Chemical Engineering 263
Numerical Tools

* Prayer

I. Course Intro

* Personal Introduction (Name, career history, research, family)
* Recruiting Pitch for UG research
* Commit to learn names (candy bag), AMA Thursday's
* Introduce TAs
* Review Syllabus & Schedule

  - Course website
  - Course description
  - Lectures & Quizzes
  * Academic Honesty
  - Homework
  - Office hours
  - Exams, grading
  - Final Exam

* This course will be hard for some of you.
  - Try HW by self first ~ ok if you are stuck
  - Avoid mentality of *just* getting HW done.
  - Do all HW is normal = B/B+ student
  - We are here to help. Everything we will cover is in a review sheet

II. Intro to Numerical computing.

A. Analytical vs. Numerical Solutions

* Engineers do math. Math is the language of Nature, and we need it to understand, predict & design engineering systems.

* A lot of math problems cannot be solved by hand.

example.

$$3x^2 + 4x - 1 = 0$$

A non-linear, algebraic equation (quadratic)

Solve via quadratic formula.

$$x = \frac{-4 \pm \sqrt{4^2 - 4(3)(-1)}}{2(3)} = \frac{-4 \pm \sqrt{16+12}}{6}$$

$$x = \frac{-4 \pm 2\sqrt{7}}{6} = -\frac{2}{3} \pm \frac{\sqrt{7}}{3} \approx (0.215, -1.549)$$

$$3x^2 + 4x - 1 = 4 \log_{10}(x+3)$$

still non-linear, algebraic equation. With the trancendental term on the RHS, we are stuck.

- Can you find an answer?

↳ see example solution : example-soln.py

(0.5636, -1.6436)

* If we can solve something by hand, we call this an analytical solution.

* If we need a computer, we are left with only a numerical solution

* Generally, we prefer an analytical solution. It is exact and usually easier to get than a numerical one. We also learn a lot about the kind of solution it is by doing analytical math. But a numerical solution is better than no solution. In this class, we will focus on how to get numerical solutions. (This compliments your analytical math classes.)

B. Classifying Math Problems

* To solve math problems, we need to be able to classify them. This will help us know what tools and methods to use to solve them.

* We can formally write many math problems like:

$$f_1(x_1, x_2, \dots, x_n) = 0$$
$$f_2(x_1, x_2, \dots, x_n) = 0$$
$$f_m(x_1, x_2, \dots, x_n) = 0$$

* If $n=m=1$, then we have a single equation if $n>1, m>1$ then we have a system of equations

* If $f_1(x_1) = 0$ then the equations are
$f_2(x_2) = 0$
$\vdots$
$f_n(x_n) = 0$

independent or uncoupled. If not, the system is coupled and all of the equations must be solved simutaneously.

* If all of the f_i's are of the form:

$$f_1 = a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n$$

then the system is linear. If not, it is non-linear. Linear systems have nice properties that make them easier to solve.

* Finally, if we replace some of the x_i's with derivatives:

$$f\left(x_1, x_2, \frac{dx_1}{dx_2}\right) = 0$$

then the equations are differential equations. If integrals appear

$$f\left(x_1, x_2, \int \phi(x_1)\,dx_2\right) = 0$$

then the equations are integral equations.

Otherwise, they are algebraic equations.

Example

* Label $3x^2+4x-1 = 4\log_{10}(x+3)$

  - single equation
  - non-linear
  - algebraic

* Label:

$$3x + 2y = 7$$
$$-4x + y = -2$$

  - system of equations, coupled
  - linear
  - algebraic

* Label:

$$\frac{dx}{dt} + x = 1$$
$$\frac{dy}{dt} - y = 4$$

  - system of equations, uncoupled
  - linear
  - differential