ChE 400: Numerical Differentiation and Integration (H-6)

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Objectives

- General:
  - Apply the concepts of this chapter for the solution of chemical engineering problems that require the calculation of integrals and derivatives numerically
- Specific objectives:
  - Use the backward, forward, and central approximations to calculate derivatives numerically
  - Use the trapezoidal rule for integration
  - Use Simpson's rule for integration
  - Use Excel and Matlab to calculate derivatives and integrals numerically

Outline

- Numerical Differentiation
  - Overview
  - Discretization of a function
  - Examples
- Numerical Integration
  - Overview
  - Trapezoidal rule
  - 1/3 Simpson's rule
- Lab Practice
  - Use of Excel
  - Use of Matlab

Numerical Differentiation

- Sometimes the function is very complex and the derivative of the function can't be evaluated analytically
- Need to use numerical methods
- Numerical differentiation methods are based on Taylor's series expansion
- Their accuracy depends on the number of terms involved in the calculation of the derivative and the profile of the function
  - Usually the more terms used in the series the better the accuracy
  - The final accuracy of the computation is strongly affected by the profile of the function

Discretization of a Function

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- Use of Excel
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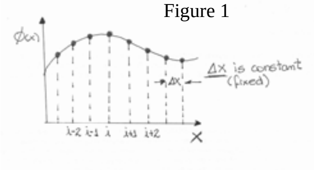
- The first step to apply numerical differentiation is to discretize the continuous function into discrete points, as shown in the figure

Figure 1



Taylor's Series

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- Using Taylor's series expansion for the points ϕ_{i+1}, ϕ_{i+2}, ϕ_{i-1}, ϕ_{i-2}

$$\phi_{i+1} = \phi_i + (\Delta x)\phi_i' + \frac{(\Delta x)^2}{2!}\phi_i'' + \frac{(\Delta x)^3}{3!}\phi_i''' + \frac{(\Delta x)^4}{4!}\phi_i^{IV} + \ldots + \quad (1)$$

$$\phi_{i+2} = \phi_i + 2(\Delta x)\phi_i' + \frac{(2\Delta x)^2}{2!}\phi_i'' + \frac{(2\Delta x)^3}{3!}\phi_i''' + \frac{(2\Delta x)^4}{4!}\phi_i^{IV} + \ldots + \quad (2)$$

$$\phi_{i-1} = \phi_i - (\Delta x)\phi_i' + \frac{(-\Delta x)^2}{2!}\phi_i'' - \frac{(\Delta x)^3}{3!}\phi_i''' + \frac{(-\Delta x)^4}{4!}\phi_i^{IV} + \ldots + \quad (3)$$

$$\phi_{i-2} = \phi_i - 2(\Delta x)\phi_i' + \frac{(-2\Delta x)^2}{2!}\phi_i'' - \frac{(2\Delta x)^3}{3!}\phi_i''' + \frac{(-2\Delta x)^4}{4!}\phi_i^{IV} + \ldots + \quad (4)$$

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Numerical Approximations

- Using a combination of equations (1) to (4) the expressions for the numerical derivatives can be obtained
- The approximations are named in accordance with the points used, e.g.,:
  - Backward approximations (uses backward points in the calculation)
  - Forward approximation (uses forward points)
  - Central approximation (uses central points)

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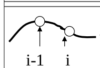
Backward Approximation
First Derivative (ϕ_i')



- Rearranging Eq. 3 to obtain the first derivative at node point i:

$$(\Delta x)\phi_i' = \phi_i - \phi_{i-1} + \frac{(-\Delta x)^2}{2!}\phi_i'' - \frac{(\Delta x)^3}{3!}\phi_i''' + \frac{(-\Delta x)^4}{4!}\phi_i^{IV} + \ldots + \quad (3.1)$$

- Dividing by (Δx):

$$\phi_i' = \frac{(\phi_i - \phi_{i-1})}{(\Delta x)} + \frac{(-\Delta x)}{2!}\phi_i'' - \frac{(\Delta x)^2}{3!}\phi_i''' + \frac{(-\Delta x)^3}{4!}\phi_i^{IV} + \ldots + \quad (3.2)$$

These are the only known points according to our figure

These terms are eliminated from the expression. They are known as the error of the approximation

