Solving Non linear equations

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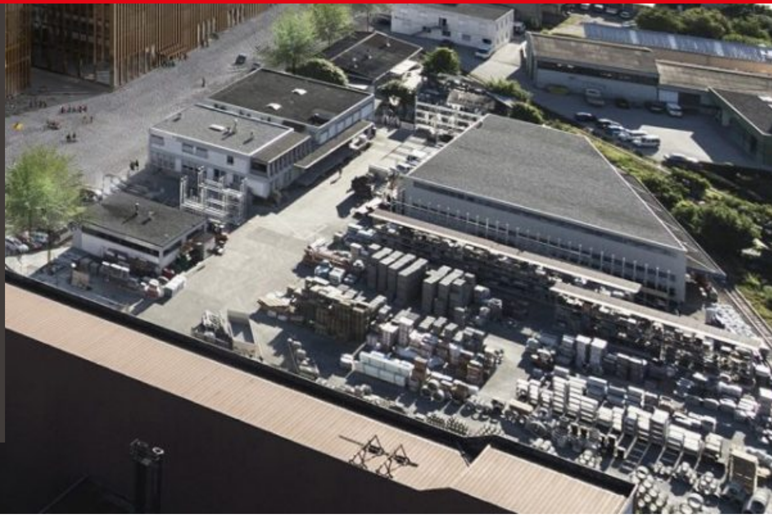


IPESE
Industrial Process
and Energy Systems
Engineering

Solving non linear equations

- The goal : *Find the value of* x^* *such that* $f(\pi_p, x^*) = 0$
  - Calculation algorithm :
    - calculates the value of $f(\pi_p, x)$ for any value of x it receives
  - Solution algorithm that is searching for the value of x^*
  - Safe guard algorithm such that
    - x^* has a meaning : i.e. $x_{min} \leq x^* \leq x_{max}$

Solving f(x)= 0 : Newton-Raphson method

TAYLOR development to approximate any function

$$f(x) = f\left(x^0\right) + \left(x - x^0\right).f'\left(x^0\right) + \frac{\left(x - x^0\right)^2}{2!}.f''\left(x^0\right) + \ldots$$

I rst order limitation (approximate with a straight line) near x^0

$$f\left(x^0\right) + \left(x^* - x^0\right).f'\left(x^0\right) \cong f\left(x^*\right) = 0$$

$$x^1 = x^0 - \frac{f\left(x^0\right)}{f'\left(x^0\right)} \Rightarrow x^{n+1} = x^n - \frac{f\left(x^n\right)}{f'\left(x^n\right)}$$

