Find the roots of

$$\left.\begin{aligned} f_1(x_1, x_2, \ldots, x_n) &= 0 \\ f_2(x_1, x_2, \ldots, x_n) &= 0 \\ &\vdots \\ f_n(x_1, x_2, \ldots, x_n) &= 0 \end{aligned}\right\} \quad \underline{f}(\underline{x}) = \underline{0}$$

Example:

$$2x_1 - x_2^2 + x_3^4 - 1 = 0$$

$$x_1^2 + x_2 - x_3^3 = 0$$

$$\sin(x_1) + \tan(x_2) + x_3 - 1 = 0$$

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

① If possible, write as a fixed point iteration

$$\underline{x} = \underline{g}(\underline{x})$$

Example: (continued from above)

$$\Rightarrow \quad x_1 = \frac{1}{2}x_2^2 - \frac{1}{2}x_3^4 - \frac{1}{2}$$

$$x_2 = -x_1^2 + x_3^3$$

$$x_3 = 1 - \sin(x_1) - \tan(x_2)$$

$$\underline{x} = \underline{g}(\underline{x})$$

$$\Rightarrow \quad \underline{x}_{i+1} = \underline{g}(\underline{x}_i)$$

Iterate until $\|\underline{x}_{i+1} - \underline{g}(\underline{x}_{i+1})\|_p < \varepsilon$

Convergence will depend on character of $\underline{g}(\underline{x})$

and also on $\underline{x}_0$

(2) Newton-Raphson Method

Focus initially on just the first equation

$$f_1(x_1, x_2, \ldots, x_n) = 0$$

iteration, not power

Given $f_1^{(i)}, x_1^{(i)}, x_2^{(i)}, \ldots, x_n^{(i)}$

Write

$$f_1^{(i+1)} = f_1^{(i)} + \frac{\partial f_1^{(i)}}{\partial x_1}\left(x_1^{(i+1)} - x_1^{(i)}\right) + \frac{\partial f_1^{(i)}}{\partial x_2}\left(x_2^{(i+1)} - x_2^{(i)}\right)$$

$$+ \ldots + \frac{\partial f_1^{(i)}}{\partial x_n}\left(x_n^{(i+1)} - x_n^{(i)}\right)$$

derivative $\frac{\partial f_1}{\partial x_n}$ evaluated at $x_1^{(i)}, x_2^{(i)}, \ldots, x_n^{(i)}$

Since the goal is to have $f_1^{(i+1)} \stackrel{!}{=} 0 \Rightarrow$

Since the goal is to have $f_1^{(i+1)} \stackrel{!}{=} 0 \Rightarrow$

$$-f_1^{(i)} = \frac{\partial f_1^{(i)}}{\partial x_1}\left(x_1^{(i+1)} - x_1^{(i)}\right) + \dots + \frac{\partial f_1^{(i)}}{\partial x_n}\left(x_n^{(i+1)} - x_n^{(i)}\right)$$

Apply this idea to every function $f_1(x), f_2(x), \dots, f_n(x)$ in $\underline{f}(\underline{x})$. Then

$$\underbrace{\begin{bmatrix} \frac{\partial f_1^{(i)}}{\partial x_1} & \cdots & \frac{\partial f_1^{(i)}}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_n^{(i)}}{\partial x_1} & \cdots & \frac{\partial f_n^{(i)}}{\partial x_n} \end{bmatrix}}_{\text{Jacobian matrix of } \underline{f}(\underline{x})} \begin{bmatrix} x_1^{(i+1)} - x_1^{(i)} \\ \vdots \\ x_n^{(i+1)} - x_n^{(i)} \end{bmatrix} = \begin{bmatrix} -f_1^{(i)} \\ \vdots \\ -f_n^{(i)} \end{bmatrix}$$

n eqns, n unknowns

$$\underline{J}^{(i)} \underline{\delta}^{(i)} = -\underline{f}^{(i)}$$

with $\underline{J}^{(i)}$: Jacobian of $\underline{f}(\underline{x})$ evaluated using information at iteration i $(\underline{x}_i)$

iteration i $(\underset{\sim}{x}_i)$

$$\underline{\delta}^{(i)} = \underline{x}^{(i+1)} - \underline{x}^{(i)}$$

$$\underline{f}^{(i)} = \underline{f}(\underline{x}^{(i)})$$ residual

Then,

$$\underline{\delta}^{(i)} = -\left(\underline{J}^{(i)}\right)^{-1} \underline{f}^{(i)}$$

