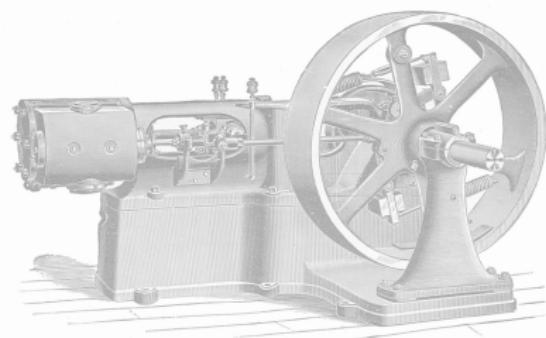


Numerical Methods

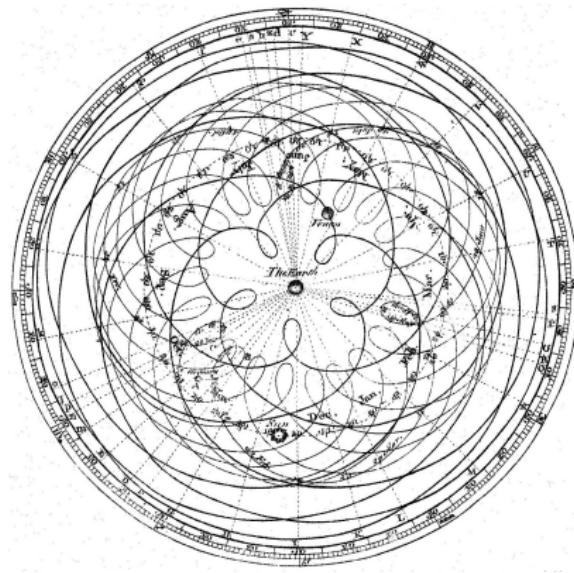
“Simulation and mathematical modeling will power the twenty-first century the way steam powered the nineteenth.”

— W.H. Press*



*Author of Numerical recipes, in “The Nature of Mathematical Modeling” by Neil Gershenfeld

Ptolemy and the Almagest



~150 AD. Development of numerical approximations to describe the motions of the heavenly bodies with accuracy matching reality sufficiently.

Some Acknowledgements



Programming

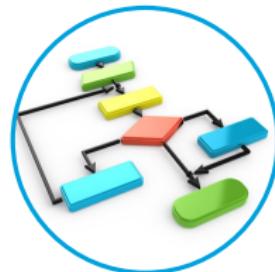
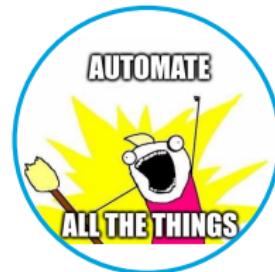
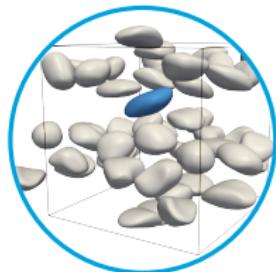
“Everybody in this country should learn to program a computer, because it teaches you to think..”

—Steve Jobs



Why?

- Scientific techniques depend in an increasing fashion upon computer programs and simulation methods
- Knowledge of programming allows you to automate routine tasks
- Ability to understand algorithms by inspection of the code
- Learn to think by dissecting a problem into smaller bits



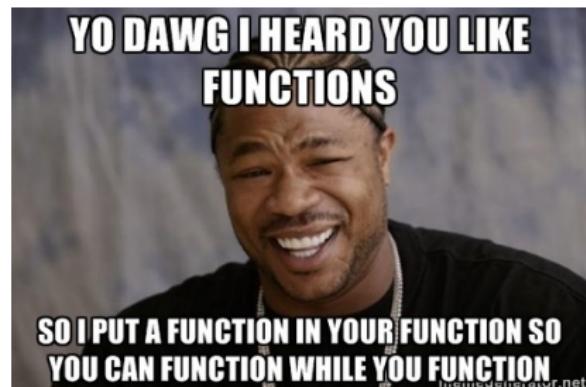
Matlab help

- Matlab documentation: `doc` or `help` function
- Canvas page
- Introduction to Numerical Methods and Matlab Programming for Engineers. T. Young and M.J. Mohlenkamp (2015). GNU-licensed document, online
- Search the web!