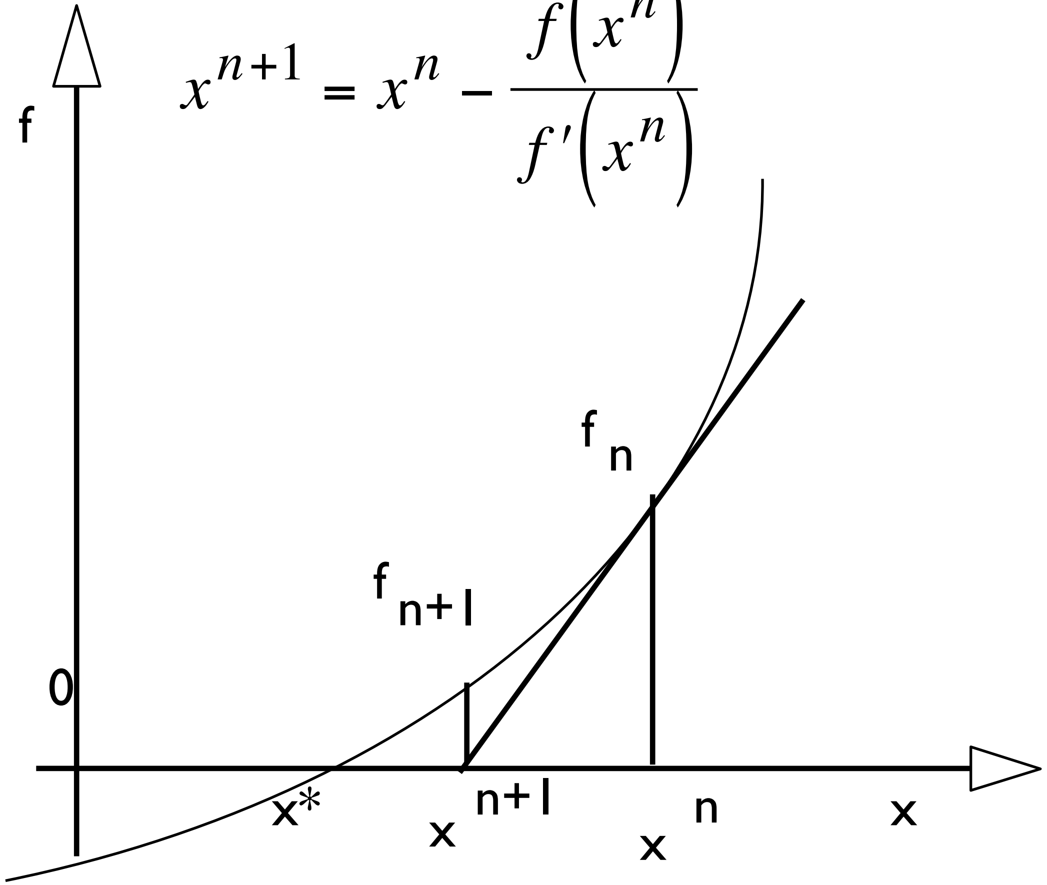
Newton Raphson algorithm

- Take x0 = guess of x*.
- Taylor development
  - f(x) = f(x0) + (x - x0) f '(x0) + 1/2 (x - x0)² f " (x0) +…
- Limit to 1rst order :
  - f(x0) + (x* - x0) . f'(x0) ≅ f(x*) = 0
- Repeat (Iterations) : $$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$
- until f(x) sufficiently close to 0

geometrical interpretation

- tangent approximation
- intersection with f=0

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



Numerical calculation of derivatives

Forward calculation

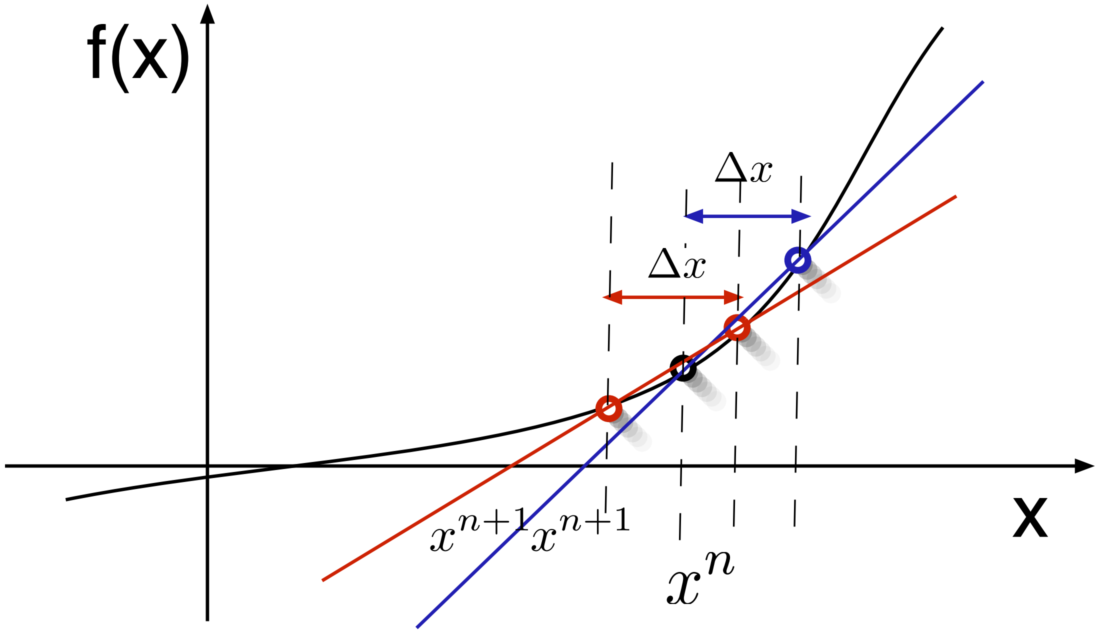
$$f'(x^n) = \left[\frac{\delta f(x)}{\delta x}\right]_{x^n} = \frac{f(x^n) - f(x^n + \Delta x)}{\Delta x}$$