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

Note: This is a set of linear algebraic equations

However, a solution is required at each iteration, because $\underline{J}$ varies between iterations

Example:

$$\left.\begin{aligned} f_1(x_1, x_2) &= x_1^2 + x_2^2 - 1 \\ f_2(x_1, x_2) &= x_1^2 - x_2 \end{aligned}\right\} \quad \underline{f}(\underline{x}) = \underline{0}$$

$$\underline{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \end{bmatrix} \quad \begin{bmatrix} 2x_1 & 2x_2 \end{bmatrix}$$

$$\underset{\sim}{J} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 & 2x_2 \\ 2x_1 & -1 \end{bmatrix}$$

Let $\underline{x}^{(0)} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, then $\underset{\sim}{J}^{(0)} = \begin{bmatrix} 2 & 2 \\ 2 & -1 \end{bmatrix}$

matrix of constants

Note: Here $\underset{\sim}{J}$ is symmetric, but need not be

Note: If the initial guess $\underline{x}^{(0)}$ is not close to the solution $\underline{x}^*$, it might not converge (just as in the single equation Newton-Raphson method)

Also, sometimes a damped Newton method is needed, such as

$$\underline{\delta}^{(i)} = -\left(\underset{\sim}{J}^{(i)}\right)^{-1} \underline{f}^{(i)}$$

but then

$$\underline{x}^{(i+1)} = \underline{x}^{(i)} + \alpha^{(i)} \underline{\delta}^{(i)} \text{ with } \alpha^{(i)} \in (0,1]$$

$$\underline{x}^{(i+1)} = \underline{x}^{(i)} + \alpha^{(i)}\underline{\delta}^{(i)} \text{ with } \alpha^{(i)} \in (0,1]$$

that moves $\underline{x}^{(i+1)}$ closer to $\underline{x}^*$

Example:

$$\underline{f}(\underline{x}) = \begin{bmatrix} x_1^2 + x_1x_2 + x_1 - 1 \\ x_1x_2 + x_2 + x_3^2 - 0.25 \\ x_1^2 + x_2^2 - 4x_3 \end{bmatrix} = \underline{0}$$

Find roots

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

For N-R, need

$$\begin{matrix} \frac{\partial f_1}{\partial x_1}, & \frac{\partial f_1}{\partial x_2}, & \frac{\partial f_1}{\partial x_3} \\ \vdots & \vdots & \vdots \\ \frac{\partial f_3}{\partial x_1}, & \dots, & \frac{\partial f_3}{\partial x_3} \end{matrix}$$

Fixed point method

$$\underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \underbrace{\begin{bmatrix} -x_1^2 - x_1x_2 + 1 \\ -x_1x_2 - x_3^2 + 0.25 \\ 0.25\,(x_1^2 + x_2^2) \end{bmatrix}}_{\underline{g}(\underline{x})}$$

Define

$$\varepsilon^i = \| \underline{f}(\underline{x}^i) \|_\infty$$

Try $\underline{x}^{(0)} = \begin{bmatrix} 1/2 \\ -1 \\ 0 \end{bmatrix}$

i	x_1	x_2	x_3	ε

1	1.25	0.75	0.3125	2.75
2	-1.5	-0.78	0.53	0.927
3	-2.42	-1.21	0.72	5.4
4	-7.83	-3.2	1.84	~77

