METHODS – Summary

Notations:

$\mathbf{f}(\mathbf{x}) = \mathbf{0}$ - The nonlinear system

$\mathbf{F}(\mathbf{x})$ = Jacobian of function $\mathbf{f}(\mathbf{x})$: $F_{ij} = \dfrac{\partial f_i}{\partial x_j}$

$\mathbf{x}^{(0)}$ = initial approximation of the solution $\boldsymbol{\alpha}$ (generally, close to $\boldsymbol{\alpha}$).

METHOD – ITERATION SCHEME

1. Fixed-Point

   For $n \geq 0$:

   $\mathbf{F}(\mathbf{x}^{(0)}) \cdot \delta\mathbf{x}^{(n+1)} = -\mathbf{f}(\mathbf{x}^{(n)})$

   $\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} + \delta\mathbf{x}^{(n+1)}$

   The Jacobian $\mathbf{F}(\mathbf{x}^{(0)})$ is updated after a number of steps (usually 3-4 steps).

   In the program:

   - The Jacobian is updated after 3 steps;
   - The Jacobian is calculated numerically (see #3), with $h = 1E-3$;

2. Newton

   For $n \geq 0$:

   $\mathbf{F}(\mathbf{x}^{(n)}) \cdot \delta\mathbf{x}^{(n+1)} = -\mathbf{f}(\mathbf{x}^{(n)})$

   $\mathbf{x}^{(n+1)} = \mathbf{x}^{(n)} + \delta\mathbf{x}^{(n+1)}$

3. Newton-Numerical (or: Discrete-Newton)

   The iteration scheme is the same as in Newton method (# 2).

   The Jacobian elements are calculated numerically (i.e. the partial derivatives are calculated by finite differences):

$$\frac{\partial f_i}{\partial x_j} = \frac{f_i(x_1, \ldots, x_j + h, \ldots, x_n) - f_i(x_1, \ldots, x_j, \ldots, x_n)}{h}$$

In the program: $h = 1E - 3$.

4. <u>Broyden-1</u> (Broyden "Good" Update)

$\mathbf{B}_k$ is the approximation of Jacobian at the step *k*.

Hereinafter we denote $\mathbf{x}_k$ instead of $\mathbf{x}^{(k)}$ (and, $\mathbf{s}_k$ instead of $\delta\mathbf{x}^{(k+1)}$).

Initialization: $\mathbf{B}_0 = \mathbf{F}(\mathbf{x}_0)$, and $\mathbf{F}(\mathbf{x}_0)$ is calculated numerically (see #3).

- Iteration Scheme:

  For $k \geq 0$:

  $\mathbf{B}_k \mathbf{s}_k = -\mathbf{f}(\mathbf{x}_k)$

  $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k$;

  $\mathbf{y}_k = \mathbf{f}(\mathbf{x}_{k+1}) - \mathbf{f}(\mathbf{x}_k)$;

  Update $\mathbf{B}_k$;

- $\mathbf{B}_k$ update formula:

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{(\mathbf{y}_k - \mathbf{B}_k \mathbf{s}_k)\mathbf{s}_k^T}{\mathbf{s}_k^T \mathbf{s}_k}$$

5. <u>Broyden-2</u> (Broyden "Bad" Update)

Same definition and initialization for $\mathbf{B}_k$.

Notation: $\mathbf{H}_k = \mathbf{B}_k^{-1}$ (inverse of $\mathbf{B}_k$).

Initialization: $\mathbf{H}_0 = \mathbf{B}_0^{-1}$

- Iteration Scheme:

  For $k \geq 0$:

$$\mathbf{s}_k = -\mathbf{H}_k \cdot \mathbf{f}(\mathbf{x}_k)$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k;$$

$$\mathbf{y}_k = \mathbf{f}(\mathbf{x}_{k+1}) - \mathbf{f}(\mathbf{x}_k);$$

Update $\mathbf{H}_k$;

- $\mathbf{H}_k$ update formula:

$$\mathbf{H}_{k+1} = \mathbf{H}_k + \frac{(\mathbf{s}_k - \mathbf{H}_k \mathbf{y}_k)\mathbf{s}_k{}^T \mathbf{H}_k}{\mathbf{s}_k{}^T \mathbf{H}_k \mathbf{y}_k}$$

Note

Broyden methods are *quasi*-*Newton* methods.

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<u>Test for iteration stopping</u>

$\| \delta \mathbf{x}^{(n+1)} \| \le eps$ or $\| \mathbf{s}_k \| \le eps$;

Number of iterations (n or k) $\le nlim$

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