Math 4543: Numerical Methods

Lecture 1 — Introduction & Bisection Method

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Introduction

First things first…

Google Classroom – 2ih7k33

Relevant Resources

- Book/Lecture notes — ***Numerical Methods with Applications*** by Professor Dr. Autar Kaw

  Link: http://nm.mathforcollege.com/NumericalMethodsTextbookUnabridged/

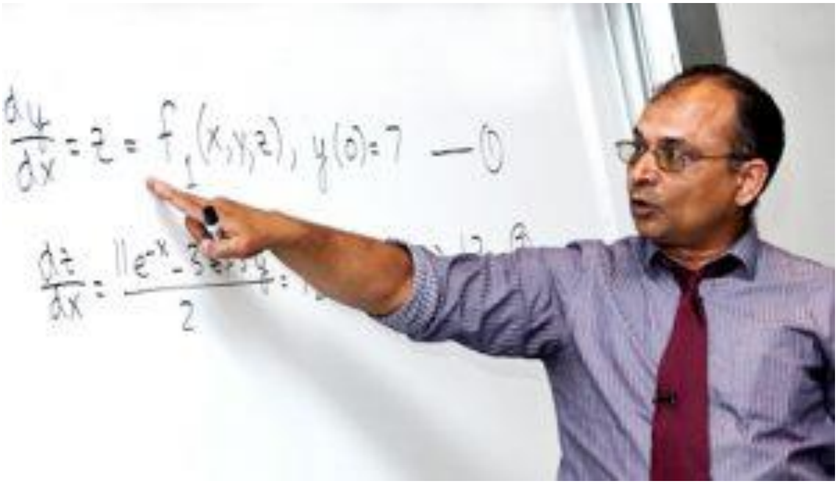
- Video Lectures — YouTube channel ***numericalmethodsguy***

  Link: https://www.youtube.com/@numericalmethodsguy

- Practise Problems — ***Holistic Numerical Methods*** website

  Link: https://nm.mathforcollege.com/physical-problems/

  Link: http://nm.mathforcollege.com/mws/che/03nle/index.html



Keep an eye on the GC for the Slides and Lectures notes.

Introduction

How to do well in this course?

For the **theory course** Math 4543 —

- Pay attention to the class lectures.
- Practise examples from the lecture notes and the *HNM* website.
- Solve previous-year questions (problems and derivations).
- Practise, practise, and practise…

For the **lab course** Math 4544 —

- Try to convert the algorithms taught in the class to pseudocode.
- Practise implementing them before attending the lab session.
- Key pre-requisite:
  - ✓ Basic knowledge about the *Python* programming language.
  - ✓ Familiarity with *Google Colab* or *Jupyter Notebook*.

Lecture Plan

The agenda for today

- What are Numerical Methods?
- Why do we need them?
- Analytical solution vs Numerical solution
- The Bisection Method of Solving a Nonlinear Equation
- The pros and cons of the method

Expect some **mini quizzes**!

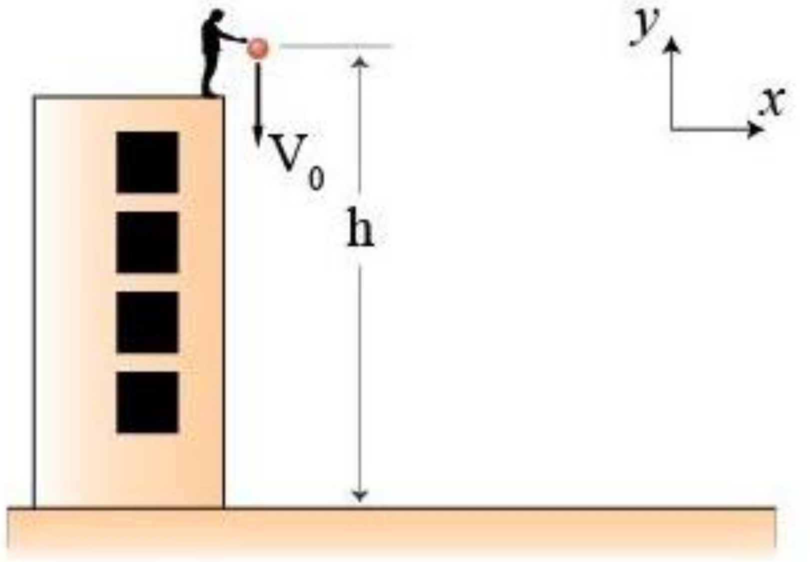
(for easy *attendance marks* bonus ☺)

Numerical Methods

What are they and why do we need them?

