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).
- W. Boehm, H. Prautzsch, "*Numerical Methods*", Universities Press (2003).
- 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

- 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.

```
# 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
```

Self-study

- 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=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^*.

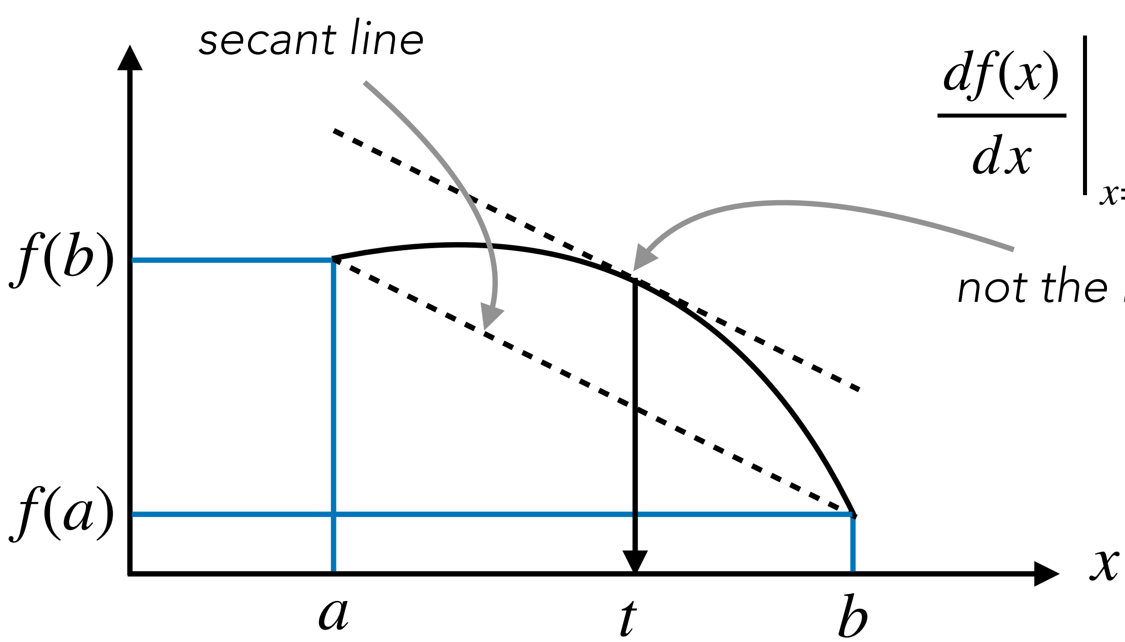
Theorems

- **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 $|g^{(1)}(x)| \le k$ 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, $|x_n - x^*| \leq k^n(b-a)$.
- 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

- 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

- 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
		...

Hands-on

- 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 $g_2(x) = -\log(1 - x/5)$.