+ 1 function evaluation

Central value

$$f'(x^n) = \left[\frac{\delta f(x)}{\delta x}\right]_{x^n} = \frac{f(x^n - \frac{\Delta x}{2}) - f(x^n + \frac{\Delta x}{2})}{\Delta x}$$

+ 2 function evaluations



Convergence criteria

- Choose a small well chosen value

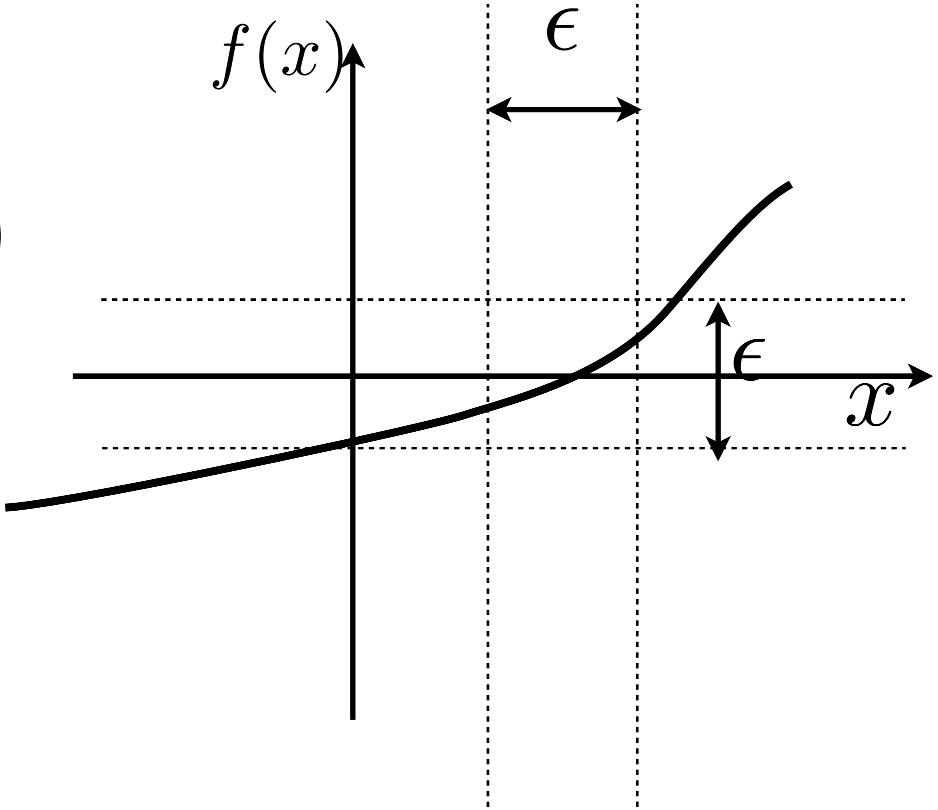
$$\epsilon = 1.0E - 06$$

- Test variable variations

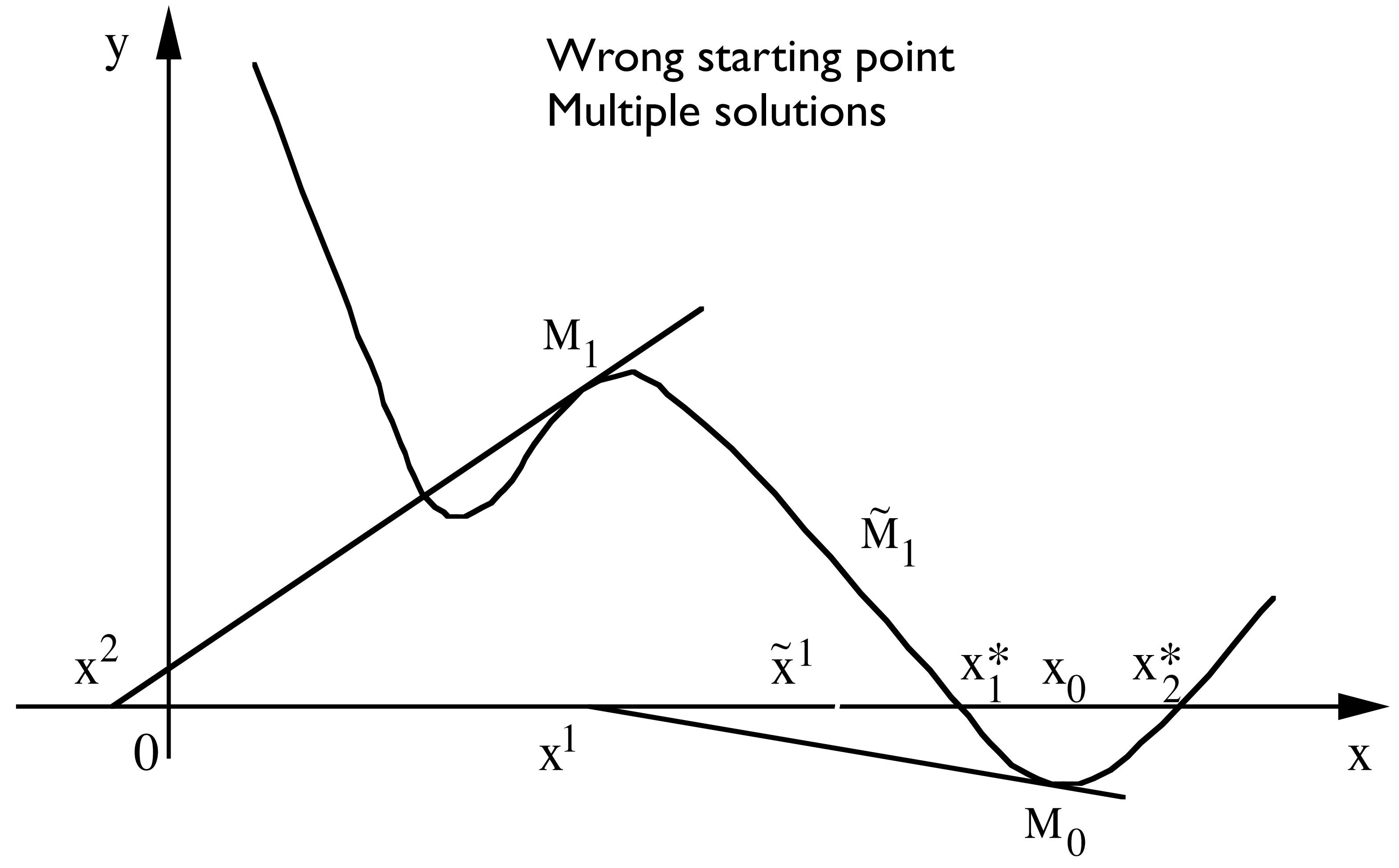
$$| x^{k+1} - x^k | \leq \epsilon * (1 + | x^k |)$$

- Test function variation

$$| f(x^k) | \leq \epsilon$$



Newton-Raphson : possible problems



Newton-Raphson : drawbacks

- Requires initial point
- Requires derivatives calculation
- divergence possible
- no step if tangent = 0

Increase robustness of solving procedure

- Use relaxation factor 0 < q < 1

$$x^{n+1} = x^n \cdot q + \tilde{x}^{n+1} \cdot (1 - q)$$

  - q=0 => full step
- Choice of q is critical ?
  - convergence speed wrt robustness
    - q >> small steps and lots of iterations
    - q << Newton step : direct convergence if linear problem
- Use past iterations to judge the need for relaxation :

is $\left|f(x^{n+1})\right| < \left|f(x^n)\right|$?

More efficient method

- 2^{nd} order development
  - $f(x)=0=c+b\,(x-x_0)+a\,(x-x_0)^2$

$$x - x_0 = \frac{-b \pm \sqrt[2]{b^2 - 4ac}}{2a}$$

  - a, b, c obtained from 3 values of f(x)