Definition: Numerical methods are techniques to ***approximate*** mathematical processes (examples of mathematical processes are integrals, differential equations, nonlinear equations).

Problem Description
↓
Mathematical Model
↓
Solution of Mathematical Model
↓
Using the Solution



Numerical methods are just one step in solving an engineering problem.

Numerical Methods

What are they and why do we need them?

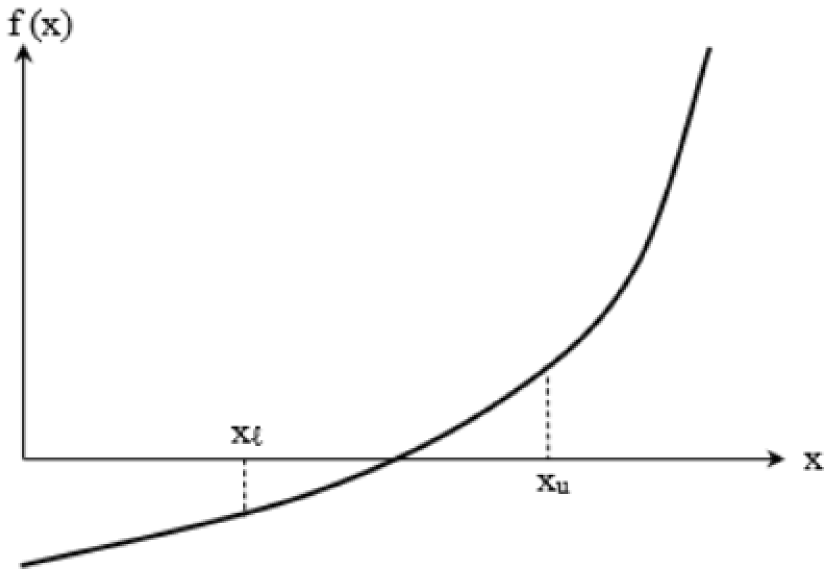
We end up with a quadratic equation (polynomial with degree 2). $ax^2 + bx + c = 0$

Solving **analytically**, using the quadratic formula

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

- ✓ Get exact solutions.
- ✓ Involves a lot of symbolic manipulations.

Solving **numerically**, using a numerical method *e.g.* the bisection method



- ✓ Get approximate solutions.
- ✓ Converge till solution *"good enough"*.

Mini Quiz

Quantifying the *goodness* of an approximation

How can we judge how good of an approximation our guess is?
(given the *ground-truth* or the value of the *guess in the previous iteration*)

Mini Quiz

Quantifying the *goodness* of an approximation

We use **absolute relative approximate error**.

Find the absolute relative approximate error as

$$|\in_a| = \left| \frac{x_m^{\text{new}} - x_m^{\text{old}}}{x_m^{\text{new}}} \right| \times 100$$

where

x_m^{new} = estimated root from present iteration

x_m^{old} = estimated root from previous iteration

Remember your physics lab experiments? (*e.g.* calculating the acceleration due to gravity using a pendulum)

