Numerical Analysis with MATLAB Application

Course Book

By

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$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix}$$

Course Overview:

Numerical analysis is a technique by which the mathematical problems are formulated, so that can be solved with arithmetic. It might be considered as a powerful problem solving tool.

Numerical analysis is the branch of mathematics that is used to find approximations to difficult problems such as finding the roots of non-linear equations, interpolation, numerical differentiation and integration and numerical solutions of the differential equations.

The manual computation required lots of time and hard work and the largest corporations could only afford them. But the applications of numerical analysis with MATLAB are indispensable for engineering students to solve the complex problems that may face in the final year project and at the work in the future.

Simulation will be the main part of this course; we intend to teach the student how to simulate engineering applications via practical examples with MATLAB.

The subjects of this course are written primarily for students who have a good background in advanced engineering mathematics.

Course Objectives:

The objectives of studying this module are to make the students familiarize with the ways of solving complicated mathematical problems numerically. In addition to make the students be able to simulate any Chemical Engineering process and produce a model to be run on MATLAB for results presentation.

Course Reading List:

Students can get benefit from all the available sources in numerical analysis and advances engineering mathematics

- Costantinis, A. and Mostoufi, N. (2001) “Numerical Methods for Chemical Engineers with MATLAB Applications”. Prentice Hall.
- Cheney, W. and Kincaid, D. (1999) “Numerical mathematics and computing” Fourth edition, Brooks / Cole Publishing Company, Pacific Grove
- Fausett, L. (1999) “Applied Numerical Analysis Using MATLAB” Prentice Hall, Upper Saddle River.
- Ali, J., Fieldhouse, J. and Talbot, C. (2011) “Numerical modelling of three-dimensional thermal surface discharges” Journal Engineering Applications of Computational Fluid Mechanics Vol. 5, No. 2.
- Abuhabaya, A., Ali, J., Fieldhouse, J. and Brown, R. (2011) “Optimization method in modelling the performance of Engine using biofuel” Proceedings of the 17th International Conference on Automation & Computing, University of Huddersfield, Huddersfield, UK, 10 September 2011

Course Content:

1. MATLAB Review
    1.1. Loops
    1.2. 1D Plot
    1.3. 2D Plot
    1.4. 3D plot
2. Introduction to Numerical Analysis
3. Error Analysis
4. *Root Approximations*
    4.1. Polynomials
    4.2. Newton -Raphson Method
    4.3. Bisection Method
    4.4. Approximation with spreadsheets
5. Matrices and determinants
    5.1. Matrices operation
    5.2. Determinants
    5.3. Solving simultaneous equations
        5.3.1. Gramer's Rule
        5.3.2. Gaussian Elimination
    5.4. 3D Grids in MATLAB
6. Finite Difference FD
    6.1. Types of Finite Difference
        6.1.1. Forward FD
        6.1.2. Backward FD
        6.1.3. Centred FD
7. Interpolation

Chapter One:

MATLAB Review:

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Objectives:

Chapter 1 is an introduction to MATLAB. The discussion is based on MATLAB Student Version 6.4 and it is also applicable to Version 7. MATLAB is an acronym for MATrix LABoratory and it is a very large computer application which is divided to several special application fields referred to as toolboxes. The chapter aims to teach students how to use the software for modelling, simulating, and analyzing dynamic systems as well as in numerical analysis.

Contents:

This chapter is contents the following subjects:

- Loops
- 1D Plot
- 2D Plot
- 3D plot

Example:

A model provided to predict the temperature decay in cooling tower in the field as function of the time. you as a process engineer determine the accuracy of the model ($z = 1.75\ e^{0.45t/T} - 1.75$) if your experimental data are (0 0.07 0.18 0.25 0.38 0.57 0.5 0.77). Find the best curve to fit the experimental measured data and a curve pass through the data.

```
t = 0:0.5:3.5;
tmax=3.5;% divide the steps time by maximum time to make the equation dimensionless
T=(1.75*exp(0.45*t./tmax))-1.75;
Te=[0 0.07 0.18 0.25 0.38 0.57 0.5 0.77];
%Draw the best curve fits the measured data
%this is one of the subjects in numerical analysis
p=polyfit(t,Te,3);
pp=polyval(p,t);
%interpolation to draw a curve passes through the measured data
tt=0:0.5:3.5;
ppp=interp1(tt,Te,t,'cubic');
plot(t,T,t,Te,'*',t,pp,tt,ppp)
```

Chapter Two:

Introduction to Numeric Analysis:

Teacher of this chapter: Dr. Jafar Abdullah Ali

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Objectives:

This chapter is studied the general aspects of numeric analysis and the differences with the analytical mathematical solution. The student will be understood the advantages and disadvantages of numeric and it is applications in engineering process.

