Nonlinear Algebraic Systems: Iterative Methods

1. Nonlinear algebraic equation systems
2. Iterative solution methods
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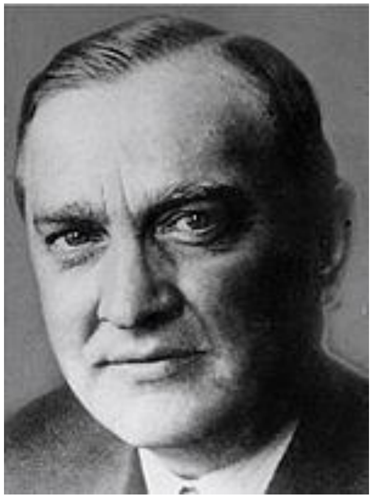

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Nonlinear Algebraic Equations: Iterative Methods

Nonlinear Algebraic Equation Systems

Nonlinear Algebraic Equations

- A single nonlinear algebraic equation in a single unknown: $f(x) = 0$
- A solution is a scalar $x = s$ for which $f(s) = 0$
- The equation may have more than one solution:

$$f(x) = x^2 + 3x + 2 = 0 \quad \Rightarrow \quad x = -1, -2$$

- The equation may have no solutions:

$$e^x = -1$$

- Typically the solution cannot be calculated analytically

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Redlich-Kwong Equation

- Redlich-Kwong equation of state:

$$P = \frac{RT}{V-b} - \frac{a}{\sqrt{T}V(V+b)}$$

  - » P = pressure
  - » V = molar volume
  - » T = temperature
  - » R = gas constant
  - » a, b = gas dependent constants

- Given P, T, R, a and b, calculate V:

$$f(V) = P - \frac{RT}{V-b} + \frac{a}{\sqrt{T}V(V+b)} = 0$$

Systems of Nonlinear Algebraic Equations

- A system of *n* nonlinear algebraic equations in *n* unknowns:

$$
\begin{aligned}
f_1(x_1, x_2, \ldots, x_n) &= 0 \\
f_2(x_1, x_2, \ldots, x_n) &= 0 \\
&\vdots \\
f_n(x_1, x_2, \ldots, x_n) &= 0
\end{aligned}
\quad \Rightarrow \quad \mathbf{f}(\mathbf{x}) = \mathbf{0} \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \mathbf{f} = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}
$$

- A solution is a vector $\mathbf{x} = \mathbf{s}$ for which $\mathbf{f}(\mathbf{s}) = \mathbf{0}$

- The system may have unique solutions, multiple solutions or no solutions

Fluid Phase Equilibria

- Two component fluid phase equilibria
  - » Assume gas phase is ideal
  - » Use the Wilson model to calculate liquid phase activity coefficients
- Equate fugacities

$$y_1 P = x_1 \gamma_1 (x_1, x_2, T) P_1^{sat}(T)$$

$$y_2 P = x_2 \gamma_2 (x_1, x_2, T) P_2^{sat}(T)$$

- Given T, P, y_1 and y_2, calculate x_1 and x_2
- Assume P_1^{sat} and P_2^{sat} have been calculated from the known temperature

Nonlinear Algebraic System Example

- Wilson activity coefficient model:

$$\ln \gamma_1 = -\ln(x_1 + x_2 G_{12}) + x_2 \left(\frac{G_{12}}{x_1 + x_2 G_{12}} - \frac{G_{21}}{x_2 + x_1 G_{21}} \right)$$

$$\ln \gamma_2 = -\ln(x_2 + x_1 G_{21}) - x_1 \left(\frac{G_{12}}{x_1 + x_2 G_{12}} - \frac{G_{21}}{x_2 + x_1 G_{21}} \right)$$

- Assume that G_{12} and G_{21} have been calculated from the known temperature
- Mole fractions must sum to unity:

$$x_1 + x_2 = 1$$

Nonlinear Algebraic System Example

- Formulate equation for total pressure

$$P = y_1 P + y_2 P = x_1\gamma_1(x_1, x_2, T)P_1^{sat}(T) + x_2\gamma_2(x_1, x_2, T)P_2^{sat}(T)$$

- Systems of 4 nonlinear equations in 4 unknowns (x_1, x_2, γ_1, γ_2)

$$f_1 = P - x_1\gamma_1(x_1, x_2, T)P_1^{sat}(T) - x_2\gamma_2(x_1, x_2, T)P_2^{sat}(T) = 0$$

$$f_2 = x_1 + x_2 - 1 = 0$$

$$f_3 = \ln\gamma_1 + \ln(x_1 + x_2 G_{12}) - x_2\left(\frac{G_{12}}{x_1 + x_2 G_{12}} - \frac{G_{21}}{x_2 + x_1 G_{21}}\right) = 0$$

$$f_4 = \ln\gamma_2 + \ln(x_2 + x_1 G_{21}) + x_1\left(\frac{G_{12}}{x_1 + x_2 G_{12}} - \frac{G_{21}}{x_2 + x_1 G_{21}}\right) = 0$$

Nonlinear Algebraic Equations: Iterative Methods

Iterative Solution Methods

Iterative Solution Methods

- Single nonlinear algebraic equation: $f(x) = 0$
- Start with an initial guess x_0 of the solution
- Algorithm generates an "improved" value x_1 of the solution from x_0
- Algorithm generates an "improved" value x_2 of the solution from x_1
- Algorithm repeated to generate sequence x_0, x_1, x_2, …
- The iterative process is convergent if the sequence x_0, x_1, x_2, … converges: $\lim_{n\to\infty}(x_{n+1} - x_n) = 0$
- In practice terminate algorithm at iteration N when we get "sufficiently close" to the solution.

