ENGT103

Introduction to Mathematics

Case study:

Analyzing the advantages,disadvantes and limitations of Numerical Methods in solving the Root Finding Problem

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1. Introduction

In the Engineering and Technology field, it is extremely important to find the roots of an equation as they are useful to study the behavior of variables. This root finding problem is resolved in various ways such as using analytical or numerical methods.

The analytical method provides exact solutions, but they become hard to use when it comes to complex equations (e.g., finding several solutions).

To overcome this problem, numerical methods are applied.

Numerical solutions involve making initial guesses to find the roots and testing whether the equation is solved. It will give approximate results, but they are acceptable as they have sufficient accuracy. Although, in some special cases these methods can fail. This can be avoided as these special cases occur under certain circumstances that are related directly to the study of a function.

In this case study, the polynomial function f(x) will be studied:

$$f(x) = x^5 + 3.8x^4 - 46.7x^3 - 43.9x^2 + 103.5x + 48.1$$

and we want to solve the equation:

$$f(x) = 0$$

It is specified that the function has 5 real roots, between x = -10 and +10.
However, as stated earlier, numerical methods find approximate results that are acceptable if they have a specific accuracy.

3 numerical methods are discussed and tested to find solutions at a stated accuracy:

- The Interval Bisection Method (to find two roots of the given function at least 3 significant figures, 3 s.f.).
- The Rearrangement Method (to find the same two roots, to at least 6 significant figures, 6 s.f.).
- The Newton-Raphson Method (to find the same two roots, to at least 9 significant figures,9 s.f.).

All advantages and disadvantages of the methods will be discussed in depth in terms of practicability and speed of convergence.
In addition to that, it will be indicated how many iterations it took to find the roots to the desired accuracy (3,6,9 s.f.).
Convergent iterations means that you will find a result as it is getting closer and closer to the point you are looking for. It is done by repeating continuously a certain process.
This case study will also show cases of each method failing, to avoid those situations.

These numerical methods have become popular with the development of computing capabilities (especially in machine learning).
Hence, in this study case Excel and an advanced graphing calculator such as Desmos will be used.

Using these programs and analyzing accurately each method keeping in mind some important considerations can lead to a successful case study.

It is extremely important to analyze the graph first before starting any method.

It is time-consuming and not recommended to start doing any calculations or iterations if you have not looked at the graph first, as you will try finding the roots without having any knowledge about them.

Look at the graph first, it will tell you if a method is going to work before you do any calculations or iterations.

Therefore, the methods remain the same but plotting the graph on desmos is the priority.
After studying the function, it is possible to program excel and start doing the calculations.

1.1 The Interval Bisection Method

Finding a root means when the function itself is equal to 0.
As our aim is to find two different roots that give us zero when substituted into f(x), we will use the interval bisection method to find if there is any interval where there is change of sign for the f(x).

In this example, the function f(x) studied will be:

$$f(x) = x^3 + x^2 - 3x - 1$$

and we want to solve the equation:

$$f(x) = 0$$

This is how the graph looks like on desmos:

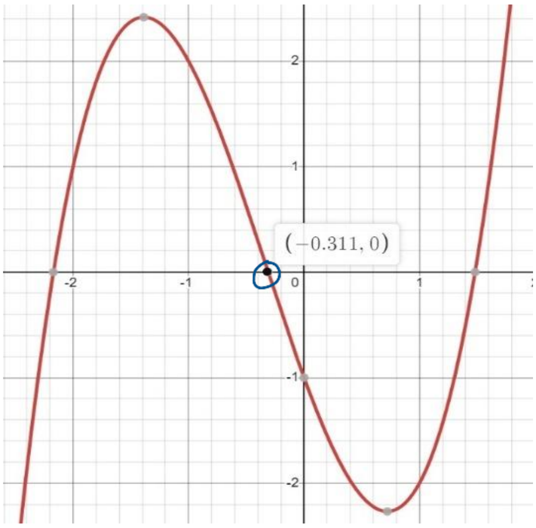

Figure 1(example for Interval bisection method)

Interval Bisection method:

- Plot the graph of f(x) on desmos and look at the desired x-intercept (-0.311).

- Plot a table with headings → x lower (xl), f(xl), x midpoint(xm), f(xm), x upper(xu), f(xu);

Lower Bound (xl)	f(xl)	Midpoint (xm)	f(xm)	Upper Bound (xu)	f(xu)
-1	+4	-0.5	+1	0	-1
-0.5	+1	-0.25	-0.125	0	-1
-0.5	+1	-0.375	0.40625	-0.25	-0.125
…	…	…	…	…	…
continue until	you find	the desired	root	with the stated	accuracy

- Choose lower bound(xl) and upper bound(xu) according to the root (e.g., we want to the circled one that is between -1 & 0).

