CHN-323

Computer Applications in Chemical Engineering

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Fixed point iteration method

- **Key idea**: Rearrange $f(x) = 0$ as $x = g(x)$ and then perform iterations as $x^{[n+1]} = g(x^{[n]})$
- Example: $f(x) = x^2 - 2x - 3 = 0$
  - Rearranging: $x^2 = 2x + 3 \rightarrow x = \sqrt{2x+3}$
  - Iteration: Let us take $x = 4$ as initial guess

$$
\begin{aligned}
x_0 &= 4, \\
x_1 &= \sqrt{11} = 3.31662, \\
x_2 &= \sqrt{9.63325} = 3.10375, \\
x_3 &= \sqrt{9.20750} = 3.03439, \\
x_4 &= \sqrt{9.06877} = 3.01144, \\
x_5 &= \sqrt{9.02288} = 3.00381,
\end{aligned}
$$

Fixed point iteration method

- Rearranging in the form of $x = g(x)$ can be done in multiple ways

- Example: $f(x) = x^2 - 2x - 3 = 0$
  - $x^2 = 2x + 3 \rightarrow x = \sqrt{2x+3}$
  - $x = (x^2 - 3\ )/2$
  - $x(x-2) = 3 \rightarrow x = 3/(x-2)$
  - $x^2 = 2x - 3 \rightarrow x = 2 - (3/x)$

Fixed point iteration method

- Let us try another rearrangement
- Example: $f(x) = x^2 - 2x - 3 = 0$
  - Rearranging: $x(x-2) = 3 \rightarrow x = 3/(x-2)$
  - Iteration: Let us take $x = 4$ as initial guess

$$x_0 = 4, \quad x_1 = 1.5, \quad x_2 = -6,$$

$$x_3 = -0.375, \quad x_4 = -1.263158, \quad x_5 = -0.919355, \quad x_6 = -1.02762, \quad x_7 = -0.990876, \quad x_8 = -1.00305,$$

Fixed point iteration method

- Let us try another rearrangement
- Example: $f(x) = x^2 - 2x - 3 = 0$
  - Rearranging: $x = (x^2 - 3\ )/2$
  - Iteration: Let us take $x = 4$ as initial guess

