



Computational Techniques

Module- I: Introduction

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About the Instructor

- Dr. Niket Kaisare
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- Research Interests
 - Catalytic micro-reactors
 - Fuel processing / Fuel Cells
 - Multi-scale modeling
 - Optimization and Control

About the Course

This course is designed to give an overview of
Computational Techniques
of interest to engineers

- Focus will be on numerical methods, their properties and analysis
- Approximately 40 one-hour modules

What You Need

For the lectures to be most effective, you need to work with me during each lecture

Keep near you:

- A pen and notebook
- A calculator
- An Excel* spreadsheet (or Google Docs* App.)

“Peer interaction” is highly recommended

*This is not an official endorsement of any product.
I personally find these Apps most suitable to this course.



Computational Techniques

An Overview of the Course

Working Definition

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use computers to solve problems by
step-wise, *repeated* and *iterative* solution methods,
which would otherwise be
tedious or *unsolvable* by hand-calculations.

Popularity

- Popularity due to availability of computers
- To solve problems for which algebraic solution cannot be obtained

Advantages

- Extremely powerful problem-solving tools
- Commercial softwares and packages available
- Can provide additional insights into various engineering problems

Historical Perspective

- Babylonian method for $\sqrt{2}$
(also called Heron's algorithm)

Iteratively calculate using the expression:

$$x^{(\text{new})} = \frac{1}{2} \left(x + \frac{2}{x} \right)$$

Layout of the Course

- Split into various modules (chapters)
- Each module → 4 to 6 one-hour lectures
 - Motivation / Overview of the topic
 - Examples
 - Graphical insight
 - Derivation and analysis
 - Summary

1. Motivation

- Why learn about Heron algorithm for $\sqrt{2}$?

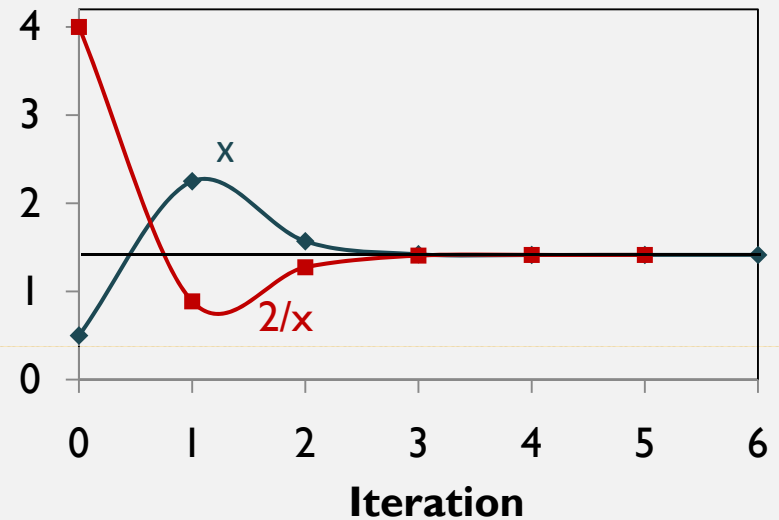
2. Example

- Start with initial guess $x = 0.5$
- Next value is $x = (0.5 + 2/0.5) \times 1/2$

iteration	x	2/x	Average
0	0.5	4	2.25
1	2.25	0.888889	1.569444
2	1.569444	1.274336	1.42189
3	1.42189	1.406578	1.414234
4	1.414234	1.414193	1.414214
5	1.414214	1.414214	1.414214
6	1.414214		

3. Graphical Insight

- For positive values, x and $2/x$ lie on either side of the true solution



4. Analysis

- Taylor's series expansion of $f(x) = (2 - x^2)$ gives us the properties of Henon algorithm (covered in Module 4)

Topics Covered in the Course

- Module 1: Introduction
- Module 2: Computation and Error Analysis
- Module 3: Linear Systems and Equations
- Module 4: Algebraic Equations
- Module 5: Regression and Curve Fitting
- Module 6: Differentiation and Integration
- Module 7: Ordinary Differential Equations (1)
- Module 8: Ordinary Differential Equations (2)
- Module 9: Partial Differential Equations