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

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 a*lgorithm* 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.

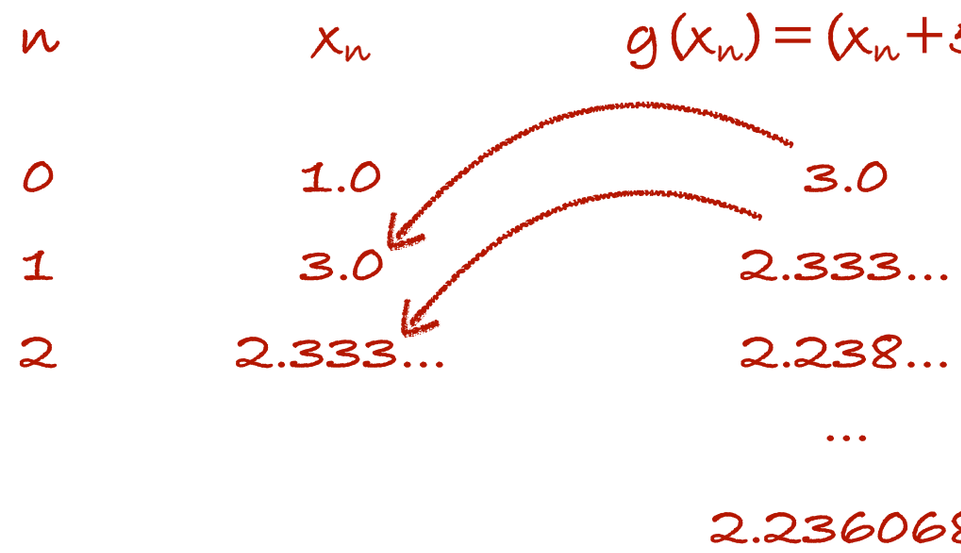
Square root by fixed-point iteration

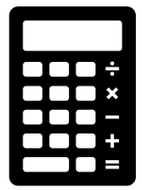
Square root of a real number

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





- 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?