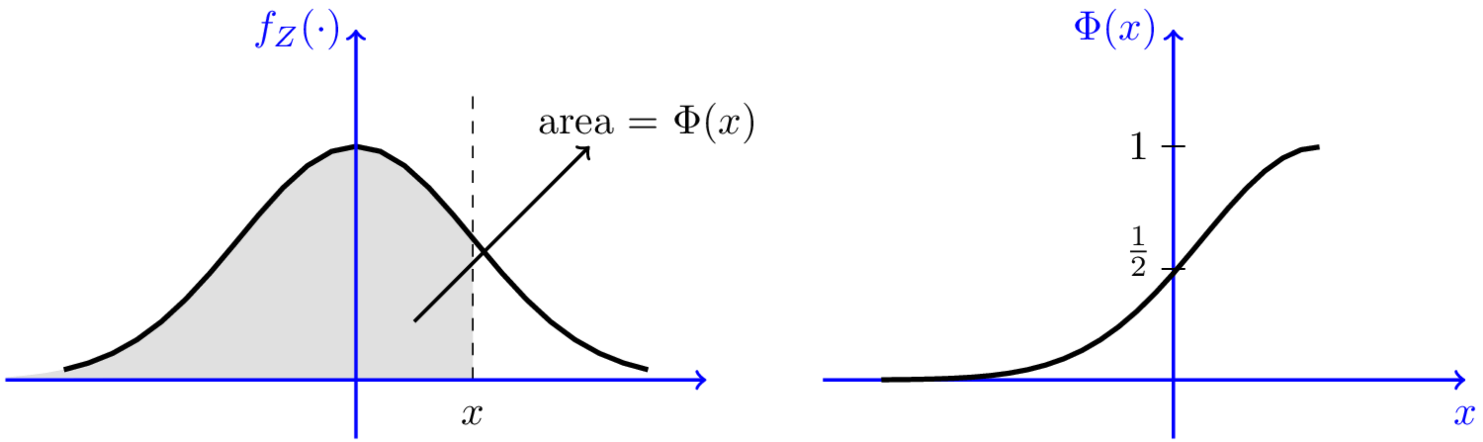
Numerical Methods

More on why we need them

We need to resort to finding approximations because —

- We cannot solve the procedure analytically, *e.g.* the standard normal cumulative distribution function (CDF)

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-t^2/2} dt$$



- The analytical method is intractable, such as solving a set of a 1000 simultaneous linear equations for a 1000 unknowns.

Bisection Method

For solving a Nonlinear Equation

One of the first numerical methods developed to find the ***root*** of a ***nonlinear equation*** $f(x) = 0$ was the bisection method (also called the *binary-search* method).

Theorem

An equation $f(x) = 0$, where $f(x)$ is a real continuous function, has at least one root between x_l and x_u if $f(x_l)f(x_u) < 0$ (See Figure 1).

Note that if $f(x_l)f(x_u) > 0$, there may or may not be any root between x_l and x_u (Figures 2 and 3). If $f(x_l)f(x_u) < 0$, then there may be more than one root between x_l and x_u (Figure 4). So the theorem only guarantees one root between x_l and x_u.

Since the method is based on finding the root between two points, the technique falls under bracketing methods.

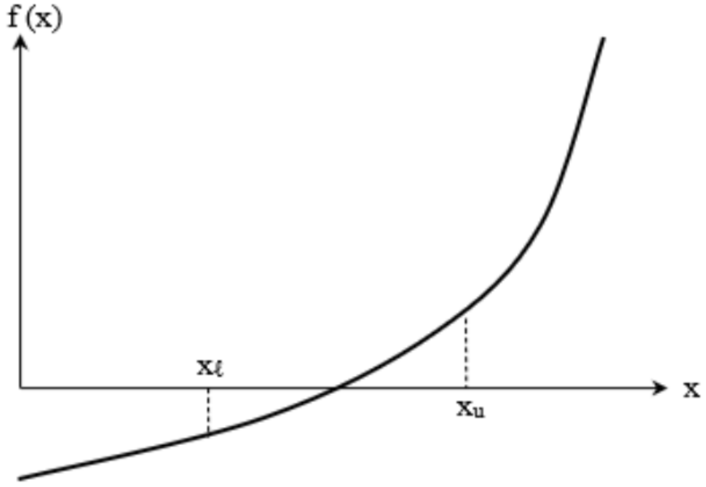


Figure 1 At least one root exists between the two points if the function is real, continuous, and changes sign.

Bisection Method

For solving a Nonlinear Equation

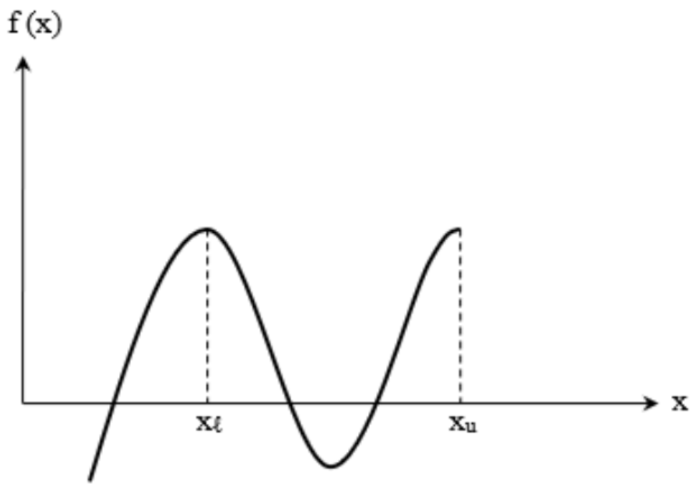


Figure 2 If the function $f(x)$ does not change the sign between the two points, roots of the equation $f(x) = 0$ may still exist between the two points.