Contents:

This chapter is contents the following subjects:

- Introduction
- What is numeric
- Comparison with analytical mathematical work
- Syllabus discussion
- Course learning outcome

Chapter Three:

Error Analysis:

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Objectives:

This chapter indicates to that the computed numerical solution is not the exact the mathematical results, i.e. there will be some error. So this subject will intend to teach the student how to calculate the error of the numerical methods.

Contents:

This chapter is contents the following subjects:

- Error
- Relative error

Example:

The absolute relative approximate error $|\in_a|$ in this example can be calculated as below:

$$|\in_a| = \left|\frac{h_m^{\text{new}} - h_m^{\text{old}}}{h_m^{\text{new}}}\right| \times 100$$

$$= \left|\frac{0.75 - 1.5}{0.75}\right| \times 100$$

$$= 100\%$$

Chapter Four:

Root Approximation:

Teacher of this chapter: Dr. Jafar Abdullah Ali

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Objectives:

This chapter is an introduction to find the roots of polynomial, using Newton's and bisection methods as well as spreadsheets for approximating roots of linear and non-linear equations. Several examples are presented to illustrate practical solutions using MATLAB and spreadsheets. The student will learn how to find the solution for complicates equations using several methods and computer program.

Contents:

This chapter is contents the following subjects:

- Polynomial
- Newton's-Raphson
- Bisection
- Spreadsheet

Example

Use the bisection method of finding roots of equations. Conduct three iterations to estimate the root of the above equation.

$$f(h) = h^3 - 9h^2 + 3.8197 = 0$$

Iteration 1

The estimate of the root is

$$h_m = \frac{h_\ell + h_u}{2}$$

$$= \frac{0+6}{2}$$

$$= 3$$

$$f(h_m) = f(3) = (3)^3 - 9(3)^2 + 3.1897 = -50.180$$

$$f(h_\ell)f(h_m) = f(0)f(3) = (3.1897)(-50.180) < 0$$

Hence the root is bracketed between h_ℓ and h_m, that is, between 0 and 3. So, the lower and upper limits of the new bracket are

$$h_\ell = 0, h_u = 3$$

At this point, the absolute relative approximate error $|\in_a|$ cannot be calculated, as we do not have a previous approximation

<u>Iteration 2</u>

The estimate of the root is

$$h_m = \frac{h_\ell + h_u}{2}$$

$$= \frac{0+3}{2}$$

$$= 1.5$$

$$f(h_m) = f(1.5) = (1.5)^3 - 9(1.5)^2 + 3.8197 = -13.055$$

$$f(h_\ell)f(h_m) = f(0)f(1.5) = (3.8197)(-13.055) < 0$$

Hence, the root is bracketed between h_ℓ and h_m, that is, between 0 and 1.5. So the lower and upper limits of the new bracket are

$$h_\ell = 0, h_u = 1.5$$

<u>Iteration 3</u>

The estimate of the root is

$$h_m = \frac{h_\ell + h_u}{2}$$

$$= \frac{0+1.5}{2}$$

$$= 0.75$$

$$f(h_m) = f(0.75) = (0.75)^3 - 9(0.75)^2 + 3.8197 = -0.82093$$

$$f(h_\ell)f(h_m) = f(0)f(0.75) = (3.8197)(-0.82093) < 0$$

Hence, the root is bracketed between h_ℓ and h_m, that is, between 0 and 0.75.

Chapter Five:

Matrices and Determinants:

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Objectives:

This chapter is an introduction to matrices and matrix operations. Determinants, Cramer's rule, and Gauss's elimination method are introduced. The student will be familiarize with making grids on a plan or a volume for modelling purposes.

Contents:

This chapter is contents the following subjects:

- Matrices operation
- Determinants
- Solving simultaneous equations
    - Gramer's Rule
    - Gaussian Elimination
- 3D Grids in MATLAB

Example:

The following example shows grid points created within a volume 6m length, 4m width and 3m height. At each grid a value 15 has been appointed, this value could be temperature, concentrations, etc.

```
>> %the following command gives 3 sets
%of matrices with 6 rows and 4 columns
U=15*ones(6,4,3)

U(:,:,1) =

    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15


U(:,:,2) =

    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15


U(:,:,3) =

    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15
    15    15    15    15
```

Chapter Six:

Finite Difference:

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Objectives:

This chapter is on finite differences, one of the wider methods in numeric analysis. It is used in interpolation which is one of its most important applications. Finite Differences form the basis of numerical analysis as applied to other numerical methods such as curve fitting, data smoothing, numerical differentiation, and numerical integration time. The student will learn how to use the finite difference methods in engineering applications.

