Numerical Methods for Natural Sciences: Foundation Topics
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Course material: https://github.com/raghurama123/nm2024

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Content

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).
- Anthony J. Pettofrezzo, "*Introductory Numerical Analysis*", Dover Publishers (1984).
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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). *See the chapters about GitHub*.
- Numpy and Scipy Documentation, https://docs.scipy.org/doc/

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 direct-method for finding a root of a polynomial of degree ≥ 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

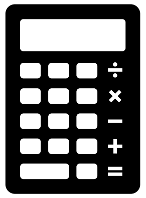
Square root of a real number

- 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 1

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

n	x_n	$g(x_n) = (x_n + 5/x_n)/2$
0	1.0	3.0
1	3.0	2.333...
2	2.333...	2.238...
		...
		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 repository[1].

[1] *https://github.com/raghurama123/nm2024*

`for` loop

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

```python
# 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=g(xold,A)
    print(n,xold,xnew)
    xold=xnew
```

```
0 1 3.0
1 3.0 2.3333333333333335
2 2.3333333333333335 2.238095238095238
3 2.238095238095238 2.2360688956433634
```

Exercise 1

- 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.

```python
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=g(xold,A)
    fstr = "{:5d} {:15.8f} {:15.8f}".format(n, xold, xnew)
    print(fstr)
    xold=xnew
```

```
    0      1.00000000      3.00000000
    1      3.00000000      2.33333333
    2      2.33333333      2.23809524
    3      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^*.

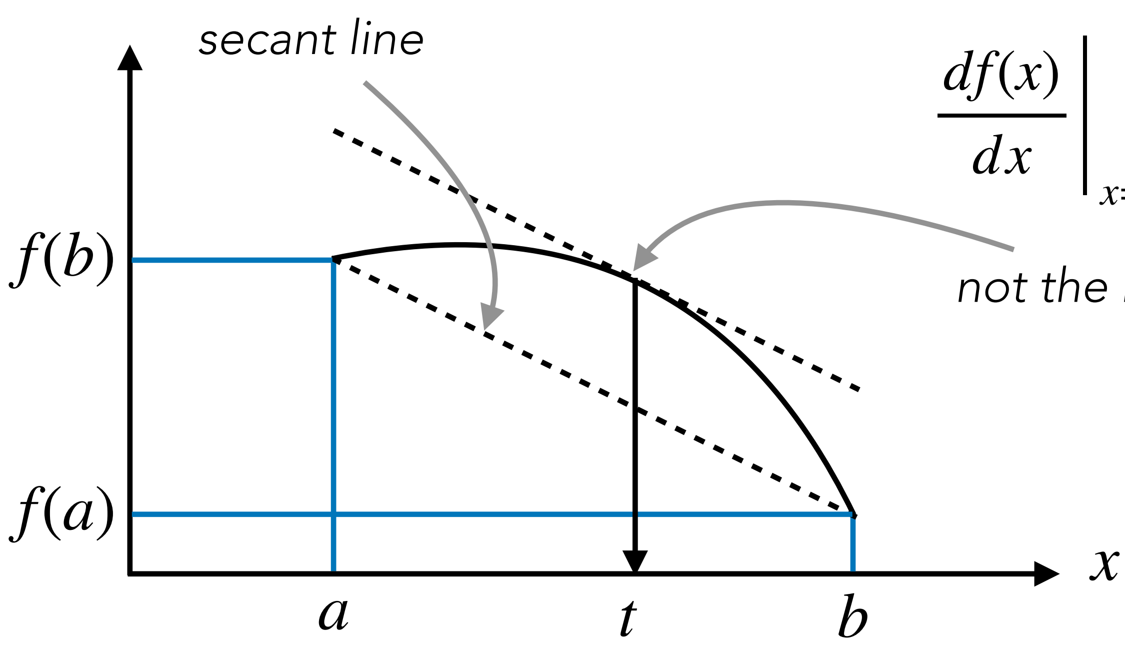
Theorems

- **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 $|g^{(1)}(x)| \leq k$ for a constant $0 \leq k < 1$ 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 $x_1, x_2, \ldots, x^* \in [a, b]$.
  - 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



$$\left.\frac{df(x)}{dx}\right|_{x=t} = f'(t) = \frac{f(b)-f(a)}{b-a}$$

- 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 $|g^{(1)}(x)| \leq k$ for some constant $0 \leq k < 1$ 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, $|x_n - x^*| \leq k^n(b-a)$.
- 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, $|g^{(1)}(x)| \leq k$ and $0 \leq k < 1$, 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 2

- 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 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
```

$0 < k \leq 1$

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 3

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

n	x_n	$g(x_n) = 5/x_n$
0	1.0	5.0
1	5.0	1.0
2	1.0	5.0
		...

