**Class 8** – **Numerical Differentiation – PART I (Chp. 4,21)**

ChE310\_Sec1\_F2019 / 9.19.19

<http://www.reuelgroup.org/numerical-methods-che-310.html>

Announcements:

* Next Tuesday is Career Fair (no class)
* 10.1 Phase 1 of project / 10.3 Midterm
* Visit <https://www.redcrossblood.org/> and search zip code “50014” for blood donation opportunities

**Warm Up Group Activity:** submit to SLACK by 2:25pm.

Velocity (m/s) of a rocket is measured over time (s):

V = [0 5 12 30 100 200]; t = [0 100 200 300 400 500];

If the acceleration is ZERO at the start and end of this recorded data, fit a spline to plot how velocity changes with time. Plot given data as ‘ro’ and fit as ‘b:’

**Outline for Class 7 Lecture**

1. Small review on splines – what did we learn?
2. Calculus is the mathematics of change



First derivative





Partial derivative



Second derivative – measure of curvature



1. Engineering (esp. ChemE) is all about rates:



1. Why do we need numerical differentiation?
2. How do we make it more accurate?
3. Taylor series – any smooth function can be approximated as a polynomial





1. Taylor series - analogy of the hill
2. Big ‘O’ notation for truncation error
	1. 
	2. Error is proportional to step size ‘h’ raised to the (n+1)th power
	3. O(h) vs. O(h2), halving the step size?
3. Derivation of numerical derivatives

 (forward)

$f^{'}\left(x\_{i}\right)= \frac{f\left(x\_{i}\right)-f(x\_{i-1})}{h}+O(h)$ (backward)

(centered)

[does it make sense that our error would improve on centered? WHY?]

1. Include MORE terms for even more exact finite differences (see tables 21.3-21.5 in Chapra)



*Real example:* Rate of protein expression vs. time?

1. What about data that is NOT sampled uniformly? (human collected)
	1. Fit with an interpolating polynomial
	2. You can do this directly w/ LaGrange



