# Numerical Methods for Natural Sciences: Foundation Topics January - April semester, 2024

Raghunathan Ramakrishnan ramakrishnan@tifrh.res.in Tata Institute of Fundamental Research Hyderabad Hyderabad, India

Course material: https://github.com/raghurama123/nm2024



# Content

		Page
References	•••	3
Chapter 1: Solutions of equations by fixed-point iteration		4

## References

#### **Textbook**

 David G. Moursund, Charles S. Duris, "Elementary Theory and Application of Numerical Analysis", Dover Publishers (1988).

#### **General References**

- Samuel D. Conte, Carl de Boor, "Elementary Numerical Analysis: An Algorithmic Approach", McGraw-Hill (1981).
- Lars Elden, Linde Wittmeyer-Koch and Hans Bruun Nielsen, "Introduction to Numerical Computing", Overseas Press (2006).
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- Richard L. Burden, J. Douglas Faires, "Numerical Analysis", Cengage Learning (2011).
- Ward Cheney, David Kincaid, "Numerical Methods and Computing", Cengage Learning (2013).
- Anne Greenbaum, Timothy P. Chartier, "Numerical Methods", Princeton Univerity Press (2012).
- William Bo Rothwell, "Linux for Developers", Pearson (2018). <u>See the chapters about GitHub</u>.
- Numpy and Scipy Documentation, <a href="https://docs.scipy.org/doc/">https://docs.scipy.org/doc/</a>

Chapter 1: Solutions of equations by fixed-point iteration

## Some definitions

## Program, algorithm, elementary operation

- A program is a set of algorithms along with statements for user interaction (i.e. input/output). An algorithm is a set of pre-defined operations to convert an input to an ouput.
- For a given problem, there may not a unique way to write a program, or the algorithms involved, or even the elementary operations involved (that comprise the algorithms).

#### Types of Numerical Methods: Direct, Iterative, and Heuristic

- Direct methods are predefined recipes (i.e. fixed algorithms with fixed elementary steps) for solving a problem. In this case, the error in the final result is only due to finite computer precision (i.e. rounding-off the numbers involved).
  - The standard formula for finding the root of a quadratic equation is a direct method.
  - It is often the case that for a given problem, a direct method may not exist (either it has not been found, or it may not even exist mathematically). A theorem in algebra says that there is no directmethod for finding a root of a polynomial of degree  $\geq 5$ .
  - We will later see that Gaussian elimination is a direct method for solving systems of linear equations.
- Iterative methods require an initial guess for the final solution of a problem. This value will be given as an input to an algorithm which will be repeated until its input and output are the same.
  - Newton-Raphson method for finding the solution of non-linear equations is an iterative method.
  - Iterative methods can be shown (using a threom) that a solution (if it exists) can be found as a limit.
- Heuristic methods are methods developed based on experience. These methods are not guarateed to give a solution.
  - Simplex method (Nelder-Mead method) for optimization is a heuristic method.

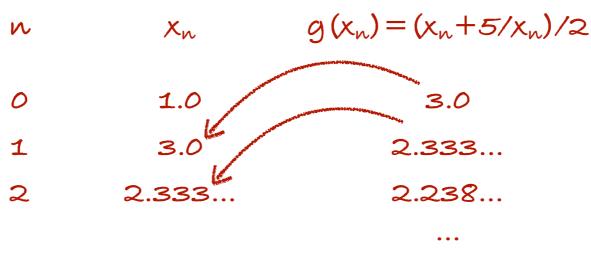
# Square root by fixed-point iteration

## Square root of a real number

The square root of a number A can be determined using the formula  $g(x) = \frac{1}{2} \left( x + \frac{A}{x} \right)$ , and using it successively. The procedure involves starting with an initial value  $x_0$  and determining  $g(x_0)$  using the formula. Now, one sets  $g(x_0)$  as  $x_1$ , and continue the process until  $g(x_n)$  (the output to the formula) is the same as  $x_n$  (the input).

# Example

■ Find the square-root of 5 by applying fixed-point iteration. Let's begin with  $x_0 = 1$ .