Exercise 2

- 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

- The equation $f(x) = 0;\ x \in [a, b]$ has a solution, $x^* \in [a, b]$ if $f(a)f(b) < 0$.

Algorithm

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

Upper bound for the error in each iteration

- The upper bound for the error in the root is given by, $|x_n - x^*| \leq (b - a)/2^n$.
- 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.

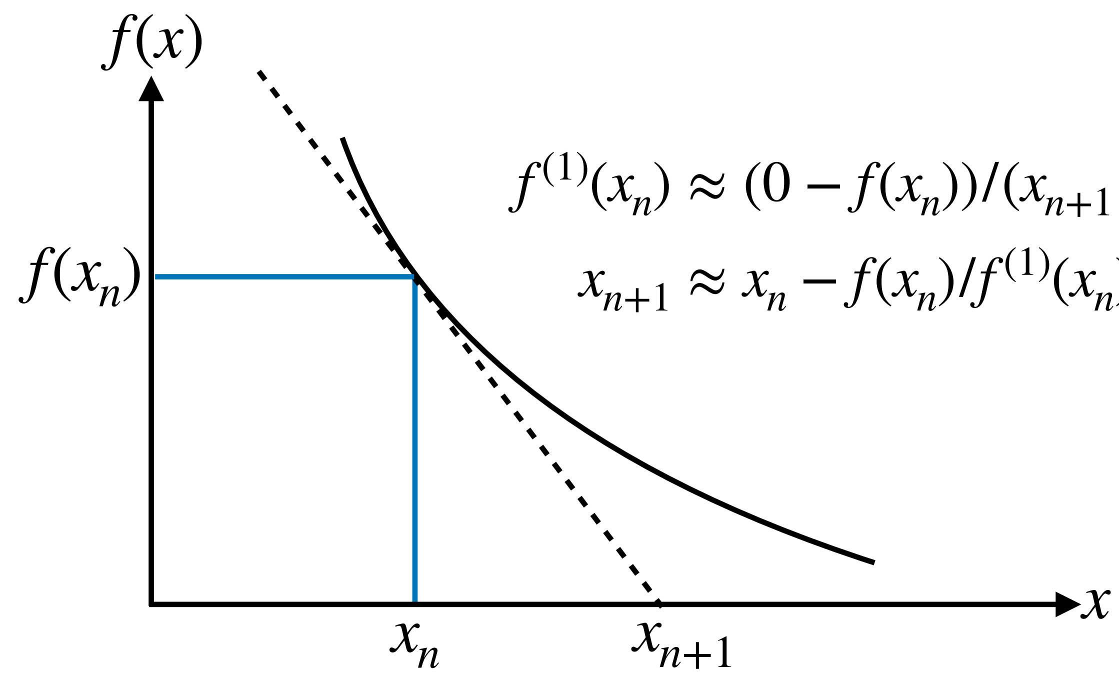
Exercise 3

- 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

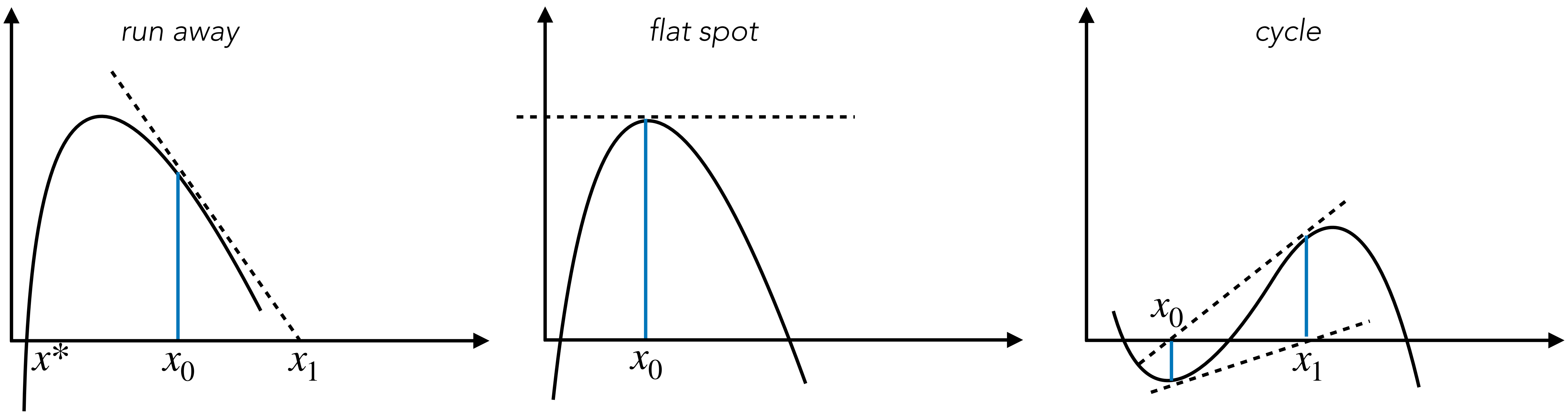
1. If $f^{(1)}(x_n) < \text{threshold}$, stop with warning.
2. If $|f(x_n)| < \text{threshold}$, $x^* = x_n$; else continue.
3. $x_{n+1} = g(x_n) \Rightarrow x_{n+1} = x_n - f(x_n)/f^{(1)}(x_n)$.