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Backward Approximation
First Derivative (ϕ_i'), continued

- Therefore, the final approximation for the first derivative using two backward points is given by:

$$\phi_i' = \frac{(\phi_i - \phi_{i-1})}{(\Delta x)} \quad (3.3)$$

- The error of the approximation is given by the truncated points from the series:

$$E(\phi_i') = \frac{(-\Delta x)}{2!}\phi_i'' - \frac{(\Delta x)^2}{3!}\phi_i''' + \frac{(-\Delta x)^3}{4!}\phi_i^{IV} + \ldots + \quad (3.4)$$

Largest term

Backward Approximation
First Derivative (ϕ_i'), continued

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- The first term in the error equation is known as the order of the approximation (O). Therefore, we can say that the two point backward approximation has an order: O (Δx)
- Notice that $0<\Delta x<1$
- The smaller Δx, the smaller the error (Eq. 3.4), therefore, the more accurate the computation of the numerical derivative (Eq. 3.3)

Procedure to Develop Numerical Approximations for the derivative

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1. Draw schematic with the discretized points involve in the calculation
2. Use Taylor's series expansions for the points involved in the calculation (See Eqs. 1 to 4)
3. Combine Eqs. 1-4 to obtain the required expression
4. Simplify the obtain expression
5. Truncate the equation containing only the known points
6. Define the error and the order of the approximation

Example 1

- Develop the backward approximation for the second derivative

Example 2

- Develop the approximation for the first derivative using central points in the computation

Table I: Summary of Useful Approximations

Approximation	Equation	Error (order of approximation)	Eqs. used in derivation
Backward	$\phi_i' = \frac{d\phi_i}{dx} = \frac{(\phi_i - \phi_{i-1})}{(\Delta x)}$	$O(\Delta x)$	Eq. (3)
	$\phi_i'' = \frac{d^2\phi_i}{dx^2} = \frac{(\phi_i - 2\phi_{i-1} + \phi_{i-2})}{(\Delta x)^2}$	$O(\Delta x)$	Eqs. (3) & (4)
Forward	$\phi_i' = \frac{d\phi_i}{dx} = \frac{(\phi_{i+1} - \phi_i)}{(\Delta x)}$	$O(\Delta x)$	Eq. (1)
	$\phi_i'' = \frac{d^2\phi_i}{dx^2} = \frac{(\phi_{i+2} - 2\phi_{i+1} + \phi_i)}{(\Delta x)^2}$	$O(\Delta x)$	Eqs. (2) & (1)
Central	$\phi_i' = \frac{d\phi_i}{dx} = \frac{(\phi_{i+1} - \phi_{i-1})}{2(\Delta x)}$	$O(\Delta x^2)$	Eqs. (1) & (3)
	$\phi_i'' = \frac{d^2\phi_i}{dx^2} = \frac{(\phi_{i+1} - 2\phi_i + \phi_{i-1})}{(\Delta x)^2}$	$O(\Delta x^2)$	Eqs. (1) & (3)

Equations valid for equal segments, that is, Δx is constant.

Table I: Summary of Useful Approximations (continued)

Approximation	Equation	Error (order of approximation)	Eqs. used in derivation
Backward (three points)	$\phi_i' = \frac{d\phi_i}{dx} = \frac{(3\phi_i - 4\phi_{i-1} + \phi_{i-2})}{(2\Delta x)}$	$O(\Delta x^2)$	Eqs. (3) & (4)
Forward (three points)	$\phi_i' = \frac{d\phi_i}{dx} = \frac{(4\phi_{i+1} - 3\phi_i - \phi_{i+2})}{(2\Delta x)}$	$O(\Delta x^2)$	Eqs. (2) & (1)

Equations valid for equal segments, that is, Δx is constant.

