ECSE 343 Numerical Methods in Engineering

Roni Khazaka

Dept. of Electrical and Computer Engineering

McGill University

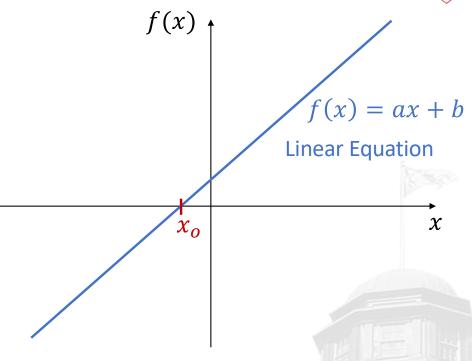


Roots of Linear Equations



Find x such that f(x) = 0

One root $x = x_o \Rightarrow f(x_0) = 0$

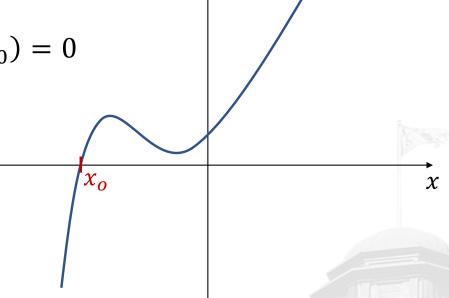


Roots of Nonlinear Equations



Find x_o such that $f(x_o) = 0$

Possibly one root $x = x_o \Rightarrow f(x_0) = 0$



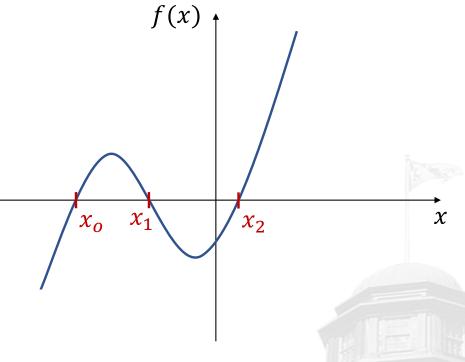
f(x)

Roots of Nonlinear Equations



Find x_o such that $f(x_o) = 0$

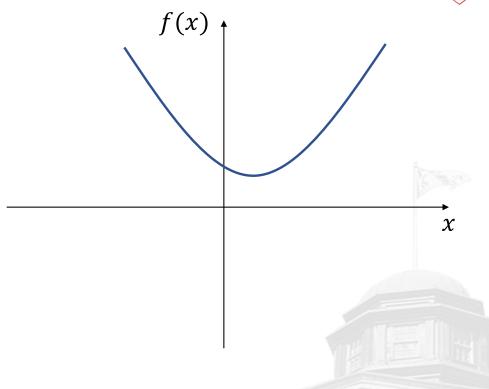
Three roots: x_0 , x_1 , and x_2



Roots of Nonlinear Equations



Find x_o such that $f(x_o) = 0$ No roots.



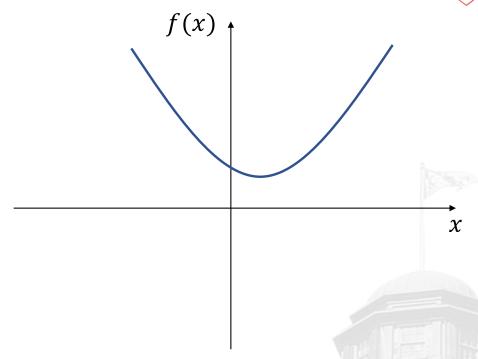
Continuous Function



$$x \to y$$

$$\downarrow$$

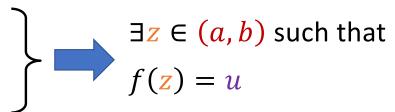
$$f(x) \to f(y)$$

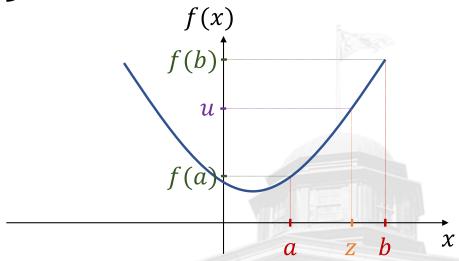


Intermediate Value Theorem



$$f(x)$$
 is continuous over interval $[a, b]$
 $f(a) < u < f(b)$ or $f(b) < u < f(a)$





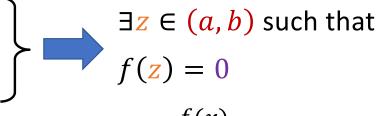
Application to Root finding

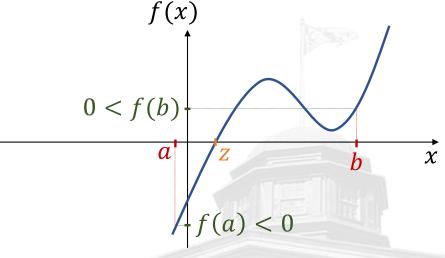


$$f(x)$$
 is continuous over interval $[a, b]$

$$f(a) < 0 < f(b) \text{ or } f(b) < 0 < f(a)$$

f(a) and f(b) have opposite signs





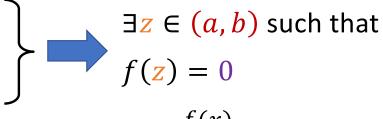
Application to Root finding

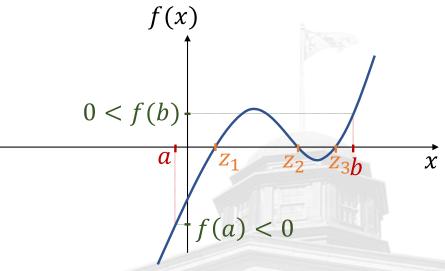


$$f(x)$$
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$$f(a) < 0 < f(b) \text{ or } f(b) < 0 < f(a)$$

f(a) and f(b) have opposite signs





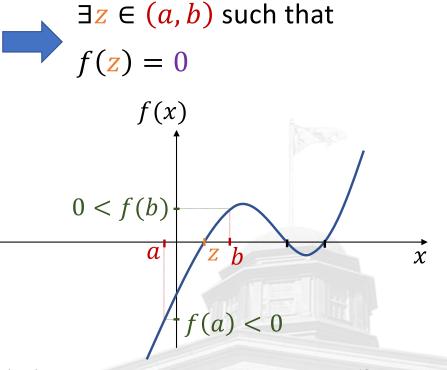
Application to Root finding



$$f(x)$$
 is continuous over interval $[a, b]$
 $f(a) < 0 < f(b)$ or $f(b) < 0 < f(a)$

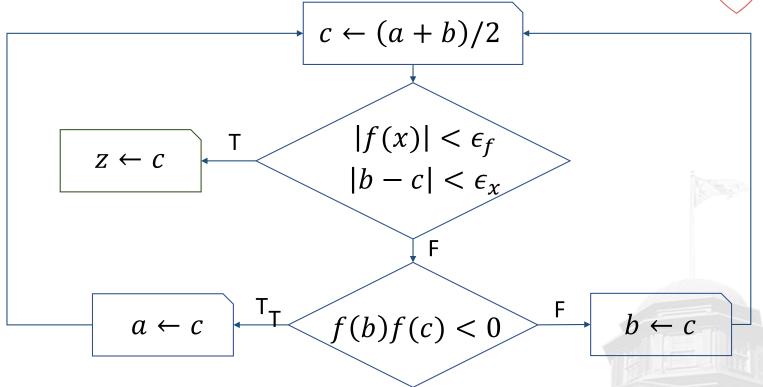
f(a) and f(b) have opposite signs

As a starting point, we need a, and b (b > a) such that: f(a) and f(b) have opposite signs.

