ChE 400: Nonlinear Algebraic Equations (H-5)

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Objectives

- General:
  - Apply the concepts of this chapter for the solution of chemical engineering problems that imply systems of non linear algebraic equations
- Specific objectives:
  - Recognize systems of nonlinear equations
  - Use the Newton Raphson method to linearize your equations
  - Use the Cramer's rule to solve for the linearize equations
  - Define appropriate guesses
  - Use Excel and Matlab to solve systems of non LAEs (fsolve and solver commands)

Outline

- Nonlinear Algebraic Equations
  - Overview
  - Uses
- Linearization
  - Method
  - Example
- Lab Practice
  - Use of Excel
  - Use of Matlab (fsolve)

Nonlinear Algebraic Equations

- Suppose that we have a set of equations as shown:

$$f_1(x_1, x_2, ..., x_n) = 0$$
$$f_2(x_1, x_2, ..., x_n) = 0$$
$$\vdots$$
$$f_n(x_1, x_2, ..., x_n) = 0$$

Where "n" is the number of equations

Nonlinear Algebraic Equations
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Nonlinear Algebraic Equations

- The system of equations is nonlinear, when it can be expressed as:

$$f(x_n)x_1 + f(x_n)x_2 + ... + f(x_n)x_n = b_1$$
$$f(x_n)x_1 + f(x_n)x_2 + ... + f(x_n)x_n = b_2$$
$$\vdots$$
$$f(x_n)x_1 + f(x_n)x_2 + ... + f(x_n)x_n = b_n$$

Where "b" are constants coefficients

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Nonlinear Algebraic Equations Conditions

- No constant coefficients
  - The coefficients are a function of the dependent variable
  - Your coefficients could be algebraic equations or transcendental equations
  - E.g., power functions of the dependent variables

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Example of nonlinear algebraic equations

$$x_1^2 + x_1 x_2 = 10$$
$$x_2 + 3x_1 x_2^2 = 57$$

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Nonlinear Algebraic Equations Uses

- Nonlinear algebraic equations are typically obtained from
  - Material Balance
  - Energy Balance
- Examples:
  - Series of flash drums
  - Series of reactors with kinetics different to first or zero order
  - Series of heat exchangers with no constant properties (e.g., conductivity a function of Temperature)
- Their solution requires the use of matrix operations and linearization methods

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Review of Mathematical form identification

- At this point you should be able to identify the following mathematical forms:
  - Differential equations (classification of them will be studied later during the course)
  - Roots of equations
  - Linear algebraic equations
  - Nonlinear algebraic equations

Linearization

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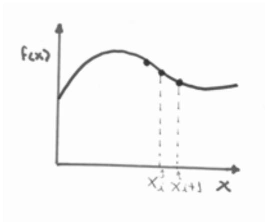
Suppose that you have a function that depends only on "x", f(x). Taylor series allows to predict the value of $f(x)|_{i+1}$ using the value of the function at the previous discretized point "$f(x)|_i$"



Linearization

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- Using Taylor Series expansion around point x_i

$$f(x_{i+1}) = f(x_i) + f^{'}(x_i)(x_{i+1} - x_i) + \frac{(x_{i+1} - x_i)^2}{2!} f^{''}(x_i) + \ldots + \frac{(x_{i+1} - x_i)^n}{n!} f^{n}(x_i)$$

Eq. 1

Linearization

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- Taking the first two terms of the series given in Eq. (1):

$$f(x_{i+1}) \approx f(x_i) + f^{'}(x_i)(x_{i+1} - x_i) \quad \text{Eq. 2}$$

Linearization

- Extending Eq. (2) for multiple "n" variables :

Eq. 3

$$f_{k,i+1} \approx f_{k,i} + \left(x_{1,i+1} - x_{1,i}\right)\frac{\partial f_k}{\partial x_1}\Big|_i + \left(x_{2,i+1} - x_{2,i}\right)\frac{\partial f_k}{\partial x_2}\Big|_i + \ldots + \left(x_{n,i+1} - x_{n,i}\right)\frac{\partial f_k}{\partial x_n}\Big|_i$$

$$\vdots$$

$$f_{n,i+1} \approx f_{n,i} + \left(x_{1,i+1} - x_{1,i}\right)\frac{\partial f_n}{\partial x_1}\Big|_i + \left(x_{2,i+1} - x_{2,i}\right)\frac{\partial f_n}{\partial x_2}\Big|_i + \ldots + \left(x_{n,i+1} - x_{n,i}\right)\frac{\partial f_n}{\partial x_n}\Big|_i$$

