ChE 310 – Computational Methods in Chemical Engineering

Spring 2019

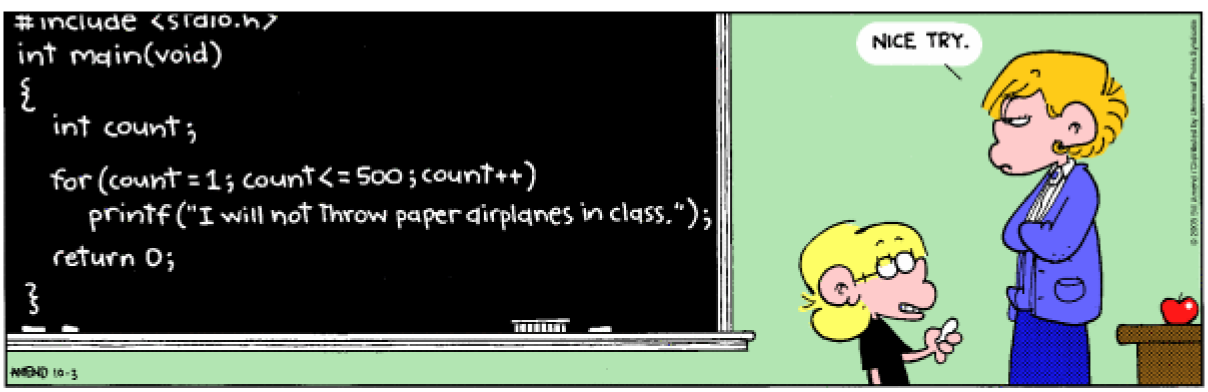
FINAL EXAM – DO NOT OPEN UNTIL INSTRUCTED

NAME: Key (NFR)

By writing my name, I certify that I have abided by all academic honesty policies.

- This portion of the exam is closed book, closed course notes. No additional resources may be consulted to complete this portion of the exam.
- This portion of the exam is worth 20 points (2 per problem).
- Write your answers to be graded in the space provided.
- You must turn in this portion of the exam before you will receive the free response portion, which is worth an additional 60 points.

Enjoy this comic while you wait:



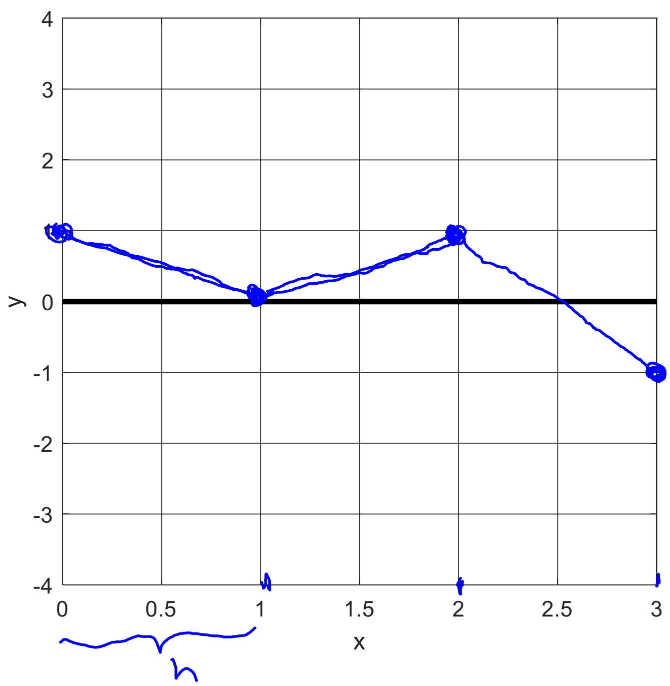
Source: Foxtrot

(1) Consider the following differential equation:

$$\frac{dy}{dx} = -y^2 + x$$

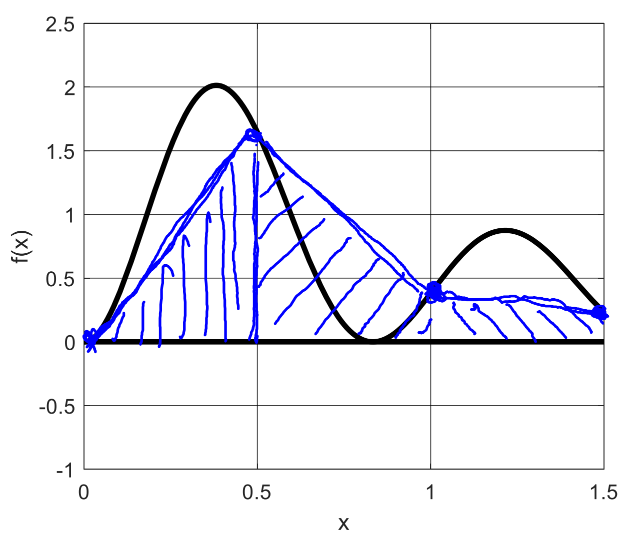
Given that $y(0) = 1$ and using a step size $h = 1$, perform two iterations of Euler's method and show on the axes below.

