Computational Techniques
Module 4: Nonlinear Algebraic Equations

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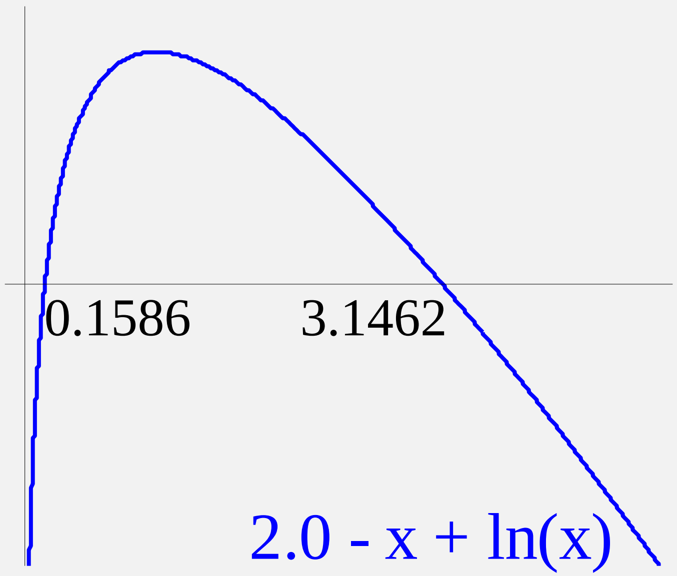
A Simple Example

- To solve the following equation:

$$2.0 - x + \ln(x) = 0$$



The solution is the location where the curve intersects the X-axis

It is possible to have multiple solutions (finite) to the problem

General Setup

- Let x be a variable of interest. The objective is to find the value of x which satisfies the following nonlinear equation

$$f(x) = 0$$

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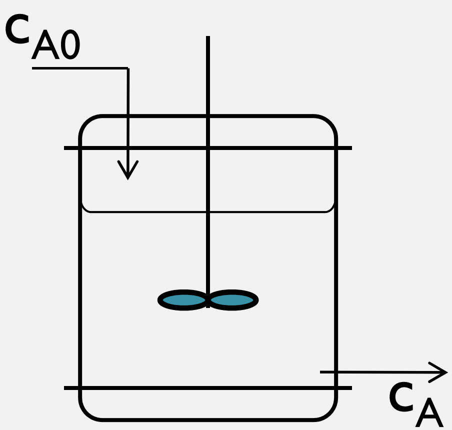
Example: Catalytic reaction in a CSTR with L-H Kinetics



$$\underbrace{\frac{C_{A0}}{\tau} - \frac{C_A}{\tau} - \frac{kC_A}{(1+KC_A)^2}}_{f(C_A)} = 0$$

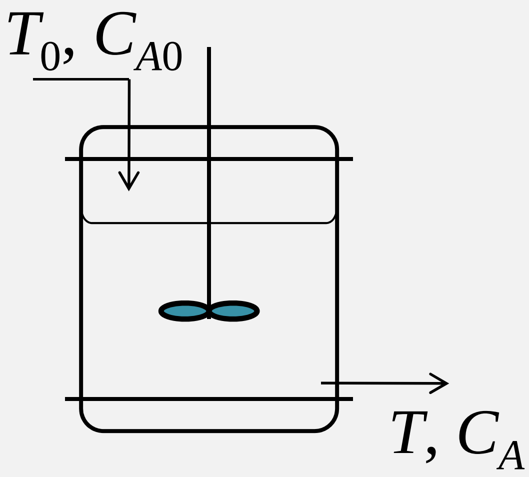
Extension to Multi-Variables

- Let x_1, x_2, …, x_n be n variables, which are described by the following coupled equations:

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

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

Example: Adiabatic CSTR



$$\underbrace{\frac{C_{A0}}{\tau} - \frac{C_A}{\tau} - k_0 e^{\left(-E/RT\right)} C_A^{1.65}}_{f_1(C_A, T)} = 0$$

$$\underbrace{\frac{T_0}{\tau} - \frac{T}{\tau} + \frac{-\Delta H}{\rho c_p}\left[k_0 e^{\left(-E/RT\right)} C_A^{1.65}\right]}_{f_2(C_A, T)} = 0$$

Outline of Non-Linear Equation

- Bracketing Methods
  - Bisection method
  - *Regula Falsi*
- Open Methods
  - Secant method
  - Fixed-point iteration
  - Newton-Raphson
- Modifications and Extensions
- Root-Finding