- Next write the values ($f_{(xl)}$; $f_{(xu)}$) that you get from substituting the lower and upper bound in f(x);

  e.g., Substitution of xu in f(x) we get f(xu) → $f(xu) = 0^3 + 0^2 - 3(0) - 1 = -1$

  - Repeat this procedure of substitution in each and every step when finding f(xl), f(xu), f(m);

- In this case, f(xl) is positive, and f(xu) is negative.
  Important consideration: as we need to know only if the value is positive or negative, it is possible to just evaluate the change of sign without substituting any value, and doing this will save even more time.

- At this point we need to verify what is happening at the midpoint (xm), but first the formula for x(m) is needed:

$$xm = \frac{(xl + xu)}{2}$$

- Once the midpoint (-0.5) is found by that formula, we found by substitution that the function f(xm) is positive.

- After that it is possible to remove the 0 as upper bound because the root (-0.311) falls within -0.5 and 0.

- Therefore 0 remains the upper bound(xu) but the lower bound(xl) now is -0.5 (considering also that f(xl) is positive, and f(xu) is negative).

- It is possible to find the midpoint again and observe if the function f(xm) is positive or negative (to see whether to substitute the lower(xl) or upper bound (xu)).

- Continue applying the same procedure until you find the desired root (-0.311).

- At last, you will find an approximate value that is near the final lower bound (xl) and upper bound (xu) as the interval bisected in each iteration becomes small.

- For the other root (e.g., we know it sits in between the lower bound 1 & upper bound 2), we do the same procedure and get that root.

A simple rule is to keep taking the middle but observe and choose always the two closest values to the root (one bigger than the root, one smaller than the root).

Knowing that the function is between the interval and that we must narrow it down a bit every time, an important consideration is needed:

- it does not give you an exact answer, it gives you intervals to help find the appropriate roots that gives you zero. We start with a wide interval and then we continue to get smaller and smaller intervals.

Advantages:

- In terms of practicability the interval bisection method is simple: we bisect continuously and change the interval where needed, until we get an accurate result for the root.

- This method is completely reliable:
  If we have the root that we want in the chosen initial interval (xl = -1, xu = 0), we are guaranteed that we will find the desired root. We can keep narrowing this down as much as we want, until we have the desired accuracy.

Disadvantages:

- Its convergence rate is slow: it means that it will take a lot of iterations to converge and therefore consume time (an initial interval close to the root improves the speed of the convergence rate).

- The method fails when:

- The signs around the root stay the same.

- Determining complex roots.

1.2 Fixed Point Iteration: The Rearrangement Method

There are a lot of different ways of applying the rearrangement method, which is one of the challenges with it. Initially, it starts rearranging in various ways for x the initial f(x), and the rearrangement will be the g(x).

In this example, the function f(x) studied will be:

$$f(x) = x^5 - 4x^4 - 5x^3 - x^2 + x + 1$$

Our 1st rearrangement will be our g(x) that will help us finding the roots of f(x):

$$g(x) = \sqrt[5]{4x^4 + 5x^3 + x^2 - x - 1}$$

(1st rearrangement)

$$g(x) = \sqrt[3]{\frac{x^5 - 4x^4 - x^2 + x + 1}{5}}$$

(2nd rearrangement)

You have an initial guess for your roots, which could be something very close to one of the intersection points, and then when you use this function g(x) as an iterative formula, it will gradually narrow down closer and closer to an intersection point.

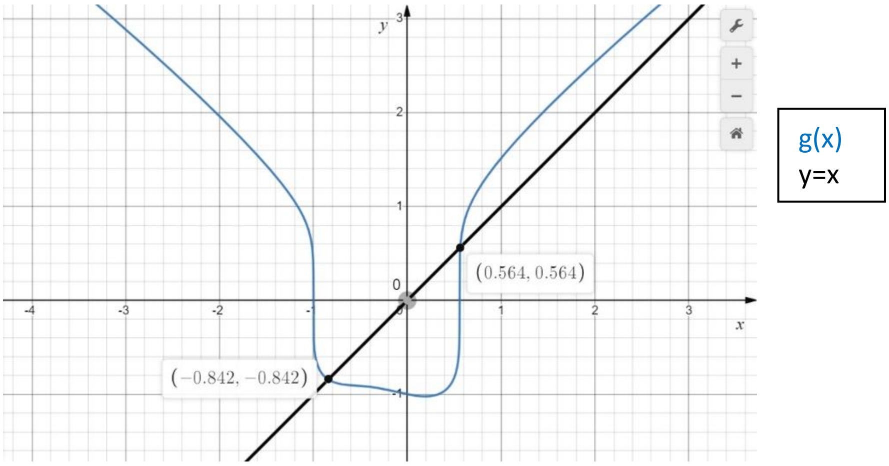

Figure 2 (1st rearrangement)