$\to \infty$

Diverges → No solution obtained

Try $\underline{x}^{(0)} = \begin{bmatrix} -1/2 \\ -1 \\ 0 \end{bmatrix}$

i	x_1	x_2	x_3	ε
1	0.25	-0.25	0.3125	1.125
2	1	0.21	0.03	1.214
3	-0.21	0.034	0.26	1.17
4	0.961	0.188	0.01	1.06

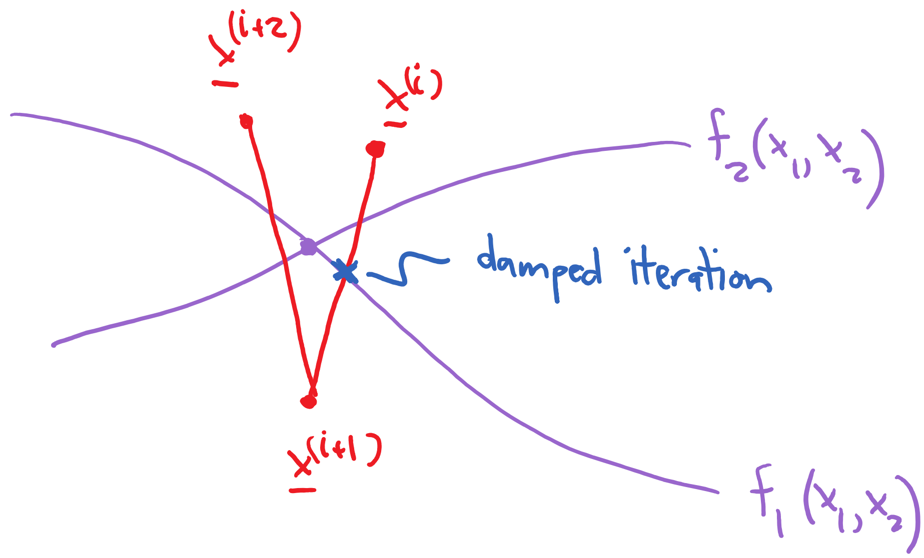
$\to \sim 1$

Does not diverge or converge

Try a damped iteration $(\alpha = \frac{1}{2})$

$$\hat{\underline{x}}^{(i+1)} = \underline{g}(\underline{x}^{(i)}) \Rightarrow \underline{x}^{(i+1)} = \frac{1}{2}\underline{x}^{(i)} + \frac{1}{2}\hat{\underline{x}}^{(i+1)}$$

i	x_1	x_2	x_3	ε
10	0.577	0.513	0.0896	1.2×10^{-3}
27	~0.577	~0.513	~0.0896	1.3×10^{-8}



Now try Newton-Raphson

$$\underset{\sim}{J} = \begin{bmatrix} 1+2x_1+x_2 & x_1 & 0 \\ x_2 & 1+x_1 & 2x_3 \\ 2x_1 & 2x_2 & -4 \end{bmatrix}$$

Note: $\underline{J}$ here is not symmetric

Try

$$\underline{x}^{(0)} = \begin{bmatrix} -1/2 \\ -1 \\ 0 \end{bmatrix}$$

i	x_1	x_2	x_3	ε
1	−1.25	−1	0.5	0.563
4	−1.0465	−0.99	0.475	0.186
6	−1	−0.99	0.49	1.3×10^{-5}

5	-1.0465	-0.94	0.915	0.106
6	-1	-0.99	0.49	1.3×10^{-5}
7	$\boxed{-1}$	$\boxed{-1}$	$\boxed{0.5}$	3×10^{-9}

Different root!

Try $\underline{x}^{(0)} = \begin{bmatrix} 1/2 \\ -1 \\ 0 \end{bmatrix}$

$i = 5$

$$\underline{x}^{(5)} = \begin{bmatrix} 0.5773 \\ 0.153 \\ 0.0893 \end{bmatrix}$$

Same root as with damped fixed point method

$$\varepsilon^{(5)} = 1.6 \times 10^{-11}$$