Where:

k: represents the equation number

n: represents the dependent variable

i: value at a guess

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Linearization

- At solution (when we solve for the system of equations) $f_{k,i+1}=0$. Substituting it into Eq. 3 (applied to all the equations in the system) and rearranging:

$$x_{1,i+1}\frac{\partial f_k}{\partial x_1}\Big|_i + x_{2,i+1}\frac{\partial f_k}{\partial x_2}\Big|_i + \ldots + x_{n,i+1}\frac{\partial f_k}{\partial x_n}\Big|_i = -f_{k,i} + x_{1,i}\frac{\partial f_k}{\partial x_1}\Big|_i + x_{2,i}\frac{\partial f_k}{\partial x_2}\Big|_i + \ldots + x_{n,i}\frac{\partial f_k}{\partial x_n}\Big|_i$$

Eq. 4

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Linearization

- Eq. 4 is now linearized.
- Since we are dealing with a system of non linear algebraic equations, we can expressed Eq. 4 in matrix form by defining the following matrices:
  - J: Jacobian Matrix
  - F: Function (or equations) vector
  - X_i: vector that contains the guesses to start the calculation
  - X_{i+1}: vector that contains the value of the variable calculated based on the guesses (x_i)

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Jacobian Matrix

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Jacobian is the matrix form by the partial derivative of the equations respect to the dependent variable, all of them evaluated at the guesses. This means that all terms in the J matrix are **known numbers**

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}_{i \text{ (evaluated at "i")}}$$

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Function Vector

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•F is the vector form by the equations evaluated at the guesses. This means that all terms in the F vector are **known numbers**

$$\{F\} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}_{i \text{ (evaluated at "i")}}$$

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X_i vector

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•X_i is the vector form by the guesses for all the dependent variables. This means that all terms in the X_i vector are **known numbers**

•Remember that we need to justify our initial guesses based on: chemical engineering principles, thermodynamics, physics, etc. Same criteria discussed in the chapter “roots of equations” apply for the definition of the initial guesses.

$$\{X_i\} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}_{i \text{ (evaluated at "i")}}$$

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X_{i+1} vector

•X_{i+1} is the vector form that contains the value of the variables calculated according to Eq. 4.

$$\{X_{i+1}\} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}_{i \text{ (evaluated at "i+1")}}$$

Linearization Equation

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- Therefore, Eq. 4 can be expressed in matrix form:

$$J\{X_{i+1}\} = -\{F\} + J\{X_i\} \quad \text{Eq. 5}$$

Linearization Procedure

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- Make all your equations equal to zero. If you **do not do** that you are solving for the **incorrect vector** “{F}”
- Apply Eq. 5 to your system
- Identify your guesses
- Calculate the Jacobians
- Substitute the Jacobians into Eq. 5 and perform matrices operations. Your matrix will be linearized by this time.

Example 1

- Linearize the following system of equations:

$$x_1^2 + x_1 x_2 = 10$$
$$x_2 + 3x_1 x_2^2 = 57$$

Solving Nonlinear Algebraic Equations

1. Linearize your system of equations (apply linearization procedure given before)
2. Since your system of equations is linearized, you can solve the system of linear algebraic equations using any of the methods that we learned (Cramer's rule, Gauss, Gauss Jordan, Inverse Matrix)
3. After finishing step 2, you will get your X_{i+1}
4. Calculate Error for each of your variables
5. If Error:
   - Less than convergence criteria stop calculation
   - Larger than convergence criteria
     - Make $X_i = X_{i+1}$ (values just calculated)
     - Go to step 2

Converge Criteria

- The error is calculated in a similar way as described in roots of equations.
- Since you have several variables you will have to calculate different errors
- All the errors should match the converge criteria before you stop your calculation

$$E_a = \left| \frac{X_r^{new} - X_r^{old}}{X_r^{new}} \right| 100$$

Example 2

- Solve the following system of equations

$$x_1^2 + x_1 x_2 = 10$$
$$x_2 + 3x_1 x_2^2 = 57$$

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Assignment

- Reproduce the results of all exercises in Tutorial 3
- Solve Homework 4 (see tentative schedule), posted on web http://www.ent.ohiou.edu/che/che400/Assignments.htm
- Quiz 3, see tentative schedule

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Summary

- Do all the exercises done in class by yourself
- Do you know how to linearize an equation?
- How do you know that the equation is linearize?
- Why is it important to define good guesses for the solution of Non LAE?
- Solve the proposed problems for the chapter
- Reproduce by yourself all the exercises given in Tutorial 3.

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