estimate the root of the equation to 6 decimal places

$$2 \sin x - x = 0$$

**Solution.** We have  $f(x) = 2 \sin x - x$ , we can start calculating the terms of the sequence

$$x_2 = x_1 - f(x_1) \frac{x_1 - x_0}{f(x_1) - f(x_0)} = 1.9 - (2 \sin(1.9) - 1.9) \frac{1.9 - 2}{(2 \sin(1.9) - 1.9) - (2 \sin(2) - 2)} = 1.895747$$

$$x_3 = x_2 - f(x_2) \frac{x_2 - x_1}{f(x_2) - f(x_1)} = 1.895747$$

Therefore the root is  $x \approx 1.895747$  correct to 6 decimal places.

# Chapter 2

## Interpolation

### 2.1 Generalities

Given a set of  $n + 1$  data points  $(x_0, f_0), \dots, (x_n, f_n)$  where

$$f_i = f(x_i)$$

for some unknown function  $f$ , the goal is to find a *polynomial* function of degree  $n$ , say  $p_n(x)$ , where its graph goes through all the datapoints. We then can use the approximation  $f(x) \approx p_n(x)$ .

**Theorem 2.1.1.** *Given a collection of  $n + 1$  data points  $(x_0, f_0), \dots, (x_n, f_n)$  in the cartesian plane such that*

$$x_0 < x_1 < x_2 < \dots < x_n$$

*Then there exists a unique polynomial of degree  $\leq n$  such that*

$$p_n(x_i) = f_i \quad \forall i \in \{0, 1, \dots, n\}$$

If we use the approximation  $f(x) \approx p_n(x)$ , then the absolute error ( $|f(x) - p_n(x)|$ ) is given by the following theorem.

**Theorem 2.1.2** (Error Formula). *The error formula with the above notation is*

$$|f(x) - p_n(x)| = |(x - x_0)(x - x_1) \cdots (x - x_n)| \frac{f^{(n+1)}(t)}{(n+1)!}$$

### 2.2 Lagrange Interpolation

Recall that our objective is approximate the function  $f(x)$  given  $n+1$  datapoints of the form  $(x_0, f_0), (x_1, f_1), \dots, (x_n, f_n)$ . Lagrange proved that the following polynomial goes through all of these points

$$p_n(x) = L_0(x)f_0 + L_1(x)f_1 + \dots + L_n(x)f_n$$

Where

$$\begin{aligned} L_0 &= \frac{(x - x_1)(x - x_2) \cdots (x - x_n)}{(x_0 - x_1)(x_0 - x_2) \cdots (x_0 - x_n)} \\ L_1 &= \frac{(x - x_0)(x - x_2) \cdots (x - x_n)}{(x_1 - x_0)(x_1 - x_2) \cdots (x_1 - x_n)} \\ L_2 &= \frac{(x - x_0)(x - x_1)(x - x_3) \cdots (x - x_n)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3) \cdots (x_2 - x_n)} \end{aligned}$$

**Example.** Consider the following 3 data points

$$(0.7, 2.2), (1.3, 3.1), (1.6, 4)$$

where  $f_i = f(x_i)$  for an unknown function  $f$ .

- (i) Find the Lagrange interpolation polynomial  $p_2(x)$ .
- (ii) Interpolate  $f(1)$ .
- (iii) If  $2 \leq |f'''(t)| \leq 3$  for all  $t \in [0.7, 1.6]$ , find an upper bound for the error in the approximation  $f(1) \approx p_2(1)$ .

