MAT 2384: Numerical Methods Lecture Notes

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Contents

Chapter 1

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

Given a continous 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 $f : [a, b] \to \mathbb{R}$ be a continous 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

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

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 $x_0 \coloneqq \sup S \in [a, b]$. We want $f(x_0) = y_0$. Consider the cases where $f(x_0) = y_0$, $f(x_0) < y_0$, and $f(x_0) \geq y_0$.

- **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 $\epsilon \coloneqq y_0 - f(x_0)$. Since f is continous 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 $\epsilon \coloneqq f(x_0) - y_0$. Since f is continous 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 δ can be arbitrarily small, and we claim $x_0 - \delta$ is an upper bound for S. To prove this, if $x > x - \delta$, 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 $f(x) \coloneqq 3x^2 + 2x - 4$, 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*)

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

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 $x_0, x_1 = g(x_0), x_2 = g(x_1), \ldots, x_n = g(x_{n-1})$ 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 striclty increasing on $[0, 2]$, so c is unique. Now using Newton's method,

$$\begin{aligned}
x_0 &= 1.8 \\
x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} &= 0.675138 \\
x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} &= 0.270469 \\
x_3 = x_2 - \frac{f(x_2)}{f'(x_2)} &= 0.248748
\end{aligned}$$

$$x_4 = x_3 - \frac{f(x_3)}{f'(x_3)} = 0.248718$$
$$x_5 = x_4 - \frac{f(x_4)}{f'(x_4)} = 0.248718$$

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

$$\begin{aligned} &f(x_1) = f(x_2) \\ \implies &x_1^3 - 2x_1 - 5 = x_2^3 - 2x_2 - 5 \\ \implies &x_1^3 - 2x_1 = x_2^3 - 2x_2 \end{aligned}$$

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,

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

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 $x \coloneqq \sqrt[3]{7.9}$, 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 $(x0, f(x0)$ 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 α. Consider employing an approximating line based on interpolation. Given 2 root estimations x_0 and x_1, then we have a linear function

$$q(x) = a_0 + a_1 x$$

with $q(x_0) = f(x_0)$, and $q(x_1) = f(x_1)$. This line is alo 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 sequnce

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

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

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 $(x_0, f_0), \ldots, (x_n, f_n)$ where

$$f_i = f(x_i)$$

for some unkown 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 $(x_0, f_0), \ldots, (x_n, f_n)$ in the cartesian plane such that*

$$x_0 < x_1 < x_2 < \cdots < x_n$$

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

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

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 $(x_0, f_0), (x_1, f_1), \ldots, (x_n, f_n)$. Lagrange proved that the following polynomial goes through all of these points

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

Where

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

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

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

So our polynomial is

$$\begin{aligned}
zp_2(x) &= (1.519x^2 - 5.3704x + 3.8519)(2.2) + (-5.6667x^2 + 12.77778x - 6.22222)(3.1) \\
&+ (3.7037x^2 - 7.4074x + 3.3704)(4) \\
&= 1.66667x - 1.83333x + 2.66667
\end{aligned}$$

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 $(x_0, f_0), \ldots, (x_n, f_n)$ 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 kth divided difference at x_i is*

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

Then, we can define Newton's Interpolation polynomial as

$$\begin{aligned} p_n(x) = f_0 &+ f(x_0, x_1)(x - x_0) \\ &+ f(x_0, x_1, x_2)(x - x_0)(x - x_1) + \cdots \\ &+ f(x_0, \ldots, x_n)(x - x_0)(x - x_1) \cdots (x - x_n) \end{aligned}$$

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 fundemental 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 satifies 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

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

So $M = 1$, then

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

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 uing 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

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

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

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

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

$$h = \frac{0.5-0}{3} = \frac{1}{6}$$

$$x_1^* = \frac{0+1/6}{2} = \frac{1}{12}$$
$$x_2^* = x_1^* + \frac{1}{6} = \frac{1}{4}$$
$$x_3^* = x_2^* + \frac{1}{6} = \frac{5}{12}$$

By the midpoint rule, we have

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

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),. . .,(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

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

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

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

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.

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

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,

$$\begin{aligned}
f(x) &= x^2 \ln x \\
f'(x) &= 2x \ln x + x \\
f''(x) &= 2 \ln x + 3 \\
f'''(x) &= \frac{2}{x} \\
f^{(4)}(x) &= -\frac{2}{x^2} \\
f^{(5)}(x) &= \frac{4}{x^3}
\end{aligned}$$

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,

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

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 $t_1, \ldots, t_n$ are not necessarily equidistant and are called the *nodes* and $w_1, \cdots w_n$ 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	-0.5773502692	1
	0.5773502692	1
3	-0.7745966692	0.555555556
	0	0.888888889
	0.7745966692	0.555555556
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

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

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

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

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

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

Chapter 4

Numerical Methods to Solving First-Order IVP's

Given a first-order IVP

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

The goal of this chapter is to explore techniques that allow us to estimate values of the function y.

4.1 Euler Method

Given a step size between our x values, Euler's method uses the formula

$$x_{n+1} = x_n + h$$

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

where h is the given step size, and $y' = f(x, y)$ for the differential equation.

Example. Consider the IVP

$$y' = 2x + y,\ y(0) = -1$$

Use Euler's method with a step size $h = 0.2$ to estimate the values of the function y on the interval $[0, 0.6]$.