Chord method : approximating derivatives

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

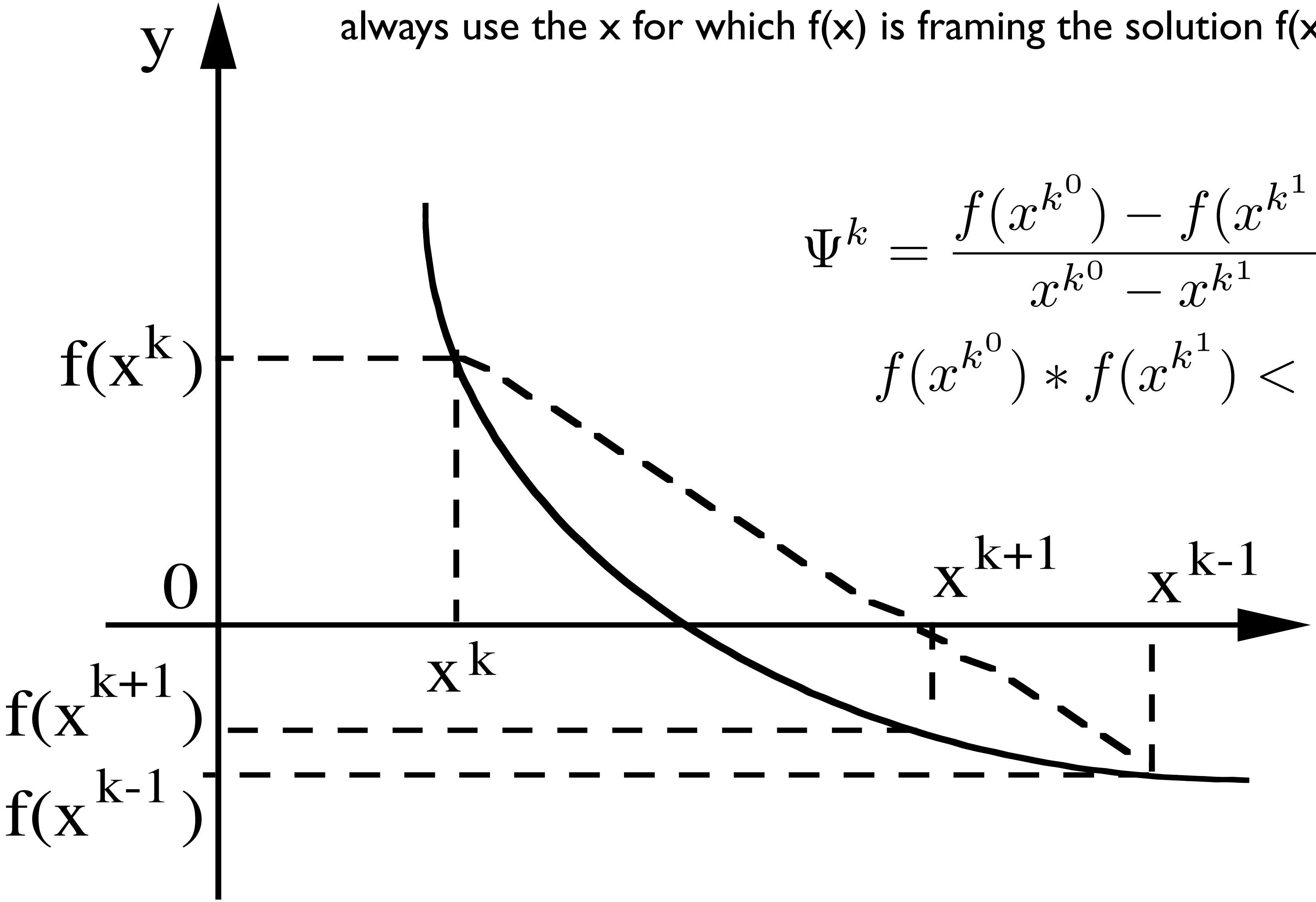
$$x^{k+1} = x^{k} - \psi^{-1} . f\left(x^{k}\right)$$

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

approximation of the derivative by the iteration step

Chord method : solving f(x)=0

always use the x for which f(x) is framing the solution f(x)=0



$$\Psi^k = \frac{f(x^{k^0}) - f(x^{k^1})}{x^{k0} - x^{k1}}$$

$$f(x^{k^0}) * f(x^{k^1}) < 0$$

Solving a set of N equations F(X)=0 : N Variables

- **Newton-Raphson n dimensions**
  - Solve F(X) = 0 (Array)

    f1(x) = f1(x1,x2,...,xn) = 0

    f2(x) = f2(x1,x2,...,xn) = 0

    . . . .

    fn(x) = fn(x1,x2,...,xn) = 0

  - Initial guess is given
  - X0 = init[x1 ... xn]