$$x_0 = 4,$$

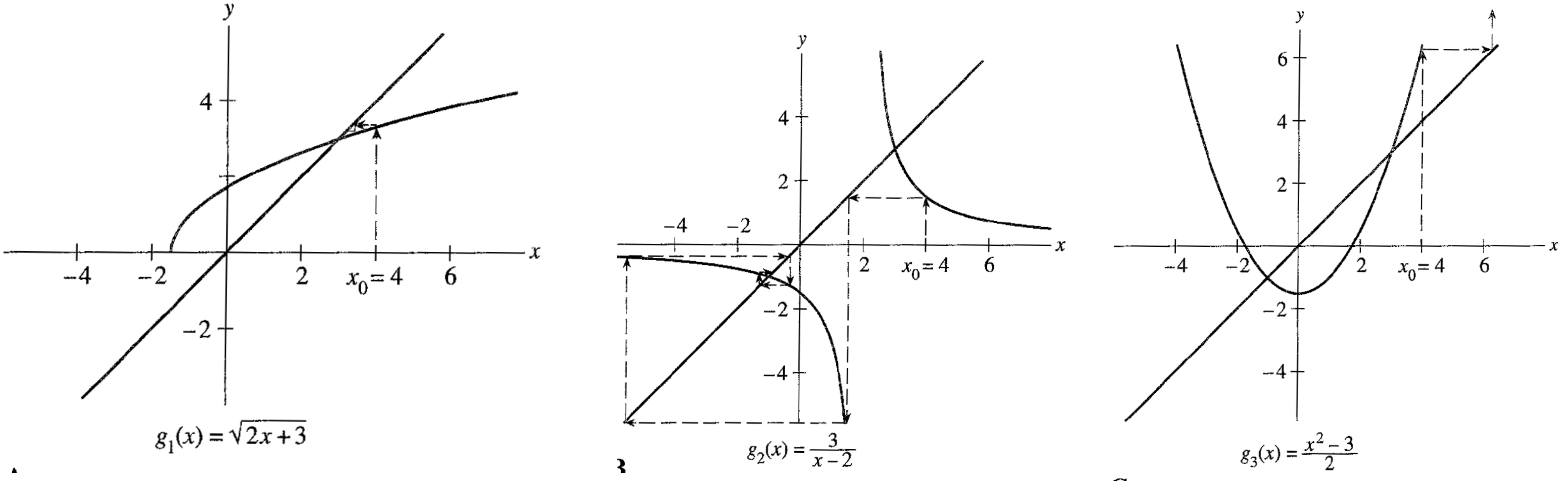
$$x_1 = 6.5,$$

$$x_2 = 19.625,$$

$$x_3 = 191.070,$$

Diverged!

Fixed point iteration method



- It appears that the different behaviors depend on whether the slope of the curve is greater, less, or of opposite sign to the slope of the line (which equals + 1).

Fixed point iteration method

- Convergence is an issue
  - Not all rearrangements lead to convergence

- Consider fixed point iteration:
  - $x^{[n+1]} = g\left(x^{[n]}\right)$
  - At convergence, $r = g(r)$

$$\rightarrow x^{[n+1]} - r = g\left(x^{[n]}\right) - g(r)$$

$$\rightarrow e^{[n+1]} = g\left(x^{[n]}\right) - g(r)$$

Fixed point iteration method

- Multiply and divide RHS with $x^{[n]} - r$
  - $e^{[n+1]} = \left(\frac{g(x^{[n]})-g(r)}{x^{[n]}-r}\right)(x^{[n]} - r)$
- With mean value theorem

$$e^{[n+1]} = g'(\xi)(x^{[n]} - r)$$

where ξ lies between $x^{[n]}$ and r

$$\rightarrow e^{[n+1]} = g'(\xi)e^{[n]}$$

1. The error will decrease with every iteration if $|g'(\xi)|<1$
2. The rate of convergence is linear since $e^{[n+1]} \propto e^{[n]}$

Error analysis for Newton's method

- $x^{[n+1]} = x^{[n]} - \frac{f\left(x^{[n]}\right)}{f'\left(x^{[n]}\right)}$
- Comparing with the fixed point iteration method (i.e., $x = g(x)$), we can say

$$g(x) = x - \frac{f(x)}{f'(x)}$$

- We have found out that the method will converge if $|g'(\xi)| < 1$

$$g'(x) = 1 - \frac{\left(f'\right)^2 - ff''}{\left(f'\right)^2} = \frac{ff''}{(f')^2}$$

- At root $(x = r)$, $f(r) = 0$ and $f'(r) \neq 0$

Thus, $g'(r) = 0$

For Newton scheme, we have |g'(r)| < 1. Therefore, with good initial guess, the Newton Scheme will converge.

System of nonlinear algebraic equations

$$
\begin{aligned}
&f_1(x_1, x_2, \cdots, x_n) = 0 \\
&f_2(x_1, x_2, \cdots, x_n) = 0 \\
&\vdots \\
&f_n(x_1, x_2, \cdots, x_n) = 0
\end{aligned}
$$

- In short form, $\underline{f}(\underline{x}) = \underline{0}$
- The equations are satisfied at the root ($\underline{x} = \underline{r}$), i.e.,
  $x_1 = r_1, x_2 = r_2, \dots, x_n = r_n$

Newton method for set of equations

- Let us consider two nonlinear equations with two unknowns

$$f_1(x_1, x_2) = 0$$
$$f_2(x_1, x_2) = 0$$

$$\underline{f}(\underline{x}) = \underline{0}$$

- Assuming that the roots $\underline{r}$ are {r1, r2}

Newton method for set of equations

- Let us revise Taylor series expansion of $f(x)$ around the point $x^{[0]}$ (for a single variable)

$$f(x) = f\left(x^{[0]}\right) + f'\left(x^{[0]}\right)\left(x - x^{[0]}\right) + \frac{f''(x^{[0]})(x - x^{[0]})^2}{2!} + \cdots$$