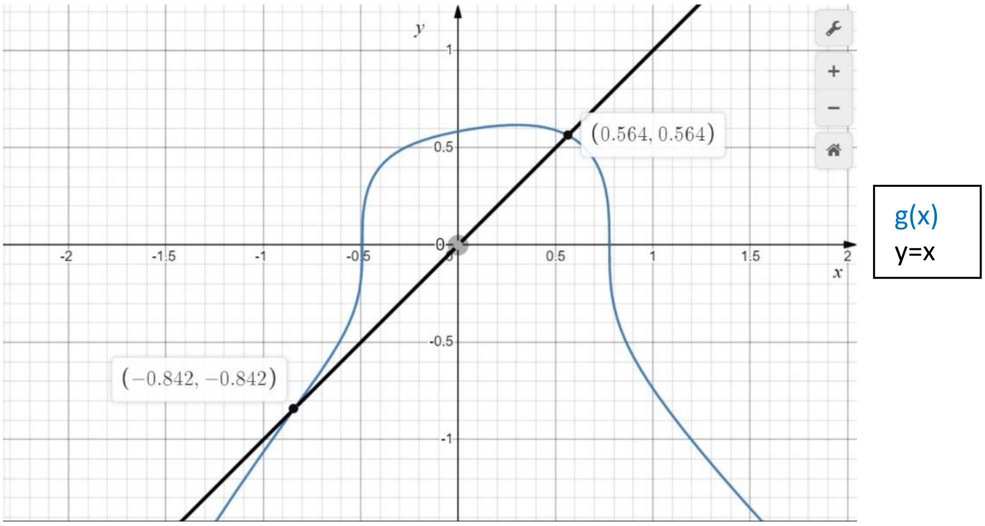

Figure 3 (2nd rearrangement)

Rearrangement method:

- Plot the graph of f(x), g(x) and a straight-line y = x on desmos and look at the desired x-intercept.
- You start with an initial value of x, that is our starting point, now you put it in f(x) and whatever value you evaluate from there, that becomes our new value of x.
- Then you put that value of x again, and just keep repeating that over and over, hopefully it will narrow down.
- From this graph it is possible to see that if you start with an initial value of x (-0.5) and put it in this iterative formula, and keep putting the answer over and over, what is happening is that you

are taking the output(y value) of g(x), and taking that as an x value and putting that back in; and you are just repeating that over and over;

- So functionally what you are doing is that you are taking an x value, then you are going into the function, and once you meet a y value you are taking that as a new x value, putting in your function, getting your new x value (that is actually the y value where it meets the graph), putting in your function again, getting your new x value, and so on.
- If it converges, it often does so in a spiral or step pattern on the graph and you can visualize it;

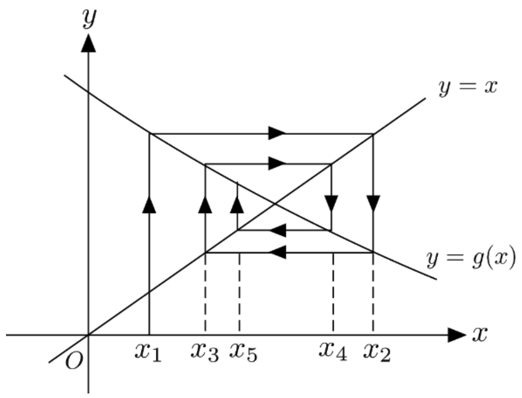

Figure 4 (spiral pattern)

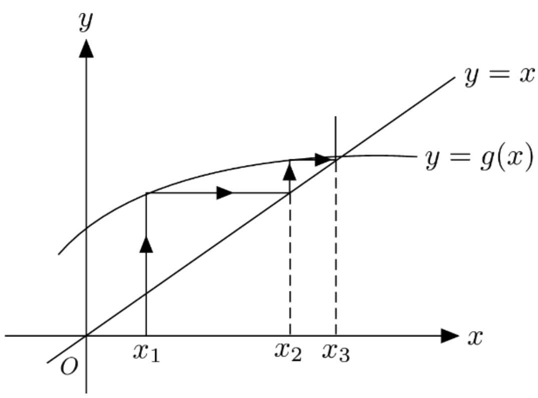

Figure 5 (step pattern)

If there is no spiral or staircase diagram that shows very clearly that it is going to converge, it is still possible to judge if the rearrangement will converge at the intersection point.

- Draw g(x) and look at the shape of the curve:
  Observe at the intersection points between the straight line and the curve, as we can consider these intersection points same as the roots of f(x) because the equations are same (just rearranged).

By looking at the shape of the curve, in particular the steepness, we need to look at to determine if it will converge or not.

It is extremely important that the gradient of the curve is less steep than the straight line.

Of course, the straight line (y = x) has a gradient (m = 1), the curve must be less steep than that.

Therefore, the gradient of the curve must be between 1 and -1 (it does not matter if the gradient is negative). If it is bigger than 1 or below -1 it is too steep, therefore it is not going to work.

The problem is that each time you put an x value into the function, you end up stepping further and further away from that intersection point instead of getting closer to it.