Computational Techniques
Summary of Module 4

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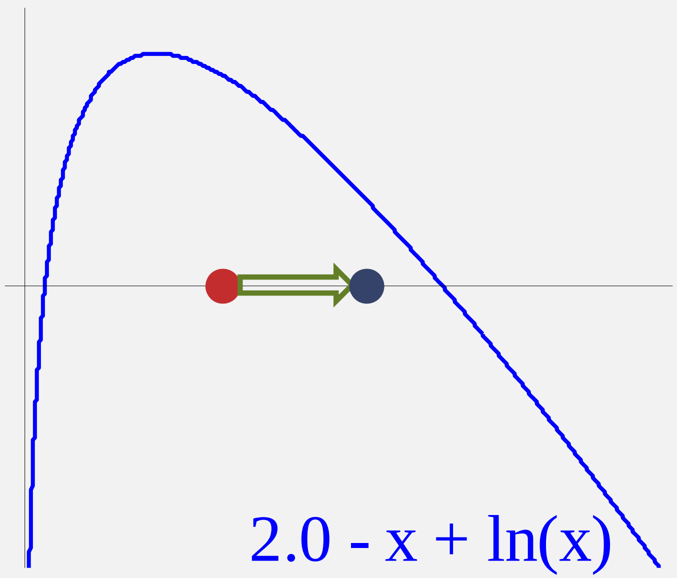
General Strategy of Solution



Start with initial guess(es)

Using a chosen strategy, move in the direction of the solution

Verify if *stopping criterion* is satisfied

Yes

Solution!

Summary (1 of 2)

Method	**# initial guesses**	$x^{(i+1)} =$	**Order Conv.**
Bisection	2; $f^{(l)} \cdot f^{(r)} < 0$	$\dfrac{x^{(l)} + x^{(r)}}{2}$	1
Regula Falsi	2; $f^{(l)} \cdot f^{(r)} < 0$	$x^{(l)} - f^{(l)} \dfrac{x^{(l)} - x^{(r)}}{f^{(l)} - f^{(r)}}$	1 to 2
Fixed Point Iteration	1	$g\left(x^{(i)}\right)$	1
Secant	2	$x^{(i)} - f^{(i)} \dfrac{x^{(i)} - x^{(i-1)}}{f^{(i)} - f^{(i-1)}}$	1 to 2
Newton-Raphson	1	$x^{(i)} - \dfrac{f\left(x^{(i)}\right)}{f'\left(x^{(i)}\right)}$	2

Summary (2 of 2)

Method	**Stability**	**Issues / Important Considerations**	**Multi-Variable**
Bisection	Guaranteed	Single variable only. $f(x)$ change sign at $\overline{x}$	No
Regula Falsi	Guaranteed	– – do – –	No
Fixed Point Iteration	Not guaranteed	Limited applicability due to stability.	Yes (easy)
Secant	Not guaranteed	Versatile and fast.	Yes (moderate)
Newton-Raphson	Not guaranteed	Most popular & fast. $x^{(1)}$ be not far from $\overline{x}$ $f'\left(x^{(i)}\right) \neq 0$	Yes (moderate)

Multi-Variable Examples:
Fixed Point Iteration

- Extension is straightforward

For all $j = 1$ to n,

$$x_j^{(i+1)} = f_j\left(x_1^{(i)}, x_2^{(i)}, \cdots, x_n^{(i)}\right)$$

$$\Downarrow$$

$$\mathbf{x}^{(i+1)} = \mathbf{f}\left(\mathbf{x}^{(i)}\right)$$

- Sufficient condition for convergence

$$\left|\frac{\partial f_j}{\partial x_1}\right| + \left|\frac{\partial f_j}{\partial x_2}\right| + \cdots + \left|\frac{\partial f_j}{\partial x_n}\right| \le 1$$

Multi-Variable Examples:
Newton-Raphson

$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \mathbf{J}^{-1}.\mathbf{f}\left(\mathbf{x}^{(i)}\right)$$

$$\mathbf{J} = \nabla \mathbf{f} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}_{\mathbf{x}^{(i)}}$$

Quadratic Rate of Convergence

Improvements developed for speed and performance

Newton-Raphson

Ralston's modifications for multiple roots

If there are *m* roots:

$$x^{(i+1)} = x^{(i)} - m\frac{f\left(x^{(i)}\right)}{f'\left(x^{(i)}\right)}$$

Improved Newton-Raphson

Roots of $f(x)$ are the same as: $h(x) = \frac{f(x)}{f'(x)}$

$$x^{(i+1)} = x^{(i)} - \frac{f\left(x^{(i)}\right)f'\left(x^{(i)}\right)}{f'\left(x^{(i)}\right)f'\left(x^{(i)}\right) - f\left(x^{(i)}\right)f''\left(x^{(i)}\right)}$$