Exercise 4

- 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 Δx, 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

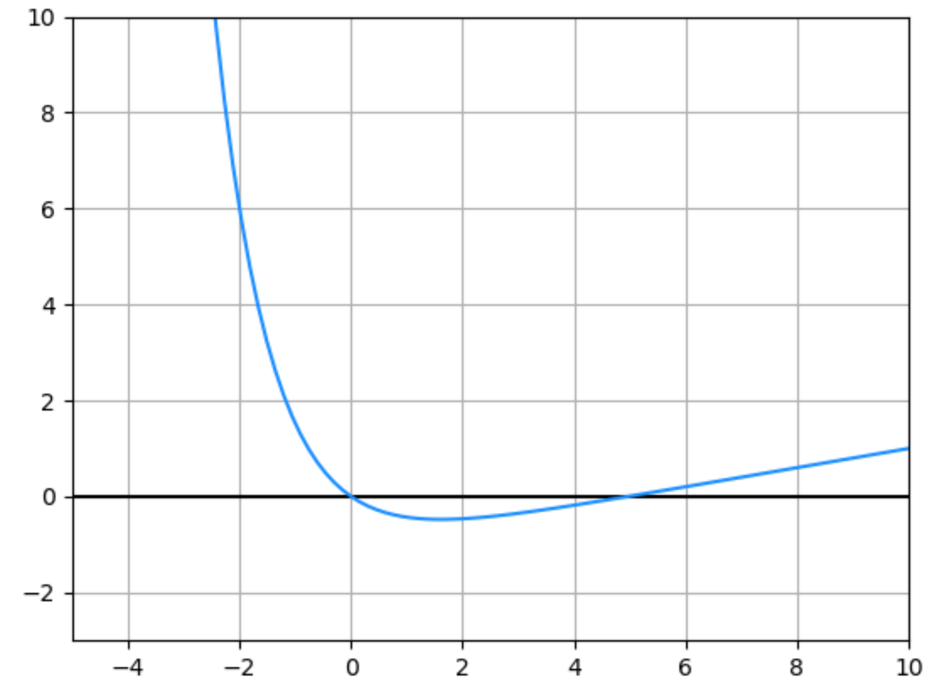
1. Basic datatypes in Python (int, float, complex, string)
2. String manipulation (splitting, splicing)
3. Python list (more commonly encountered datatype during string processing)
4. String concatenation and list appending (building larger strings)
5. For loop (to iterate over a list)
6. While loop (when the number of cycles is unknown *a priori*)
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 5

- 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.
- Go through the content in (*Python_Matplotlib.ipynb*) provided in the course repository.