2.236068

- You can repeat these steps by a manual calculation with the help of a pocket-calculator, smart phone, or a computer.
- Now, you are ready to try these steps in Python. Try the notebook (*Chapter01\_Fixed\_Point\_Iteration.ipynb*) provided in the course repository¹.

## for loop

You can refine the simple steps given in the notebook into a neat program as follows.

#### Exercise

- Learn about Python's built-in function **range**, and **for** loops in Python.
- Learn what a Python module is. In the following, we are calling a procedure (sqrt) from a module (numpy). Learn about how to use an alias for a module or a procedure while importing in your code.

```
import numpy
print(numpy.sqrt(5))
```

2.23606797749979

# Pretty print

You should always use formatted strings to display any output.

```
# Number, whose square root we want to find
A=5
# Maximum number of steps
MaxIter=4
# Start with a guess
xold=1
# Iterate
for n in range(MaxIter):
    xnew=q(xold,A)
    fstr = "{:5d} {:15.8f} {:15.8f}".format(n, xold, xnew)
    print(fstr)
    xold=xnew
           1.00000000
                            3.00000000
    0
    1
           3.00000000
                            2.33333333
           2.33333333
                            2.23809524
           2.23809524
                            2.23606890
```

- How does this code differ from the one given in the previous page?
- You may also try the following two lines to print the output in the same format.

```
output = "{val1:5d} {val2:15.8f} {val3:15.8f}"
print(output.format(val1=n, val2=xold, val3=xnew))
```

■ In this code, we have limited the number of iterations to a fixed number. Suppose we do not know how many iterations. we will require. How will you modify this code by introducing a **while** loop?

# Fixed-point iteration: Statement, Algorithm, and Theorem

#### Statement of the method

The solution of f(x) = 0; where f(x) is single-valued, can be determined by rewriting the equation in the form x = g(x) and starting with an initial value  $x_0$ . Then, under certain conditions, the sequence  $x_1 = g(x_0), x_2 = g(x_1), \ldots$  will converge to one of the solutions of x = g(x), denoted as  $x^* = \lim_{n \to \infty} x_n$ .

## Algorithm

- 1. Define the function g(x).
- 2. Initialize x to a real number, let's call it  $x_0$ .
- 3. Generate the sequentially improved estimates for the root through the formula  $x_{n+1} = g(x_n)$ .
- 4. Stop when  $|x_{n+1} x_n|$  is below a threshold and return  $x_n$  as the solution  $x^*$ .

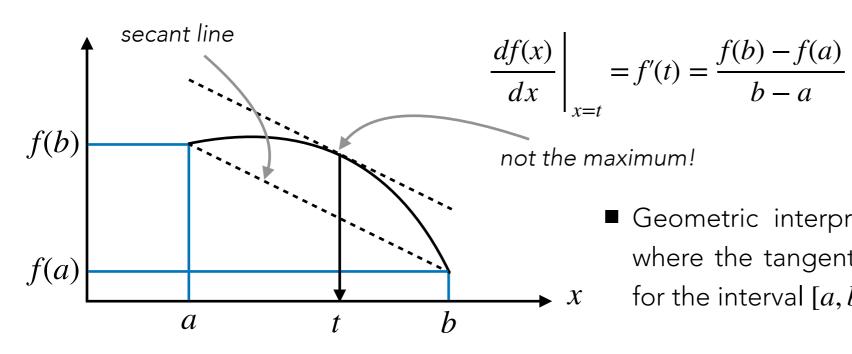
#### **Theorems**

- **Theorem 1:** The equation x = g(x) has a solution for some value of x, which we call  $x^* \in [a, b]$ , provided  $g(x) \in C([a, b])$  has its range contained in the same closed interval [a, b].
  - The theorem does not tell us if we will have one solution (a unique solution) or the equation has multiple solutions.
- Theorem 2 (Uniqueness): If the same g(x) (obeying conditions stated above) further satisfies  $|g^{(1)}(x)| \le k$  for a constant  $0 \le k < 1$  in the open interval (a, b), then x = g(x) has exactly one root in [a, b].
  - The previous theorem stated that the domain of g(x) is [a,b] (and its range is also contained in this interval). Hence, if  $x_0 \in [a,b]$ , then  $g[x_0] \in [a,b]$ , and by induction  $x_1, x_2, ..., x^* \in [a,b]$ .
  - In both the theorems, instead of the closed interval [a,b], we can consider a symmetric interval  $[x^* \delta, x^* + \delta]$ , where  $x^*$  is a solution of the x = g(x), and  $\delta > 0$ .