Contents:

This chapter is contents the following subjects:

- Types of Finite Difference
    - Forward FD
    - Backward FD
    - Centred FD

Example:

Form a difference table showing the values of given x as 1, 2, 3, 4, 7 and 9 , the values of f(x) corresponding to $y = x^3$, and the first through the fourth divided differences

x	$f(x)$			
x_0	$f(x_0)$			
		$f(x_0, x_1)$		
x_1	$f(x_1)$		$f(x_0, x_1, x_2)$	
		$f(x_1, x_2)$		$f(x_0, x_1, x_2, x_3)$
x_2	$f(x_2)$		$f(x_1, x_2, x_3)$	
		$f(x_2, x_3)$		
x_3	$f(x_3)$			

Function		***Divided Differences***			
x	$f(x) = x^3$	***First***	***Second***	***Third***	***Fourth***
0	***0***				
		1			
1	***1***		*4*		
		13		*1*	
3	***27***		*8*		*0*
		37		*1*	
4	***64***		*14*		*0*
		93		*1*	
7	***343***		*20*		
		193			
9	***729***				

Chapter Seven:

Interpolation:

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Objectives:

This chapter is studied the interpolation by using different methods. Interpolation is a method of constructing new data points within the range of a discrete set of known data points. The subject discuss in details all advantage and disadvantages of each method separately. The student will be able to identify the method that is suitable to compute a certain process.

Contents:

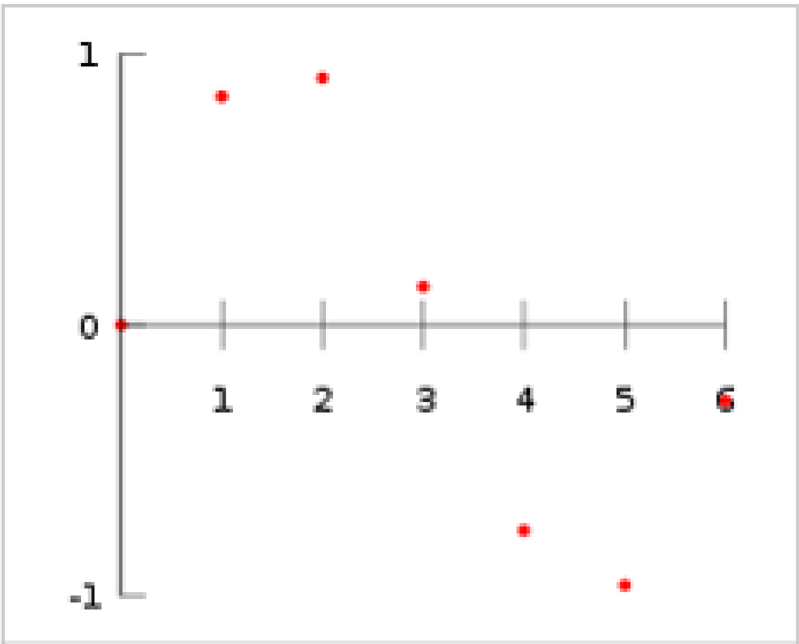
This chapter is contents the following subjects:

- Interpolation methods
  - Linear Interpolation
  - Polynomial Interpolation
  - Newton's Interpolation
  - Spline Interpolation

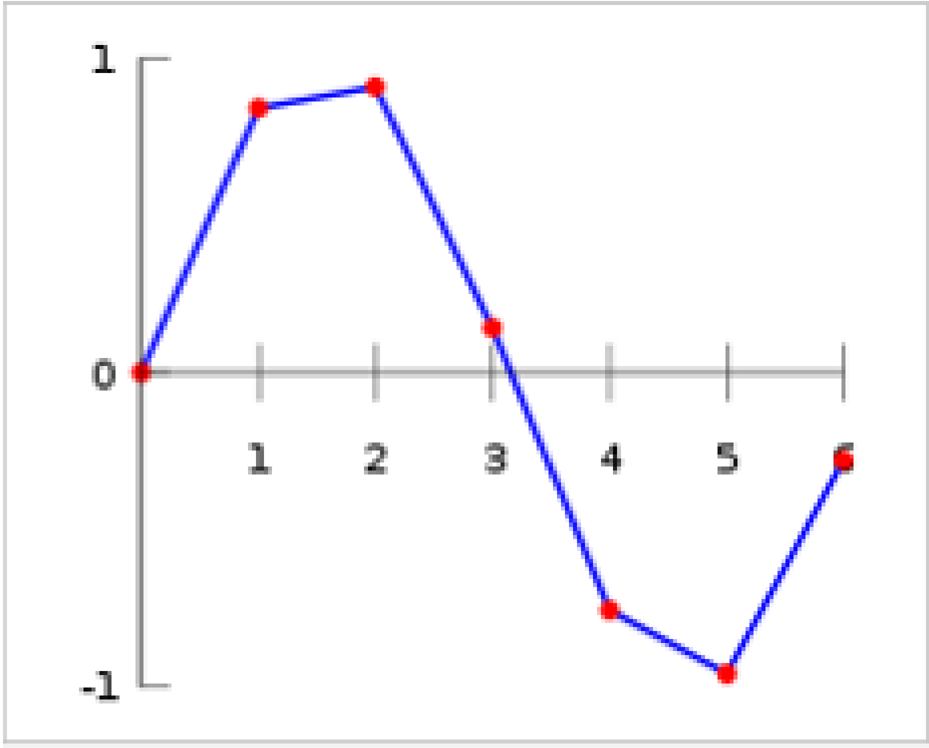
Example 1:

For example, suppose we have a table like this, which gives some values of an unknown function *f*. interpolate the given data use linear and polynomial methods.

x	*f*(*x*)
0	0
1	0.8415
2	0.9093
3	0.1411
4	−0.7568
5	−0.9589
6	−0.2794



Example 2:



Chapter Eight:

Curve Fitting:

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Objectives:

This chapter is an introduction to regression and procedures for finding the best curve to fit a set of data. We will discuss linear and parabolic regression, and regression with power series approximations. The objective of this chapter is to let the students able to create equations from set of measured data (modelling). The produced equation will predict theoretical data that can be used in the engineering application. We will illustrate their application with several examples, as well as with excel spreadsheet.

Contents:

This chapter is contents the following subjects:

- Regression
- Linear Regression
- Parabolic Regression
- Curve Fitting with Excel

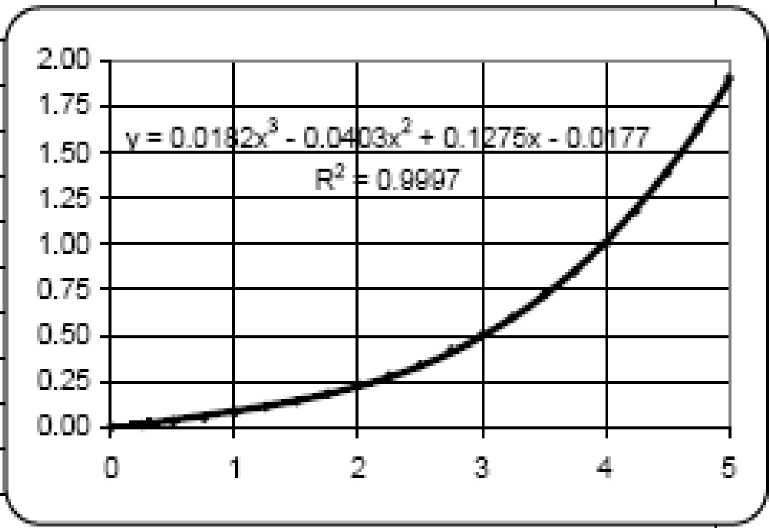
Example:

The voltages (volts) shown on Table 1 were applied across the terminal of a non-linear device and the current ma (milliamps) values were observed and recorded. Use Excel's *Add Trendline* feature to derive a polynomial that best approximates the given data.

Experimental Data											
Volts	0.00	0.25	0.50	0.75	1.00	1.25	1.50	1.75	2.00	2.25	2.50
ma	0.00	0.01	0.03	0.05	0.08	0.11	0.14	0.18	0.23	0.28	0.34
Volts	2.75	3.00	3.25	3.50	3.75	4.00	4.25	4.50	4.75	5.00	
ma	0.42	0.50	0.60	0.72	0.85	1.00	1.18	1.39	1.63	1.91	

Solution: We enter the given data on the spreadsheet where, for brevity, only a partial list of the given data is shown. However, to obtain the plot, we need to enter all data in Columns A and B.

	A	B	C	D
1				
2	Volts	Amps		
3				
4	0.00	0.00		
5	0.25	0.01		
6	0.50	0.03		
7	0.75	0.05		
8	1.00	0.08		
9	1.25	0.11		
10	1.50	0.14		
11	1.75	0.18		
12	2.00	0.23		
13	2.25	0.28		
14	2.50	0.34		



Chapter Nine:

Differential Equations:

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Objectives:

Many situations in the physical world are concerned with the rates of changes of quantities, some are in the form of mathematical work which involves the derivatives of one quantity with respect to another. All these should be represented as differential equations. An example is Newton's law of cooling, which relates the change of the temperature of a cooling liquid to the temperature itself. In general a differential equation is an equation in an unknown function, say y(x), where the equation contains various derivatives of y and various known functions of x. The problem is to find the unknown function.