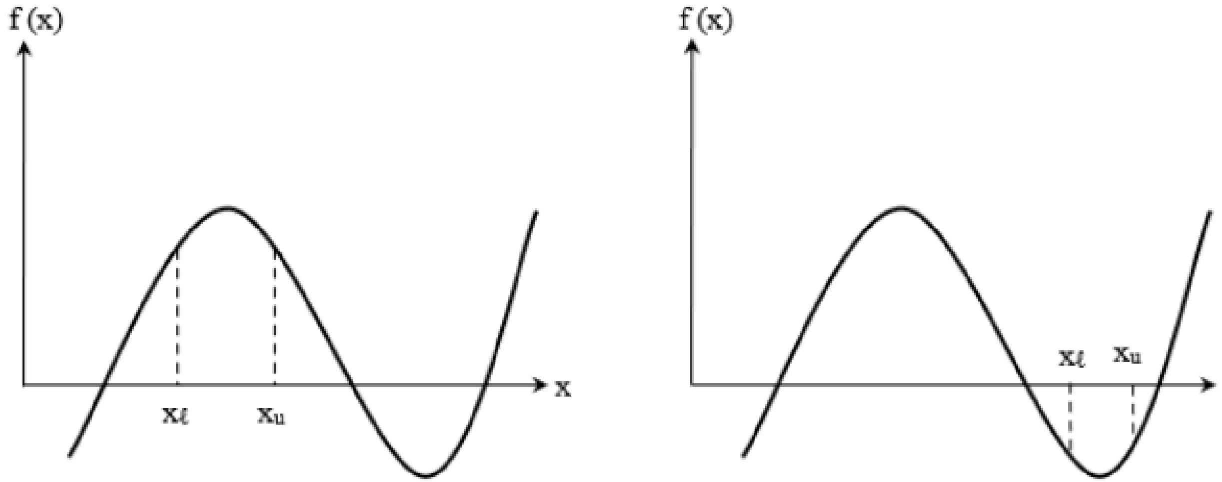


Figure 3 If the function $f(x)$ does not change the sign between two points, there may not be any roots for the equation $f(x) = 0$ between the two points.