**Solution.**

- (i) We know that our polynomial is of the form

$$p_2(x) = L_0(x)f_0 + L_1(x)f_1 + L_2(x)f_2$$

Where  $f_0, f_1, f_2$  are given. We can calculate the  $L_i$ 's as follows

$$\begin{aligned} L_0 &= \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} \\ &= \frac{(x - 1.3)(x - 1.6)}{(0.7 - 1.3)(0.7 - 1.6)} \\ &= 1.519x^2 - 5.3704x + 3.8519 \\ L_1 &= \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \\ &= \frac{(x - 0.7)(x - 1.6)}{(1.3 - 0.7)(1.3 - 1.6)} \\ &= -5.6667x^2 + 12.77778x - 6.22222 \\ L_2 &= \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} \\ &= \frac{(x - 0.7)(x - 1.3)}{(1.6 - 0.7)(1.6 - 1.3)} \\ &= 3.7037x^2 - 7.4074x + 3.3704 \end{aligned}$$

So our polynomial is

$$\begin{aligned} zp_2(x) &= (1.519x^2 - 5.3704x + 3.8519)(2.2) + (-5.6667x^2 + 12.7778x - 6.2222)(3.1) \\ &\quad + (3.7037x^2 - 7.4074x + 3.3704)(4) \\ &= 1.66667x - 1.83333x + 2.66667 \end{aligned}$$

We can check that this polynomial does go through all our points.

- (ii) We can interpolate  $f(1)$  by plugging in  $x = 1$  into our polynomial, so we have

$$f(1) \approx p_2(x) = 2.50000$$

- (iii) We can use the error formula to find an upper bound for the error,

$$\begin{aligned} |f(1) - p_2(1)| &= \left| (1 - 0.7)(1 - 0.13)(1 - 1.6) \frac{f'''(t)}{3!} \right| = 0.009|f'''(t)| \\ 0.0009(2) = 0.0018 &\leq |f(1) - p_2(1)| \leq 0.009(3) = 0.027 \end{aligned}$$

Therefore our lower bound is 0.0018 and our upper bound is 0.027.

**Example.** Consider the 4 points  $(x_i, f_i)$ ,

$$(0, 1), (1, 0.765), (2, 0.224), (3, -0.260)$$

- (i) Find the Interpolation polynomial  $p_3(x)$  using your Lagrange. Round your answer to 3 decimal places.
- (ii) Interpolate a value for  $f(2.5)$
- (iii) Given that  $0.75 \leq |f^{(4)}(t)| \leq 1.17$  for any  $t \in [0, 3]$ , give an upper and a lower bound for the error in the approximation  $f(2.5) \approx p_3(2.5)$ .

**Solution.**

- (i) We start with the Lagrange polynomial

$$p_3(x) = L_0(x)f_0 + L_1(x)f_1 + L_2(x)f_2 + L_3(x)f_3$$

$$\begin{aligned}
L_0(x) &= \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} \\
&= \frac{(x-1)(x-2)(x-3)}{(0-1)(0-2)(0-3)} \\
&= -0.167x^3 + x^2 - 1.833x + 1 \\
L_1(x) &= \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} \\
&= \frac{(x-0)(x-2)(x-3)}{(1-0)(1-2)(1-3)} \\
&= 0.5x^3 - 2.5x^2 + 3x \\
L_2(x) &= \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} \\
&= \frac{(x-0)(x-1)(x-3)}{(2-0)(2-1)(2-3)} \\
&= -0.5x^3 + 2x^2 - 1.5x \\
L_3(x) &= \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} \\
&= \frac{(x-0)(x-1)(x-2)}{(3-0)(3-1)(3-2)} \\
&= 0.167x^3 - 0.5x^2 + 0.33x
\end{aligned}$$

Then,

$$\begin{aligned}
p_3(x) &= (-0.167x^3 + x^2 - 1.833x + 1)(1) + (0.5x^3 - 2.5x^2 + 3x)(0.765) \\
&\quad + (-0.5x^3 + 2x^2 - 1.5x)(0.224) \\
&\quad + (0.167x^3 - 0.5x^2 + 0.33x)(-0.260) \\
&= 0.061x^3 - 0.335x^2 + 0.040x + 1
\end{aligned}$$

(ii) Then we can calculate  $f(2.5) \approx p_3(2.5)$

$$p_3(2.5) = 0.061(2.5)^3 - 0.335(2.5)^2 + 0.040(2.5) + 1 = -0.048$$

(iii) Then the error is given by

$$\begin{aligned}
|f(2.5) - p_3(2.5)| &= \left| (2.5-0)(2.5-1)(2.5-2)(2.5-3) \frac{f^{(4)}(t)}{4!} \right| \\
&= 0.039 |f^{(4)}(t)|
\end{aligned}$$