Newton-Raphson

Modifications to improve stability

"Line-Search":

$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \omega.\mathbf{J}^{-1}\mathbf{f}\left(\mathbf{x}^{(i)}\right)$$

$0 < \omega \leq 1$ is like under-relaxation parameter

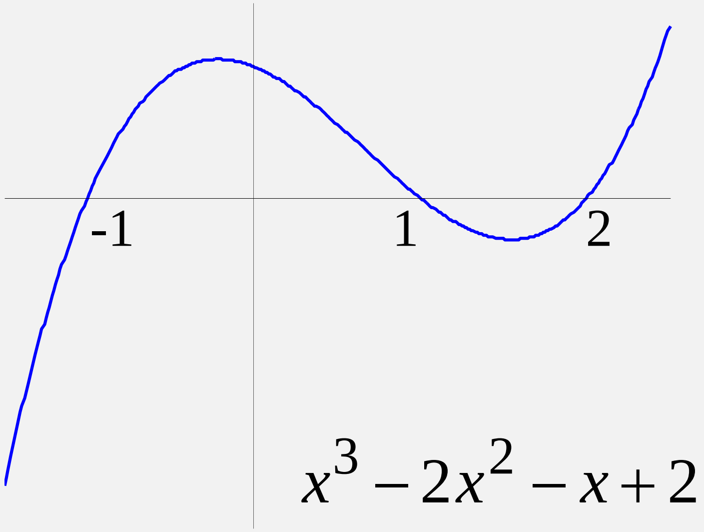
Levenberg-Marquardt modification

Motivation: Root of $f(x)$ is a minimum of $[f(x)]^2$

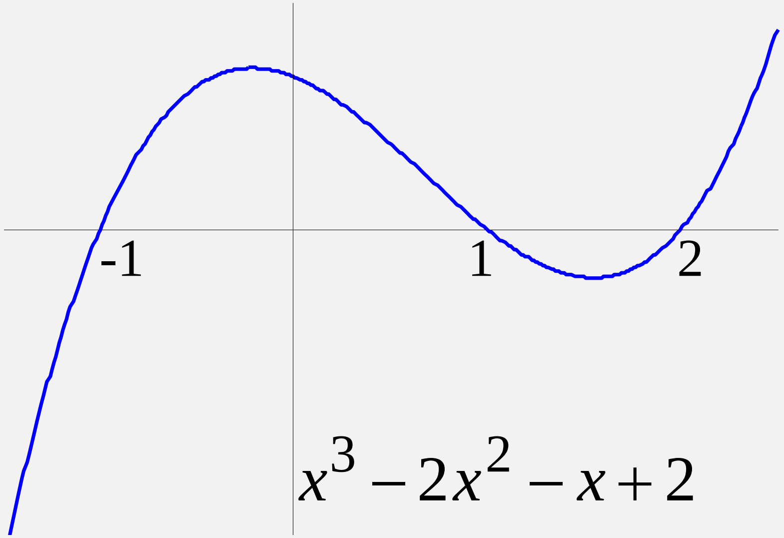
$$\mathbf{x}^{(i+1)} = \mathbf{x}^{(i)} - \left[\mathbf{J}^T\mathbf{J} + \beta\mathbf{I}\right]^{-1}\mathbf{J}^T\ \mathbf{f}\left(\mathbf{x}^{(i)}\right)$$

Root Finding

- Aim is to find all roots of a polynomial
- i.e., all solutions to $f(x) = 0$
  where f is a polynomial function



Root Finding



- Bairstow's method

$$a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

$$\Downarrow$$

$$\underbrace{\left[b_0 + b_1 x + b_2 x^2 + \cdots + b_{n-2} x^{n-2}\right]}_{P_{n-2}} \underbrace{\left[x^2 + px + q\right]}_{Q} + \underbrace{\left[c_1 x + c_0\right]}_{R}$$

$$\Downarrow$$

$$P_n = Q P_{n-2} + R$$

Q is a factor of P_n if $R = 0$

Additional Reading

- Gupta S.K. (1995), *Numerical Methods for Engineers*, New Age International
- Chapra S.C. and Canale R.P. (2006), *Numerical Methods for Engineers*, 5th Ed., McGraw Hill
- Press W.H., Teukolsky S.A., et al. (2007), *Numerical Recipes: The Art of Scientific Computing*, Cambridge University Press, 3rd Edition.
- Online version at the Numerical Recipes website: http://www.nr.com/