# Proof of the uniqueness theorem

#### Mean-value theorem

■ If  $f(x) \in C([a,b])$ , and if f(x) is differentiable in (a,b), then there is a point  $t \in (a,b)$  such that



■ Geometric interpretation: There is a point  $t \in (a, b)$  where the tangent of f(x) is parallel to its secant line for the interval [a, b].

## Proof-by-contradiction for the uniqueness theorem

- Suppose g(x) defined in Theorem 2 has two roots p and q in [a,b]. At the roots, we have g(p) = p, and g(q) = q.
- Hence, according to the mean-value theorem there must be a point  $t \in [p,q]$  such that  $g'(t) = \frac{g(q) g(p)}{q p} = \frac{q p}{q p} = 1$ .
- This violates our assumption that  $|g^{(1)}(x)| \le k$  for some constant  $0 \le k < 1$  in the open interval (p,q).

# Convergence of fixed point iteration

## Upper bound for the error in each iteration

- In the Textbook, Theorem1-5-3 and its corollary are proved using the mean-value theorem. This theorem states that at the n-th iteration, the upper bound for the error in the root is given by,  $|x_n x^*| \le k^n(b a)$ .
- So, for a given problem, if we select the domain [a,b] appropriately, and find k, we can estimate the maximum error that one can expect in each iteration.
- With the known information,  $|g^{(1)}(x)| \le k$  and  $0 \le k < 1$ , we can find an approximate value of k. To do this, we can use  $(x_0, g_0)$ , and  $(x_1, g_1)$  and estimate k as the finite derivative  $(g_1 g_0)/(x_1 x_0)$ .

## Example

Let's find the error bound for finding the square-root of 5. Let's begin with  $x_0 = 1$ , and assume the domain to be [1,3]. The following results are obtain using the notebook (Chapter01\_Fixed\_Point\_Iteration.ipynb) provided in the course repository.

actual error

			in ea	in each iteration	
n	x_n	x_(n+1)	x_n-x^*	upper-bound	
0	1.00000000	3.00000000	1.23606798		
1	3.00000000	2.33333333	0.76393202		
2	2.33333333	2.23809524	0.09726536	0.11111111	
3	2.23809524	2.23606890	0.00202726	0.03703704	
4	2.23606890	2.23606798	0.00000092	0.01234568	
5	2.23606798	2.23606798	0.00000000	0.00411523	
6	2.23606798	2.23606798	0.00000000	0.00137174	
7	2.23606798	2.23606798	0.00000000	0.00045725	
8	2.23606798	2.23606798	0.00000000	0.00015242	
9	2.23606798	2.23606798	0.00000000	0.00005081	

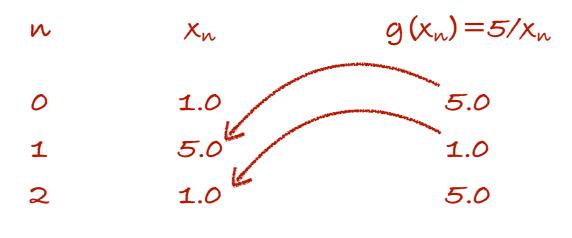
Error bound estimated using k = 0.3333

# Choice of g(x) and initial guess

- To find the square root of a number, the equation we want to solve is  $x = \sqrt{A} \rightarrow x^2 = A \rightarrow x^2 A = 0$ . This equation is of the known form f(x) = 0. To apply fixed-point iteration (see p.9), we have to rewrite the equation in the form x = g(x). Let's look at some choices of g(x).
- Choice-1:  $x^2 A = 0 \rightarrow x^2 = A \rightarrow x = A/x$ . Now,  $g_1(x) = A/x$ .
- Choice-1:  $x^2 A = 0 \rightarrow x^2 = A \rightarrow x = A/x \rightarrow 2x = x + A/x \rightarrow x = (x + A/x)/2$ . Now,  $g_2(x) = (x + A/x)/2$ .