Procedure to Calculate Numerical Derivatives

1. Draw schematic with the discretized points involve in the calculation, around the "i" value that your are interested in evaluating
2. Use the appropriate equation from the ones given in Table I for the calculation of the derivative
3. Calculate the derivative

Need to use this procedure all the time, for homework, exams, etc (**all the steps**)

Remarks

- First order approximations usually good for functions that have a flat profile
- Second order approximations usually good for functions that have a steep profile
- The trend is to use high order approximations with small number of nodes. This approach saves time but may provide the wrong answer

Example 3

- Calculate the first derivative of the given function $f(x) = x^2 + 3x - 2$ at x = 1, using:
  - Backward approximation
  - Forward approximation
  - Central approximation
  - Compare your results with the analytical solution

Example 4

- The following data were collected when a large oil tanker was loading:

t, min	0	15	30	45	60	90	120
V, 10^6 barrels	0.5	0.65	0.73	0.88	1.03	1.14	1.30

- Calculate the flow rate Q for each time to the order $E=O(\Delta t^2)$

Numerical Integration

- Suppose that we have to integrate the function F(x):

$$I = \int_{x_0}^{x_n} F(x)dx$$

- The idea of numerical methods of integration is to substitute the function F(x) by an equivalent function "y(x)", that is easier to integrate. Usually y(x) is a polynomial

Overview

- Therefore:

$$I = \int_{x_0}^{x_n} F(x)dx \approx \int_{x_0}^{x_n} y(x)dx$$

- Methods to approximate function:
  - Newton-cotes methods
    - Equally spaced points
    - Modified for unequal spaced points
  - Gauss quadrature (unequally spaced points)

Newton-cotes methods

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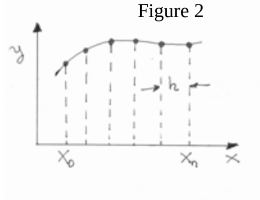
- Using Gregory-Newton Interpolation formula, the function is discretized into several segments of width "h", between the desired interval $[x_0,x_n]$, as shown:

Figure 2



Gregory-Newton interpolation

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- Then, the function can be expressed as a product of polynomials:

$$y = y_0 + \frac{(x-x_0)}{h}\Delta y_0 + \frac{(x-x_0)(x-x_1)}{2!h^2}\Delta^2 y_0 + \frac{(x-x_0)(x-x_1)(x-x_2)}{3!h^3}\Delta^3 y_0 + \ldots +$$

Eq. (5)

Trapezoidal Rule

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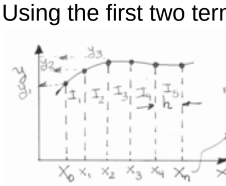
- Using the first two terms of Eq. (5)

Figure 3



$$I_1 = \int_{x_0}^{x_1}\left[y_0 + \frac{(x-x_0)}{h}\Delta y_0\right]dx + \int_{x_0}^{x_1} R_n(x)\,dx$$

Eq. (6)

Error

Trapezoidal rule (continued)

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Integrating Eq. (6) and separating the error:

$$I_1 \approx \frac{(y_0 + y_1)}{2} h \qquad \text{Eq. (7)}$$

$$\text{Error} \approx \left[-\frac{1}{12} h^3 y_0'' + \frac{h^4}{24} y_0''' + \ldots + \right] \Rightarrow \text{Error} \approx O(h^3)$$

Eq. (8)

Trapezoidal rule (continued)

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- Generalizing Eq. (7) for any trapezoid in the curve (see Figure 3):

$$I_i \approx \frac{(y_{i-1} + y_i)}{2} h \qquad \text{Eq. (9)}$$

- Finally the total integral is obtained by adding each of the trapezoids shown in Figure 3:

$$I \approx \sum_{i=1}^{n} I_i = I_1 + I_2 + I_3 + \ldots + I_n \qquad \text{Eq. (10)}$$

- The error of the total integral is Error=O(h^2)

Trapezoidal Rule Procedure Constant "h"

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1. Draw schematic with the discretized points involved in the calculation (showing the trapezoids):
   1. Indicate the integrating range [x_0,x_n] and the value of "h". h = (x_n-x_0)/n where "n" is number of trapezoids
   2. Use as many trapezoids as possible (small "h"), this will make your calculation more accurate
2. Calculate the area of each trapezoid (I_i) using Eq. 9
3. Calculate the value of the Integral (I) by adding the area of the different trapezoids using Eq. (10)
   1. Sometimes programmers use the direct formula:

$$I \approx \frac{h}{2}\left[y_0 + y_n + 2\sum_{i=1}^{n-1} y_i \right]$$

4. Recommendation: It is ideal to perform these calculations using a table format. In the future (real work), it will be most likely that you will be solving numerical integrals by using an Excel spreadsheet that you write with the equations given in this procedure