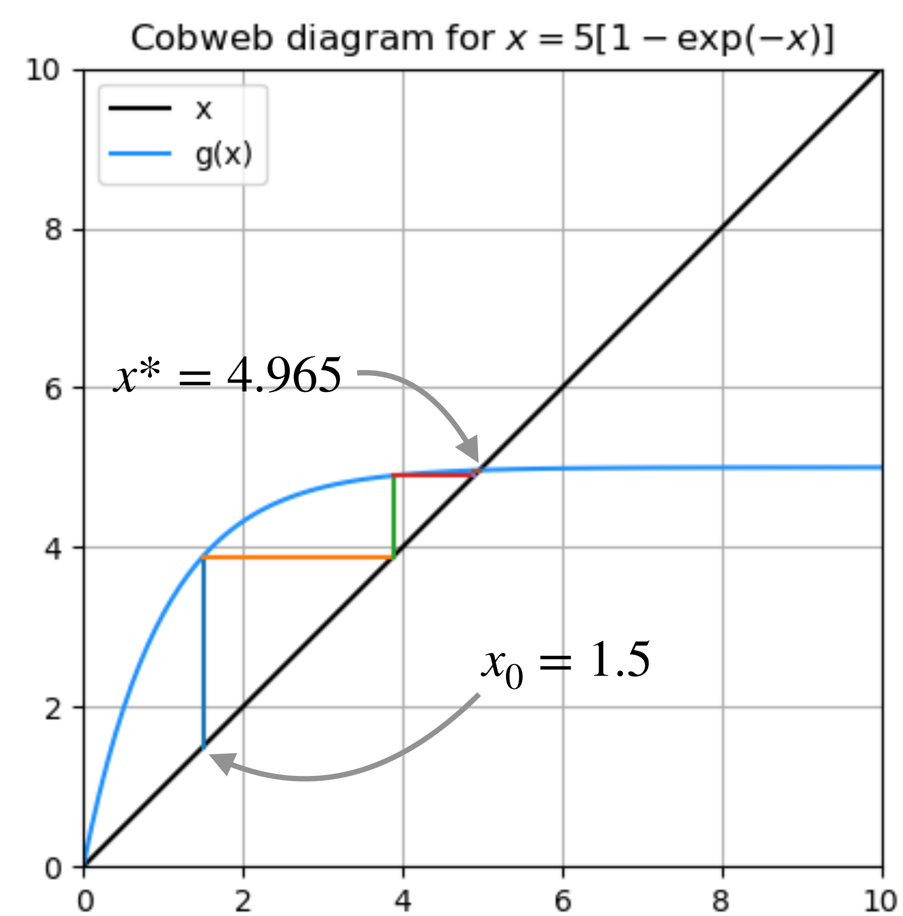
Graphical solution

- Graphically, the solution(s) of an equation can be determined by plotting $f(x) = 0$, and inspecting where $f(x)$ crosses the x-axis. In fixed point iteration, we solve $x = g(x)$, where we can plot both the L.H.S. and the R.H.S. and inspect the point(s) of intersection.
- The plots shown here were obtained using the notebook (*Chapter01_Fixed_Point_Iteration.ipynb*) provided in the course repository.



Graphical representation of fixed-point iteration using cobweb diagram

- Mark the point $\{x_0, 0\}$; find $g(x_0)$, which is x_1
- Connect $\{x_0, x_0\}$ to $\{x_0, x_1\}$ (vertical line)
- Connect $\{x_0, x_1\}$ to $\{x_1, x_1\}$ (horizontal line)
- Connect $\{x_1, x_1\}$ to $\{x_1, x_2\}$ (vertical line)
- Connect $\{x_1, x_2\}$ to $\{x_2, x_2\}$ (horizontal line)
- Repeat until you Connect $\{x_{n-1}, x_n\}$ to $\{x_n, x_n\}$ (horizontal line)



Exercise 6

- Find example equations to show using fixed-point iteration: (i) monotonous convergence, (ii) monotonous divergence, (iii) oscillatory convergence, (iv) oscillatory divergence. Present your results in the form of cobweb diagrams.