## Example

■ Let's find the square-root of 5 using  $x_0 = 1$  and  $g_1(x)$ .





#### Exercise

- To prevent the code from running indefinetly, one can estimate k and decide whether the loop should run beyond iteration, n = 1. For  $g_1(x) = A/x$ , we can see that k = 1 violating our assumption about g(x).
- Include such a condition in your code.
- The equation  $e^{-x} + x/5 1 = 0$  is encountered in the derivation of Wien's displacement law. Write this equation in the form x = g(x) and apply fixed-point iteration. Analyse how the choice of initial value affects the convergence to a desired value of  $x^*$  for  $g_1(x) = 5(1 e^{-x})$  and  $g_2(x) = -\log(1 x/5)$ .

#### **Bisection method**

#### Statement of the method

■ If  $f(x) \in C[a,b]$ , and f(a)f(b) < 0, then the equation f(x) = 0 has a solution,  $x^* \in [a,b]$ .

#### Algorithm

- 1. Determine f(a) and f(b), verify  $sign f(a) \neq sign f(b)$ . If sign f(a) = sign f(b), exit.
- 2. Determine c = (a + b)/2.
- 3. If |a-b| < threshold,  $x^* = c$ ; else continue.
- 4. Determine f(c) and f(a)f(b).
- 5. If sign f(c) = sign f(a), set a = c, else if sign f(c) = sign f(b), set b = c.
- 6. Repeat 2, then the sequence  $c_0, c_1, \dots, c_n \in [a, b]$  will converge to  $x^*$ .

## Upper bound for the error in each iteration

- The upper bound for the error in the root is given by,  $|x_n x^*| \le (b a)/2^n$ .
- Bisection method is guaranteed to find  $x^*$  how ever with a slower convergence compared to other iterative methods. Often bisection method is used to find an initial guess for a solution in an interval.

#### Exercise

■ Write a Python program to find the square-root of 5 by solving the equation  $x^2 - 5 = 0$  using the bisection method in the interval [1,3]. How many iterations does it take to reach |a - b| < 0.001 and compare with the number of iterations taken in fixed-point-iteration method to reach  $|x_{n+1} - x_n| < 0.001$ .

# Newton-Raphson method

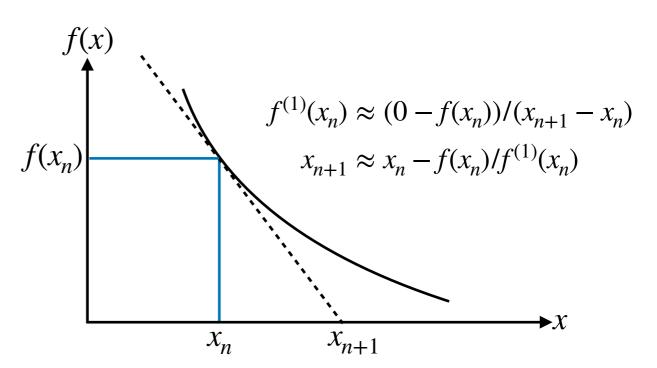
#### Statement of the method

- Newton-Raphson method is a variant of the fixed-point iteration method for solving f(x) = 0, in the form x = g(x) and starting with an initial value  $x_0$ , where  $g(x) = x f(x)/f^{(1)}(x)$ .
- The iteration predicts  $x_{n+1}$  where the function is estimated to vanish.

# Algorithm

- 1. If  $f^{(1)}(x_n)$  < threshold, stop with warning.
- 2. If  $|f(x_n)| < \text{threshold}$ ,  $x^* = x_n$ ; else continue.