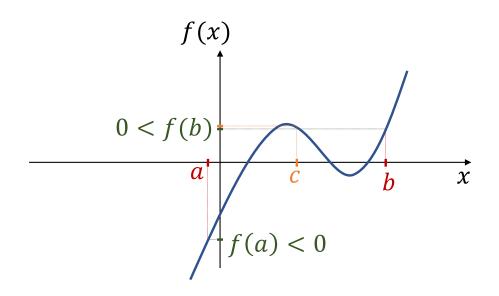


Bisection Method







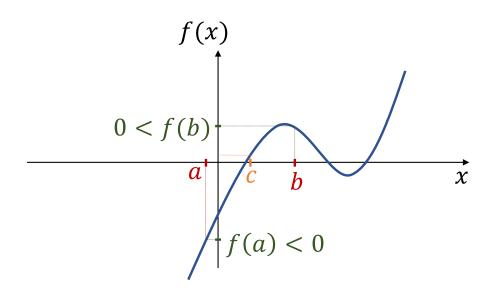


$$c \leftarrow (a+b)/2$$

$$f(b)f(c) < 0$$

$$b \leftarrow c$$

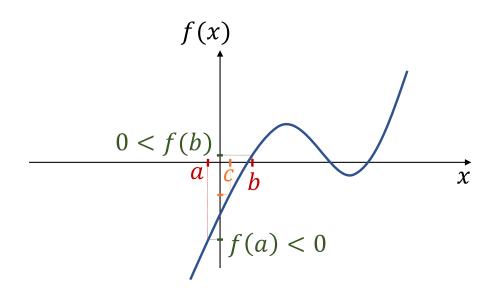




$$c \leftarrow (a+b)/2$$

$$f(b)f(c) < 0$$

$$b \leftarrow c$$



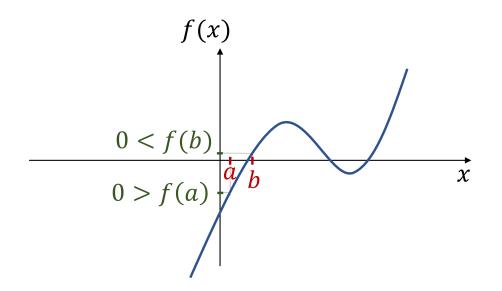


$$c \leftarrow (a+b)/2$$

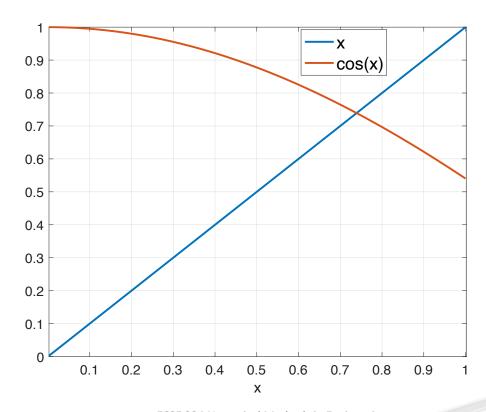
$$f(b)f(c) < 0$$

$$a \leftarrow c$$

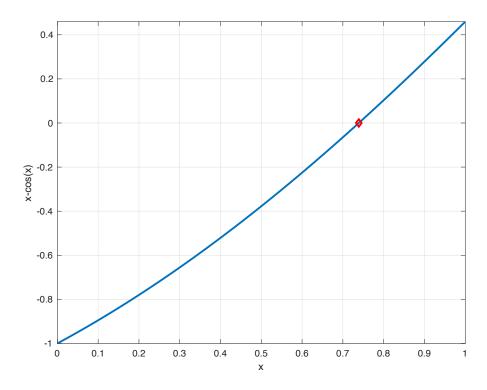




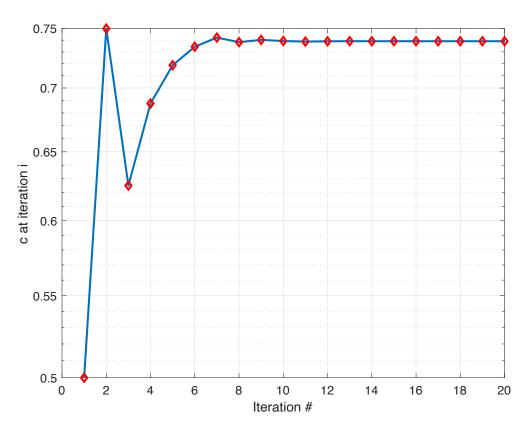






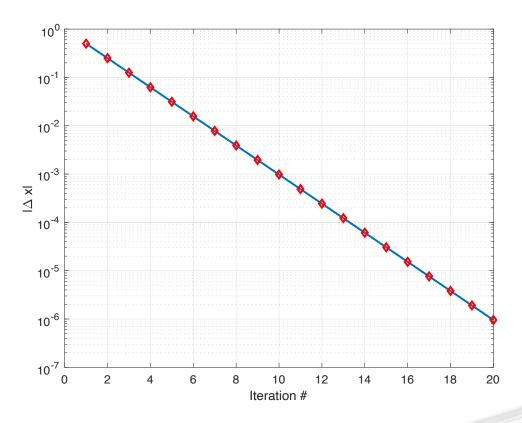




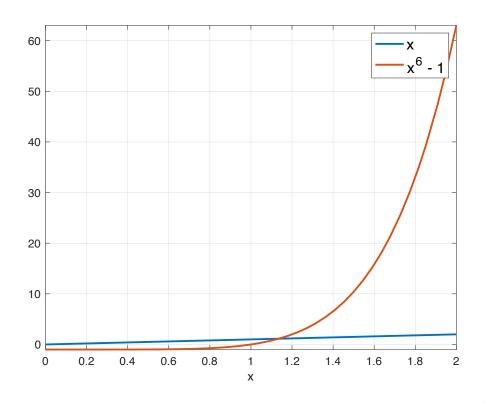


$$z = 0.7391$$

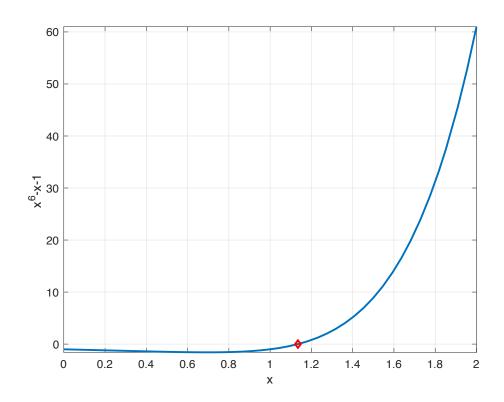




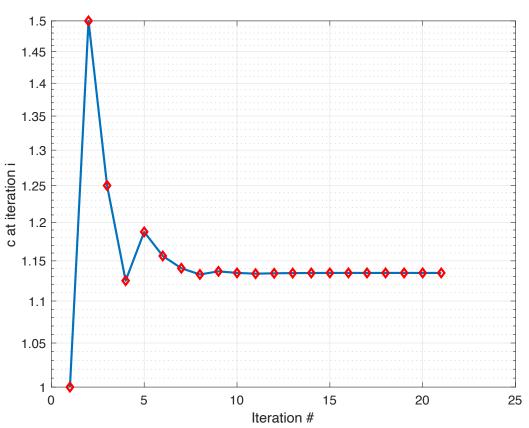