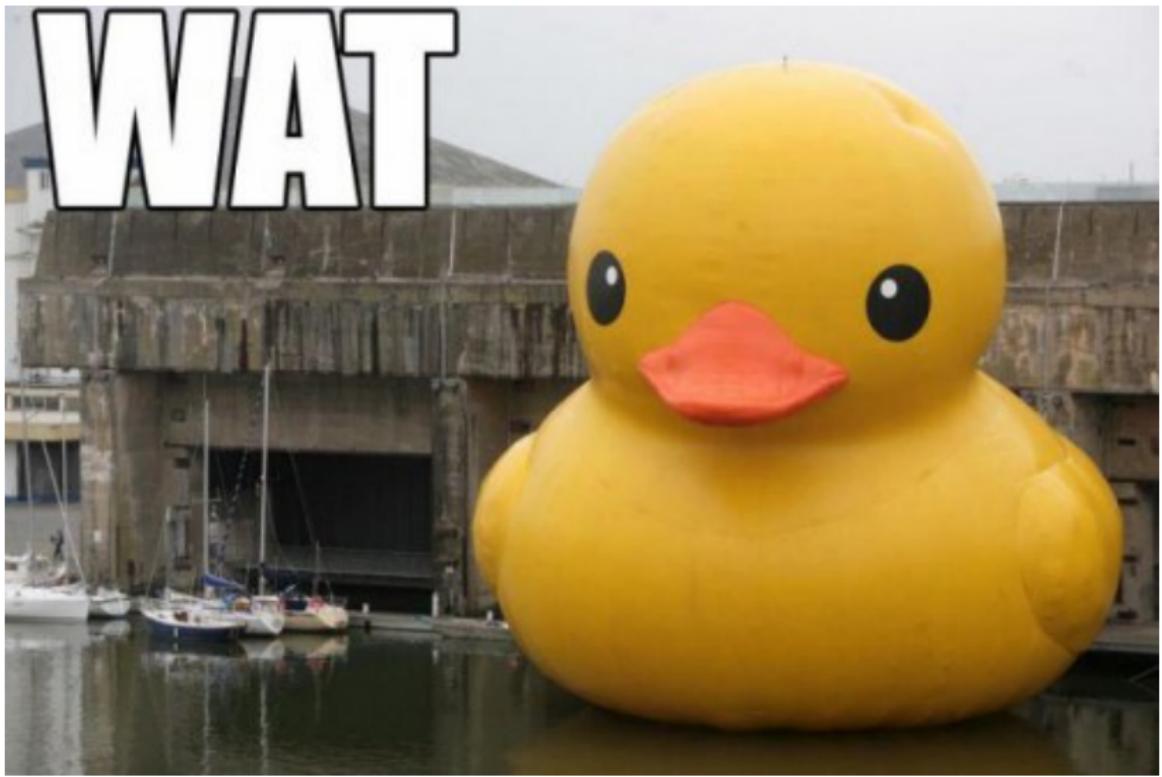


Recursion

- In order to understand recursion, one must first understand recursion
- A recursive function is called by itself (a function within a function)
 - This could lead to infinite calls;
 - A base case is required so that recursion is stopped;
 - Base case does not call itself, simply returns.



WAT



Errors in computer programs

Computer programs often contain errors (bugs): buildings collapse, governments fall, kittens will die.



Representation of real (floating point) numbers

- Formally, a real number is represented by the following bit sequence

$$x = \sigma \left(2^{-1} + c_2 2^{-2} + \dots + c_m 2^{-m} \right) 2^{e-1023}$$

Here, σ is the sign of x and e is an integer value.