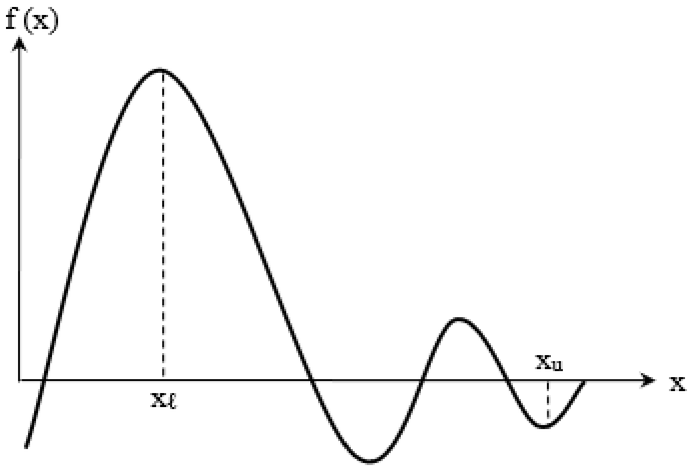
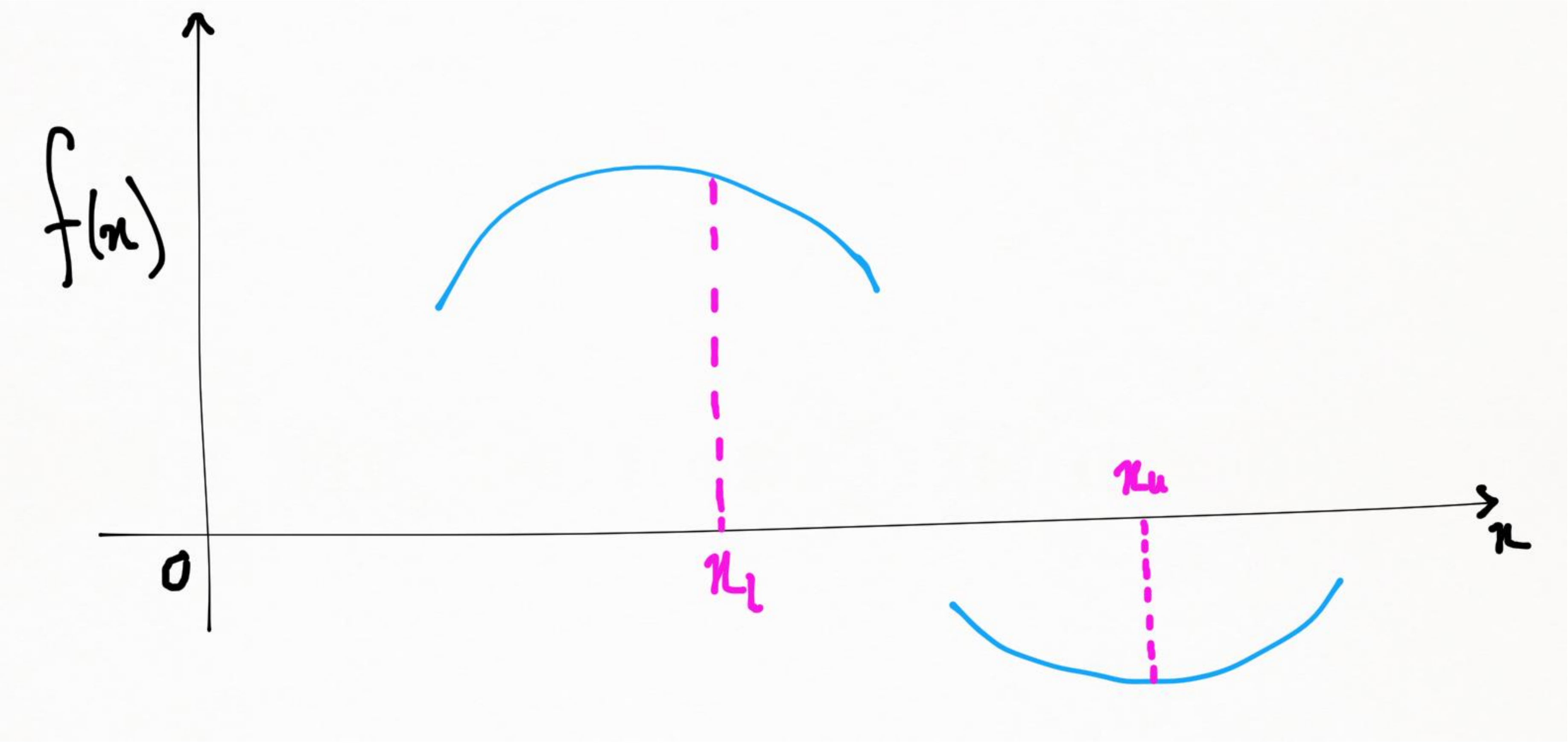


Figure 4 If the function $f(x)$ changes the sign between the two points, more than one root for the equation $f(x) = 0$ may exist between the two points.

Mini Quiz

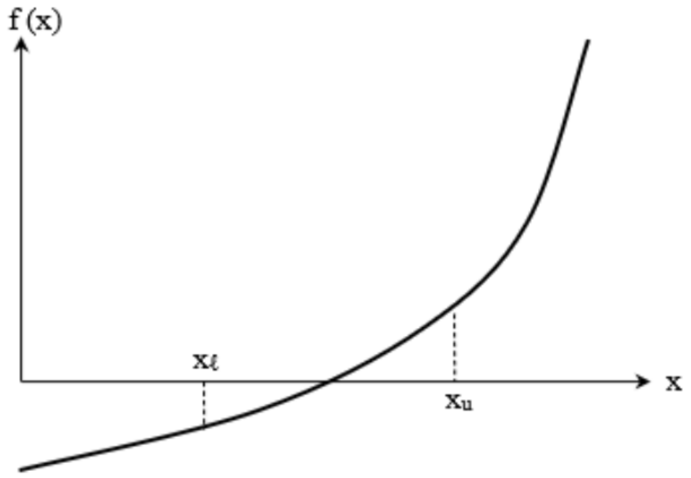
An edge case?

Does the theorem fail in this case?



Bisection Method

The algorithm



The steps to apply the bisection method to find the root of the equation $f(x) = 0$ are

Choose x_l and x_u as two guesses for the root such that $f(x_l)f(x_u) < 0$, or in other words, $f(x)$ changes sign between x_l and x_u.