Example 5

- Solve the integral given below using trapezoidal rule. Compare your solution with the analytical solution.

$$I = \int_0^{0.8} F(x)dx$$

$$F(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

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Trapezoidal Rule variable "h"

- You will encounter a variable h most of the time in your calculations, especially when you are using experimental data.
- The procedure is very similar to the one described for constant "h", except that you will have to calculate a new "h" all the time

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Trapezoidal Rule Procedure Variable "h"

1. Draw schematic with the discretized points involved in the calculation (showing the trapezoids):
   1. Indicate the integrating range $[x_0,x_n]$
   2. Use as many trapezoids as possible (small "h"), this will make your calculation more accurate
2. Calculate the area of each trapezoid:
   1. Calculate your "h" for each trapezoid: $h_i=(x_i-x_{i-1})$
   2. Calculate "I_i" using Eq. 9
3. Calculate the value of the Integral (I) by adding the area of the different trapezoids using Eq. (10)
4. Recommendation: It is ideal to perform these calculations using a table format. In the future (real work), it will be most likely that you will be solving numerical integrals by using an Excel spreadsheet that you write with the equations given in this procedure

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Example 6

- Solve the exercise given in example 5 using unequal segments for the trapezoidal rule

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Simpson's 1/3 Rule

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- Uses the first three terms of Gauss-Newton Interpolation (Eq. 5)
- It uses two segments of width h, therefore, integration is done faster
- It only works with an even number of segments (e.g., n= 2, 4, 6, 8,…, etc)
- Only applies for equal segments of h

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Simpson's 1/3 Rule continued

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- The area of each two segments is calculated by:

$$I_{2i} \approx \frac{h}{3}\left(y_{2[i-1]} + 4y_{2i-1} + y_{2i}\right) \quad \text{Eq. (11)}$$

- The total integral is calculated by:

$$I \approx \sum_{i=1}^{n/2} I_{2i} = I_2 + I_4 + I_6 + ... + I_n \quad \text{Eq. (12)}$$

Where "n" is an even number

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Simpson's 1/3 Rule continued

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- The error is order: Error O(h^4). More accurate than trapezoidal rule
- Programmers can also use the following expression to calculate the total integral:

$$I \approx \frac{h}{3}\left(y_0 + y_n + 4\sum_{i=1}^{n/2} y_{2i-1} + 2\sum_{i=1}^{n/2-1} y_{2i} \right) \quad \text{Eq. (13)}$$

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Simpson's 1/3 Rule Procedure

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1. Draw schematic with the segment points involved in the calculation (showing the individual areas):
   1. Divide your curve in "n" even number of segments
   2. Indicate the integrating range [x_0,x_n] and the value of "h". h = (x_n-x_0)/n where "n" is number of segments
   3. Use as many segments as possible (small "h"), this will make your calculation more accurate
2. Calculate the area of each two segments (I_{2i}) using Eq. (11)
3. Calculate the value of the Integral (I) by adding the area of the different segments using Eq. (12)
4. Recommendation: It is ideal to perform these calculations using a table format. In the future (real work), it will be most likely that you will be solving numerical integrals by using an Excel spreadsheet that you write with the equations given in this procedure

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Example 7

- Solve the integral given below using Simpson's 1/3 rule (with 4 segments). Compare your solution with the analytical solution.

$$I = \int_0^{0.8} F(x)dx$$

$$F(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

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- The way to use excel to solve for numerical integrals is by developing a spreadsheet that will use the equations shown in this handout
- It is not automatic. It is a very organized way to perform your calculation, instead of using a calculator

Use of Matlab

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- Numerical integration using "quad" function
- Symbolic integration using "int" function

Assignment

- Reproduce the results of all exercises in Tutorial 4
- Solve Homework 5 (due 10/16/06), posted on web http://www.ent.ohiou.edu/che/che400/Assignments.htm
- Quiz 4, 10/16/06

Summary

- Do all the exercises done in class by yourself
- Review and know all the methods given in this handout
- Reproduce by yourself all the exercises given in Tutorial 4
- Do by yourself the homework assignment
- Solve the proposed problems for the chapter