This chapter is the main one in this course, the student will learn how to deal with the major equations in engineering and how to simulate any process using the PDE. Heat diffusion, wave and transport equations are among those that students model.

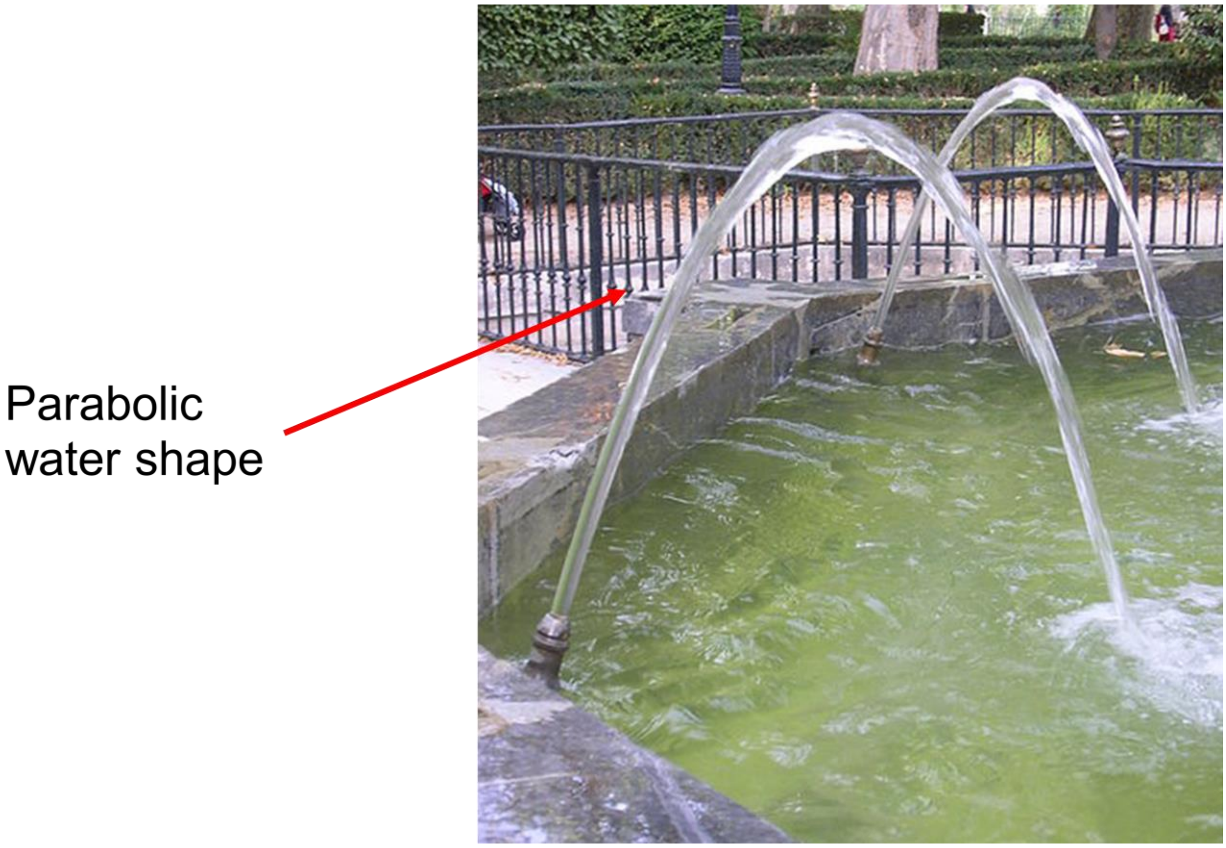
<u>Contents</u>:

This chapter is contents the following subjects:

- Introduction to differential equations
- Ordinary Differential Equation ODE
- Solution of ODE
    - Euler's Method
    - Runge-Kutta Method
- Partial Differential Equation PDE
- Solution of PDE
- Modelling, heat equation, transport equation and wave equation