Then using  $0.75 \leq |f^{(4)}(t)| \leq 1.17$ , we have

$$0.039(0.75) \leq |f(2.5) - p_3(2.5)| \leq 0.039(1.17)$$

## 2.3 Newton's Divided Difference Interpolation Polynomial

Similar to Lagrange Interpolation, we start with  $n$  datapoints  $(x_0, f_0), \dots, (x_n, f_n)$  where  $f_i = f(x_i)$  for some unknown function  $f$ .

**Definition 2.3.1.** Given a node  $x_i$ ,

1. The first divided difference at  $x_i$  is defined as

$$f(x_i, x_{i+1}) = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

2. The second divided difference at  $x_i$  is

$$f(x_i, x_{i+1}, x_{i+2}) = \frac{f(x_{i+1}, x_{i+2}) - f(x_i, x_{i+1})}{x_{i+2} - x_i}$$

3. In general, the  $k$ th divided difference at  $x_i$  is

$$f(x_i, x_{i+1}, \dots, x_{i+k}) = \frac{f(x_{i+1}, \dots, x_{i+k}) - f(x_i, \dots, x_{i+k-1})}{x_{i+k} - x_i}$$

Then, we can define Newton's Interpolation polynomial as

$$\begin{aligned} p_n(x) &= f_0 + f(x_0, x_1)(x - x_0) \\ &\quad + f(x_0, x_1, x_2)(x - x_0)(x - x_1) + \dots \\ &\quad + f(x_0, \dots, x_n)(x - x_0)(x - x_1) \dots (x - x_{n-1}) \end{aligned}$$

**Example.** Given 3 datapoints,

$$(1.2, 4.5), (1.7, 5.9), (2.1, 7.4)$$

Calculate the interpolation polynomial using Newton's Divided Difference method and approximate  $f(1.8)$ .

**Solution.** We start by calculating *all* the first divided differences,

$$f(x_0, x_1) = \frac{f_1 - f_0}{x_1 - x_0} = \frac{5.9 - 4.5}{1.7 - 1.2} = 2.8$$

$$f(x_1, x_2) = \frac{f_2 - f_1}{x_2 - x_1} = \frac{7.4 - 5.9}{2.1 - 1.7} = 3.75$$

Now we can calculate all the second divided differences, in this case there is only one

$$f(x_0, x_1, x_2) = \frac{f(x_1, x_2) - f(x_0, x_1)}{x_2 - x_0} = \frac{3.75 - 2.8}{2.1 - 1.2} = 1.05556$$

So the Newton's Interpolation polynomial is

$$\begin{aligned} p_2(x) &= f_0 + f(x_0, x_1)(x - x_0) + f(x_0, x_1, x_2)(x - x_0)(x - x_1) \\ &= 4.5 + 2.8(x - 1.2) + 1.05556(x - 1.2)(x - 1.7) \\ &= 1.05556x^2 - 0.26111x + 3.29333 \end{aligned}$$

Then we can use this polynomial to approximate  $f(1.8)$ ,

$$f(1.8) \approx p_2(1.8) = 6.24333$$

## Chapter 3

# Numerical Integration

The fundamental theorem of calculus states that if  $f$  is continuous on  $[a, b]$ , then

$$\int_a^b f(x)dx = F(b) - F(a)$$

where  $F'(x) = f(x)$ . In practice, it is often difficult to find an antiderivative of  $f(x)$ , so the goal of this chapter is to explore numerical methods to estimate the value of the integral.

