Chapter 4

4.1. Cramer's rule and matrix inversion-multiplication offer alternative techniques to solve a system of linear algebraic equations. Conduct a literature search to collect information about these two techniques and the elimination and iteration techniques discussed in this chapter. Compare the various techniques regarding the complexity of algorithms, ease of implementation, and potential errors.

No solution will be given.

4.2. The Newton-Raphson technique may not converge to a solution. Inspecting equation 4.16, in what other possible way can the technique fail?

Equation 4.16 is:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

The technique will not yield a solution, if the absolute value of the second term on the right hand side does not tend to approach 0 with increasing number of iterations. However, the technique will also fail at any point where $f'(x_n) = 0$. The second term becomes indeterminate at this point and no further evaluations are possible.

4.3. Roots of any equation can be found using what is known as the *bracketing technique*. Conduct a literature search and explain the principle behind such solution techniques.

No solution will be given.

4.4. The following data were obtained in an experiment where the concentration of a substance was monitored as a function of time. Calculate the first derivative of the concentration with respect to time for all possible times using the forward difference formula. Can the second derivative also be calculated numerically?

Time, s	Concentration
0	0
10	0.5
20	1.0
30	2.0
40	4.0
50	5.5
60	6.5
70	7.0
90	7.7

The first derivative of concentration is calculated using equation 4.18. Further application of the principle yields the following forward difference formula for the second derivative:

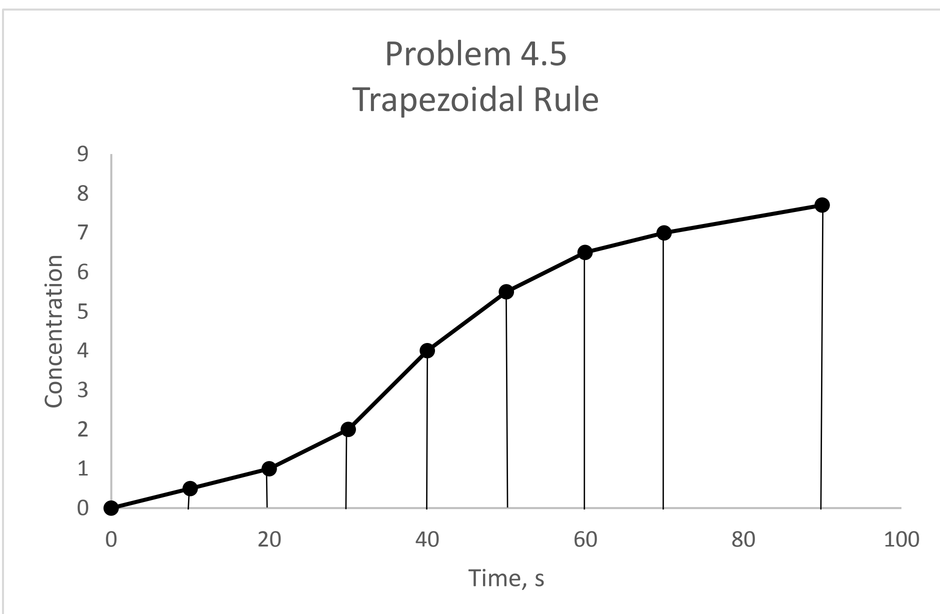
$$\frac{d^2C}{dt^2} = \frac{\Delta}{\Delta t}\left(\frac{\Delta C}{\Delta t}\right) = \frac{C_{i+2} - 2C_{i+1} + C_i}{\left(t_{i+1} - t_i\right)^2}$$

Excel calculations for the first and second derivatives of concentration are shown below in columns 4 and 6, respectively.

Time, s	Concentration	$\Delta C = C_{i+1} - C_i$	$\boldsymbol{\Delta C/\Delta t}$	$\Delta(\Delta C/\Delta t)$	$\boldsymbol{\Delta(\Delta C/\Delta t)/\Delta t}$
0	0	0.5	**0.05**	0	**0**
10	0.5	0.5	**0.05**	0.05	**0.005**
20	1	1	**0.1**	0.1	**0.01**
30	2	2	**0.2**	-0.05	**-0.005**
40	4	1.5	**0.15**	-0.05	**-0.005**
50	5.5	1	**0.1**	-0.05	**-0.005**
60	6.5	0.5	**0.05**	-0.015	**-0.0015**
70	7	0.7	**0.035**		
90	7.7				

4.5. What is the area under the concentration-time curve obtained from the data shown for problem 4.4? Use the trapezoid method. An alternative technique is to use the rectangle method. What is the difference in the areas if the area is calculated using the rectangle method?

A plot of the concentration-time data is shown below. Also shown are the trapezoids formed between any two adjacent date points by the straight line between the two data points, the time-axis, and the two ordinates. The total area under the curve is found by calculating the area of each trapezium and adding all such areas. The trapezoidal rule yields an area of 377 concentration units-seconds.



A simpler alternative is to draw rectangles as shown in the figure below. The area under curve in this case is 419 concentration units-seconds. This is clearly an overestimate, as it assumes that the concentration in any time interval is constant and equal to the concentration at the end of the interval. If on the other hand, it is assumed that the concentration in any time interval is equal to the concentration at the beginning of that interval, the area obtained would be 335 concentration units-seconds, a clear underestimate. However, all three values will tend to converge to a single value as the frequency of measurements increases or the time interval between measurements decreases to a very small value.