MAT 2384: Numerical Methods Lecture Notes

Last Updated:

June 28, 2023

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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

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

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 $f(x_0) \geq y_0$.

- **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 $\epsilon := y_0 - f(x_0)$. 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 $\epsilon := f(x_0) - y_0$. 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 arbitrarly 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.

$\square$

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. $\square$

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,

$$\begin{aligned}
x_0 &= 1.8 \\
x_1 &= x_0 - \frac{f(x_0)}{f'(x_0)} = 0.675138 \\
x_2 &= x_1 - \frac{f(x_1)}{f'(x_1)} = 0.270469 \\
x_3 &= x_2 - \frac{f(x_2)}{f'(x_2)} = 0.248748 \\
x_4 &= x_3 - \frac{f(x_3)}{f'(x_3)} = 0.248718 \\
x_5 &= x_4 - \frac{f(x_4)}{f'(x_4)} = 0.248718
\end{aligned}$$

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,

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

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 $x \coloneqq \sqrt[3]{7.9}$, 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 $(x_0, f_0), \dots, (x_n, f_n)$ 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 $(x_0, f_0), \dots, (x_n, f_n)$ 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

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

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

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

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

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

So our polynomial is

$$\begin{aligned} p_2(x) &= (1.519x^2 - 5.3704x + 3.8519)(2.2) + (-5.6667x^2 + 12.77778x - 6.22222)(3.1) \\ &\quad + (3.7037x^2 - 7.4074x + 3.3704)(4) \\ &= 1.66667x - 1.83333x + 2.66667 \end{aligned}$$

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,

$$|f(1) - p_2(1)| = \left|(1 - 0.7)(1 - 0.13)(1 - 1.6)\frac{f'''(t)}{3!}\right| \quad = 0.009|f'''(t)|$$

$$0.0009(2) = 0.0018 \leq |f(1) - p_2(1)| \leq 0.009(3) = 0.027$$

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,

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

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

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

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*

$$f(x_i, x_{i+1}, x_{i+2}) = \frac{f(x_{i+1}, x_{i+2}) - f(x_1, x_{i+1})}{x_{i+2} - x_i}$$

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 $f(1.8)$,

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