### 3.1 Midpoint Method

The idea is to divide the interval  $[a, b]$  into  $n$  subintervals of equal length, and approximate the function  $f(x)$  with the constant function  $y = f(x_i^*)$  on  $[x_i, x_{i+1}]$  where

$$x_i^* = \frac{x_i + x_{i+1}}{2}$$

is the mid point of the sub interval. The length of each subinterval is

$$h = \frac{b - a}{n}$$

So we approximate the integral with

$$\int_a^b f(x)dx \approx h[f(x_1^*) + f(x_2^*) + \cdots + f(x_n^*)]$$

The error in the midpoint rule satisfies the following inequality

$$|E_m| \leq \frac{M(b-a)^3}{24n^2}$$

where  $M$  is an upper bound for  $|f''(t)|$  for  $t \in [a, b]$ . To find an upperbound  $|f''(x)|$ , it might be useful to compute  $f'''(x)$  to see if  $f''(x)$  is decreasing or



increasing. If  $f''(x)$  is decreasing, then we can use  $f''(a)$  as an upper bound, and if  $f''(x)$  is increasing, then we can use  $f''(b)$  as an upper bound.

**Example.** Consider the integral

$$I = \int_1^2 x \ln x dx$$

Use the midpoint rule to estimate the value of  $I$  with a maximum error of 0.001.

**Solution.** We first need to divide the interval  $[1, 2]$  into  $n$  subintervals of length  $h = \frac{1}{n}$ . Then we can calculate the value for  $n$  to meet the error requirement,

$$f(x) = x \ln x$$

$$f'(x) = \ln x + 1$$

$$f''(x) = \frac{1}{x}$$

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

The third derivative is negative on  $[1, 2]$  so  $f''(x)$  is decreasing, therefore

$$f''(2) \leq f''(x) \leq f''(1) \implies |f''(x)| \leq 1$$

So  $M = 1$ , then

$$|E_m| \leq \frac{1(2-1)^3}{24n^2} \leq 0.001 \implies n \geq 6.45$$

We take  $n = 7$  to have an error at most 0.001. Then we can calculate  $h$

$$h = \frac{b-a}{n} = \frac{1}{7}$$

$$x_1^* = \frac{1 + 8/7}{2} = \frac{15}{14}$$

$$x_2^* = x_1^* + \frac{1}{7} = \frac{17}{14}$$

$$x_3^* = x_2^* + \frac{1}{7} = \frac{19}{14}$$

$$x_4^* = x_3^* + \frac{1}{7} = \frac{21}{14}$$

$$x_5^* = x_4^* + \frac{1}{7} = \frac{23}{14}$$

$$x_6^* = x_5^* + \frac{1}{7} = \frac{25}{14}$$

$$x_7^* = x_6^* + \frac{1}{7} = \frac{27}{14}$$

Then we can calculate the approximation of the integral,

$$\begin{aligned}\int_1^2 x \ln x &\approx h[f(x_1^*) + \cdots + f(x_7^*)] \\ &= \frac{1}{7} \left[ \frac{15}{14} \ln \left( \frac{15}{14} \right) + \cdots + \frac{27}{14} \ln \left( \frac{27}{14} \right) \right] \\ &= 0.63571\end{aligned}$$

**Example.** Estimate the value of the following integral using the midpoint rule with a maximal absolute error of 0.001.

$$I = \int_0^{0.5} x \cos x dx$$

**Solution.** We have to first find  $n$

$$f(x) = x \cos x$$

$$f'(x) = \cos x - x \sin x$$

$$f''(x) = -\sin x - \sin x - x \cos x = -2 \sin x - x \cos x$$

We can see that

$$\begin{aligned}| -2 \sin x - x \cos x | &\leq | -2 \sin x | + | -x \cos x | \\ &= 2 | \sin x | + | x | | \cos x | \\ &\leq 2 + | x | \\ &\leq 2.5\end{aligned}$$

Thus  $M = 2.5$ , then by the error formula we have

$$|E_m| \leq \frac{2.5(0.5-0)}{24n^2} \leq 0.001 \implies n \geq \sqrt{\frac{2.5(0.5)^3}{24(0.001)}} = 2.79$$

We take  $n = 3$ . Then we can calculate  $h$ ,

$$\begin{aligned}h &= \frac{0.5-0}{3} = \frac{1}{6} \\ x_1^* &= \frac{0+1/6}{2} = \frac{1}{12} \\ x_2^* &= x_1^* + \frac{1}{6} = \frac{1}{4} \\ x_3^* &= x_2^* + \frac{1}{6} = \frac{5}{12}\end{aligned}$$