Looking at the shape of that graph, the intersection point (0.564) that is one of the roots of f(x) would be a solution of the equation f(x) = 0, but the iteration will not work because the g(x) is too steep. Therefore, if that root (0.564) of our function is one of the roots we are aiming to find, this rearrangement will not work. (figure 2)

Even if we start with an initial value of x that is close to the intersection point, it will still not work. For example, if we start with an initial value of x (e.g., 0.64), we are still very close to that intersection point but this time the spiral assumes a step pattern. It is going to converge up there as the curve is less steep on that intersection point.

Instead, we can get the other one (-0.842) because the gradient is less steep than the straight line.

However, we can still get that intersection point by trying a different rearrangement (2nd rearrangement) for a different term (e.g., $5x^3$).

First, double check if the rearrangement is done correctly. We can do that by checking the rearrangement but also by checking if the intersection points are the same as they were in f(x). In this case, it is confirmed that they are the same (0.564, -0.842).

Notice this time, the graph has changed. We have all the same intersection points, so they are all roots of that function, but the shape of g(x) is different.

In this rearrangement, the intersection points -0.842 will not converge as the curve is too steep (it is steeper than the line y=x), but the other one that we want (0.564) will. We can see that the curve is less steep than the straight-line y = x, so the method should be able to converge there (figure 3).

There are some cases in which when you start quite close to the intersection point it is not going to converge. But stepping away from it, it starts converging there where is the curve is less steep.

Advantage:

- Often when it converges, it does quickly.
- It is a quick method to find a root, but as it can fail, it is a long process.
- If lucky, with one rearrangement you can find two roots.

Disadvantage:

- It can fail.
- It can be problematic as it depends on the steepness of the curve.
- Technically it can be the most complicated one.

1.3 Fixed Point Iteration: The Newton-Raphson Method

The Newton Raphson method:

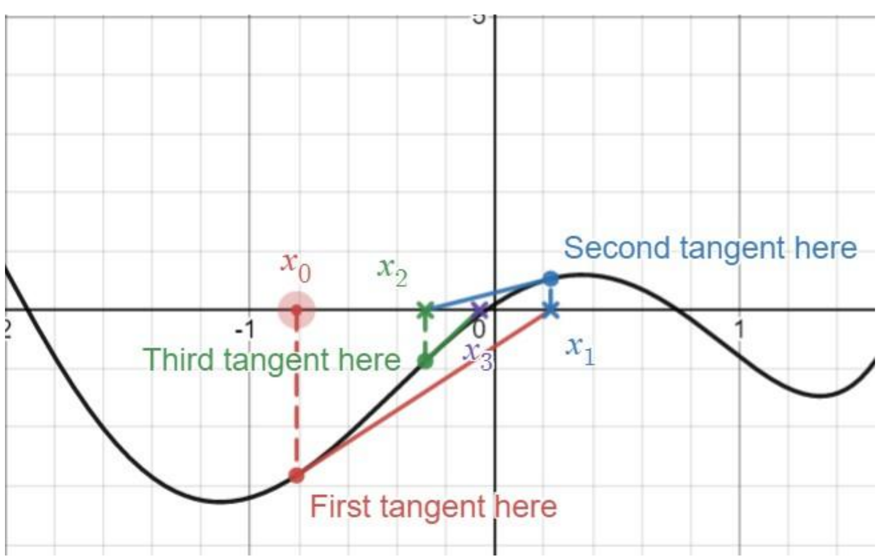

Figure 6 6(e.g., for Newton Raphson method)

- Plot the curve of f(x).
- Start choosing one root that you would like to find (do not start too far away from it).
- This is our starting point (x_0), and from there we are going up until it meets the curve, then we plot a tangent to the curve at that point.
- To find the equation of that tangent, we need the x value, the value of f(x) and the gradient.
- As gradient is required, we need to differentiate the function.
- We put our initial x value in the function to get the y value. Then we want to know the gradient of the function as well so we can draw a tangent.
- Therefore, we get the gradient by substituting the x value in the derivative of f.
- Then we can plot the tangent, which crosses the x-axis somewhere. We can calculate this intersection.
- Whatever the result is, it is our new x value (x_1) because we started with x_0.
- To find the formula of the Newton-Raphson method with which this procedure is much faster, we first write down the equation of the tangent.

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

- And this is the rearranged formula, the Newton-Raphson formula, that we use for the iterations:

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

- That rearranged equation for x_1 is giving us the x-intercepts of the first tangent we made. Now we substitute x_1 in the same formula at the place where x_0 was before. The result is our new x value, x_2. We repeat this procedure over and over again.
- We carry on, and if we are lucky it will converge for the root that we try to find because the tangents will cross the x-axis closer and closer to the root.
- But the method is not always converging.

This method is very reliable in a way, as it converges for sure somewhere. But even if our starting point is near to the root, it might not convert. This is a drawback of this method.
But, if it converges, it is usually the quickest method with the fastest convergence rate.

However, you can end up jumping over to a completely different part of the curve (depending on what shape) with one iteration if you choose a not suitable starting point.