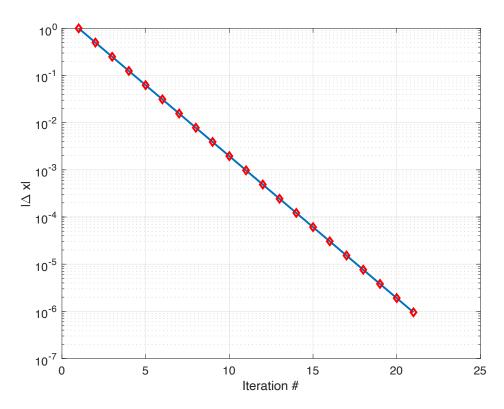


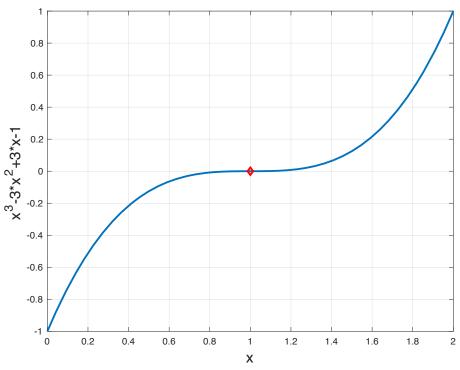




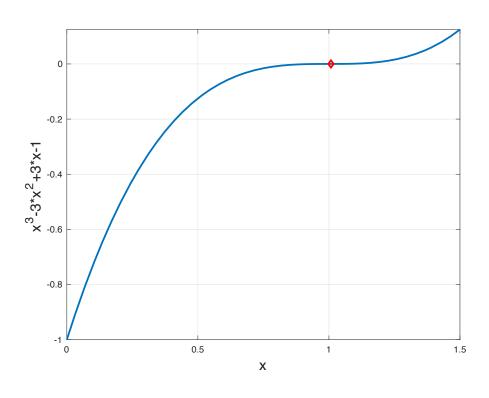
$$z = 0.1.1347$$





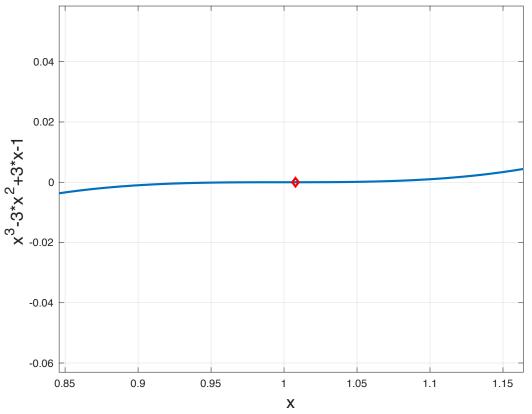


$$z = 1$$



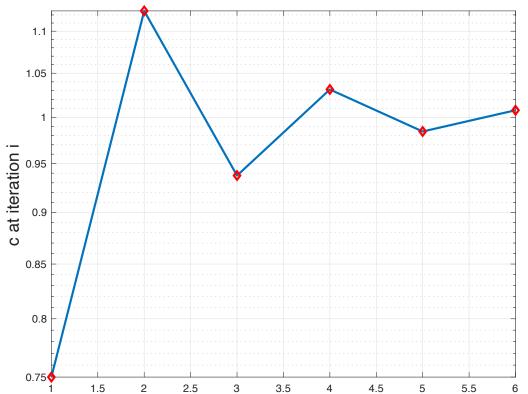
$$z = 1.0078$$





$$z = 1.0078$$

$$f(z) = 4.7684 \times 10^{-7}$$



Iteration #

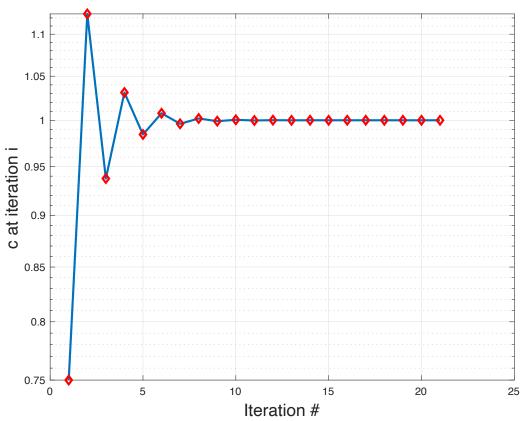
Solution converges to:

$$z = 1.0078$$

$$f(z) = 4.7684 \times 10^{-7}$$

Stop if:

$$\epsilon_f < 10^{-6}$$
 or $\epsilon_x < 10^{-6}$



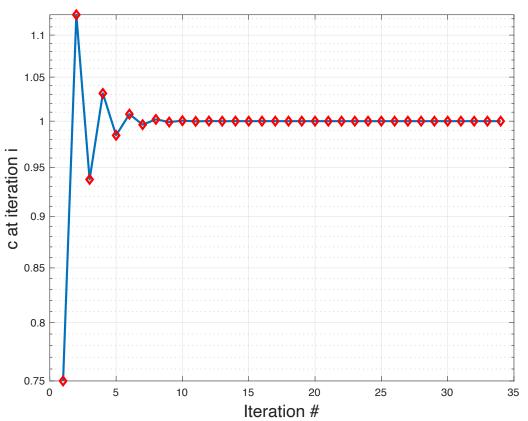
Solution converges to:

$$z = 0.999985$$

$$f(z) = 3.1 \times 10^{-15}$$

Stop if:

$$\begin{array}{c} \epsilon_f < 10^{-6} \\ \text{AND } \epsilon_\chi < 10^{-6} \end{array}$$