x	Slope
0	$-(1)+0 = -1$
1	$-(0)+1 = 1$
2	$-(2)^2+2 = -2$



(2) Consider the following function. Sketch the following integral using the composite trapezoid method, with $h = 0.5$.

$$\int_0^{1.5} f(x)\,dx$$



(3) We are given a large set of evenly spaced, highly accurate and precise measurements of reaction rate as a function of *T* and *P*. We wish to determine the reaction rate at a value T_A and P_A for which we don't have a tabulated rate, although T_A and P_A are between values that we have already in our data set.

Should we use *interpolation* or *regression* to determine our unknown rate, and why?

Interpolation is used for finding points between values of accurate, tabulated data.

(4) Assume $f(x)$ is a smooth, continuous, differentiable function of a single variable x. If x_{min} represents a value such that f has a **global minimum** value at $x = x_{min}$, which of the following is always true?

(A) MATLAB's `fminsearch` function in open mode will always find x_{min}.

(B) The function evaluated at x_{min} is equal to zero; i.e., $f(x_{min}) = 0$

(C) x_{min} is also a root of $f(x)$

(D) The first derivative of f evaluated at x_{min} is equal to zero; i.e., $f'(x_{min}) = 0$

(5) Consider the following nonlinear equation; we obtain measurements of k as a function of c. Rearrange the expression to a format suitable for linear regression, i.e. the format $y = a_0 + a_1 x$. What would you plot as your 'x' and 'y'? After regression, how can you obtain k_m and c_s from your linear fit?

$$k = \frac{k_m c^2}{c_s + c^2}$$

$k(c_s + c^2) = k_m c^2$

$\frac{c_s + c^2}{c^2} = \frac{k_m}{k}$

$\frac{c_s}{c^2} + 1 = \frac{k_m}{k} \Rightarrow \underbrace{\frac{c_s}{k_m}}_{m}\underbrace{\left(\frac{1}{c^2}\right)}_{x} + \underbrace{\frac{1}{k_m}}_{b} = \underbrace{\left(\frac{1}{k}\right)}_{y}$

You should plot $\left(\frac{1}{c^2}\right)$ as x and $\left(\frac{1}{k}\right)$ as y for your data. Then use the regressed slope (m) and intercept (b):

$k_m = \frac{1}{b}$ and $c_s = k_m \cdot m$

(6) What is the value of n after running the following code? n = 6

```
n = 0;
for ii = 1:2:5
    for jj = linspace(1,2,2)
        n = n+1;
    end
end
```

[1, 3, 5]

[1, 2]

Because nested

$3 \cdot 2 = 6$

(7) You are in charge of optimizing a new process that is affected by multiple input variables. What are the key advantages (list two) of using design of experiments (DoE) to tackle this problem?

(1) Efficient resource use - a reduced # of experimental trials needed

(2) You'll be able to observe interactions between variables.

(8) What does the $O(h^n)$ notation refer to in a table of numerical derivatives? Why does it matter?

This refers to truncation error. It arises from approximating any function as a taylor series, and showing which terms are neglected. The 'h' is your step size and refers to how much your error will reduce based on change in step size. A higher "n" refers to a MORE accurate method.

(9) Using elements of the following matrix 'M', write a Matlab expression that would give you: ans = 6 (there are MANY correct answers for this problem…)

Note to grader.
There are lots of them.

$$M = \begin{matrix} 1 & 2 & 3 \\ 5 & 7 & 4 \\ 8 & 9 & 10 \end{matrix}$$

examples

M(1,2) + M(1,1)

M(3,3) - M(2,3)

(10) Given an ODE and initial value, and the algorithm options below, in which order would you attempt them? What is the difference between each?

Algorithm	**Order**	**Unique features of this algorithm**
Euler method or rk4sys	3	Not efficient method, but harder to diverge, especially if you have a small step size.
ode23s	2	Used to solve STIFF problems.
ode45	1	Robust runge kutta method, typically works and is most efficient.