In the Newton Raphson Method, you have the function and the derivative of your function. You put a starting point in there and then you start iterating, therefore the only factor you can adjust is where you start. Hence, that makes it simpler as there is only one thing you can change.

So that is a factor you must try out and adjust. This is the only thing that can go wrong with the Newton-Raphson method.

It is clearer to see if we look at the graph. If we start near a turning point, we end up with a tangent that takes us far away from the root because the tangent is very flat. So, starting somewhere near the turning point is not a good idea because that first tangent is going to take us way over to some other part of the curve due to its gentile gradient.

This is a disadvantage because depending on the position of the root, we need to choose a starting point near to a turning point. And maybe the method ends up converging for a different root.

So even in this case look at the graphs first, moving the starting point where it is the best.

2. Results and Analysis

Now we apply the three numerical methods and analyze the results.
To start, we will do the Rearrangement method, then the Newton-Raphson method and at last the interval bisection method.

2.1 Rearrangement method

First, we have to find some rearrangement of our function in order to apply the method:

$$g(x) = \sqrt[5]{-3.8x^4 + 46.7x^3 + 43.9x^2 - 103.5x - 48.1}$$

(1st rearrangement)

$$g(x) = \sqrt[3]{\frac{x^5 + 3.8x^4 - 43.9x^2 + 103.5x + 48.1}{46.7}}$$

(2nd rearrangement)

$$g(x) = \sqrt[2]{\frac{x^5 + 3.8x^4 - 46.7x^3 + 103.5x + 48.1}{43.9}}$$

(3rd rearrangement)

We plotted the 1st and the 2nd rearrangement on desmos.
The 2nd rearrangement already seems to converge for two roots of our function (figure 9). Therefore, we do not need to check the 3rd rearrangement because we only need two roots.

Figure 7 shows the graph of the 2nd rearrangement. As we can see that the graph is not too steep at (1.3948/1.3948). Therefore, we can assume that this rearrangement will converge for x=1.3948.

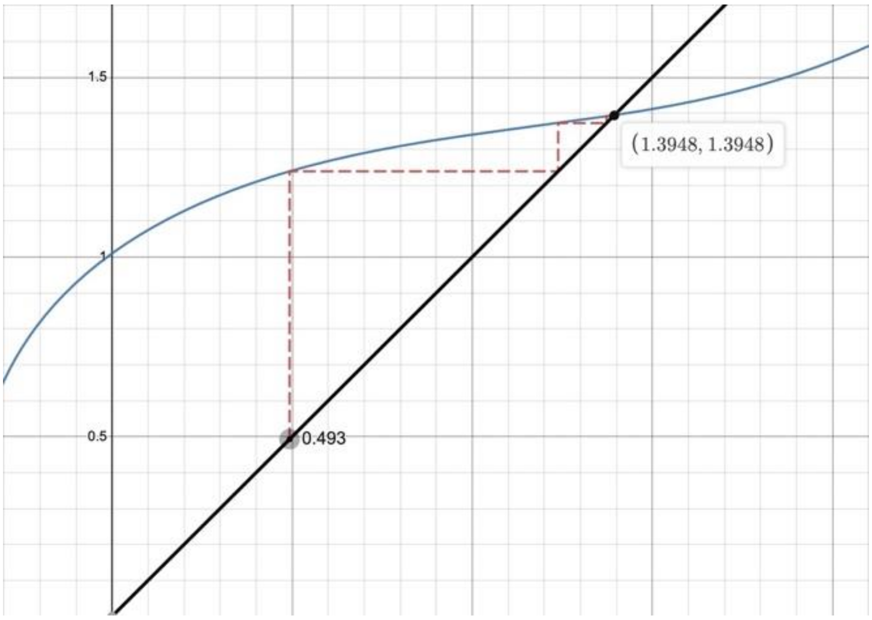

Figure 7 (2nd rearrangement, 1.3948)

In addition to that, the 2nd rearrangement looks like it is convergent for x = -1.74, too (figure 9, step pattern). That means we have already found two roots, which we can investigate.

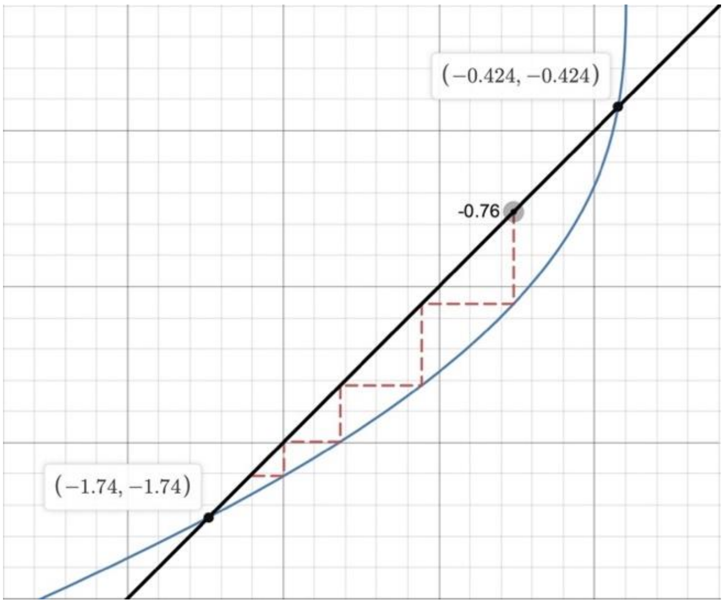

Figure 8 (2nd rearrangement, -1.74)