Solution converges to:

$$z = 0.999985$$

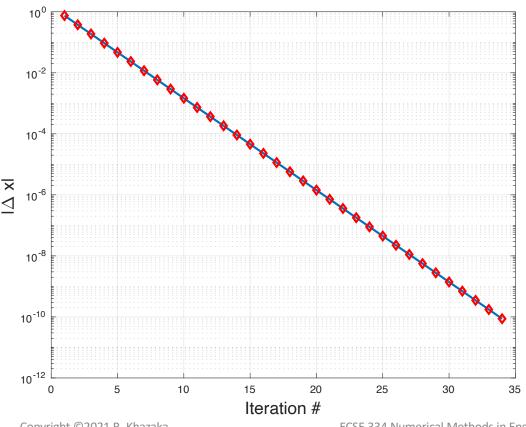
$$f(z) = 3.1 \times 10^{-15}$$

Stop if:

$$\begin{array}{c} \epsilon_f < 10^{-10} \\ \text{AND } \epsilon_\chi < 10^{-10} \end{array}$$

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Solution converges to:

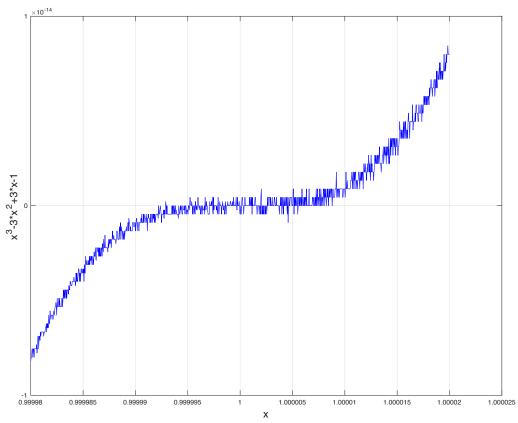
$$z = 0.999985$$

$$f(z) = 3.1 \times 10^{-15}$$

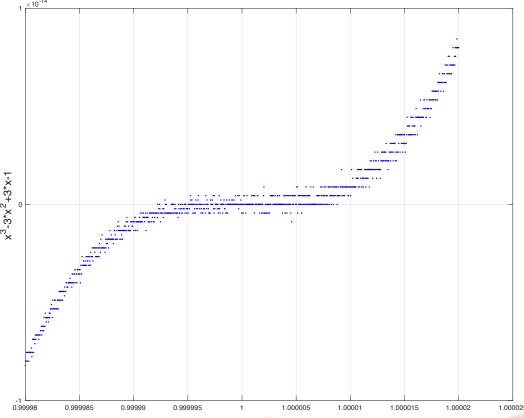
Stop if:

$$\begin{array}{c} \epsilon_f < 10^{-10} \\ \text{AND } \epsilon_{\chi} < 10^{-10} \end{array}$$

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Lipschitz Continuous Functions



$$\exists c; |g(x) - g(y)| \le c|x - y|$$

$$\forall x, y$$

g(x) must be continuous, but not necessarily differentiable. Lipschitz functions are limited in their rate of change.

Contractions



$$\exists 0 < c < 1; |g(x) - g(y)| \le c|x - y|$$

 $\forall x, y$

The distance between x and y contacts when operated on by $g(\).$

Hence the name contraction.

Fixed Point Iteration



Find the fixed point of g(.):

$$g(x) = x$$

Equivalent to finding a root of f(.):

$$f(x) = g(x) - x$$

Fixed Point Iteration



Choose initial guess: $\chi^{(0)}$

Update guess $x^{(1)} = g(x^{(0)})$

Update guess $x^{(2)} = g(x^{(1)})$

Update guess $x^{(k)} = g(x^{(k-1)})$

Until: $x^{(n+1)} = x^{(n)}$

Converges if g(x) is a contraction.

Fixed Point Iteration



Assume that x^* is the fixed-point solution.

Then: $g(x^*) = x^*$

Note, as per the algorithm: $x^{(k+1)} = g(x^{(k)})$

Distance between guess and x^* : $E_k = |x^{(k)} - x^*|$ g(x) is a contraction:

$$|g(x^{(k)}) - g(x^*)| < |x^{(k)} - x^*|$$

Fixed Point Iteration

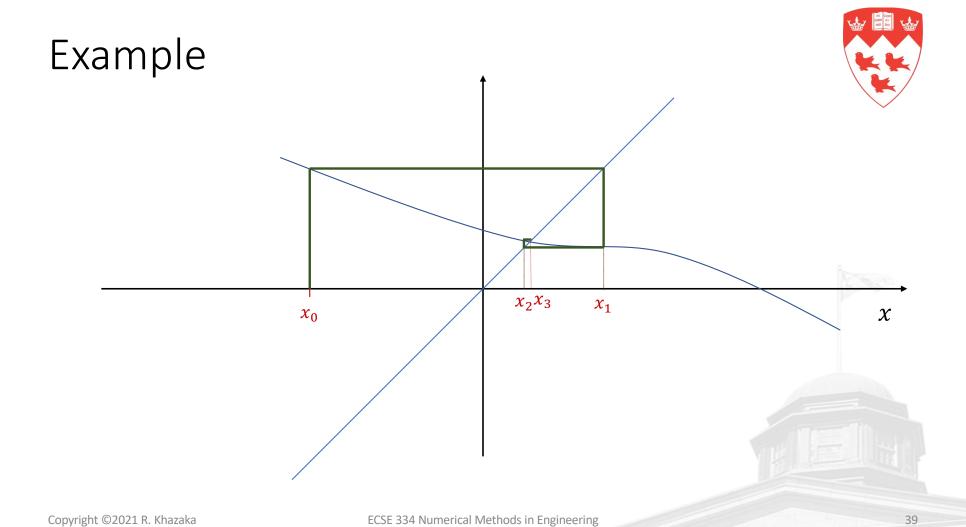


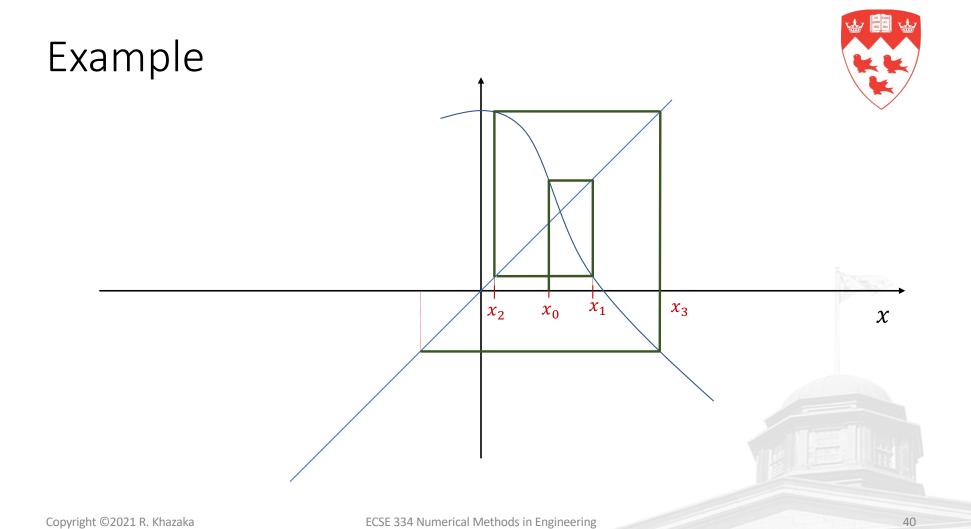
$$|g(x^{(k)}) - g(x^*)| < |x^{(k)} - x^*|$$

$$|x^{(k+1)} - x^*| < |x^{(k)} - x^*|$$

$$E_{k+1} < E_k$$







Key Advantage Compared to Bisection



Fixed point iteration can be easily applied to systems of nolinear equations

Find the fixed point of
$$g(.)$$
: $g(x) = x$

$$g(x) \in \mathbb{R}^n \qquad x \in \mathbb{R}^m$$

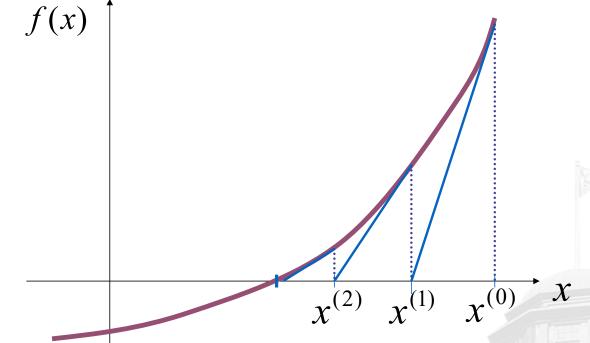
Can easily apply:
$$x^{(k)} = g(x^{(k-1)})$$





Find *x* such that:

$$f(x) = 0$$





Current guess: $x^{(0)}$

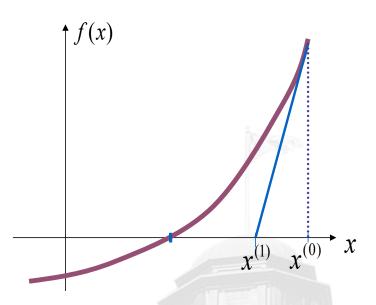
Taylor expansion at $x^{(0)}$:

$$f(x) = f(x^{(0)}) + f'(x^{(0)})(x - x^{(0)}) + \frac{1}{2}f''(x^{(0)})(x - x^{(0)})^2 + \cdots$$

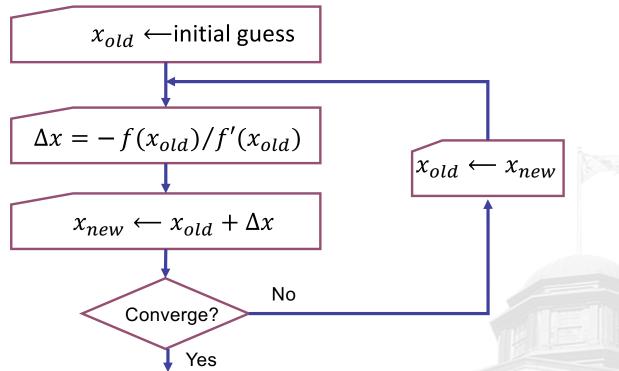
Linear Approximation:

$$f(x) \cong f(x^{(0)}) + f'(x^{(0)})(x - x^{(0)})$$

Find the root:
$$x^{(1)} = x^{(0)} - \frac{f(x^{(0)})}{f'(x^{(0)})}$$









Solve:
$$\frac{2}{3}x + e^{40x} - \frac{5}{3} = 0$$

Find x such that:
$$f(x) = \frac{2}{3}x + e^{40x} - \frac{5}{3} = 0$$

Note:
$$f'(x) = \frac{2}{3} + 40e^{40x}$$





Start with initial guess: $x^{(0)} = 0.1$

$$f(x^{(0)}) = \frac{2}{3} \times 0.1 + e^{40 \times 0.1} - \frac{5}{3} = 52.998$$

$$f'(x^{(0)}) = \frac{2}{3} + 40e^{40 \times 0.1} = 2184.6$$

$$\Delta x^{(0)} = -\frac{f(x^{(0)})}{f'(x^{(0)})} = -2.426 \times 10^{-2}$$



$$x^{(1)} = x^{(0)} + \Delta x^{(0)} = 0.1 - 2.426 \times 10^{-2} = 7.574 \times 10^{-2}$$

$$f(x^{(1)}) = \frac{2}{3} \times 7.574 \times 10^{-2} + e^{40 \times 7.574 \times 10^{-2}} - \frac{5}{3} = 1.9073 \times 10^{1}$$

$$f'(x^{(1)}) = \frac{2}{3} + 40e^{40 \times 7.574 \times 10^{-2}} = 8.2823 \times 10^{2}$$

$$\Delta x^{(1)} = -\frac{f(x^{(1)})}{f'(x^{(1)})} = -2.30285 \times 10^{-2}$$



$$x^{(2)} = x^{(1)} + \Delta x^{(1)} = 7.574 \times 10^{-2} - 2.30285 \times 10^{-2} = 5.271 \times 10^{-2}$$

$$f(x^{(2)}) = \frac{2}{3} \times x^{(2)} + e^{40 \times x^{(2)}} - \frac{5}{3} = 6.60403$$

$$f'(x^{(2)}) = \frac{2}{3} + 40e^{40 \times x^{(2)}} = 3.3009 \times 10^2$$

$$\Delta x^{(2)} = -\frac{f(x^{(2)})}{f'(x^{(2)})} = -2.00068 \times 10^{-2}$$



$$x^{(3)} = x^{(2)} + \Delta x^{(2)} = 3.2705 \times 10^{-2}$$

$$f(x^{(3)}) = \frac{2}{3} \times x^{(3)} + e^{40 \times x^{(3)}} - \frac{5}{3} = 2.0546$$

