CS323 LECTURE NOTES - LECTURE 3

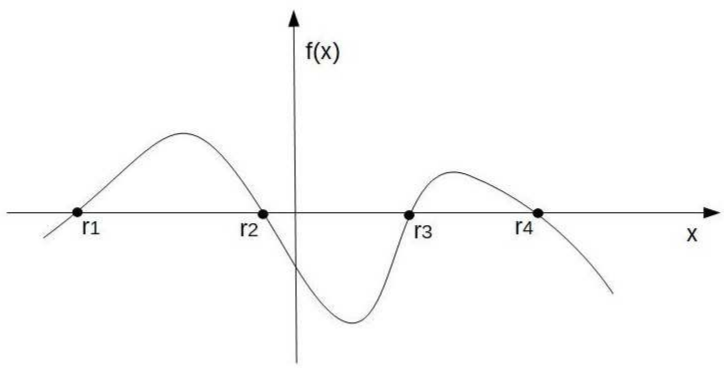
1 Roots of Real Valued Functions

1.1 Introduction

The problem that we will solve in this section consists of finding the roots of the following type of functions:

$$f : \mathbb{R} \to \mathbb{R}$$

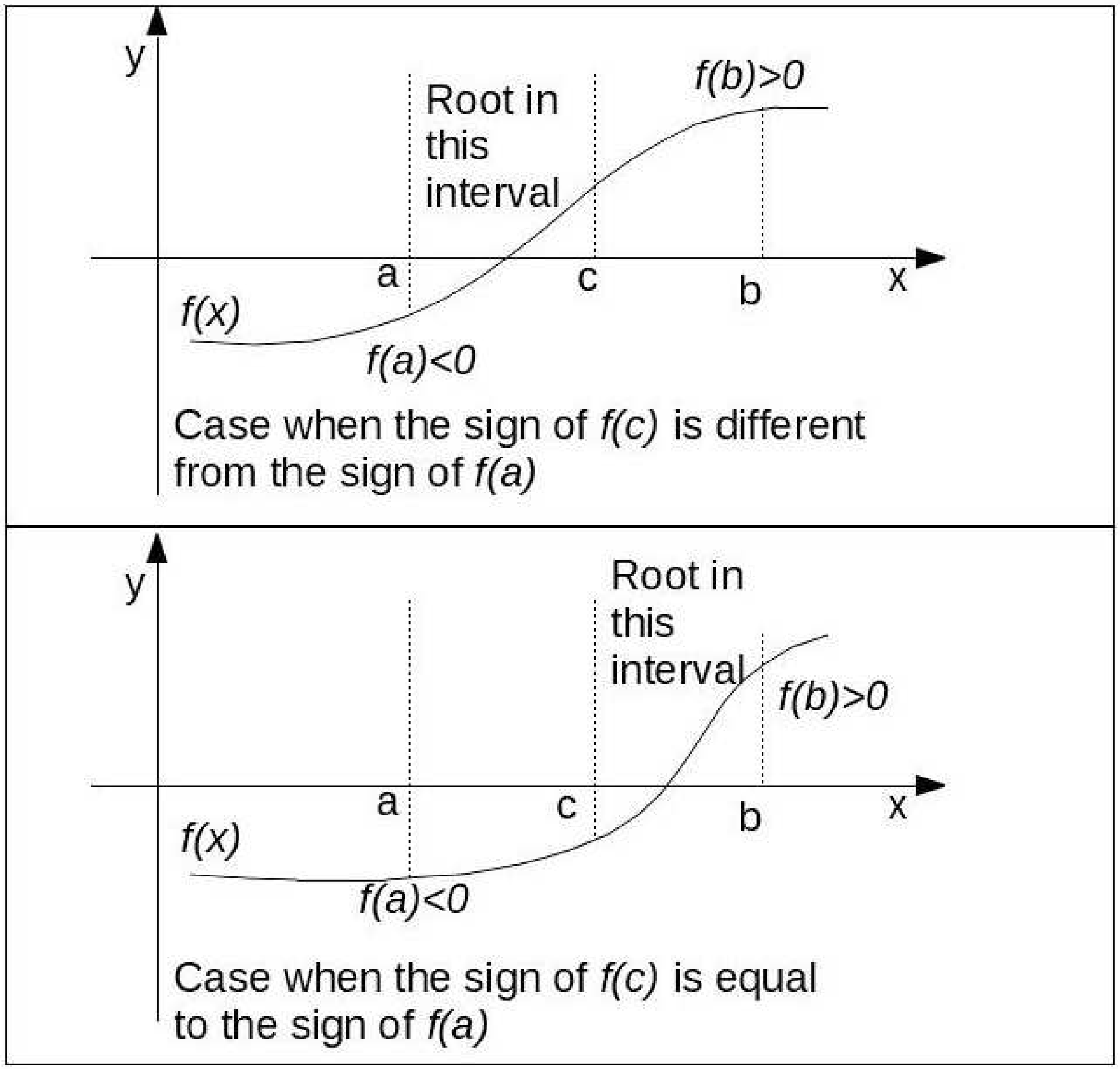
We can plot these functions:



What we want is to find at least one of the points where the graph of $f(x)$ intersects the x axis. These points are the roots of the function. In the example given in the figure we would like to find at least one of the points $(r_1, 0), (r_2, 0), (r_3, 0), (r_4, 0)$. However, we will also discuss later a method to obtain more than one root.

1.2 The Bisection Method

In this method the goal is to "trap" one of the roots between two real numbers that can be as close to each other as we want. If the function is continuous in $[a, b]$ and the sign of $f(a)$ is not the same as the sign of $f(b)$ then, the *Intermediate Value Theorem* tells us that there must be a real number $x \in [a, b]$ such that $f(x) = 0$.



Using this argument we obtain the bisection algorithm by starting with two values a and b such that the sign of $f(a)$ is different from the sign of $f(b)$. Using a and b we can compute the mid point between a and b

$$c = \frac{a+b}{2}$$

assuming that $f(c) \neq 0$ we observe the sign of $f(c)$, and notice that there are two cases:

- If the sign of $f(c)$ different from the sign of $f(a)$, then we know that there must be a root of $f(x)$ in the interval $[a, c]$ (because we assume $f(x)$ to be continuous in $[a, b]$)
- Otherwise (sign of $f(c)$ is the same as the sign of $f(a)$) the root must be in $[c, b]$ as show in the figure.

In this way we have a new interval half the length of the original one, that we can split in half again. This interval will be divided in half again, and again. This process could continue forever, but the algorithm would never stop, therefore it is necessary to provide a minimum interval length (ϵ), so that the algorithm stops as soon as it finds an interval smaller than ϵ. This value (ϵ) is the precision that we want our solution to have and is called the *error tolerance*. The error tolerance must always be provided by the end user as one of the values taken as input by the algorithm. We must also make sure that the function ($f(x)$) must be continuous in the interval $[a, b]$ for the algorithm to work correctly. The algorithm cannot verify the continuity of $f(x)$, so the user is responsible for providing such a function.

Let us proceed to write pseudocode for the algorithm.

BISECTION ALGORITHM

```
INPUT: function f : ℝ → ℝ
          a, b, ϵ ∈ ℝ
repeat
     c ← (a+b)/2
     if (f(c) = 0)
          print "The solution is " c
          stop
     else if (f(a)f(c) < 0)
          b ← c
     else
          a ← c
until |b − a| < ϵ
print "The root is in" [a, b]
```

Notice that $f(a)$ and $f(c)$ have distinct sign if and only if $f(a)f(c) <$ 0

EXAMPLE

Use the *Bisection Algorithm* to find one root of the function $f(x) = x^2 - 2$ with an error tolerance of 10^{-2}

We still need to provide the initial interval $[a, b]$ to the algorithm. This means that we need to find two points where the function has different sign. We can mentally find those starting points in the case of simple functions, or we can tabulate the function. In the case of the example let us tabulate the function for those values of $x \in \{0, 1, 2\}$.

x	$x^2 - 2$
0	-2
1	-1
2	2

From this table we can see that there is a sign change in the interval $[1, 2]$, which implies that one of the roots must be in that interval because $f(x) = x^2 - 2$ is continuous. In summary, the input values given to the algorithm are: $a = 1$, $b = 2$, $\epsilon = 0.01$

Now let us trace the bisection algorithm on the example given. It is a good exercise to take a calculator and do all the computation by hand to get a feel of how the algorithm works.