By the midpoint rule, we have

$$\begin{aligned}\int_0^{0.5} x \cos x dx &\approx h[f(x_1^*) + f(x_2^*) + f(x_3^*)] \\ &= \frac{1}{6} \left[ \frac{1}{12} \cos \left( \frac{1}{12} \right) + \frac{1}{4} \cos \left( \frac{1}{4} \right) + \frac{5}{12} \cos \left( \frac{5}{12} \right) \right]\end{aligned}$$

## 3.2 Trapezoidal Rule

Similar to the mid-point rule, we start by dividing the interval for the integral

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

into  $n$  subintervals  $(x_0, x_1), (x_1, x_2), \dots, (x_{n-1}, x_n)$ . The length of the intervals  $h$  is

$$h = \frac{b-a}{n}$$

we approximate  $f(x)$  with the linear function to calculate the areas of the trapezoids that are formed by the graph of  $f(x)$  and the  $x$ -axis. So

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

**Theorem 3.2.1.** *The absolute error  $|E_T|$  in the Trapezoidal rule satisfies*

$$|E_T| \leq \frac{M(b-a)^3}{12n^2}$$

**Example.** Use the Trapezoidal rule with a maximal absolute error of 0.01 to estimate the value of the integral

$$\int_0^1 e^{-x^2} dx$$

**Solution.** First we compute  $n$ ,

$$f(x) = e^{-x^2}$$

$$f'(x) = -2xe^{-x^2}$$

$$f''(x) = -2e^{-x^2} + 4x^2e^{-x^2}$$

$$f'''(x) = -2e^{-x^2} + 4x^2e^{-x^2}$$

$$f''''(x) = 8xe^{-x^2} + (-2 + 4x^2)(-2xe^{-x^2}) = e^{-x^2}4x(3 - 2x^2)$$

From the third derivative we see that  $f'''(x)$  is always positive on  $[0, 1]$ , so  $f''(x)$  is increasing, therefore

$$f''(0) \leq f''(x) \leq f''(1) \implies -2 \leq f''(x) \leq -2e^{-1} + 4e^{-1}$$

Thus we can take  $M = 2$ . Then by the error formula we have

$$\frac{2}{12n^2} \leq 0.01 \implies n \geq \sqrt{\frac{1}{6(0.01)}} \approx 4.08$$

Then we take  $n = 5$ . So our length of each subinterval is

$$h = \frac{1-0}{5} = 0.2$$

Now we can approximate the integral

$$\begin{aligned} \int_0^1 e^{-x^2} dx &\approx \frac{0.2}{2} [f(0) + 2f(0.2) + 2f(0.4) + 2f(0.6) + 2f(0.8) + f(1)] \\ &= 0.1 \left( 1 + 2e^{-0.2^2} + 2e^{-0.4^2} + 2e^{-0.6^2} + 2e^{-0.8^2} + 2e^{-1} \right) \end{aligned}$$

### 3.3 Simpson's Rule

We start by subdividing  $[a, b]$  into an *even* number of subintervals. The idea is to estimate the function  $f(x)$  in every subinterval with a polynomial of degree 2.

$$\int_a^b f(x) \approx \frac{h}{3} [f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + f(b)]$$

where  $h = \frac{b-a}{n}$  and  $n$  is the number of subintervals. The error in Simpson's rule is given by

$$|E_S| \leq \frac{M(b-a)^5}{180n^4}$$

Where  $M$  is the upperbound for the fourth derivative of  $f(x)$ .