$$f'(x^{(3)}) = \frac{2}{3} + 40e^{40 \times x^{(3)}} = 1.4865 \times 10^2$$

$$\Delta x^{(3)} = -\frac{f(x^{(3)})}{f'(x^{(3)})} = -1.3822 \times 10^{-2}$$



$$x^{(4)} = x^{(3)} + \Delta x^{(3)} = 1.8883 \times 10^{-2}$$

$$f(x^{(4)}) = \frac{2}{3} \times x^{(4)} + e^{40 \times x^{(4)}} - \frac{5}{3} = 4.7417 \times 10^{-1}$$

$$f'(x^{(4)}) = \frac{2}{3} + 40e^{40 \times x^{(4)}} = 8.5797 \times 10^{1}$$

$$\Delta x^{(4)} = -\frac{f(x^{(4)})}{f'(x^{(4)})} = -5.5267 \times 10^{-3}$$



$$x^{(5)} = x^{(4)} + \Delta x^{(4)} = 1.3356 \times 10^{-2}$$

$$f(x^{(5)}) = \frac{2}{3} \times x^{(5)} + e^{40 \times x^{(5)}} - \frac{5}{3} = 4.8376 \times 10^{-2}$$

$$f'(x^{(5)}) = \frac{2}{3} + 40e^{40 \times x^{(5)}} = 6.8912 \times 10^{1}$$

$$\Delta x^{(5)} = -\frac{f(x^{(5)})}{f'(x^{(5)})} = -7.0199 \times 10^{-4}$$



$$x^{(6)} = x^{(5)} + \Delta x^{(5)} = 1.2654 \times 10^{-2}$$

$$f(x^{(6)}) = \frac{2}{3} \times x^{(6)} + e^{40 \times x^{(6)}} - \frac{5}{3} = 6.6636 \times 10^{-4}$$

$$f'(x^{(6)}) = \frac{2}{3} + 40e^{40 \times x^{(6)}} = 6.7022 \times 10^{1}$$

$$\Delta x^{(6)} = -\frac{f(x^{(6)})}{f'(x^{(6)})} = -9.9424 \times 10^{-6}$$



$$x^{(7)} = x^{(6)} + \Delta x^{(6)} = 1.2644 \times 10^{-2}$$

$$f(x^{(7)}) = \frac{2}{3} \times x^{(7)} + e^{40 \times x^{(7)}} - \frac{5}{3} = 1.31169 \times 10^{-7}$$

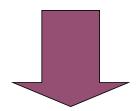
$$f'(x^{(7)}) = \frac{2}{3} + 40e^{40 \times x^{(7)}} = 6.6996 \times 10^{1}$$

$$\Delta x^{(7)} = -\frac{f(x^{(7)})}{f'(x^{(7)})} = -1.9579 \times 10^{-9}$$





$$x^{(8)} = x^{(7)} + \Delta x^{(7)} = 1.2644 \times 10^{-2}$$



Exit Iteration

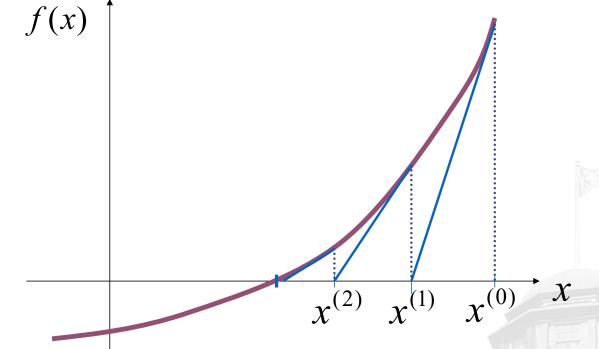
k	$\boldsymbol{\mathcal{X}}^{(k)}$	$\Delta x^{(k-1)}$
1	7.574×10^{-2}	-2.426×10^{-2}
2	5.2712×10^{-2}	-2.3029×10^{-2}
3	3.2705×10^{-2}	-2.0007×10^{-2}
4	1.8883×10^{-2}	-1.3822×10^{-2}
5	1.3356×10^{-2}	-5.5267×10^{-3}
6	1.2654×10^{-2}	-7.0199×10^{-4}
7	1.2644×10^{-2}	-9.9424×10^{-6}
8	1.2644×10^{-2}	-1.9579×10^{-9}





Find *x* such that:

$$f(x) = 0$$





Current guess: $x^{(0)}$

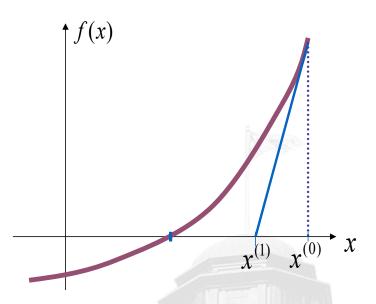
Taylor expansion at $x^{(0)}$:

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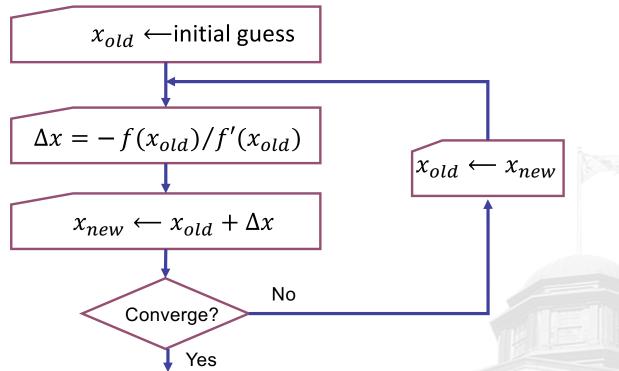
Linear Approximation:

$$f(x) \cong f(x^{(0)}) + f'(x^{(0)})(x - x^{(0)})$$

Find the root:
$$x^{(1)} = x^{(0)} - \frac{f(x^{(0)})}{f'(x^{(0)})}$$









Solve:
$$\frac{2}{3}x + e^{40x} - \frac{5}{3} = 0$$

Find x such that:
$$f(x) = \frac{2}{3}x + e^{40x} - \frac{5}{3} = 0$$

Note:
$$f'(x) = \frac{2}{3} + 40e^{40x}$$





Start with initial guess: $x^{(0)} = 0.1$

$$f(x^{(0)}) = \frac{2}{3} \times 0.1 + e^{40 \times 0.1} - \frac{5}{3} = 52.998$$

$$f'(x^{(0)}) = \frac{2}{3} + 40e^{40 \times 0.1} = 2184.6$$

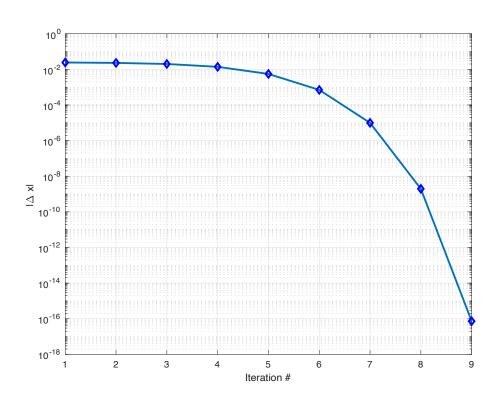
$$\Delta x^{(0)} = -\frac{f(x^{(0)})}{f'(x^{(0)})} = -2.426 \times 10^{-2}$$