- A floating point number hence contains sections that contain the sign, the exponent and the mantissa

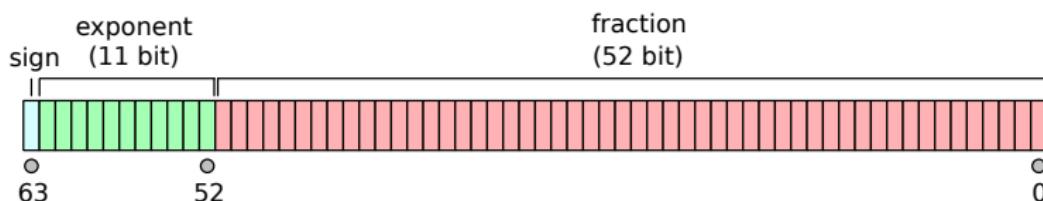


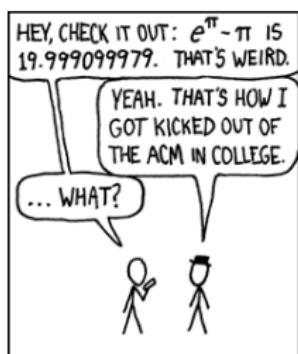
Image: Wikimedia Commons CC by-SA

Example 2

Start your calculation program of choice (Excel, Matlab, ...)

Calculate the result of y :

$$y = e^\pi - \pi = 19.999099979 \neq 20$$



DURING A COMPETITION, I TOLD THE PROGRAMMERS ON OUR TEAM THAT $e^\pi - \pi$ WAS A STANDARD TEST OF FLOATING-POINT HANDLERS -- IT WOULD COME OUT TO 20 UNLESS THEY HAD ROUNDING ERRORS.
I

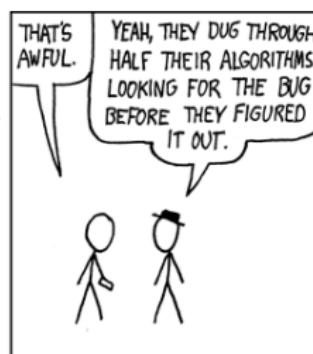
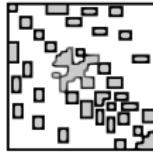
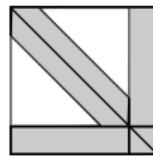
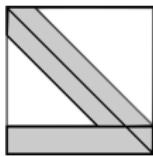
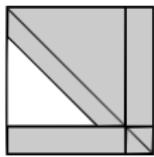
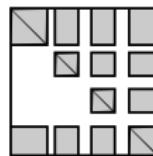
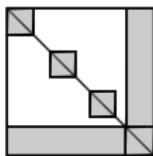
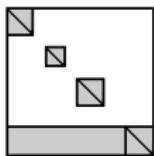
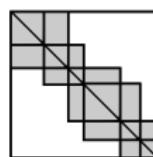
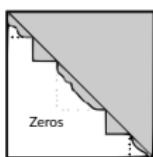
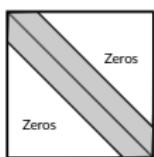


Image: [xkcd](#)

Sparse matrix layout examples



Numerical methods for Chemical Engineers:

Non-linear equations

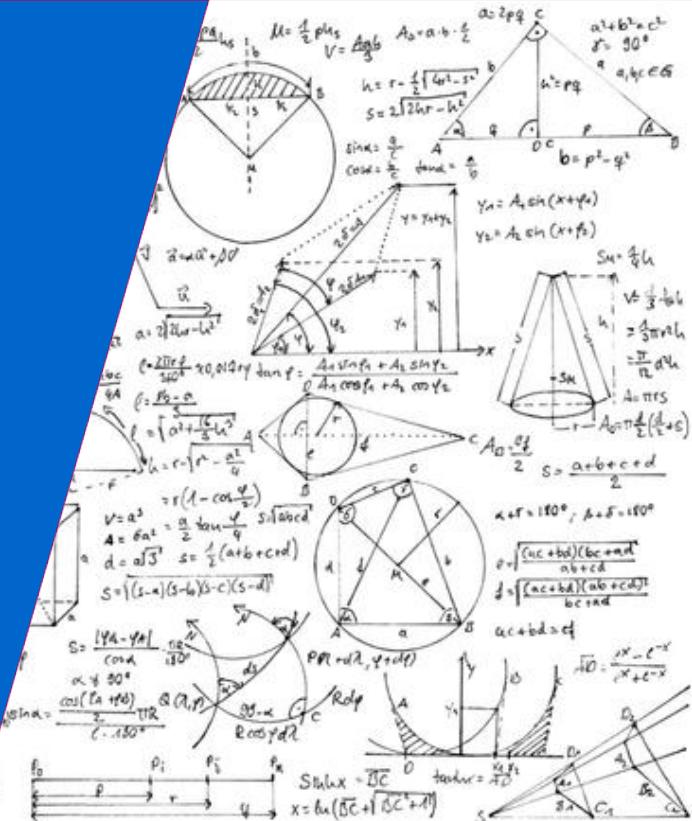
Prof.dr.ir. Martin van Sint Annaland
Dr.ir. Ivo Roghair