Figure 9 shows an example of failure. It is the graph of the 2nd rearrangement, and it is clear to see, that it does not converge for x = -0.424 because the graph is too steep there. And, even if we move the starting point of the iterations near that value, it still converges for x = 1.395.

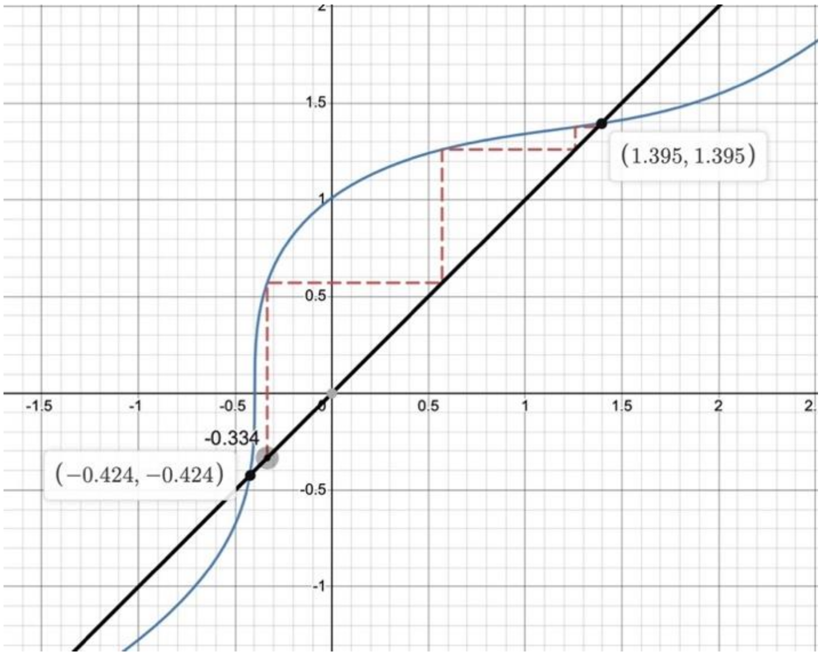

Figure 9 (example of failure in 2nd rearrangement)

Figure 10 is another example of failure and shows the 1st rearrangement. As we can see in the figure, the rearrangement does not convert for x = -1.731 because the graph is too steep around that x value, and it is converging away from that point.

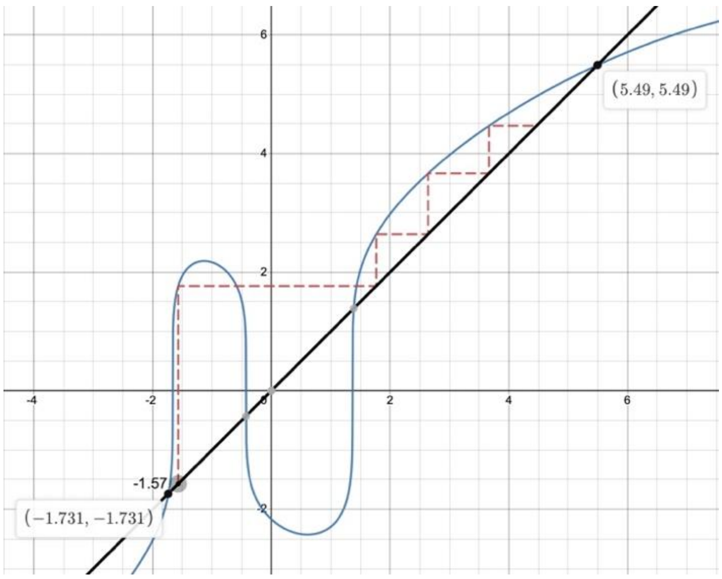

Figure 10 (example of failure in 1st rearrangement)

Instead, the 1st rearrangement converges to x = 5.49, which we can already assume from figure 5 because the iterations are moving up to this point with a step pattern.