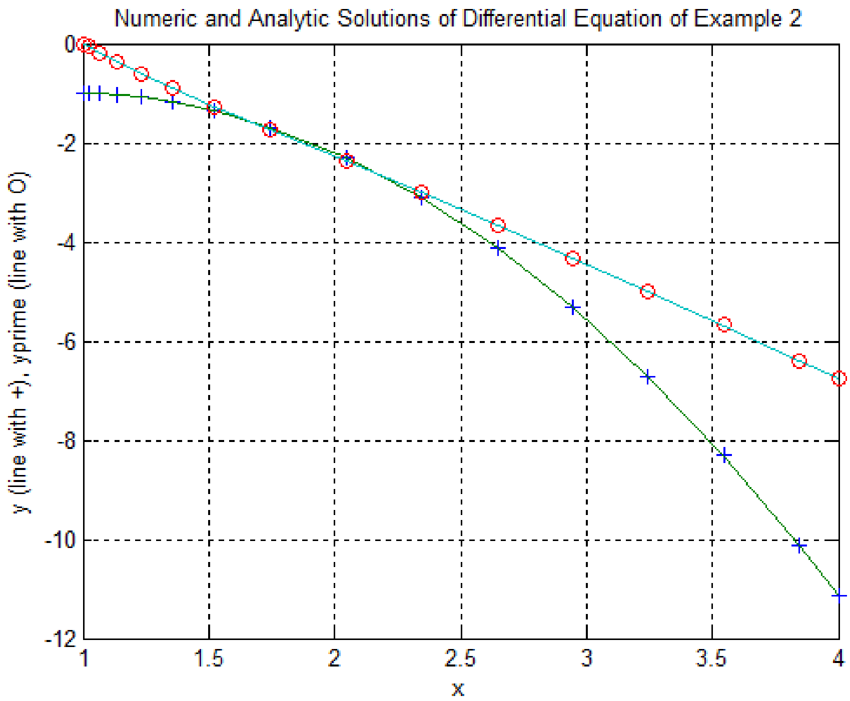
<u>Example 1:</u>

Parabolic partial differential equation shape presented in the figure below:



Example 2:

Comparison of numeric and analytic solution of a differential equation shows in figure below:



Chapter Ten:

Integration by numerical methods:

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Objectives:

This chapter is an introduction to numerical methods for integrating functions which are very difficult or impossible to integrate using analytical means. We will discuss the trapezoidal rule that computes a function f(x) with a set of linear functions, and Simpson's rule that computes a function f(x) with a set of quadratic functions.

<u>Contents</u>:

This chapter is contents the following subjects:

- The Trapezoidal Rule
- Simpson's Rule
- Examples and Exercises in chemical engineering field

Example 1:

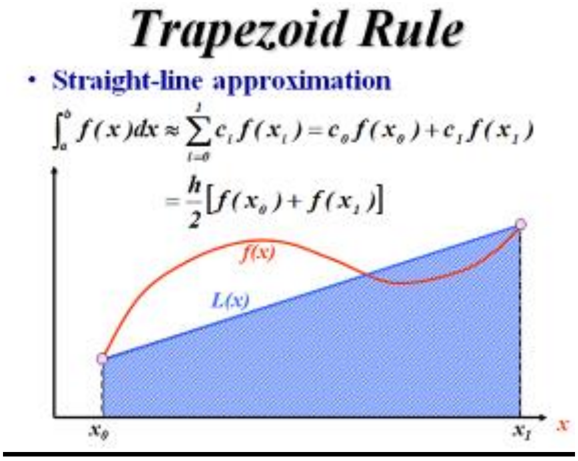
Evaluate the integral: $\int_0^4 xe^{2x}dx$

- Exact solution:

$$\int_0^4 xe^{2x}dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4$$
$$= \frac{1}{4}e^{2x}(2x-1)\Big|_0^1 = 5216.926477$$

- Trapezoidal rule:

$$I = \int_0^4 xe^{2x}dx \approx \frac{4-0}{2}\left[f(0)+f(4)\right] = 2(0+4e^8) = 23847.66$$
$$\varepsilon = \frac{5216.926 - 23847.66}{5216.926} = -357.12\%$$



Example 2:

Use Simpson rule to evaluate the integral: $\int_0^4 xe^{2x}dx$

$$I = \int_0^4 xe^{2x}dx \approx \frac{h}{3}[f(0) + 4f(2) + f(4)]$$

$$= \frac{2}{3}\left[0 + 4(2e^4) + 4e^8\right] = 8240.411$$

$$\varepsilon = \frac{5216.926 - 8240.411}{5216.926} = -57.96\%$$

Chapter Eleven:

Differentiation by Numerical Method:

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Objectives:

This chapter is an introduction to numerical methods for differentiation functions which are very difficult or impossible to solve using analytical means. However this chapter is less likely to be given to the students, but the objective of it to show them how the numeric analysis sort the differentiation out.