Chemical process Intensification

TU/e

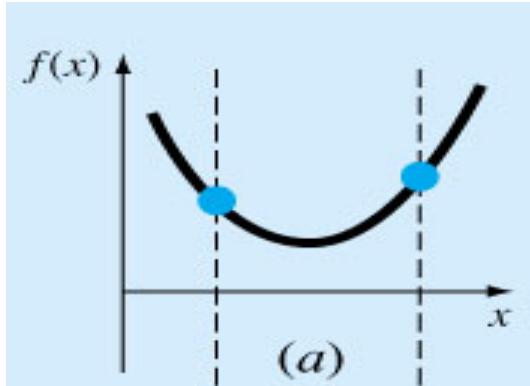
Technische Universiteit
Eindhoven
University of Technology

Where innovation starts

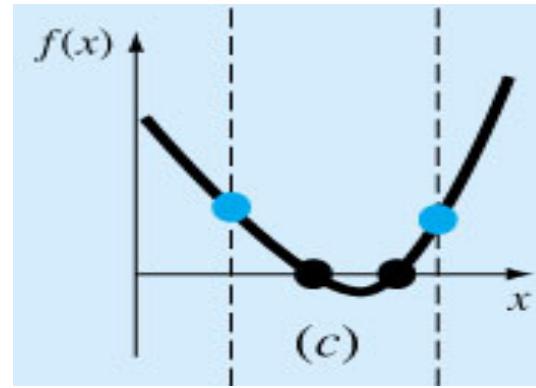


General idea

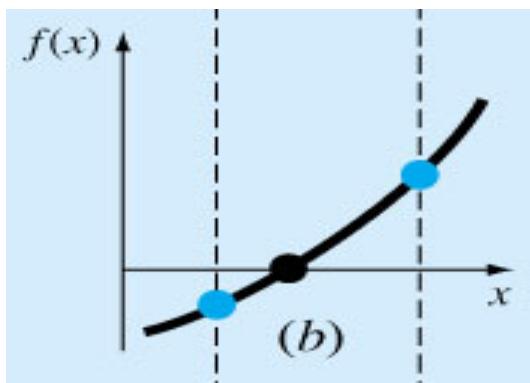
- Examples of pitfalls of root finding...



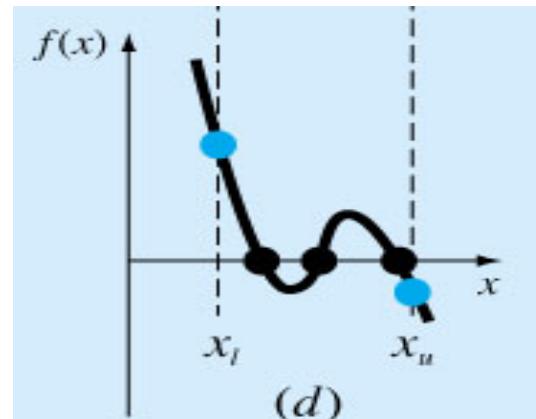
No answer (no root)



Oops!! (two roots!!)



Nice case (one root)



Three roots (might work for a while!)

Optimization Spectrum

Problem	Method	Solvers
LP	Simplex method Barrier methods	Linprog (Matlab) CPLEX (GAMS, AIMMS, AMPL, OPB)
NLP QP	Lagrange multiplier method	Fminsearch/fmincon (Matlab)
	Successive linear programming	MINOS (GAMS, AMPL)
	Quadratic programming	CONOPT (GAMS)
MIP	Branch and bound	
MILP	Dynamic programming	Bintprog (Matlab)
MINLP MIQP	Generalized Benders decomposition	DICOPT (GAMS)
	Outer approximation method Disjunctive programming	BARON (GAMS)