Chapter 2: Matrix computations and solution of linear equations

System of linear equations

Finding simultaneous solution of *N* equations

- We have discussed methods for solving an equation of the form $f(x) = 0$. Here x is a scalar variable and the function $f(x)$ is also scalar-valued.
- Suppose we have an equation containing two variables: $f(x, y) = 0$, then it is possible that we may not be able to find the solution (x^*, y^*) using information contained in one equation. It may however be possible to find the solution if we have two equations in the same variables: $f_1(x, y) = 0$ and $f_2(x, y) = 0$. We call these two equations as a system of two equations in two unknowns. We can write these equations in many ways as follows:

$$\begin{aligned} f_1(x, y) &= 0 \\ f_2(x, y) &= 0 \end{aligned}$$

$$\mathbf{f}(\mathbf{x}) = 0$$

Here $\mathbf{x} = [x, y]^{\mathrm{T}}$ and $\mathbf{f} = [f_1(x, y), f_2(x, y)]^{\mathrm{T}}$, where T indicates a transpose because we normally denote these vector valued variables and functions as column vectors. For simplicity, the RHS is not written in bold face, 0 indicates a 0-vector.

Finding simultaneous solution of *N* linear equations

- If the functions involve only the first power (or lower, which is a constant) of the independent variables, we have a linear equation. For example, $f(x, y) = ax + by + c$. Suppose we have $f_1(x, y) = a_{11}x + a_{12}y + b_1 = 0$ and $f_1(x, y) = a_{21}x + a_{22}y + b_2 = 0$, we can write the equations in the matrix form as follows

$$\begin{aligned} f_1(x, y) &= b_1 \\ f_2(x, y) &= b_2 \end{aligned}$$

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{11} & a_{12} \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

$$\mathbf{Ax} = \mathbf{b}$$

- In Ch. 2, we will discuss methods to solve systems of linear equations and in Ch.3, we will discuss methods for non-linear equations.

- The formula to calculate the matrix-vector multiplication, $\mathbf{Ax} = \mathbf{b}$, is $b_i = \sum_j A_{i,j} x_j$. In the matrix notation, we can define b_i as $\mathbf{A}_{i,} \cdot \mathbf{x}$, where $\mathbf{A}_{i,}$ is the $\boldsymbol{i}$-th row of $\mathbf{A}$ and $\mathbf{x}$ is the column vector, which we can calculate using the `np.dot` function. This is usually the convention we will follow.
- One can also think of $\mathbf{Ax}$ as a linear combination of columns of $\mathbf{A}$ with the elements of $\mathbf{x}$ as the linear expansion coefficient, $b_i = \mathbf{x}^{\mathrm{T}} \cdot \mathbf{A}_{,j}$
- For mutliplying two matrices A and B, we will use the `np.dot` function as `C=np.dot(A,B)`

Exercise 6

- Go through the content in *Chapter02_Matrix_Computations.ipynb* provided in the course repository.
- Write a Python function for reading a matrix from a file if the elements are listed sequentially, one below another. Use `reshape` function to convert a 1D array into a 2D array (matrix).

Exercise 7

- As you have seen in the example code, the computational complexity of addition of two matrices is $\mathcal{O}(N^2)$, and for multiplication it is $\mathcal{O}(N^3)$. Write Python functions to
  (1) add two circulant matrices with a computational complexity of $\mathcal{O}(N)$, i.e., a linear scaling procedure.
  (2) multiply two circulant matrices with a computational complexity of $\mathcal{O}(N^2)$, i.e., a quadratically scaling procedure.
  You can figure out the definition of a circulant matrix by printing a square Toeplitz matrix using the `scipy.linalg.toeplitz` function and passing the first row of the matrix as the argument.

```
toeplitz([1,2,3])
```

```
array([[1, 2, 3],
       [2, 1, 2],
       [3, 2, 1]])
```

```
toeplitz([1,1,3])
```

```
array([[1, 1, 3],
       [1, 1, 1],
       [3, 1, 1]])
```

```
toeplitz([1,2,3,4])
```

```
array([[1, 2, 3, 4],
       [2, 1, 2, 3],
       [3, 2, 1, 2],
       [4, 3, 2, 1]])
```