DEPARTMENT OF CHEMICAL ENGINEERING

Numerical Methods in ChE Engineering (BTCH-21405)

Tutorial Sheet # 1

Topics: Significance of Numerical Methods in Chemical Engineering & Errors

Q1. What is meant of “Computational techniques” or “Numerical Methods” Why this techniques are gaining popularity in modern era? State the advantages of Computational techniques.

Q2. Solve using Babylonian method for √2 using Heron’s algorithm.

Hint: $x^{(new)} = 1/2\{x+2/x\}$

Q3. Suppose that you have the task of measuring the lengths of a bridge and a rivet and come up with 9999 and 9 cm, respectively. If the true values are 10,000 and 10 cm, respectively, compute (a) the true error and (b) the true percent relative error for each case.

Q4. In mathematics, functions can often be represented by infinite series. For example, the exponential function can be computed using

$$e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!}$$

Thus, as more terms are added in sequence, the approximation becomes a better and better estimate of the true value of e^x. Equation   is called a Maclaurin series expansion. Starting with the simplest version, $e^x = 1$, add terms one at a time to estimate $e^{0.5}$. After each new term is added, compute the true and approximate percent relative errors, respectively. Note that the true value is $e^{0.5}=1.648721$ Add terms until the absolute value of the approximate error estimate ε_a falls below a prespecified error criterion ε_s conforming to three significant figures.

Q5. The exponential function $y = e^x$ is given by the infinite series

$$e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{3!} + \cdots + \frac{x^n}{n!}$$

is given by the infinite series

Evaluate this function for x = 10 and x = − 10, and be attentive to the problems of round- off error.

DEPARTMENT OF CHEMICAL ENGINEERING

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Tutorial Sheet # 2

Topics: Linear & Non Linear Methods in Chemical Engineering

Q1. (a) Use the bisection method to determine the drag coefficient c needed for a parachutist of mass m = 68.1 kg to have a velocity of 40 m/s after free-falling for time t = 10 s. Note: The acceleration due to gravity is 9.8 m/s^2

(Hint: $f(c) = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right) - v$)

(b) Continue Q1 (a) until the approximate error falls below a stopping criterion of ε_s = 0.5%.

Q2. Use the false-position method to determine the root of the same equation investigated in Q1(a)

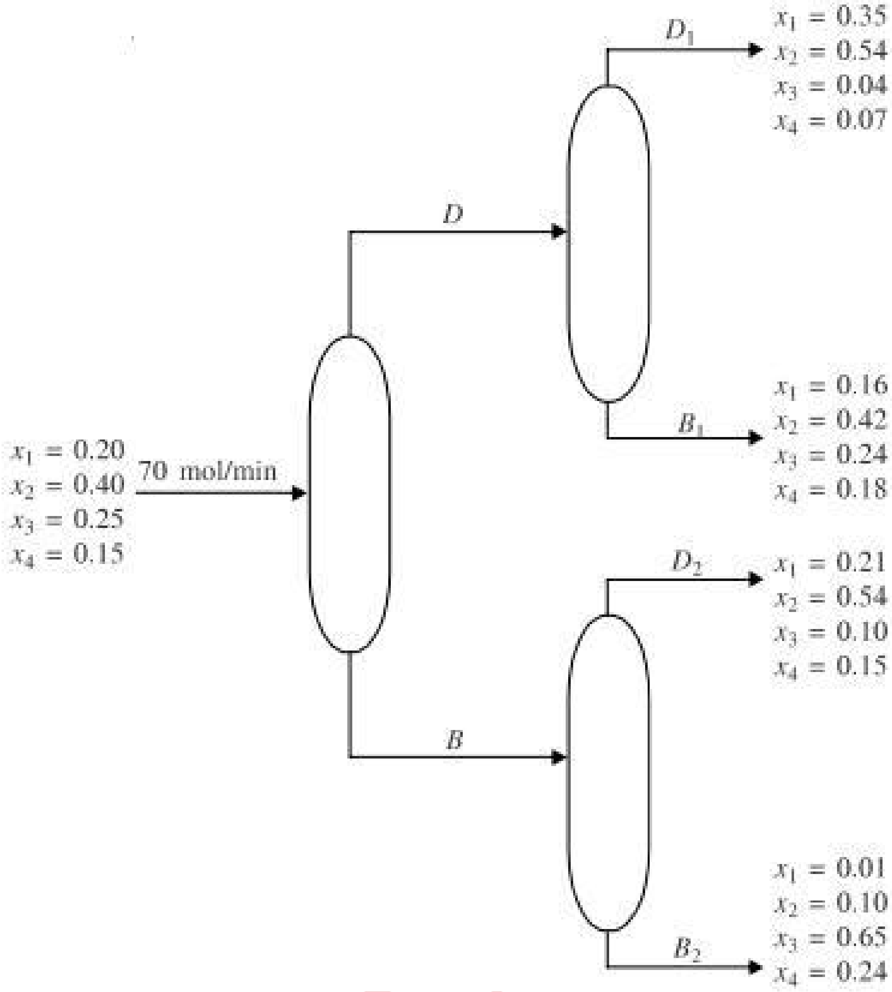
Q3. Use the Newton-Raphson method to estimate the root of $f(x) = e^{-x} - x$, employing an initial guess of $x_0 = 0$.