Estimate the root x_m of the equation $f(x) = 0$ as the mid-point between x_l and x_u as

$$x_m = \frac{x_l + x_u}{2}$$

Now check the following

If $f(x_l)f(x_m) < 0$, then the root lies between x_l and x_m; then $x_l = x_l$ and $x_u = x_m$.

If $f(x_l)f(x_m) > 0$, then the root lies between x_m and x_u; then $x_l = x_m$ and $x_u = x_u$.

If $f(x_l)f(x_m) = 0$; then the root is x_m. Stop the algorithm if this is true.

Find the new estimate of the root

$$x_m = \frac{x_l + x_u}{2}$$

Find the absolute relative approximate error as

$$|\in_a| = \left| \frac{x_m^{new} - x_m^{old}}{x_m^{new}} \right| \times 100$$

where

$$x_m^{new} = \text{estimated root from the present iteration}$$

$$x_m^{old} = \text{estimated root from the previous iteration}$$

Compare the absolute relative approximate error $|\in_a|$ with the pre-specified relative error tolerance $\in_s$. If $|\in_a| > \in_s$, then go to Step 3, else stop the algorithm. Note one should also check whether the number of iterations is more than the maximum number of iterations allowed. If so, one needs to terminate the algorithm and notify the user about it.

Bisection Method

An example problem

Use the bisection method to find the root of the nonlinear equation

$$x^3 = 20$$

Use initial lower and upper guesses of 1 and 4, respectively.

Conduct three iterations to estimate the root of the equation.

Find the absolute relative approximate error at the end of each iteration.

Find the number of significant digits that are at least correct at the end of each iteration.

Bisection Method

An example problem

Solution

Rewrite the equation $x^3 = 20$ in the form $f(x) = 0$ that gives

$$f(x) = x^3 - 20 = 0$$

Check if the function changes the sign between the two initial guesses, x_l and x_u. The initial guesses are given as $x_l = 1$ and $x_u = 4$

$$\begin{aligned} f(x_l) &= f(1) \\ &= 1^3 - 20 \\ &= -19 \end{aligned}$$

$$\begin{aligned} f(x_u) &= f(4) \\ &= 4^3 - 20 \\ &= 44 \end{aligned}$$

Hence

$$\begin{aligned} f(x_l)f(x_u) &= f(1)f(4) \\ &= (-19)(44) < 0 \end{aligned}$$

This change in sign tells us that the initial bracket of $[1, 4]$ given to us is valid.

Bisection Method

An example problem

<u>Iteration 1</u>

$$x_l = 1,\ x_u = 4$$

The estimate of the root is

$$\begin{aligned} x_m &= \frac{x_l + x_u}{2} \\ &= \frac{1+4}{2} \\ &= 2.5 \end{aligned}$$

Bisection Method

An example problem

Iteration 2

Find the value of the function at the midpoint from the previous iteration and use it to determine the new bracket.

$$\begin{aligned} f(x_m) &= f(2.5) \\ &= (2.5)^3 - 20 \\ &= -4.375 \end{aligned}$$

$$\begin{aligned} f(x_l)f(x_m) &= f(1)f(2.5) \\ &= (-19)(-4.375) > 0 \end{aligned}$$

Since $f(x_l)f(x_m) > 0$, the root does not lie between x_l and x_m, but between x_m and x_u, that is, 2.5 and 4.

$$x_l = 2.5,\ x_u = 4$$

Bisection Method

An example problem

The estimate of the root is

$$\begin{aligned} x_m &= \frac{x_l + x_u}{2} \\ &= \frac{2.5 + 4}{2} \\ &= 3.25 \end{aligned}$$

The absolute relative approximate error $|\varepsilon_a|$ at the end of Iteration 2 is

$$\begin{aligned} |\varepsilon_a| &= \left| \frac{x_m^{new} - x_m^{old}}{x_m^{new}} \right| \times 100 \\ &= \left| \frac{3.25 - 2.5}{3.25} \right| \times 100 \\ &= 23.1\% \end{aligned}$$

None of the significant digits are at least correct in the estimated root of the equation because the absolute relative approximate error is greater than 5%.