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k	$\boldsymbol{\chi}^{(k)}$	$\Delta x^{(k-1)}$
1	7.574×10^{-2}	-2.426×10^{-2}
2	5.2712×10^{-2}	-2.3029×10^{-2}
3	3.2705×10^{-2}	-2.0007×10^{-2}
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5	1.3356×10^{-2}	-5.5267×10^{-3}
6	1.2654×10^{-2}	-7.0199×10^{-4}
7	1.2644×10^{-2}	-9.9424×10^{-6}
8	1.2644×10^{-2}	-1.9579×10^{-9}

N-R Convergence Rate



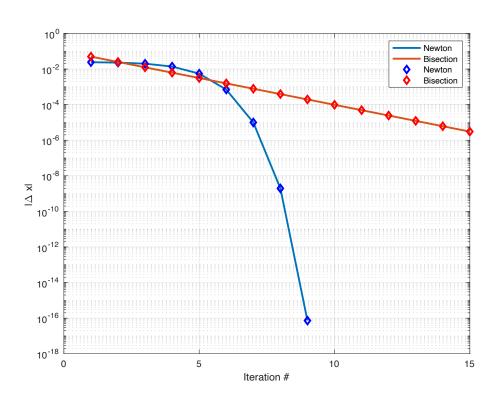


$$f(x) = \frac{2}{3}x + e^{40x} - \frac{5}{3}$$

Initial Guess
$$x_0 = 0.1$$

Bisection vs N-R





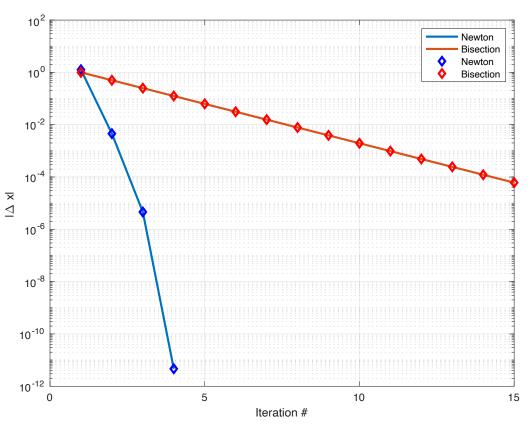
$$f(x) = \frac{2}{3}x + e^{40x} - \frac{5}{3}$$

Initial Guess $x_0 = 0.1$

Initial Interval [0, 0.1]

Bisection vs N-R





$$f(x) = x - \cos(x)$$

Initial Guess $x_0 = 0.1$

Initial Interval [0, 0.1]

Secant Method



Newton Update:
$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

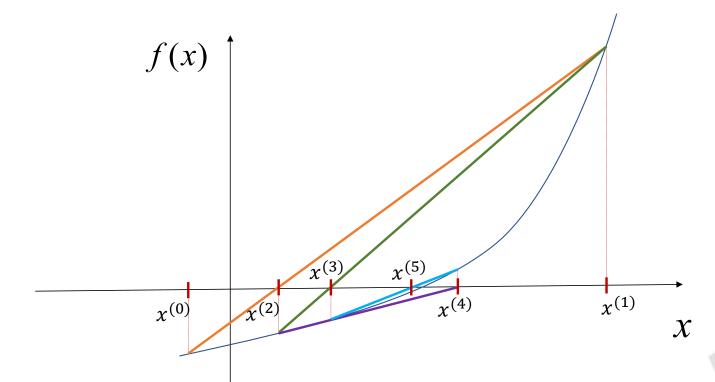
Approximate:
$$f'(x^{(k)}) \approx \frac{f(x^{(k)}) - f(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}$$

Secant Method:
$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})(x^{(k)} - x^{(k-1)})}{f(x^{(k)}) - f(x^{(k-1)})}$$

Need two starting points.

Secant Method





Multi-variate Case



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

Find the roots of f(x)



Newton-Raphson



Update method, starting with guess $x^{(k)}$ Approximate f(x) with:

$$f(x) \approx f(x^{(k)}) + \left(\frac{d}{dx}f(x^{(k)})\right)(x - x^{(k)})$$

Solve:

$$f(x^{(k)}) + \left(\frac{d}{dx}f(x^{(k)})\right)(x - x^{(k)}) = 0$$

Newton-Raphson



Solve:
$$f(x^{(k)}) + J_k(x - x^{(k)}) = 0$$

$$J_{k} = \frac{d}{dx} f(x^{(k)}) = \begin{bmatrix} \frac{\partial f_{1}}{\partial x_{1}} & \frac{\partial f_{1}}{\partial x_{2}} & \cdots & \frac{\partial f_{1}}{\partial x_{n}} \\ \frac{\partial f_{2}}{\partial x_{1}} & \frac{\partial f_{2}}{\partial x_{2}} & \cdots & \frac{\partial f_{2}}{\partial x_{n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_{n}}{\partial x_{1}} & \frac{\partial f_{n}}{\partial x_{2}} & \cdots & \frac{\partial f_{n}}{\partial x_{n}} \end{bmatrix}_{x=x^{(k)}}$$

Solution is $x^{(k+1)}$

Newton-Raphson



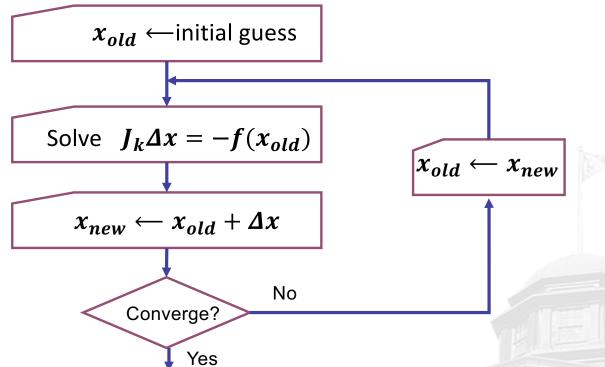
$$f(x^{(k)}) + J(x^{(k+1)} - x^{(k)}) = 0$$

$$Jx^{(k+1)} = Jx^{(k)} - f(x^{(k)})$$

$$x^{(k+1)} = x^{(k)} - J_k^{-1} f(x^{(k)})$$

$$J_k \Delta x = -f(x^{(k)})$$
 System of Linear Equations





Broyden's Method



Just like the secant method avoided computing the derivative, Broyden's method allow us to avoid computing the Jacobian.