- Taylor series expansion of $\underline{f}(\underline{x})$ around the point $\left(x_1^{[0]}, x_2^{[0]}\right)$ (for two variables)

$$f_1(x_1, x_2) = f_1\left(x_1^{[0]}, x_2^{[0]}\right) + \left[\frac{\partial f_1}{\partial x_1}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)}\left(x_1 - x_1^{[0]}\right) + \left[\frac{\partial f_1}{\partial x_2}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)}\left(x_2 - x_2^{[0]}\right) + \cdots$$

$$f_2(x_1, x_2) = f_2\left(x_1^{[0]}, x_2^{[0]}\right) + \left[\frac{\partial f_2}{\partial x_1}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)}\left(x_1 - x_1^{[0]}\right) + \left[\frac{\partial f_2}{\partial x_2}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)}\left(x_2 - x_2^{[0]}\right) + \cdots$$

Newton method for set of equations

- Consider $\underline{x} = \underline{r}$ (roots)

$$f_1(r_1, r_2) = f_1\left(x_1^{[0]}, x_2^{[0]}\right) + \left[\frac{\partial f_1}{\partial x_1}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \left(r_1 - x_1^{[0]}\right) + \left[\frac{\partial f_1}{\partial x_2}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \left(r_2 - x_2^{[0]}\right)$$

$$f_2(r_1, r_2) = f_2\left(x_1^{[0]}, x_2^{[0]}\right) + \left[\frac{\partial f_2}{\partial x_1}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \left(r_1 - x_1^{[0]}\right) + \left[\frac{\partial f_2}{\partial x_2}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \left(r_2 - x_2^{[0]}\right)$$

- But $\underline{f}(\underline{r}) = \underline{0}$

$$0 = f_1\left(x_1^{[0]}, x_2^{[0]}\right) + \left[\frac{\partial f_1}{\partial x_1}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \left(r_1 - x_1^{[0]}\right) + \left[\frac{\partial f_1}{\partial x_2}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \left(r_2 - x_2^{[0]}\right)$$

$$0 = f_2\left(x_1^{[0]}, x_2^{[0]}\right) + \left[\frac{\partial f_2}{\partial x_1}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \left(r_1 - x_1^{[0]}\right) + \left[\frac{\partial f_2}{\partial x_2}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \left(r_2 - x_2^{[0]}\right)$$

Newton method for set of equations

- Let us introduce $\delta_1 = r_1 - x_1^{[0]}$ and $\delta_2 = r_2 - x_2^{[0]}$

$$0 = f_1\left(x_1^{[0]}, x_2^{[0]}\right) + \left[\frac{\partial f_1}{\partial x_1}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \delta_1 + \left[\frac{\partial f_1}{\partial x_2}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \delta_2$$

$$0 = f_2\left(x_1^{[0]}, x_2^{[0]}\right) + \left[\frac{\partial f_2}{\partial x_1}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \delta_1 + \left[\frac{\partial f_2}{\partial x_2}\right]_{\left(x_1^{[0]}, x_2^{[0]}\right)} \delta_2$$

- In matrix form

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}_{\left(x_1^{[0]}, x_2^{[0]}\right)} + \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix}_{\left(x_1^{[0]}, x_2^{[0]}\right)} \begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix}$$

- In compact form

$$\underline{0} = \underline{f}^{[0]} + \underline{\underline{J}}^{[0]}\underline{\delta} \qquad \rightarrow \underline{\delta} = -\left[\underline{\underline{J}}^{[0]}\right]^{-1} \underline{f}^{[0]}$$

The improved guess $\underline{x}^{[1]}$ is obtained as $\underline{x}^{[0]} + \underline{\delta}$. Continue iterations until convergence.

Newton method for set of equations

- In general, we can write

$$\underline{\delta}^{[n]} = -\left[\underline{\underline{J}}^{[n]}\right]^{-1} \underline{f}^{[n]}$$

$$\underline{x}^{[n+1]} = \underline{x}^{[n]} + \underline{\delta}^{[n]}$$

Example

- 5 CSTR Of equal volume operating in series at steady state. Reaction (A→B) in CSTR is second order, reaction rate constant is unity. Volumetric flow rate at inlet of 1st reactor is 200 m^3/s. In the figure below, x denotes concentration of A. Find Volume of each reactor.