Bisection Method

An example problem

Iteration 3

Find the value of the function at the midpoint from the previous iteration and use it to determine the new bracket.

$$\begin{aligned} f(x_m) &= f(3.25) \\ &= (3.25)^3 - 20 \\ &= 14.3281 \end{aligned}$$

$$\begin{aligned} f(x_l)f(x_m) &= f(2.5)f(3.25) \\ &= (-4.375)(14.3281) < 0 \end{aligned}$$

Since $f(x_l)f(x_m) < 0$, the root does lie between x_l and x_m, that is, 2.5 and 3.25.

$$x_l = 2.5, x_u = 3.25$$

Bisection Method

An example problem

The estimate of the root is

$$x_m = \frac{x_l + x_u}{2}$$
$$= \frac{2.5 + 3.25}{2}$$
$$= 2.875$$

The absolute relative approximate error $|\varepsilon_a|$ at the end of Iteration 3 is

$$|\epsilon_a| = \left| \frac{x_m^{new} - x_m^{old}}{x_m^{new}} \right| \times 100$$
$$= \left| \frac{2.875 - 2.5}{2.875} \right| \times 100$$
$$= 13.0\%$$

Still, none of the significant digits are at least correct in the estimated root of the equation as the absolute relative approximate error is greater than 5%.

Bisection Method

The pros and cons

Advantages of the bisection method

a) The bisection method is always convergent. Since the technique brackets the root, the procedure is guaranteed to converge.

b) As iterations are conducted, the interval gets halved. So, one can guarantee the error in the solution of the equation.

Bisection Method

The pros and cons

Drawbacks of bisection method

a) The convergence of the bisection method is slow as it is based on halving the interval.

b) If one of the initial guesses is closer to the root, it will take a larger number of iterations to reach the root.

c) If a function $f(x)$ is such that it just touches the x-axis (Figure 1) such as

$$f(x) = x^2 = 0$$

it will be unable to find the lower guess, x_l, and upper guess, x_u, such that

$$f(x_l)f(x_u) < 0$$

d) For functions $f(x)$ where there is a singularity, and it reverses the sign at the singularity, the bisection method may converge on the singularity (Figure 2). An example includes

$$f(x) = \frac{1}{x}$$

where $x_l = -2$, $x_u = 3$ are valid initial guesses which satisfy

$$f(x_l)f(x_u) < 0$$

However, the function is not continuous, and the theorem that a root exists is also not applicable.

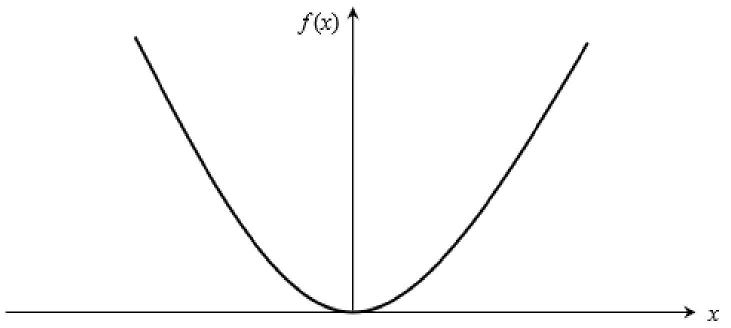


Figure 1 The equation $f(x) = x^2 = 0$ has a single root at $x = 0$ that cannot be bracketed.

A singularity in a function is defined as a point where the function becomes infinite. For example, for a function such as $1/x$, the point of singularity is $x = 0$ as it becomes infinite.

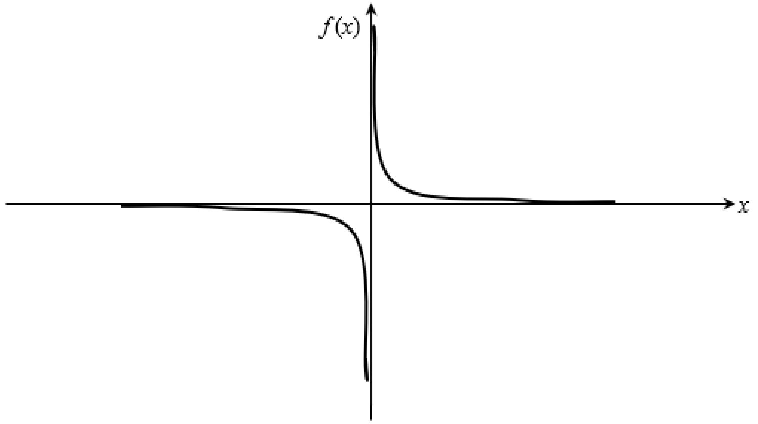


Figure 2 The equation $f(x) = \dfrac{1}{x} = 0$ has no root but changes sign.