BME695 Numerical Methods in BME

Final Exam

5/6, 10:30 -- noon

Please review these notes before you start!

1. There will be three sections in this exam.
2. Section 1 includes a few filling-the-blank questions asking you to demonstrate you have acquired basic knowledge on simulation modeling and analysis, as well as numerical analysis in general.
3. Section 2 includes two calculation questions asking you to follow two algorithm statements and construct spreadsheets by hand or simple computational tools. You are expected to demonstrate you have acquired the skill of understanding algorithms effectively from scratch, which is the prerequisite to computer implementation of algorithms.
4. Section 3 is the coding task, which is what I assigned to you last week.
5. Turn in all your work by Thursday noon. I will check your work of Section 3 during the one-on-one meeting on Friday and Saturday. But you MUST not modify your work between Thursday noon and then.

Your Name: __*Andrew Sivaprakasam*_____________________________________

<u>Section 1</u>. Filling the Blanks (40 pts)

1. What are the three types of computational analysis tasks we have covered this semester? (6 pts)
   a. _____Sensitivity Analysis_______________________
   b. _____Metamodeling/surrogate modeling______________________
   c. _____Model Calibration______________________

2. Write out a general first-order IVP with respect to *t*. (2 pts)

$$y' = \frac{t}{2y}, y(0) = -1$$

(written with https://latex2image.joeraut.com/, since my word processor doesn't handle equations well)

3. What are the numerical approximation methods for solving the initial value problem of first-order ODEs? Name two (2 pts)
   a. _____Euler's Method______________________
   b. __________Runge Kutta, either 2^{nd} or 4^{th} order__________________

4. Write out the SIR model (3 pts)
   (again using latex2image}

$$\frac{dS}{dt} = -\frac{\beta IS}{N}$$
$$\frac{dI}{dt} = \frac{\beta IS}{N} - \gamma I$$
$$\frac{dR}{dt} = \gamma I$$

Where S = susceptible, I = Infected, R = recovered.

5. Write out the Markovian property (2 pts)

   Stochastic processes are memoryless.

6. Name three common non-parametric sampling schemes (3 pts)
   a. _______Random Sampling_________________________
   b. _______Latin Hypercube Sampling________________________
   c. _______Orthogonal Sampling__________________________

7. What are some of the numerical techniques for sensitivity analysis beyond doing scatterplots? Name four (4 pts)
   a. _______Rank Transformations________________________
   b. _______Pattern-based Gridding________________________
   c. _______Regression Analysis_________________________
   d. _______Correlation_________________________

8. What are two common response surface designs? (2 pts)
    a. ______CCD______________________
    b. ______Box-Behnken______________________

9. What is bias-variance dilemma? (2 pts)

Minimizing both bias and variance is complicated because minimizing the two prevents proper generalization of learning algorithms...i.e. can cause under-fitting or overfitting-fitting of the model to the data.

10. Name two Machine Learning based surrogate models? (2 pts)
    a. ____SVR – Support Vector Regression________________________
    b. ____ANN – Artificial Neural Networks________________________

11. What are two advanced **interpolating** methods in metamodeling? (2 pts)
    a. _______Kriging______________________
    b. _______Simulation Metamodeling – i.e. using Bayesian Networks______________________

12. What is MCMC? (2 pts)

Markov Chain Monte Carlo- using Markov Chain structure to randomly sample based on a previous random sample. Allows you to vary pdfs you are sampling from at various points in the chain.

13. What are three categories of uncertainty? (3 pts)
    a. ______Physical_______________
    b. ______Modeling________________
    c. ______Statistical________________

14. Write out the mathematical formulation for the optimization-based model calibration problem? (2 pts)

$$\min X_e f(Y_{obs}, Y_{pre}(X_a, X_e))$$

...can change min to max depending on whether you want to minimize the error or maximize the correlation/agreement.

15. What are common measures applicable to compare two PDFs? Name three (3 pts)
    a. ____Minkowski Measures______(i.e. Euclidean distance)____________
    b. ____L1 Family (i.e. Sorenson)__________________
    c. ____Intersection family (i.e. Wave Hedges)__________________

*Practically speaking, MSE, City block, or Chebyshev (all in Minkowski family) typically do just fine...not sure what’s common in practice since I’m new to this

<u>Section 2</u>. Constructing Algorithm Spreadsheet (30 pts)

Problem 2-1.

Page 66 of the book by Burden and Faires, “Numerical Analysis”. Follow the Newton’s algorithm (Algorithm 2.3) on Page 67 and work out the spreadsheet for the following foot-finding problem instance.

Approximate the root for the function $f(x) = 1 - \sin x - x$, which lies in $[0, \pi/2]$. Please perform the algorithm by hand for 5 or more iterations, i.e., calculate p1, p2, p3, …, and construct Table 2.4.

f’: -cos(x) - 1

Iteration	f	f’	p_n
0	N/A	N/A	0.5
1	0.0205744614	-1.877582562	0.510957953
2	2.897609E-05	-1.872276456	0.5109734294
3	5.856449E-11	-1.872268888	0.5109734294
4	0	-1.872268888	0.5109734294
5	0	-1.872268888	0.5109734294
6	0	-1.872268888	0.5109734294

(looks sloppy unless I paste as image…so see my spreadsheet for proper detail, and more precision)

Problem 2-2.

Page 256 of the same book by Burden and Faires. Following the Euler’s algorithm (Algorithm 5.1) on Pages 257 – 258 and work out the spreadsheet for the following IVP-ODE problem instance.

Approximate the root for the initial-value problem

$y' = \cos 2t + \sin 3t$, $0 \leq t \leq 1$, $y(0) = 1$, with $h = 0.25$ (i.e., $N = 4$).

Please perform the algorithm by hand for 5 or more iterations, i.e., calculate t_i, w_i, $y_i = y(t_i)$, $|y_i - w_i|$.

Next, given the actual solution $y(t) = 1/2 * \sin 2t - 1/3 * \cos 3t + 4/3$ add one more column to compare the actual error at each step to the error bound and construct Table 5.1.

t	w	y	Y-w	Actual error
0	1	1	0	0.0003333333
0.25	1.25	1.5592213219	0.3092213219	0.2298276126
0.5	1.6398053305	1.5377972925	0.102008038	0.1927160451
0.75	2.0242546536	0.8488103986	1.175444255	1.1924522444
1	2.2364572532	-0.275026828	2.5114840817	2.3926763766
1.25	2.1677005461	-1.372704934	3.5404054804	3.2785206057

<u>Section 3.</u> Refine your Response Surface Optimization Methodology (20 pts)

Show your algorithm on the Rosenbrock function with *n* = 2 and *n* = 3.

I had issues with Rosenbrock specifically...even after passing other test cases.

Here is a 3D visualization of what is happening. The linear optimization gets it close...but the quadratic optimization does not seem to work. Maybe it is due to setting improper bounds…the minimum found is [-0.0295, 0.7878] when it should be [1,1]. I could not get this working for higher dimension functions like n = 3 unfortunately. Here are some other figures that show the optimization works for other common test functions (sphere/levi, can show this in one-on-one discussion).