Q4. Use the secant method to estimate the root of $f(x) = e^{-x} - x$. Start with initial estimates of $x_{-1} = 0$ and $x_0 = 1.0$.

5. Oil droplets of diameter 2 mm are to be settled from air at 25°C and 1 atm. The density of oil is 900 kg/m^3. Calculate the terminal settling velocity of the particles. For air at these conditions, $\mu = 1.85 \times 10^{-5}$ kg/m-s. C_D is given by $C_D = \frac{24}{Re_p}(1 + 0.15 Re_p^{0.687})$.

6. Air at 25°C and 1 atm flows through a 4 mm diameter tube with an average velocity of 50 m/s. The roughness is s = 0.0015 mm. Calculate the friction factor using the Colebrook equation: $\frac{1}{\sqrt{f}} = -2.0 \log\left(\frac{\varepsilon/D}{3.7} + \frac{2.51}{Re\sqrt{f}}\right)$. Determine the pressure drop in a 1 m section of the tube using the relation: $\Delta P = \frac{f * L * V * \rho}{2D}$. Density of air at 25°C and 1 atm is 1.23 kg/m^3 and viscosity is 1.79×10^{-5} kg/m-s.

Q7. Benzene (1), toluene (2), styrene (3), and xylene (4), are to be separated in the sequence of distillation columns shown in Figure. Determine molar flow rates of streams D_1, B_1, D_2, and B_2. The composition of the feed stream and the stream D_1, B_1, D_2, and B_2 is shown in the figure. Also determine the molar flow rates and compositions of streams B and D. The molar flow rate of the feed stream is 70 mol/min.



x1 = 0.20
x2 = 0.40
x3 = 0.25
x4 = 0.15
70 mol/min
D
B
D1
x1 = 0.35
x2 = 0.54
x3 = 0.04
x4 = 0.07
B1
x1 = 0.16
x2 = 0.42
x3 = 0.24
x4 = 0.18
D2
x1 = 0.21
x2 = 0.54
x3 = 0.10
x4 = 0.15
B2
x1 = 0.01
x2 = 0.10
x3 = 0.65
x4 = 0.24

DEPARTMENT OF CHEMICAL ENGINEERING

Numerical Methods in ChE Engineering (BTCH-21405)