Newton's Update:
$$x^{(k+1)} = x^{(k)} - J_k^{-1} f(x^{(k)})$$

$$J_k = \frac{d}{dx} f(x^{(k)})$$

How do we approximate J_k ? Not easy for multidimensional problems



$$J_k = \frac{d}{dx} f(x^{(k)})$$

$$J_k$$
 must satisfy: $J_k(x^{(k)} - x^{(k-1)}) = f(x^{(k)}) - f(x^{(k-1)})$

The above formula is not enough to compute J_k It constrains the action of J_k only in one direction: $(x^{(k)} - x^{(k-1)})$



$$J_k = \frac{d}{dx} f(x^{(k)})$$

$$J_k$$
 must satisfy: $J_k(x^{(k)} - x^{(k-1)}) = f(x^{(k)}) - f(x^{(k-1)})$

Assume that we know J_{k-1}

Find J_k such that: $||J_k - J_{k-1}||_F$ is minimum

Subject to
$$J_k(x^{(k)} - x^{(k-1)}) = f(x^{(k)}) - f(x^{(k-1)})$$



$$J_{k} = J_{k-1} + \frac{\left(f(x^{(k)}) - f(x^{(k-1)}) - J_{k-1}(x^{(k)} - x^{(k-1)})\right)}{\|x^{(k)} - x^{(k-1)}\|_{2}^{2}} (x^{(k)} - x^{(k-1)})^{T}$$

Rank 1 Update

$$\Delta \boldsymbol{J} = \boldsymbol{J}_k - \boldsymbol{J}_{k-1} = \boldsymbol{u}\boldsymbol{v}^T$$

In the absence of better information, we use: $J_0 = U$



Just like the secant method avoided computing the derivative, Broyden's method allow us to avoid computing the Jacobian.

Broyden's Update:
$$x^{(k+1)} = x^{(k)} - J_k^{-1} f(x^{(k)})$$

Broyden's method allow us to approximate J_k We still need to solve the system $J_k \Delta x = -f(x^{(k)})$



Sherman-Morisson Formula



$$(A + uv^{T})^{-1} = A^{-1} - \frac{A^{-1}uv^{T}A^{-1}}{1 + v^{T}A^{-1}u}$$



Update Inverse Instead



$$J_{k}^{-1} = J_{k-1}^{-1} + \frac{x^{(k)} - x^{(k-1)} - J_{k-1}^{-1} \left(f(x^{(k)}) - f(x^{(k-1)}) \right)}{(x^{(k)} - x^{(k-1)})^{T} J_{k-1}^{-1} \left(f(x^{(k)}) - f(x^{(k-1)}) \right)} \left(\left(x^{(k)} - x^{(k-1)} \right)^{T} J_{k-1}^{-1} \right)$$

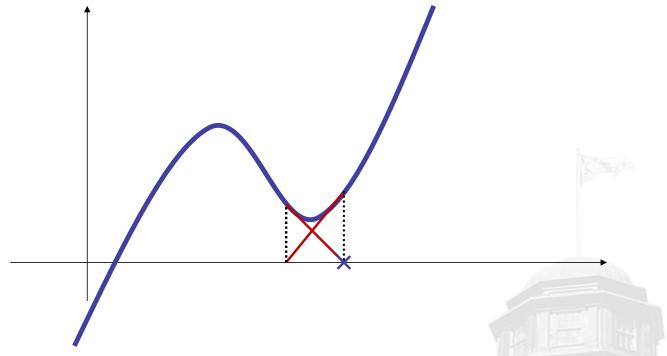
If we use $J_0 = U$

The inverse of \boldsymbol{J}_0 is trivial



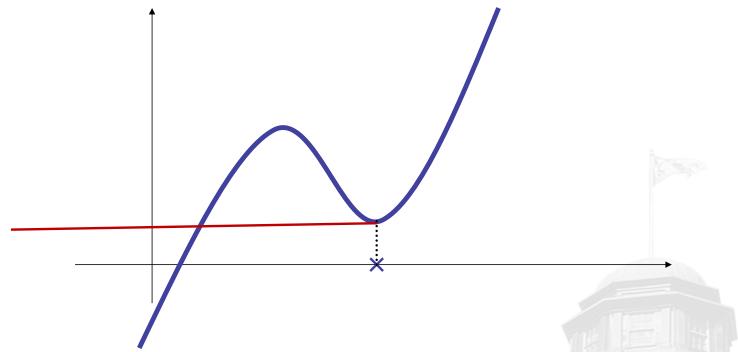
Convergence Problems





Convergence problems





Continuation Methods (Homotopy)



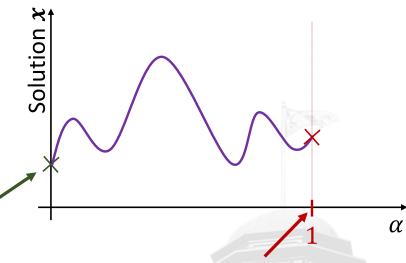
Initial Problem: f(x) = 0

Embed parameter α

Modified Problem:

$$g(x, \alpha) = 0$$

Solution of g(x, 0) = 0 is trivial



$$g(x,1) = f(x)$$

Example



$$f(x) = \frac{2}{3}x + e^{40x} - \frac{5}{3}$$
$$g(x, \alpha) = \frac{2}{3}x + \alpha e^{40x} - \frac{5}{3}$$

$$g(x,\alpha) = \frac{2}{3}x + \alpha e^{40x} - \frac{5}{3}$$

$$g(x,0) = \frac{2}{3}x - \frac{5}{3}$$

$$g(x,1) = \frac{2}{3}x + e^{40x} - \frac{5}{3} = f(x)$$

Example



$$f(x) = x^3 - 6x^2 + 1$$

$$g(x,\alpha) = x^3 - 6\alpha x^2 + 1$$

$$g(x,0) = x^3 + 1$$

$$g(x, 1) = x^3 - 6x^2 + 1$$

$$g(x,\alpha) = x^3 - 6x^2 + \alpha$$

$$g(x,0) = x^3 - 6x^2$$

$$g(x,1) = x^3 - 6x^2 + 1$$

Homotopy Transformation



Initial Problem:
$$f(x) = 0$$

Embed parameter α

Modified Problem:

$$\Psi(x,\alpha) = \alpha f(x) + (1 - \alpha)g(x)$$

$$\Psi(x,\mathbf{0})=g(x)$$

$$\Psi(x,1)=f(x)$$