Solution. We have $f(x, y) = 2x + y$, $x_0 = 0$, $y_0 = -1$, and $h = 0.2$. Now we can caluclate each step

$$x_1 = x_0 + h = 0.2$$

$$y_1 = y_0 + hf(x_0, y_0) = -1 + 0.2(-1) = -1.2$$

$$x_2 = x_1 + h = 0.4$$

$$y_2 = y_1 + hf(x_1, y_1) = -1.2 + 0.2(2(0.2) - 1.2) = -1.36$$

$$x_3 = x_2 + h = 0.6$$

$$y_3 = y_2 + hf(x_2, y_2) = -1.36 + 0.2(2(0.4) - 1.36) = -1.472$$

4.2 Improved Euler Method

The improved Euler method consists of using Euler's method to "predict" the value for y, then "correct" it at each step to have a more accurate value. Given a first order IVP

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

We have the x values at each step

$$x_{n+1} = x_n + h$$

Then the y values are

$$y^c_{n+1} = y^c_n + \frac{h}{2}\left[f(x_n, y^c_n) + f(x_{n+1}, y^p_{n+1})\right]$$

where y^p is the predicted y value obtained from the standard Euler method.

Example. Consider the previous IVP with the improved Euler method,

$$y' = 2x + y,\ y(0) = -1$$

We're given $f(x,y) = 2x + y$, $h = 0.2$, $y_0 = -1$, and $x_0 = 0$, then

$$x_1 = x_0 + h = 0.2$$
$$y_1^p = y_0 + hf(x_0, y_0) = -1 + 0.2(-1) = -1.2$$
$$y_1^c = y_0 + \frac{h}{2}\left[f(x_0, y_0) + f(x_1, y_1^p)\right] = -1 + 0.1\left[-1 + 2(0.2) - 1.2\right] = -1.18$$
$$x_2 = x_1 + h = 0.4$$
$$y_2^p = y_1^c + hf(x_1, y_1^c) = -1.18 + 0.2(2(0.2) - 1.18) = -1.336$$
$$y_2^c = y_1^c + \frac{h}{2}\left[f(x_1, y_1^c) + f(x_2, y_2^p)\right] = -1.18 + 0.1\left[2(0.2) - 1.18 + 2(0.4)\right] = -1.3116$$
$$x_3 = x_2 + h = 0.6$$
$$y_3^p = y_2^c + hf(x_2, y_2^c) = -1.3116 + 0.2(2(0.4) - 1.3116) = -1.41392$$
$$y_3^c = -1.3116 + 0.1\left[2(0.4) - 1.18 + 2(0.6) - 1.413192\right] = -1.384152$$

4.3 Runge-Kutta Method of Order 4

Given a first order ODE

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

In the improved Euler method, we had "2 steps" with "predicting" and "correcting" each term. The Runge-Kutta method of order 4 concists of "4 steps" to compute y_{n+1}. The formula is as follows. Note that the step size is given as h,

$$y' = f(x,y);\ y(x_0) = y_0$$
$$x_{n+1} = x_n + h$$
$$k_1 = hf(x_n, y_n)$$
$$k_2 = hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_1\right)$$
$$k_3 = hf\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}k_2\right)$$
$$k_4 = hf\left(x_n + h, y_n + k_3\right)$$
$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k3 + k_4)$$

Example. Conisder the IVP

$$y' = y - x^2 + 1;\ y(0) = \frac{1}{2}$$

Use Runge-Kutta Method of Order 4 to estimate the values of the function y, on the interval $[0,1]$, using a step size $h = 0.5$.

Solution. We have $x_0 = 0$, and $y_0 = \frac{1}{2}$, and $f(x,y) = y - x^2 + 1$. Now we can compute with a step size $h = 0.5$,

$$x_1 = x_0 + h = 0.5$$
$$k_1 = hf(x_0, y_0) = 0.5(\frac{1}{2} - 0 + 1) = 0.75$$
$$k_2 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1\right) = 0.5f(0.25, 0.875) = 0.90625$$
$$k_3 = hf\left(x_0 + \frac{h}{2}, y_0 + \frac{1}{2}k_2\right) = 0.5f(0.25, 0.953125) = 0.9453125$$
$$k_3 = hf\left(x_0 + h, y_0 + k_3\right) = 0.5f(0.5, 1.4453125) = 1.09765625$$

Then,

$$y_1 = y_0 + \frac{1}{6}(k_1 + 2k_2 + 3k_2 + k_4) = 1.4251306$$

So we get the new point

$$(x_1, y_1) = (0.5, 1.4251302)$$

Then we continue

$$\begin{aligned}
&x_2 = x_1 + h = 1 \\
&k_1 = hf(x_1, y_1) = 1.087561 \\
&k_2 = hf\left(x_1 + \frac{1}{2}h, y_1 + \frac{1}{2}k_1\right) = 1.2032014 \\
&k_3 = hf\left(x_1 + \frac{1}{2}h, y_1 + \frac{1}{2}k_2\right) = 1.2321167 \\
&k_4 = hf(x_1 + h, y_1 + k_3) = 1.3286235 \\
&y_2 = y_1 + \frac{1}{6}(k_1 + 2k_2 + 3k_2 + k_4) = 2.6396027
\end{aligned}$$

This gives us our final point

$$(x_2, y_2) = (1, 2.6396027)$$