Contents:

This chapter is contents the following subjects:

- Definition
- Solutions
- Applications

Example:

$$x^2 + 3y^2 = k_1 \quad (1)$$

$$3y = k_2 x^3 \quad (2)$$

Implicit differentiation of (1) yields

$$2x + 6y\frac{dy}{dx} = 0$$

or

$$\frac{dy}{dx} = -\frac{1}{3} \cdot \frac{x}{y} \quad (3)$$

Differentiation of (2) yields

$$\frac{dy}{dx} = \frac{3k_2 x^2}{3} = k_2 x^2 \quad (4)$$

From (2),

$$k_2 = \frac{3y}{x^3}$$

and by substitution into (4) we get

$$\frac{dy}{dx} = \frac{3y}{x^3} \cdot x^2 = 3\frac{y}{x} \quad (5)$$

Chapter Twelve:

Optimization methods:

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Objectives:

This chapter introduces a method for maximizing or minimizing some function in order to achieve the optimum solution. The method discusses in detail the financial and engineering economic problems. Our intent here is to introduce the method with the basic ideas to make the student be able to solve some economic problem which might face in future at field.

Contents:

This chapter is contents the following subjects:

- Linear Programming
- Dynamic Programming
- Examples and Exercises in chemical engineering field

Example:

A large oil distributor can buy *Grade A* oil which contains 7 % lead for $25.00pb (per barrel) from one oil refinery company. He can also buy *Grade B* oil which contains 15% lead for $20.00pb per barrel from another oil refinery company. The Environmental Protection Agency (EPA) requires that all oil sold must not contain more than 10% lead. How many barrels of each grade of oil should he buy so that after mixing the two grades can minimize his cost while at the same time meeting EPA's requirement? Solve this problem graphically and check your answers with Excel's *Solver*.

Solution:

Let x be the number of barrels of Grade A oil and y be the number of barrels of Grade B oil. The objective is to minimize $z = \$25.00x + \$20.00y$ or, for simplicity,

$$z = 25x + 20y \quad (1)$$

We want to minimize (1) because it represents a cost, not a profit.

Each barrel to be sold must not contain more than 10% lead and since Grade A contains 7% and Grade B 15%, we must have

$$0.07x + 0.15y \leq 0.10 \quad (2)$$

The oil of Grade A and Grade B used in each barrel to be sold must be equal to unity. Thus,

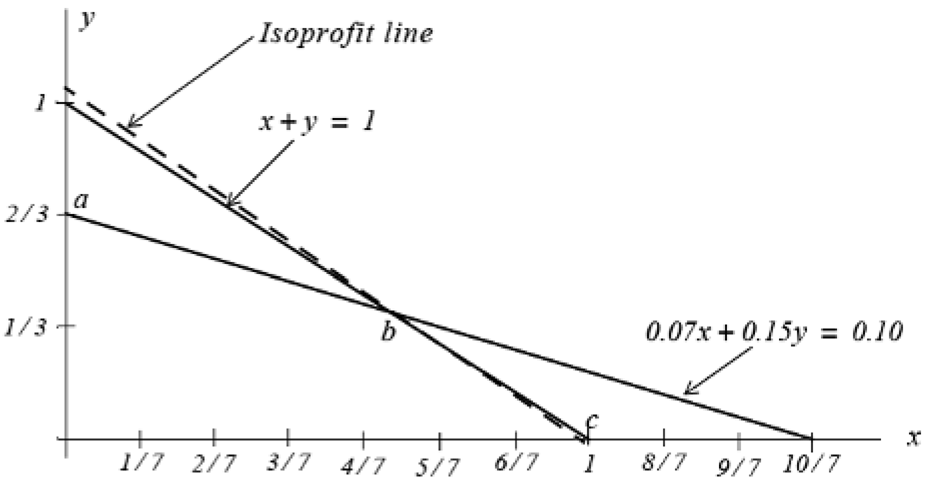
$$x + y = 1 \quad (3)$$

Moreover, x and y cannot be negative numbers, therefore

$$x \geq 0 \qquad y \geq 0 \quad (4)$$

The problem then can be stated as:

Minimize (1) subject to the constraints of (2), (3), and (4). To determine the feasible region we plot (2) and (3) where the x and y crossings are found by first setting $x = 0$ and then $y = 0$. Thus from (2), if $x = 0$, $y = 0.10/0.15 = 2/3$ and if $y = 0$, $x = 0.10/0.07 = 10/7$. Likewise, from (3), if $x = 0$, $y = 1$, and if $y = 0$, $x = 1$.