Iterative Solution Methods

- Key issues is developing an iterative solution method for nonlinear algebraic equations include:
  - » What is the iterative algorithm that generates x_{n+1} from x_n?
  - » How can we ensure that the algorithm converges to a correct answer?
  - » How is the initial guess x_0 made?
  - » What are the criteria for stopping the algorithm?
- We will study three iterative algorithms:
  - » Fixed point method (today)
  - » Newton-Raphson method (next lecture)
  - » Secant method (next lecture)

Fixed Point Method

- Single nonlinear algebraic equation:

$$f(x) = 0 \quad \Rightarrow \quad x = f(x) + x = g(x)$$

- Generate an iterative equation:

$$x_{n+1} = f(x_n) + x_n = g(x_n)$$

- A value $x = s$ that satisfies $s = g(s)$ is called a fixed point
- The fixed point also is a solution of $f(s) = 0$
- The function $g(x)$ is not unique

Convergence of the Fixed-Point Method

- Let $x = g(x)$ have a solution $x = s$ and assume that $g(x)$ has a continuous first-order derivative on some interval J containing s.
- Then the fixed-point iteration converges for any x_0 in J and the limit of the sequence $\{x_n\}$ is s if:

$$\left|\frac{\partial g}{\partial x}\right| \le K < 1 \quad x \in J$$

- A function satisfying the theorem is called a contraction mapping:

$$\left|g(x) - g(v)\right| \le K\left|x - v\right| \quad K < 1$$

- K determines the rate of convergence

Nonlinear Algebraic Equations: Iterative Methods

Fixed-point Iteration Examples

Fixed Point Example 1

- Nonlinear equation:

$$f(x) = x^2 - 3x + 1 = 0 \quad \Rightarrow \quad x = 0.3820, 2.618$$

- Fixed point iteration:

$$3x = x^2 + 1 \quad \Rightarrow \quad x_{n+1} = \tfrac{1}{3}(x_n^2 + 1) = g(x_n)$$

Iteration	$x_0 = 1$	$x_o = 3$
1	0.6667	3.333
2	0.4815	4.037
3	0.4106	5.766
4	0.3895	11.42
8	0.3820	6.171×10^9

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Fixed Point Example 1

- Nonlinear equation:

$$f(x) = x^2 - 3x + 1 = 0 \quad \Rightarrow \quad x = 0.3820, 2.618$$

- Fixed point iteration:

$$x - 3 + \frac{1}{x} = 0 \quad \Rightarrow \quad x_{n+1} = 3 - \frac{1}{x_n} = g(x_n)$$

Iteration	$x_0 = 3$	$x_o = 1$
1	2.667	2.000
2	2.625	2.500
3	2.619	2.600
4	2.618	2.615
5	2.618	2.618

Fixed Point Example 2

- Redlich-Kwong equation:

$$P = \frac{RT}{V-b} - \frac{a}{\sqrt{T}V(V+b)}$$

- Given P, R, T, a and b, calculate V
- Iterative equation 1:

$$V_{n+1} = V_n - P + \frac{RT}{V_n - b} - \frac{a}{\sqrt{T}V_n(V_n+b)} = g_1(V_n)$$

Fixed Point Example 2

- Data for argon
  - » $a = 16.82\ \mathrm{L^2 \cdot bar \cdot mol^{-2} \cdot K^{1/2}}$
  - » $b = 0.02219\ \mathrm{L/mol}$
- Conditions
  - » $P = 174$ bar
  - » $T = 390$ K
- Gas constant: $R = 0.08314\ \mathrm{L \cdot bar \cdot mol^{-1} \cdot K^{-1}}$

Iteration	$v_0 = 1$	$v_o = 0.1$
1	-140	173
2	-315	-0.187
3	-489	-357
4	-663	-530
5	-837	-704

Fixed Point Example 2

- Redlich-Kwong equation: $P = \dfrac{RT}{V-b} - \dfrac{a}{\sqrt{T}V(V+b)}$
- Iterative equation 2:

$$V_{n+1} = \frac{RTV_n}{(V_n - b)P} - \frac{a}{\sqrt{T}P(V_n + b)} = g_2(V_n)$$

Iteration	$v_0 = 1$	$v_0 = 0.1$
1	0.1861	0.1997
2	0.1884	0.1879
3	0.1883	0.1883
4	0.1883	0.1883
5	0.1883	0.1883

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Fixed Point Example 3

- 2 coupled nonlinear algebraic equations

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} x_1^2 + x_2^2 - 2 \\ x_1 x_2 - 1 \end{bmatrix} = \mathbf{0}$$

- Iterative equations

$$\begin{bmatrix} x_{1,n+1} \\ x_{2,n+1} \end{bmatrix} = \begin{bmatrix} \dfrac{2 - x_{2,n}^2}{x_{1,n}} \\ \dfrac{1}{x_{1,n}} \end{bmatrix}$$

Fixed Point Example 3

Iteration	$x_{1,0} = 1$	$x_{2,0} = 1$
1	1	1
2	1	1
3	1	1

Iteration	$x_{1,0} = 1.1$	$x_{2,0} = 1.1$
1	0.718	0.909
2	1.63	1.39
3	0.0375	0.612
4	43.4	26.7
5	-16.4	0.0230

- No iterative equations worked for any initial condition other than the solution

Nonlinear Algebraic Equations: Iterative Methods

In-class Exercise