**Example.** Using Simpson's rule, with a maximal error of 0.001, estimate the value of the integral

$$\int_{0.5}^{1.5} x^2 \ln x dx$$

**Solution.** We start by computing  $n$ ,

$$f(x) = x^2 \ln x$$

$$f'(x) = 2x \ln x + x$$

$$f''(x) = 2 \ln x + 3$$

$$f'''(x) = \frac{2}{x}$$

$$f^{(4)}(x) = -\frac{2}{x^2}$$

$$f^{(5)}(x) = \frac{4}{x^3}$$

The fifth derivative is always positive so  $f^{(4)}$  is increasing, therefore

$$f^{(4)}(0.5) \leq f^{(4)}(x) \leq f^{(4)}(1.5) \implies |f^{(4)}(x)| \leq 8$$

So we can take  $M = 8$ . Then by the error formula we have

$$\frac{8(1.5 - 0.5)}{180n^4} \implies n \geq \sqrt[4]{\frac{8}{180(0.001)}} \approx 2.58$$

We need an even  $n$  so we take  $n = 4$ . Then we can calculate  $h$ ,

$$\begin{aligned} h &= \frac{1}{4} \\ x_0 &= 0.5 \\ x_1 &= 0.5 + \frac{1}{4} = 0.75 \\ x_2 &= 0.75 + \frac{1}{4} = 1 \\ x_3 &= 1 + \frac{1}{4} = 1.25 \\ x_4 &= 1.25 + \frac{1}{4} = 1.5 \end{aligned}$$

Then we can approximate the integral,

$$\begin{aligned} \int_{0.5}^{1.5} x^2 \ln x dx &\approx \frac{0.25}{3} [f(0.5) + 4f(0.75) + 2f(1) + 4f(1.25) + f(1.5)] \\ &= \frac{1}{12} [0.5^2 \ln 0.5 + 4(0.75)^2 \ln 0.75 + 2(1)^2 \ln 1 + 4(1.25)^2 \ln 1.25 + (1.5)^2 \ln 1.5] \\ &\approx 0.123915 \end{aligned}$$

### 3.4 Gaussian Quadrature

The Gaussian Quadrature of order  $n$  consists of estimating the integral

$$\int_{-1}^1 f(t) dt$$

using an expression of the form

$$\int_{-1}^1 f(t) dt \approx w_1 f(t_1) + \cdots w_n f(t_n)$$

where  $t_1, \dots, t_n$  are not necessarily equidistant and are called the *nodes* and  $w_1, \dots, w_n$  are constants called the coefficients. The approximation becomes an equality if  $f(t)$  is a polynomial of degree  $2n-1$ . In general, to convert  $\int_a^b f(x) dx$  to  $\int_{-1}^1 g(t) dt$ , we use the following change of variables

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

We then use a table of values to find the nodes and coefficients.

Order $n$	Nodes $t_i$	Coefficients $w_i$
1	0	2
2	$\pm\sqrt{\frac{1}{3}}$	1
3	$\pm\sqrt{\frac{3}{5}}$ 0	$\frac{5}{9}$ $\frac{8}{9}$
4	-0.8611363116	0.3478548451
	-0.3399810436	0.6521451549
	0.3399810436	0.6521451549
	0.8611363116	0.3478548451
5	-0.9061798459	0.2369268850
	-0.5384693101	0.4786286705
	0.0	0.5688888889
	0.5384693101	0.4786286705
	0.9061798459	0.2369268850

**Example.** Use Gaussian Quadrature of order 4 to estimate the value of

$$\int_0^1 \sin(x^2) dx$$

**Solution.** First we substitute  $x$  with

$$x = \frac{b-a}{2}t + \frac{b+a}{2} = \frac{1}{2}t + \frac{1}{2}$$

$$\frac{dx}{dt} = \frac{1}{2} \implies dx = \frac{dt}{2}$$

$$\int_0^1 \sin(x^2) dx = \int_{-1}^1 \sin\left(\frac{(t+1)^2}{4}\right) \frac{1}{2} dt$$

Then we can use Gaussian Quadrature of order 4 to estimate the value of the integral,

$$\begin{aligned} \int_{-1}^1 \sin\left(\frac{(t+1)^2}{4}\right) \frac{1}{2} dt &\approx w_1 f(t_1) + w_2 f(t_2) + w_3 f(t_3) + w_4 f(t_4) \\ &= 0.3479 f(-0.8611) + 0.6521 f(-0.3399) \\ &\quad + 0.6521 f(0.3399) + 0.3479 f(0.8611) \end{aligned}$$