ME201 Advanced Calculus

Project #1: Numerical Integration and Least Squares Analysis

Assigned date: February 6, 2017 Due date: March 3, 2017

Project Requirements

Numerical integration and the least squares method are two numerical analysis techniques that are used extensively in engineering physics, particularly for reducing and interpreting experimental data. In the following project you will perform least squares/numerical analyses of data sets for two different examples. While it is recommended that Microsoft Excel be used to perform all calculations and data presentation, other software tools may be used if you find them more convenient.

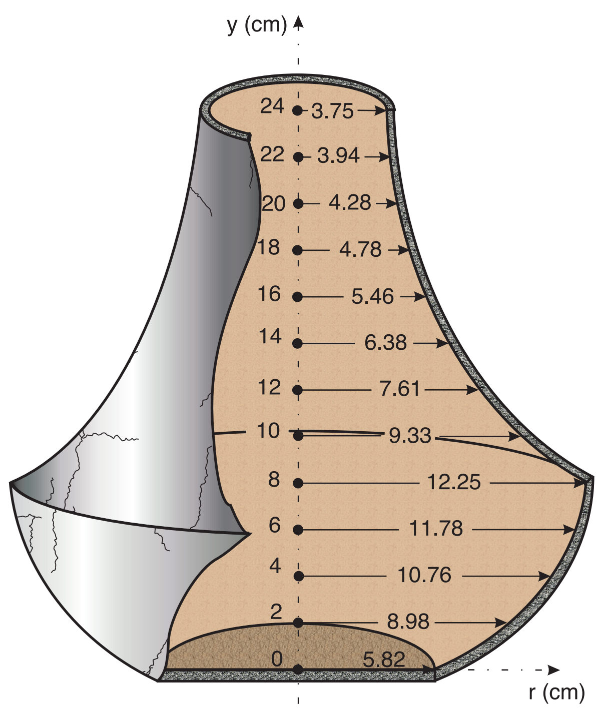
Reports will be submitted on an individual basis. **Due date: Friday, March 3.**

Present your analysis and results in a clear, concise report, typed or neatly handwritten. The report should explain the techniques used, summarize the analyses, describe any problems encountered, and present the results. Your Excel worksheets should be included in an appendix and referred to in the main body of the report.

Detailed Description

Part 1:

During an archeological dig, workers unearthed pottery shards of a water jug from an ancient civilization. Despite the fact that the complete jug was not recovered, enough pieces were recovered to take the measurements shown on the adjoining figure. The interior radius measurements were taken every $2\ cm$ from the bottom of the jug. In this exercise, you will use these radius measurements to approximate the interior volume of the water jug.



In Section 7.2 of Trim (4th ed.) the following formula (Eq. 7.8) is presented for calculating the volume of a region formed by rotating the function $f(y)$ about the $y-$axis from a to b.

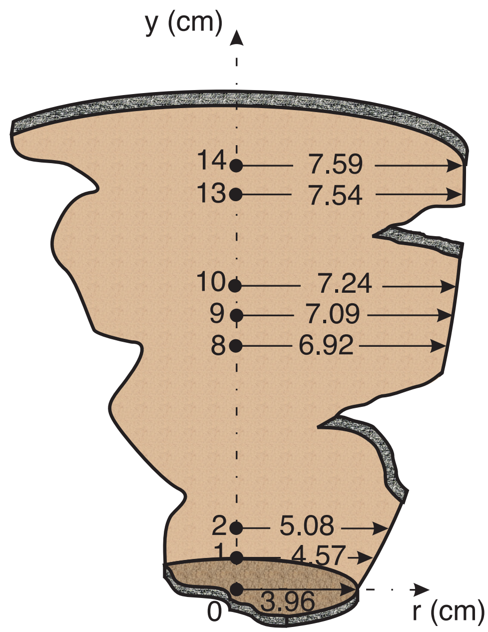
$$V = \int_a^b \pi \ [f(y)]^2 \ dy$$

i) Using Trapezoidal and Simpson's rule methods, derive equations to approximate the volume of the water jug (*in litres*). Present all equation development, your calculations, and your final results.

ii) Program these equations using Excel to implement Trapezoidal and Simpson's rule and solve for the volume of the water jug. Provide a copy of your worksheet as an appendix to your report and place a copy of your code in the Learn dropbox.

iii) Provide a thorough discussion of your results including the details of the methods used, an estimate of the error and any problems in implementing the techniques.

Another shard is discovered in the same location and a similar volume calculation is required. However, the radius measurements cannot be made at uniform intervals. The volume can still be calculated using the volume of rotation equation (as before), but the integral cannot be solved directly using our simple numerical integration techniques. Instead, a function based on a least squares fit of the data will be used as the integrand where our irregularly spaced data will be mapped to second order polynomial that can be used to predict regularly spaced data points.



iv) Derive the equations for the least squares method for a 2nd order polynomial.

$$r = ay^2 + by + c$$

Present the complete development of these equations in your report.

v) Use Excel to implement the least squares method for the correlation function, r. Then using the polynomial curve fit, generate data at regularly spaced intervals that can be used in a Trapezoidal rule calculation to find the volume, similar to the procedure in part i). Present the generated data points in a clearly labeled table along with the Trapezoidal rule calculations and your final results. Plot the fit of the irregularly spaced data points and present the equation of the curve fit using the polynomial function along with the residual for the curve fit.