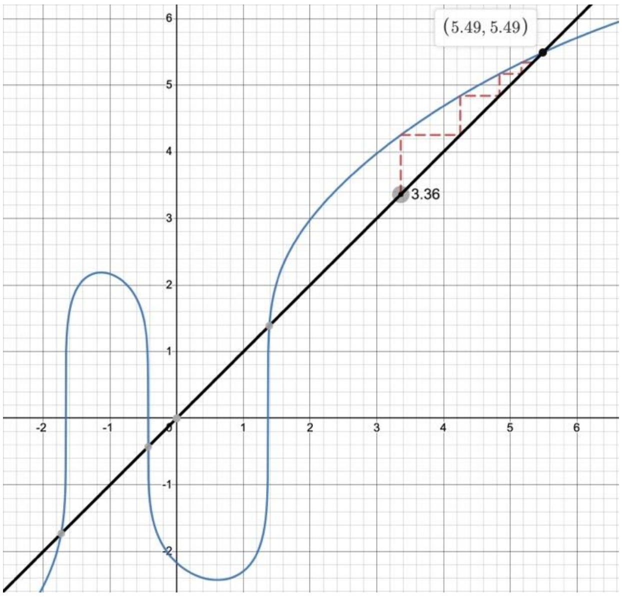

Figure 11 (1st rearrangement, 5.49)

After we looked at the graphs of the 1st and 2nd rearrangement, we calculated the roots to a certain accuracy by using excel.
As predicted earlier, we found a result of 1.395 with the 2nd rearrangement. This result is exact for 11 significant figures because we can see in figure 12 that the last number gets repeated. That means, that the method needed 10 iterations and is exact to 11 significant figures.

iteration	
n	X_n
0	1,395
1	1,39481224945
2	1,39478386056
3	1,39477956853
4	1,39477891965
5	1,39477882155
6	1,39477880671
7	1,39477880447
8	1,39477880413
9	1,39477880408
10	1,39477880407
11	1,39477880407

Figure 12 (2nd rearrangement, 1.3948)

When we calculated the other root with excel, we got a result of 11 significant figures, too. But this time, as we can see in figure 11, the convergence rate was slower, and it took us 24 iterations to find our result.

iteration	
n	X_n
0	-1,74
1	-1,74000521957
2	-1,74000795173
3	-1,74000938187
4	-1,74001013046
5	-1,74001052231
6	-1,74001072742
7	-1,74001083479
8	-1,74001089099
9	-1,74001092041
10	-1,74001093580
11	-1,74001094386
12	-1,74001094808
13	-1,74001095029
14	-1,74001095145
15	-1,74001095205
16	-1,74001095237
17	-1,74001095254
18	-1,74001095262
19	-1,74001095267
20	-1,74001095269
21	-1,74001095270
22	-1,74001095271
23	-1,74001095271
24	-1,74001095272
25	-1,74001095272

Figure 13 (2nd rearrangement, -1.74)

2.2 Fixed Point Iteration: The Newton-Raphson

The next method we analyze is the Newton-Raphson method. We also have to check the convergence for this method. We use desmos again to check the convergence by plotting our function and setting some tangents, that represent the iterations of the method. We adjust our starting point so that the tangents converge as close as possible. In figure 14 we can see the graph of our function g(x) (2^{nd} rearrangement) and the tangents. It seems like this method converges for x = 1.395. Moreover, the third tangent looks like it crosses the x-axis close to the root. Therefore, we assume that the convergence rate is fast.

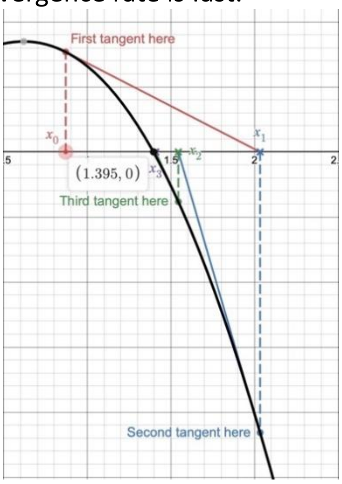

Figure 14 (Newton Raphson Method, 1.3948)

Furthermore, also for x = -1.74 the tangents are moving closer to the root. The method is probably also convergent at this point. Hence, we can find the same two roots as in the rearrangement method (figure 15).

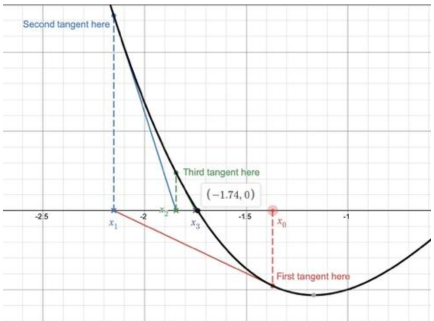

Figure 15 (Newton Raphson Method, -1.74)

At this point we use excel to calculate the two roots. We found a result for x = -1.74 and x = 1.395, which were also exact to 11 significant figures. Also, the speed of the convergence rate was very high as only two iterations were needed to obtain the result. The results are the same as the ones that we got with the rearrangement method and newton Raphson method.

iteration	root estimate		
n	X_n	f(X_n)	f ' (X_n)
0	-1,74	002213974400024	-202,136916
1	-1,74001095285	0,00000002594	-202,14165253051
2	-1,74001095272	-0,00000000000	-202,14165247501
3	-1,74001095272	-0,00000000000	-202,14165247501