iteration	a	b	c	$f(a)$	$f(c)$	sign $f(a)f(c)$	$\|b-a\|$
0	1	2	1.5	-1	0.25	negative	1
1	1	1.5	1.25	-1	-0.4375	positive	0.5
2	1.25	1.5	1.375	-0.4375	-0.109375	positive	0.25
3	1.375	1.5	1.4375	-0.109375	0.06640625	negative	0.125
4	1.375	1.4375	1.40625	-0.109375	-0.0224609375	positive	0.0625
5	1.40625	1.4375	1.421875	-0.0224609375	0.0217285156	negative	0.03125
6	1.40625	1.421875	1.4140625	-0.0224609375	-0.0004272461	negative	0.015625
7	1.4140625	1.421875	1.41796875	-0.0004272461	0.010635376	negative	0.0078125

Let us describe what is going on during the first couple of iterations:

- Initially, the middle value between $a = 1$ and $b = 2$ is $c = 1.5$, and since there is a sign change between a and c (the sign of $f(a)f(c)$ is negative, then there must exist a root between a and c, therefore, the new value of b assigned in this first iteration is 1.5.
- During the first iteration the middle value between $a = 1$ and $b = 1.5$ is $c = 1.25$, and since there is no change of sign between a and c (the sign of $f(a)f(c)$ is positive then there must be a root between c and b, therefore, the new value of a assigned in this iteration is 1.25.
- The algorithm continues working in the same way until $|b - a| < 0.01$, and the algorithm terminates in the eighth iteration showing that a root exists in the interval $[1.4140625, 1.421875]$

The equation of this example can easily be solved algebraically since we only want to find the value of x for which $f(x) = 0$, i.e., $x^2 - 2 = 0$ which has a solution $x = \sqrt{2} = 1.414241$.
NUMBER OF ITERATIONS
If we want to determine how efficient this algorithm is, we need to compute the number of iterations required to solve a given equation. Notice that the algorithm starts by trying to find a root in an interval of length $b - a$, and after the first iteration, the interval length is reduced by $1/2$, i.e. $\frac{b-a}{2}$. In each iteration, the length of the candidate interval is reduced to $1/2$ of its previous length. Using this fact we can build the following table:

Iteration	Interval length $(b-a)$
0	$b-a$
1	$\frac{b-a}{2}$
2	$\frac{b-a}{2^2}$
3	$\frac{b-a}{2^3}$
$\vdots$	$\vdots$
n	$\frac{b-a}{2^n}$

We know that the algorithm stops when the length of the interval is less than ϵ, i.e.

$$\frac{b-a}{2^n} < \epsilon$$

Solving for n we get

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

and finally, since n must be integer,

$$n = \left\lceil \log_2 \frac{b-a}{\epsilon} \right\rceil$$

In the example of the previous section we started with an interval $[1, 2]$ and an $\epsilon = 0.01$,

$$n = \left\lceil \log_2 \frac{2-1}{0.01} \right\rceil = 7$$

Therefore, the number of iteration necessary to find a root with the given error tolerance is 7, which matches the tracing that we performed on the algorithm.

Assuming that $b - a = 1$, we show a table with the number of iterations that are necessary to find a root with the desired error tolerance $= \epsilon$.

ϵ	iterations
0.01	7
0.001	10
0.0001	14
0.00001	17
0.000001	20
0.0000001	24
0.00000001	27
0.000000001	30

2 Taylor Series Remainder

In many of the algorithms covered in the course we will need to use Taylor Series and in order to computed the error bounds we will need to make use of the Taylor's Theorem that computes the remainder.

Recall that Taylor Series can be use to approximate the value of $f(x)$ when a value of f and all the derivatives of f can be computed for a point x_0 "close to x.

$$f(x) = f(x_0)+f'(x_0)(x-x_0)+\frac{f''(x_0)}{2!}(x-x_0)^2+\frac{f'''(x_0)}{3!}(x-x_0)^3+\ldots$$