Tutorial Sheet # 3

Topics: Regression and Interpolation

1. Answer true or false to each of the following:

a	Collocation is used when the data are known to be accurate	T F
b	The polynomial of degree n passing through n+1 points is unique	T F
c	Collocation functions are commonly used for interpolation	T F
d	Spline functions cannot be used for interpolation	T F
e	The derivation of Lagrange interpolation function does not require the solution of a set of linear equations	T F
f	In general, a low order piece-wise polynomial is better than a single higher order polynomial to interpolate n data points	T F

g	Numerical differentiation is inherently more accurate that numerical integration	T F
h	Any interpolation polynomial can be used to derive the finite-difference formulas	T F
i	Higher order accuracy finite difference formulas can be derived by retaining more terms in Taylor's series expansion	T F
j	Numerical integration is also known as quadrature	T F
k	In general, Simpson's method is more accurate than the trapezoidal method	T F
l	The error in trapezoidal rule is proportional to h^2	T F

2. Match the following:

1. Collocation	(a) Piecewise polynomial
2. Regression	(b) Useful to represent any periodic function
3. Interpolation	(c) Curve passing thorough every data point
4. Inverse Interpolation	(d) Curve passing through n+1 data points
5. Splines	(e) Curve made to represent the general trend of the data
6. n^{th} degree polynomial	(f) Estimation of the value of a function between known data points
7. Fourier Series	(g) Estimation of the value of independent variable for a specified value of the function

3. Select the most appropriate answer out of the multiple choices given:

a The following type of functions are most commonly used for interpolation
(i) polynomials (ii) splines (iii) Fourier series

b All previous computations can still be used when new data points are added in the following type of polynomials
(i) Lagrange's (ii) Splines (iii) Newton's

c The second derivative of a function represents the
(i) curvature (ii) slope (iii) continuity

d The method of least squares is useful for
(i) interpolation (ii) collocation (iii) linear regression

4. The data on the variation of the ratio of stagnation pressure to static pressure (r) with Mach number (M) for the flow through a duct are as follows:

i	1	2	3	4	5
M_i	0.2	0.4	0.6	0.8	1.0
r_i	1.05	1.1	1.3	1.55	1.9

Fit a fourth-degree polynomial to the data.

5. The power developed by a hydraulic impulse turbine (P) by changing the penstock diameter (D) is found to be as follows:

i	1	2	3	4
D_i (m)	0.4	0.6	0.8	1.0
P_i (MW)	20	50	105	180

Fit a cubic polynomial to the data.

6. The kinematic viscosity of SAE 30 oil with variation in temperature was found to be as follows:

i	1	2	3	4	5	6	7
Temperature, T_i (^0C)	1	20	40	60	80	100	120
Viscosity μ_i (m^2/s)	$2.5x10^{-3}$	$5.5x10^{-4}$	$1x10^{-4}$	$5x10^{-5}$	$2x10^{-5}$	$1.2x10^{-5}$	$6x10^{-6}$

Develop a relationship between the two parameters of the form $\mu_i = ae^{(b/T)}$

7. Derive the Lagrange interpolation polynomial that passes through the following points

x	-4	-3	-2	-1	0
y	5	0	3	2	9

8 The variation of heat transfer coefficient per unit area (q) during the boiling of water under pressure (p) has been found to be as follows:

q , (MW/m^2)	1.1	2.4	3.4	3.9	4.0	3.8	3.0	1.2
p (MPa)	0	1	2	4	6	10	15	20

Develop a suitable polynomial relation between *q* and *p*.

9. The drag coefficient (C) with Reynolds number (Re) for a smooth sphere is found to vary according to the following data:

Re_i	0.1	1	10	100	1000	10000
C_i	210	30	4	1	0.5	0.4

Develop a suitable relationship between Re and C.

DEPARTMENT OF CHEMICAL ENGINEERING

Numerical Methods in ChE Engineering (BTCH-21405)

Tutorial Sheet # 4

Topics: Numerical Differentiation & Integration

Q1. Compute from following table the value of the derivative of y=f(x) at $x = 1.7485$:

x	1.73	1.74	1.75	1.76	1.77
y	1.772844100	1.155204006	1.737739435	1.720448638	1.703329888

Q2. Using only the first term in the formula show that

$$f'(x_0) \approx \frac{y_1 - y_{-1}}{2h}.$$

Compute from following table the value of the derivative of $y = e^x$ at $x = 1.15$:

x	1.05	1.15	1.25
e^x	2.8577	3.1582	3.4903

3. Retaining only the first two terms in the formula, show that

$$f'(x_0) \approx \frac{-3y_0 + 4y_1 - y_2}{2h}.$$

Hence compute the derivative of $y = e^x$ at $x = 1.15$ from the following table:

x	1.15	1.20	1.25
e^x	3.1582	3.3201	3.4903

Also compare your result with the computed value in the Q2. & Q3.