$$3. x_{n+1} = g(x_n) \Rightarrow x_{n+1} = x_n - f(x_n) / f^{(1)}(x_n).$$

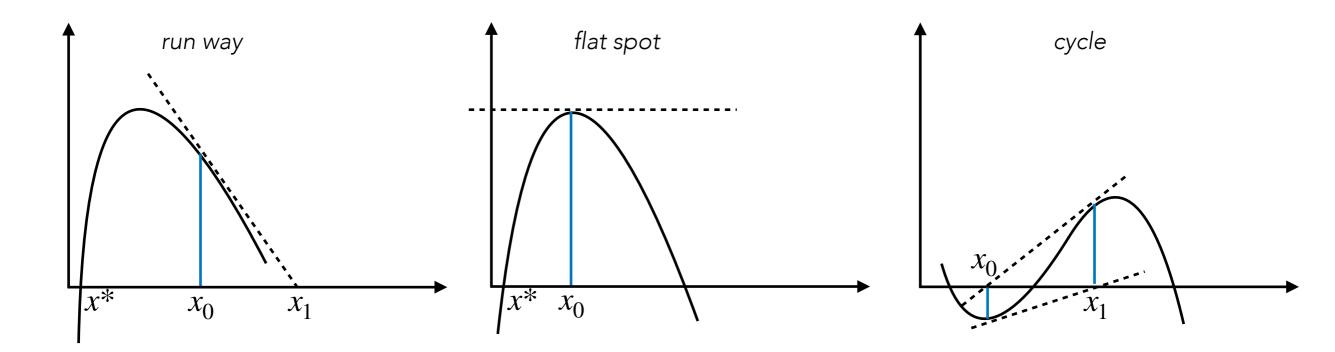


#### **Exercise**

- In general for the fixed point iteration method, show that  $|x^* x_{n+1}| = |g^{(1)}(t)| |x^* x_n|$ , where  $t \in (x_n, x^*)$ . Show that for the Newton-Raphson method,  $|x^* x_{n+1}| = (g^{(2)}(t)/2) |x^* x_n|^2$  (i.e., the error converges quadratically).
- Write a Python program to find the square-root of 5 by solving the equation  $x^2 5 = 0$  using the Newton-Raphson method starting with  $x_0 = 1$ . How many iterations does it take to reach  $|x_{n+1} x_n| < 0.001$ .
- Multiple roots: If f(x) has more than one root at  $x = x^*$  (for example,  $f(x) = (x x^*)^M$ ), then show that Newton-Raphson iteration fails to converge. Show that in this case, the modified Newton-Raphson iteration given below works

$$x_{n+1} = x_n - \frac{f(x_n)f^{(1)}(x_n)}{\left[f^{(1)}(x_n)\right]^2 - f(x_n)f^{(2)}(x_n)}$$

# Problematic initial guesses for Newton-Raphson



# Quasi-Newton-Raphson method (Secant method)

- Nearly in all practical applications of root-finding or minimization problems (especially in higher-dimensional problems such as geometry optimization in computational chemistry research), a variant of Newton-Raphson method, called as the quasi-Newton-Raphson method is used. In one-dimension, it is called as the Secant method.
- The word 'quasi' implies that  $f^{(1)}(x)$  is estimated through finite derivatives and an explicit formula for it is not requried. This makes the method very useful for problems where the analytic derivative of f(x) is not amenable.
- Along with  $x_0$ , the approach requires a small increment  $\Delta x$ , and  $x_1$  is set as  $x_0 + \Delta x$ . Then,  $f^{(1)}(x_1)$  is estimated as  $(f(x_1) f(x_0))/\Delta x$ .
- At the *n*-th iteration,  $f^{(1)}(x_n)$  is estimated as  $(f(x_n) f(x_{n-1}))/(x_n x_{n-1})$ .

# Python basics

## 10 things in Python to know

- 1. Basic datatypes in Python (int, float, complex, string)
- 2. String manipulation (splitting, splicing)
- 3. Python list (more commonly encountered datatype during string processing)
- 4. String concatenation and list appending (building larger strings)
- 5. For loop (to iterate over a list)
- 6. While loop (when the number of cycles is unknown apriori)
- 7. Break vs. continue (gracefully exiting a loop)
- 8. Functions (writing custom functions, doc string, help)
- 9. Module (importing modules, math, numpy, numpy arrays.)
- 10. Input/output (Read from/Write in a file, formatted printing)

#### **Exercise**

- Go through the content in (*Python\_Basics.ipynb*) provided in the course repository.
- Go through the content in (*Python\_NumpyBasics.ipynb*) provided in the course repository.