Since we can effectively compute the series only for a finite number n of terms, we can write it as:

$$f(x) = f(x_0) + \sum_{i=1}^{n} \frac{f^{(i)}(x_0)}{i!}(x - x_0)^i + R_n(x)$$

Where $R_n(x)$ is called *the remainder*, and it can be very useful to compute the error in Taylor series approximations. We are interested in finding out if the remainder can be written in such a way that looks like the term of degree $n + 1$ of the Taylor series, i.e. we will try to find a constant R such that the remainder can be written as:

$$R_n(x) = \frac{R}{(n+1)!}(x - x_0)^{n+1}$$

In order to find the R, we will find useful to define $f(x)$ written as a series (above) as a function of x_0, but in order not to be confused with the notation, I will use ξ instead of x_0, so we will rewrite $f(x_0)$ as $F(\xi)$,

$$F(\xi) = f(\xi) + \sum_{i=1}^{n} \frac{f^{(i)}(\xi)}{i!}(x - \xi)^i + \frac{R}{(n+1)!}(x - \xi)^{n+1}$$

Notice that $F(x_0)$ is exactly the same as the Taylor series, so its value is $f(x)$, and if we compute $F(x)$, all the terms $x - \xi$ are equal to 0. Therefore we have that:

$$
\begin{aligned}
F(x_0) &= f(x) \\
F(x) &= f(x)
\end{aligned}
$$

Since $x_0 \neq x$, we see that the function has the same value $y = f(x)$ for two different values of the x axis. So, we can use Rolle's Theorem (from calculus), which says that if a function $g(x)$ satisfies standard continuity conditions and $g(a) = g(b) \quad a \neq b$, then there exists a point $\xi \in [a, b]$ such that $g'(\xi) = 0$ (its derivative is 0).

So, in order to compute the value of the constant R we will use the equation given by Rolle's Theorem:

$$F'(\xi) = 0$$

where ξ is between x_0 and x.

Computing $F'(\xi)$ we have:

$$
\begin{aligned}
F'(\xi) &= f'(\xi) + \sum_{i=1}^{n} \left(\frac{f^{(i+1)}(\xi)}{i!}(x-\xi)^i + \frac{f^{(i)}(\xi)}{i!} i (x-\xi)^{i-1}(-1) \right) \\
&\quad + \frac{R}{(n+1)!}(n+1)(x-\xi)^n(-1)
\end{aligned}
$$

Simplifying the factorials since $a! = a(a-1)!$, we have

$$F'(\xi) = f'(\xi) + \sum_{i=1}^{n} \left(\frac{f^{(i+1)}(\xi)}{i!}(x-\xi)^i - \frac{f^{(i)}(\xi)}{(i-1)!}(x-\xi)^{i-1} \right) - \frac{R}{n!}(x-\xi)^n$$

To make clear that the summation is a telescoping series, notice that if we define

$$C_i = \frac{f^{(i+1)}(\xi)}{i!}(x-\xi)^i$$

clearly

$$C_{i-1} = \frac{f^{(i)}(\xi)}{(i-1)!}(x-\xi)^{i-1}$$

So, the summation is equal to

$$\begin{aligned}\sum_{i-1}^{n}(c_i - c_{i-1}) &= (c_1 - c_0) + (c_2 - c_1) + (c_3 - c_2) + \ldots (c_n - c_{n-1}) \\ &= -c_0 + c_n\end{aligned}$$

Therefore, the summation is equal to

$$-f'(\xi) + \frac{f^{n+1}(\xi)}{n!}(x-\xi)^n$$

Substituting the summation in $F'(\xi)$ we get

$$\begin{aligned}F'(\xi) &= f'(\xi) - f'(\xi) + \frac{f^{(n+1)}}{n!}(x-\xi)^n - \frac{R}{n!}(x-\xi)^n \\ &= \frac{(x-\xi)^n}{n!}(f^{(n+1)}(\xi) - R)\end{aligned}$$

Back to Rolle's Theorem, we have that there exists a ξ between x_0 and x, such that $F'(\xi) = 0$, so we have that

$$\frac{(x-\xi)^n}{n!}(f^{(n+1)}(\xi) - R) = 0$$

since $(x-\xi) \neq 0$, $n! \neq 0$, we can solve for R

$$R = f^{(n+1)}(\xi)$$

substituting R in the remainder

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)^{n+1}$$

So we can write down our complete Taylor Series:

$$f(x) = \sum_{i=0}^{n}\frac{f^{(i)}(x_0)}{i!}(x-x_0)^i + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)^{n+1}$$