Newton Raphson : N dimension

- Taylor development
-

$$f_i(\underline{x}) = f_i(\underline{x_0}) + \sum_{j=1}^{n} \left(\frac{\partial f_i}{\partial x_j} \right) \Delta x_j = 0$$

i = 1, n

Matrix representation

Jacobian matrix
matrix of derivatives

function evaluated for x0

$$
\begin{vmatrix}
\frac{\delta f_1}{\delta x_1} & \cdots & \frac{\delta f_1}{\delta x_j} & \cdots & \frac{\delta f_1}{\delta x_n} \\
\cdots & & \cdots & & \cdots \\
\frac{\delta f_i}{\delta x_1} & \cdots & \frac{\delta f_i}{\delta x_j} & \cdots & \frac{\delta f_i}{\delta x_n} \\
\cdots & & \cdots & & \cdots \\
\frac{\delta f_n}{\delta x_1} & \cdots & \frac{\delta f_n}{\delta x_j} & \cdots & \frac{\delta f_n}{\delta x_n}
\end{vmatrix}
\cdot
\begin{vmatrix} \Delta x_1 \\ \cdots \\ \Delta x_j \\ \\ \Delta x_n \end{vmatrix}
+
\begin{vmatrix} f_1(\underline{x}^0) \\ \cdots \\ f_i(\underline{x}^0) \\ \cdots \\ f_n(\underline{x}^0) \end{vmatrix}
=
\begin{vmatrix} f_1(\underline{x}) \\ \cdots \\ f_i(\underline{x}) \\ \cdots \\ f_n(\underline{x}) \end{vmatrix}
$$

$$ {}^t\underline{\underline{J}}\,\underline{\Delta x} + \underline{F}\left(\underline{x}^0\right) = \underline{F}\left(\underline{x}\right) $$

Newton -Raphson (N dimensions)

$$^{t}\underline{J}\,\underline{\Delta x} + \underline{F}\left(\underline{x}^{0}\right) = \underline{F}\left(\underline{x}\right)$$

$$\underline{F}(\underline{X}) = 0$$

$$\underline{x}^{1} = \underline{x}^{0} - {}^{t}\underline{J}_{\underline{x}^{0}}^{-1}\,\underline{F}\left(\underline{x}^{0}\right)$$

Iteration n :

$$\underline{x}^{n+1} = \underline{x}^{n} - {}^{t}\underline{J}_{\underline{x}^{n}}^{-1}\,\underline{F}\left(\underline{x}^{n}\right)$$

Convergence criteria

- At iteration k
  - Variables variations

$$\mid x^{k+1} - x^{k} \mid \leq \epsilon * (1 + \mid x^{k} \mid)$$

  - Functions variation

$$\mid f(x^{k}) \mid \leq \epsilon$$

Scaling variables and equations

- Variables

Original problem

$$| f^{k+1} | \leq \epsilon$$
$$| x^{k+1} - x^k | \leq \epsilon * (1 + | x^k |)$$

Scaling $F(X) = 0 \rightarrow \Phi(\Xi) = 0$

$$\Xi = Scale_x \cdot X$$
$$\Phi = Scale_f \cdot F(X)$$

All equations and variables are compared with the same reference value

New problem

$$| \chi_j^{k+1} - \chi_j^k | \leq \epsilon * (1 + | \chi_j^k |) \quad \forall j$$
$$| \phi_j^{k+1}(\chi) - \phi_j^k(\chi) | \leq \epsilon \quad \forall j$$

Calculating derivatives

- Forward numerical estimation

$$\frac{\partial f}{\partial x_i} = \frac{f(X + \Delta x_i) - f(X)}{\Delta x_i} \quad \forall i = 1, \ldots, n_X + 1$$

- Computation time cost !
  - central derivatives avoided
  - Matrix Inversion
    - the matrix $J_{x^n}^{-1}$ is reused and not re-evaluated at each iteration

- Numerical noise (is the derivative a derivative ?)
- $\Delta f(X) = |F(X)_0 - F(X)_{n_X+1}|$

Newton-Raphson n dimensions ;Drawbacks

- Initial guess
- Matrix inversion + derivatives
- Matrix inversion at each iteration n*n derivatives,
- Relaxation may be applied :

$$\underline{\tilde{x}}^{n+1} = \underline{\tilde{x}}^{n} - {}^{t}\underline{\underline{J}}^{-1}_{\underline{x}^{n}} \underline{F}\left(\underline{\tilde{x}}^{n}\right).(1-q)$$