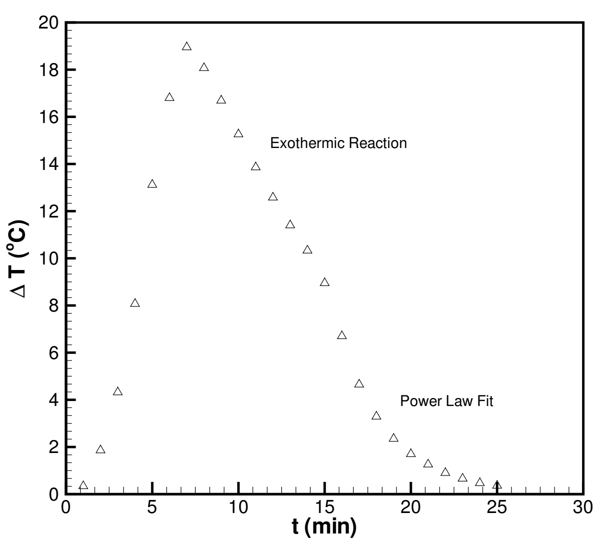
vi) Provide a thorough discussion of your results including the details of the methods used, an estimate of the error and any problems in implementing the techniques.

Part 2:

Differential thermal analysis is a specialized technique that can be used to determine transition temperatures and the thermodynamics of chemical reactions. In this method, the temperature of a sample of the material being studied is compared to the temperature of an inert reference material, when both are heated simultaneously under identical conditions. The furnace housing the two materials is heated such that the temperature, $\boldsymbol{T_f}$, increases linearly with time, $\boldsymbol{t}$, and the difference between the temperatures of the sample and the reference, $\boldsymbol{\Delta T}$, is recorded. A typical data set for this type of test is as follows:

$t\ (min)$	0	1	2	3	4	5	6	7	8	9	10	11	12
$\Delta T\ (°C)$	0.00	0.34	1.86	4.32	8.07	13.12	16.80	18.95	18.07	16.69	15.26	13.86	12.58
$T_f\ (°C)$	86.2	87.8	89.4	91.0	92.7	94.3	95.9	97.5	99.2	100.8	102.3	103.9	105.5
$t\ (min)$	13	14	15	16	17	18	19	20	21	22	23	24	25
$\Delta T\ (°C)$	11.40	10.33	8.95	6.70	4.65	3.29	2.35	1.70	1.26	0.90	0.66	0.47	0.36
$T_f\ (°C)$	107.1	108.6	110.2	111.8	113.5	115.1	116.8	118.4	120.0	121.6	123.2	124.9	126.5

The temperature difference data, $\boldsymbol{\Delta T}$ values, increase to a maximum and then decreases due to the heat evolved in an exothermic reaction. Once the reaction is complete, the $\boldsymbol{\Delta T}$ data begins to decrease as a *power law function*, as shown in the figure below. A unique feature of a power law function is that it is transformed into a linear relationship when plotted on a log-log scale as $\boldsymbol{\Delta T\ vs.\ t}$.



The objective in this problem is to determine the precise time when the reaction is complete. This can be achieved in an approximate manner by plotting the data on a log-log plot and determining the inflection point in the $\boldsymbol{\Delta T\ vs.\ t}$ curve, where the data first becomes linear.

Or for a more accurate determination of this point, you can curve fit the data using a power law formulation to find the subset of the data that best fits this relationship. By selectively excluding points outside the region of interest, the precise point at which the reaction is complete can be determined.

i) Present your $log(\Delta T)$ versus $\log(time)$ data in an Excel table and plot the data in Excel using a log-log scale. By inspection from this graph, find the approximate time when the reaction ends. Clearly demonstrate how you determined the inflection point. Label all relevant points including those regions that map to a linear fit, the actual point of inflection, and the value of time at this point.

ii) Derive the equations for a least squares analysis of the data using a power law fit,

$$y = a\, x^b$$

Present a complete development of these equations in your report.

iii) In Excel, use the least squares method to determine a correlation of $\log(\Delta T)$ versus $\log(time)$ for data from the table above. Given that we are trying to determine where the exothermic reaction ends, limit your range of data to the general region, where the inflection point occurs i.e. $t = 10 \rightarrow t = 20$ minutes.

iv) By selectively moving the starting point of your curve fit from $t = 10$ to $t = 11$ to $t = 12$ and so on, find the power law curve fit for each of these cases. Once the curve fit includes only data in the power law region you will notice a significant improvement in the curve fitting residual. Using this method you should be able to determine where the exothermic reaction ends. Present a table that indicates the starting point value, a, b, the residual and the difference between successive values of the residual. Based on this parametric study, find the time when the reaction ends and compare to your results from Part i).

Provide a thorough discussion of your results including the details of the methods used, an estimate of the uncertainty ($\pm$) in your time, any assumptions made, and any problems in implementing the techniques.