Chemical Engineering 263 – Numerical Tools

Outline
I. Syllabus & schedule
II. Intro to numerical computing

I. Syllabus & Schedule

* See syllabus & schedule!

II. Introduction to Numerical Computing

A. Analytical vs. Numerical Solutions

* As engineers we need math!
* Lots to do by hand!

Ex. $3x^2 + 4x - 1 = 0$ ← a nonlinear (quadratic) algebraic Eq.

$a = 3,\ b = 4,\ c = -1$

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$= \frac{-4 \pm \sqrt{4^2 - 4 \cdot 3 \cdot (-1)}}{2 \cdot 3}$$

$16 + 12 = 28 = 4 \cdot 7$

$$= -\frac{2}{3} \pm \frac{1}{3}\sqrt{4 + 3}$$

$$= -\frac{2}{3} \pm \frac{\sqrt{7}}{3}$$

Ex2. $3x^2 + 4x - 1 = 4\log_{10}(x+3)$ ← a nonlinear algebraic Eq.

???

- No way to isolate 'x'
- Implicit ↗

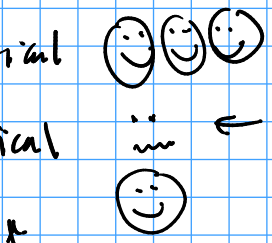
→ (0.5636, −1.6436) 2 solutions

We could not do this by hand!

* By hand → "analytical solution"
* Need Computer → "numerical solution"

* In general

- analytical ----> cheap / quick / Infinite Precision
- numerical ← this class ---> Finite Precision, Costly, Big computers?



At least we get one!

B. Classifying Math Problems

* To solve a problem, you first need to classify it!

* Many problems will have this general form:

$$f_1(x_1, x_2, x_3 \cdots x_n) = 0$$

$$f_2(x_1, x_2, \cdots x_n) = 0$$

$$\vdots$$

$$f_m(x_1, x_2, \cdots, x_n) = 0$$

① single vs system

If $n = m = 1$ ⇒ single equation

If $n \geq 1, m > 1$ ⇒ system of equations

② independent vs. coupled

If $f_1(x_1) = 0$

$f_2(x_2) = 0$

$\vdots$

$f_n(x_n) = 0$ → independent or uncoupled

$f_1(x_1, x_2) = 0$

$f_2(x_1, x_2) = 0$ → dependent or coupled

Ex: $x+y=3$ ✓ system $n=2$

$x^2+y^2=7$ ✓ coupled. $m=2$

↳ $x+y-3=0 = f_1$

$x^2+y^2-7=0 = f_2$

Ex2. $x=3$ ✓ system $n=2,\ m=2$

$y^2+y-7=0$ ✓ uncoupled

(3) Linear vs. Nonlinear

If all f's have the form:

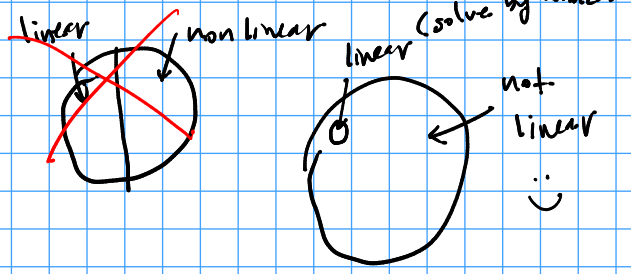
$$f_1 = a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n$$

(a_{1n}: Const coeffs; x_n: no powers, no products)

then I am linear.

$h(ax+by) = ah(x)+bh(y)$

All other cases are nonlinear



(4) Algebraic vs. Differential

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

($\frac{dx_1}{dx_2}$: differential) → Differential Equation $\frac{d^2y}{dt^2} = -g$

No differentials → algebraic Eq. → $x^2-2x+1=0$ ✓

(there are others)

- $f\left(x_1, x_2, \int \phi(x_1)\,dx_2\right) = 0$ (integral Eq.)
- $f\left(x_1, x_2, \frac{dx_1}{dx_2}, \int \phi(x_1)\,dx\right) = 0$ (integro-differential Ex)

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

1. single
2. x only for a system
3. non-linear
4. algebraic

Example: $3x + 2y = 7$

$-4x + y = -2$

1. system
2. coupled
3. linear
4. algebraic

Example: $\frac{dx}{dt} + x = 1$ $\times \frac{dx}{dt}$ NL.

$\frac{dy}{dt} - y = 4$

1. system
2. uncoupled
3. linear
4. differential