Figure 16 (Newton Raphson method, Excel, -1.74)

iteration	root estimate		
n	X_n	f(X_n)	f ' (X_n)
0	1,395	,05118106575313	231,42052189687
1	1,39477883955	-0,00000820849	-231,34629112813
2	1,39477880407	-0,00000000000	-231,34627921922
3	1,39477880407	-0,00000000000	-231,34627921922

Figure 17 (Newton Raphson method, Excel, 1.3948)

2.3 The Interval Bisection

As stated in the introduction, the Interval Bisection method always converges. Therefore, we can directly use excel to calculate our roots and we do not need to see if it converges on the graph. We were successful and found our two roots. But the convergence rate was really slow because we needed 37 and 40 iterations to find the desired result. On the other hand, it converged to 14 significant figures instead of only 11 numbers. However, we can assume that the rate would be still slow even if we converge until 11 iterations.

30	1,39477880407127	0,0000000039323693083595	1,39477880407221
31	1,39477880407221	0,0000000017581050014214З	1,39477880407268
32	1,39477880407268	0,00000000006705121053971 82	1,39477880407291
33	1,39477880407291	0,00000000001383328916548 14	1,39477880407303
34	1,39477880407291	0,0000000000138332891654814	1,39477880407297
35	1,39477880407291	0,0000000000138332891654814	1,39477880407294
36	1,39477880407294	0,00000000000689416807507909	1,39477880407296
37	1,39477880407296	0,00000000000226670327010685	1,39477880407297
38	1,39477880407296	0,00000000000226670327010685	1,39477880407297

Figure 18 (Interval bisection , 1.3948)

30	-1,74001095270741	-0,0000000196375990053215	-1,74001095271672
31	-1,74001095271672	-0,00000000008180372006927 29	-1,74001095272138
32	-1,74001095271672	-0,0000000000818037200692729	-1,74001095271905
33	-1,74001095271672	-0,0000000000818037200692729	-1,74001095271789
34	-1,74001095271672	-0,0000000000818037200692729	-1,74001095271731
35	-1,74001095271672	-0,0000000000818037200692729	-1,74001095271702
36	-1,74001095271702	-0,0000000000211585796997209	-1,74001095271717
37	-1,74001095271702	-0,0000000000211585796997209	-1,7400109527171
38	-1,7400109527171	-0,00000000000497752429628563	-1,74001095271714
39	-1,7400109527171	-0,00000000000497752429628563	-1,74001095271712
40	-1,74001095271712	-0,000000000000963635348102725	-1,74001095271713
41	-1,74001095271712	-0,000000000000963635348102725	-1,74001095271713

Figure 19 (Interval bisection, -1.74)

3. Conclusions

As stated in the introduction, it is extremely important to analyze the graph first before starting any method. Looking at the graph first, helps to visualize it and observe which intersection point can converge.

This is particularly important for the Rearrangement Method, as a particular rearrangement would work for one, two or three of the roots, but will not work for all of them.

The rearrangement method often converges quickly if it does converge. For our results for example, the method took only 10, which is quite fast.
If lucky, with one rearrangement you can find two roots. In our case we had the 2nd rearrangement with which we had already found our two roots.

The disadvantage is that technically it can be the most complicated and longer one.
Moreover, the disadvantage is that it can fail as it depends on the steepness of the curve. For instance, our 1st rearrangement failed for most of the roots.

On the other hand, the interval bisection cannot go wrong because the method always converges.
In terms of practicability the interval bisection method is simple as we bisect continuously in the middle and change the interval where needed, until we get an accurate result for the root.

The interval bisection method is also completely reliable.
If we have the root that we want in the chosen initial interval, we are guaranteed that we will find the desired root. We can keep narrowing this down as much as we want, until we have the accuracy we desire.

For example, a problem comes when you choose your lower and upper bound without any knowledge of where the roots are, as you do not know which root you are going to converge. It will converge on a root eventually, but without looking at the graph we would not be able to choose a root and we would lose time. That is why it is important to analyze the graph first.

The convergence rate of the Interval bisection method is slow as it takes a lot of iterations to converge. Therefore, it consumes time. This could be overcome by choosing an initial interval close to the root but in this case, study even choosing close lower and upper bound (e.g., 1.394 & 1.396) close to the root (1.3948) took us 37 iterations to converge.

However, the bisection method can fail when the signs around the root stay the same or when determining complex roots.

The Newton Raphson's method compared to the other two methods, has a really fast convergence rate. This is a big advantage of this method. However, we should be careful on adjusting the starting point as the rate of convergence depends on that. On the other hand, as it is the only factor that can change, it makes the Newton Raphson's method simpler.
However, compared to the interval bisection it is still a bit more difficult.

To improve the accuracy of this investigation more methods can be applied such as Brent's Method, Secant Method, and Steffensen's Method. More importantly, these methods can be applied to more functions as we could have a wider range of comparability between functions and numerical methods for root finding problems.

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