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

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

S is a subset of [a, b] so it is bounded,  $a \in S$  since  $f(a) \le y_0$ . Therefore  $S \ne \emptyset$ . 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  $f(x_0) \ge y_0$ .

- 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  $f(x_0) < y_0 \le f(b)$ , 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  $\delta$  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.

**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

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

Therefore, the sequence converges.

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

$$x_0 = 1.8$$

$$x_1 = g(x_0) = \frac{3 - 1.8^2}{12} = -0.236000$$

$$x_2 = g(x_1) = \frac{3 - (0.236)^2}{12} = 0.251095$$

$$x_3 = g(x_2) = \frac{3 - (0.251095)^2}{12} = 0.24861$$

$$x_4 = g(x_3) = \frac{3 - (0.24861)^2}{12} = 0.248718$$

$$x_5 = g(x_4) = \frac{3 - (0.248718)^2}{12} = 0.248718$$

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

$$f(0) = -3$$
 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.

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

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 (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  $\alpha$ . Consider employing an approximating

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

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

with  $q(x_0) = f(x_0)$ , and  $q(x_1) = f(x_1)$ . This line is all 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 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  $(x_0, f_0), \ldots, (x_n, f_n)$  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

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

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.

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

### 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

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  $2 \le |f'''(t)| \le 3$  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

$$L_0 = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

$$= \frac{(x - 1.3)(x - 1.6)}{(0.7 - 1.3)(0.7 - 1.6)}$$

$$= 1.519x^2 - 5.3704x + 3.8519$$

$$L_1 = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$

$$= \frac{(x - 0.7)(x - 1.6)}{(1.3 - 0.7)(1.3 - 1.6)}$$

$$= -5.6667x^2 + 12.77778x - 6.22222$$

$$L_1 = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

$$= \frac{(x - 0.7)(x - 1.3)}{(1.6 - 0.7)(1.6 - 1.3)}$$

$$= 3.7037x^2 - 7.4074x + 3.3704$$

So our polynomial is

$$p_2(x) = (1.519x^2 - 5.3704x + 3.8519)(2.2) + (-5.6667x^2 + 12.77778x - 6.22222)(3.1) + (3.7037x^2 - 7.4074x + 3.3704)(4)$$
  
= 1.66667x - 1.83333x + 2.66667

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,

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

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

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

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

$$L_0(x) = \frac{(x - x_1)(x - x_2)(x - x_3)}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)}$$

$$= \frac{(x - 1)(x - 2)(x - 3)}{(0 - 1)(0 - 2)(0 - 3)}$$

$$= -0.167x^3 + x^2 - 1.833x + 1$$

$$L_1(x) = \frac{(x - x_0)(x - x_2)(x - x_3)}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)}$$

$$= \frac{(x - 0)(x - 2)(x - 3)}{(1 - 0)(1 - 2)(1 - 3)}$$

$$= 0.5x^3 - 2.5x^2 + 3x$$

$$L_2(x) = \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)}$$

$$= \frac{(x - 0)(x - 1)(x - 3)}{(2 - 0)(2 - 1)(2 - 3)}$$

$$= -0.5x^3 + 2x^2 - 1.5x$$

$$L_3(x) = \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)}$$

$$= \frac{(x - 0)(x - 1)(x - 2)}{(3 - 0)(3 - 1)(3 - 2)}$$

$$= 0.167x^3 - 0.5x^2 + 0.33x$$

Then.

$$p_3(x) = (-0.167x^3 + x^2 - 1.833x + 1)(1) + (0.5x^3 - 2.5x^2 + 3x)(0.765)$$

$$+ (-0.5x^3 + 2x^2 - 1.5x)(0.224)$$

$$+ (0.167x^3 - 0.5x^2 + 0.33x)(-0.260)$$

$$= 0.061x^3 - 0.335x^2 + 0.040x + 1$$

(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

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

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

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

Then, we can define Newton's Interpolation polynomial as

$$p_n(x) = f_0 + f(x_0, x_1)(x - x_0) + f(x_0, x_1, x_2)(x - x_0)(x - x_1) + \cdots + f(x_0, \dots, x_n)(x - x_0)(x - x_1) \cdots (x - x_n)$$

Example. Given 3 datapoints,

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

$$p_2(x) = f_0 + f(x_0, x_1)(x - x_0) + f(x_0, x_1, x_2)(x - x_0)(x - x_1)$$

$$= 4.5 + 2.8(x - 1.2) + 1.05556(x - 1.2)(x - 1.7)$$

$$= 1.05556x^2 - 0.26111x + 3.29333$$

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

$$\int_{a}^{b} f(x)dx \approx h[f(x_{1}^{*}) + f(x_{2}^{*}) + \dots + f(x_{n}^{*})]$$

The error in the midpoint rule satisfies the following inequality

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

where M is an upper bound for |f''(t)| for  $t \in [a, b]$ .