Q4. Retaining only the first two terms in the formula show that

$$f'(x_0) \approx \frac{y_{-2} - 8y_{-1} + 8y_1 - y_2}{12h}.$$

Hence compute from following table the value of the derivative of $y = e^x$ at $x = 1.15$:

x	1.05	1.10	1.15	1.20	1.25
e^x	2.8577	3.0042	3.1582	3.3201	3.4903

Q5. Following table gives the values of $y = f(x)$ at the tabular points $x = 0 + 0.05 \times k$, $k = 0, 1, 2, 3, 4, 5.$

x	0.00	0.05	0.10	0.15	0.20	0.25

y	0.00000	0.10017	0.20134	0.30452	0.41075	0.52110

Compute (i)the derivatives y' and y'' at $x = 0.0$ by using the formula Lagrange's interpolating

Q6. Compute from following table the value of the derivative of $y = f(x)$ at $x = 0.6$:

x	0.4	0.6	0.7
y	3.3836494	4.2442376	4.7275054

Q7. Using Trapezoidal rule compute the integral $\int_0^1 e^{x^2} dx,$ where the table for the values of $y = e^{x^2}$ is given below:

x	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
y	1.00000	1.01005	1.04081	1.09417	1.17351	1.28402	1.43332	1.63231	1.89648	2.2479	2.71828

Q8. Repeat the problem 7 using Simpson's rule. Also estimate the error in its calculation and compare it with the error using Trapezoidal rule.

Q9. Compute the integral $\int_{0.05}^{1} f(x)dx$, where the table for the values of $y = f(x)$ is given below:

0.05	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.0785	0.1564	0.2334	0.3090	0.4540	0.5878	0.7071	0.8090	0.8910	0.9511	0.9877	1.0000

Q10. Compute the integral $\int_0^{1.5} f(x)dx$, where the table for the values of $y = f(x)$ is given below:

x	0.0	0.5	0.7	0.9	1.1	1.2	1.3	1.4	1.5
y	0.00	0.39	0.77	1.27	1.90	2.26	2.65	3.07	3.5

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Tutorial Sheet # 5

Topics: ODE & Initial Value Theorem

Q1. Find y(1.0) using RK method of order four by solving the IVP $y' = -2xy^2$, $y(0) = 1$ with step length 0.2. Also compare the solution obtained with RK methods of order three and two.

Q2. Find y in [0,3] by solving the initial value problem $y' = (x - y)/2$, $y(0) = 1$ using RK method of order four with h = 1/2 and 1/4. Solution

Q3.Using RK method of order four find y(0.1) for $y' = x - y^2$, $y(0) = 1$.

Q4. Using RK method of order four find y at x = 1.1 and 1.2 by solving $y' = x^2 + y^2$, $y(1) = 2$.

Q5. Consider a reaction A→B, carried out in batch reactor. The differential equation for species A is $\frac{dC_A}{dt} = -k * C_A$. The initial conditions is at time t=0, C_A= 1mol/m^3. The reaction rate constant (*k*) is 1s^{-1}. Using Runge-Kutta fourth order method, determine the concentration of A at 3 sec.

Q6. Apply Runge-Kutta method to find an approximate value of *y* for *x* = 0.2 in steps of 0.1, if $\frac{dy}{dx} = x + y^2$ given that *y* =1 , where *x*=0.

Q7. Solve the equation $y'' = x + y$ with boundary conditions $y(0) = y(1) = 0$.