The isoprofit line passes through point b and its coordinates are found by simultaneous solution of (2) and (3). For convenience, we use the following MATLAB code:

```
syms x y; [x,y]=solve(0.07*x+0.15*y–0.10, x+y–1)
x =
 5/8

y =
 3/8
```

Therefore, the distributor should buy Grade A oil at the ratio $x = 5/8$ and Grade B at the ratio $y = 3/8$ and by substitution into (1)

$$z = 25 \times \frac{5}{8} + 20 \times \frac{3}{8} = \frac{185}{8} = \$23.125$$

and this represents his cost per barrel. The isoprofit line is

$$z = 25x + 20y = 23.125$$

and the y-intercept is found by setting x in the equation above to zero and we find that

$$y - intercept = 23.125/20 = 1.1563$$

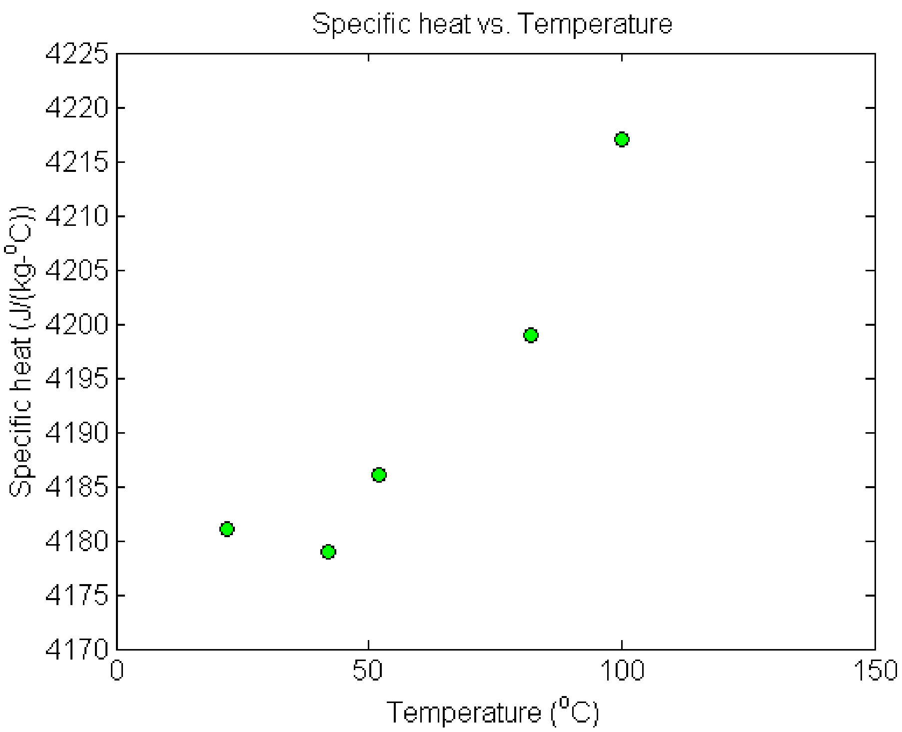
Chapter Thirteen:

Exam Samples:

To find how much heat is required to bring a kettle of water to its boiling point, you are asked to calculate the specific heat of water at $61°\text{C}$. The specific heat of water is given as a function of time in Table 1.

Table 1 Specific heat of water as a function of temperature.

Temperature, T $(°\text{C})$	Specific heat, C_p $\left(\frac{\text{J}}{\text{kg} - °\text{C}}\right)$
22	4181
42	4179
52	4186
82	4199
100	4217



Determine the value of the specific heat at $T = 61°\text{C}$ using Newton's divided difference method of interpolation and a first order polynomial.

Solution

For linear interpolation, the specific heat is given by

$$C_p(T) = b_0 + b_1(T - T_0)$$

Since we want to find the velocity at $T = 61°\text{C}$, and we are using a first order polynomial we need to choose the two data points that are closest to $T = 61°\text{C}$ that also bracket $T = 61°\text{C}$ to evaluate it. The two points are $T = 52$ and $T = 82$.

Then

$$T_0 = 52, \quad C_p(T_0) = 4186$$

$$T_1 = 82, \quad C_p(T_1) = 4199$$

gives

$$b_0 = C_p(T_0)$$

$$= 4186$$

$$b_1 = \frac{C_p(T_1) - C_p(T_0)}{T_1 - T_0}$$

$$= \frac{4199 - 4186}{82 - 52}$$

$$= 0.43333$$

Hence

$$C_p(T) = b_0 + b_1(T - T_0)$$
$$= 4186 + 0.43333(T - 52), \qquad 52 \le T \le 82$$

At $T = 61$,

$$C_p(61) = 4186 + 0.43333(61 - 52)$$
$$= 4189.9 \frac{\text{J}}{\text{kg} - ^\circ\text{C}}$$

If we expand

$$C_p(T) = 4186 + 0.43333(T - 52), \qquad 52 \le T \le 82$$

we get

$$C_p(T) = 4163.5 + 0.43333T, \qquad 52 \le T \le 82$$

and this is the same expression as obtained in the direct method.