Chapter 10
Numerical Solutions of Nonlinear Systems of Equations

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Section 10.1
Fixed Points for Functions of Several Variables

Objective

To solve a system of nonlinear equations of the form

$$\begin{cases} f_1(x_1, x_2, \cdot, x_n) = 0, \\ f_2(x_1, x_2, \cdot, x_n) = 0, \\ \vdots \\ f_n(x_1, x_2, \cdot, x_n) = 0, \end{cases} \tag{1}$$

where each $f_i : \mathbb{R}^n \to \mathbb{R}$ is a (nonlinear) function for $i = 1, 2, \ldots, n$. The unknown vector $x = [x_1, x_2, \cdots, x_n]^T \in \mathbb{R}^n$ is called **a solution** to the nonlinear system (1).

Reformulation of the Nonlinear System

Consider a vector-valued function $F:\mathbb{R}^n \to \mathbb{R}^n$ defined by

$$F(x) = [f_1(x), f_2(x), \cdots, f_n(x)]^T \in \mathbb{R}^n \quad \forall x \in \mathbb{R}^n.$$

- The system of nonlinear equations (1) can be represented as

$$F(x) = \mathbf{0}, \quad x = [x_1, x_2, \cdot, x_n]^T \in \mathbb{R}^n. \tag{2}$$

- The functions $f_1, f_2, \cdots, f_n$ are called the **coordinate functions (坐標函數) of** F.

Two Vector Norms (向量的範數)

Definition (常用的向量範數)

Let $v = [v_1, v_2, \cdots, v_n]^T \in \mathbb{R}^n$.

- T he l_2-**norm (or Euclidean norm)** of v is defined by

$$\|v\|_2 = \sqrt{v^T v} = \sqrt{\sum_{i=1}^{n} v_i^2}.$$

- T he l_∞-**norm** of v is defined by $\|v\|_\infty = \max_{1 \le i \le n} |v_i|$.

MATLAB Command: `norm(v, 2)` or `norm(v)` is used for $\|v\|_2$, and `norm(v, 'inf')` is used for $\|v\|_\infty$.

Example 1, p. 631

Place the following nonlinear system

$$\begin{cases} 3x_1 - \cos(x_2x_3) - \frac{1}{2} = 0 \\ x_1^2 - 81(x_2+0.1)^2 + \sin x_3 + 1.06 = 0 \\ e^{-x_1x_2} + 20x_3 + \frac{10\pi-3}{3} = 0 \end{cases} \tag{3}$$

in the form (2).

Solution

Rewrite the nonlinear system (3) as

$$\begin{aligned} F(x_1, x_2, x_3) &\equiv [f_1(x_1, x_2, x_3), f_2(x_1, x_2, x_3), f_3(x_1, x_2, x_3)]^T \\ &= [0, 0, 0]^T = \mathbf{0} \in \mathbb{R}^3, \end{aligned}$$

where the coordinate functions are defined by

$$\begin{aligned} f_1(x_1, x_2, x_3) &= 3x_1 - \cos(x_2 x_3) - \frac{1}{2}, \\ f_2(x_1, x_2, x_3) &= x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06, \\ f_3(x_1, x_2, x_3) &= e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3}. \end{aligned}$$

Fixed-Point Forms

- As in Chap. 2, we shall transform the root-finding problem (2) into a fixed-point problem

$$x = G(x), \quad x \in D,$$

where $G : D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ is some vector-valued function with domain

$$D = \{[x_1, x_2, \cdots, x_n]^T \mid a_i \leq x_i \leq b_i,\ i = 1, 2, \cdots, n\} \qquad (4)$$

for some constants $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$.

- **Fixed-Point Iteration (FPI)** with an initial vector $x^{(0)} \in D$:

$$x^{(k)} = G(x^{(k-1)}), \quad k = 1, 2, \ldots,$$

provided that $x^{(k)} \in D \quad \forall\, k \geq 1$.

Def 10.5

The vector-valued function $G : D \subseteq \mathbb{R}^n \to \mathbb{R}^n$ has a fixed point at $p \in D$ if $G(p) = p$.

Questions

- Under what conditions does the sequence of vectors $\{x^{(k)}\}_{k=0}^{\infty}$ generated by FPI converge to the **unique** fixed point $p \in D$?
- What is the error bound for the absolute error $\|x^{(k)} - p\|_\infty$?
- What is the rate of convergence for FPI?

We may write

$$G(x) = [g_1(x), g_2(x), \cdots, g_n(x)]^T,$$

where each g_i is the ith component function of G for $i = 1, 2, \ldots, n$.

Thm 10.6

Let G be **conti.** on D with $G(D) \subseteq D$, where the domain D is defined as in (4). Then

(1) G has at least one fixed point in D.

(2) If, in addition, $\exists\, 0 < K < 1$ s.t. each component function g_i has **conti.** partial derivatives with

$$\left|\frac{\partial g_i(x)}{\partial x_j}\right| \le \frac{K}{n}, \quad \text{whenever } x \in D,$$

for $i, j = 1, 2, \ldots, n$, then with **any** $x^{(0)} \in D$ conv. to the **unique** fixed point $p \in D$, and

$$\|x^{(k)} - p\|_\infty \le \frac{K^k}{1-K} \|x^{(1)} - x^{(0)}\|_\infty \quad \forall\, k.$$

Thm 10.4 (分量函數的連續性)

Let $g : D \subseteq \mathbb{R}^n \to \mathbb{R}$ be a function and $x_0 \in D$. If $\exists\, \delta > 0$ and $M > 0$ s.t. the partial derivatives of g exist on $N_\delta(x_0) \cap D$ with

$$\left| \frac{\partial g(x)}{\partial x_j} \right| \le M \qquad \forall\, x \in N_\delta(x_0) \cap D,$$

for $j = 1, 2, \ldots, n$, then g is conti. at x_0.

Continuity of G

- G is conti. at $x_0 \in D \Longleftrightarrow$ each component function g_i is conti. at x_0 for $i = 1, 2, \ldots, n$.
- G is conti. on $D \Longleftrightarrow$ each g_i is conti. on D for $i = 1, 2, \ldots, n$.

Example 2, p. 633

(a) Place the nonlinear system in **Example 1**

$$\begin{cases} 3x_1 - \cos(x_2x_3) - \frac{1}{2} = 0 \\ x_1^2 - 81(x_2+0.1)^2 + \sin x_3 + 1.06 = 0 \\ e^{-x_1x_2} + 20x_3 + \frac{10\pi-3}{3} = 0 \end{cases}$$

in a **fixed-point form** $x = G(x)$, $x \in D$, and show that there is a **unique** sol. on

$$D = \{[x_1, x_2, x_3]^T \mid -1 \le x_i \le 1,\ i = 1, 2, 3\}.$$

(b) Perform the FPI with $x^{(0)} = [0.1, 0.1, -0.1]^T$ and the stopping criterion $\|x^{(k)} - x^{(k-1)}\|_\infty < 10^{-5}$.

Solving the ith eq. of (3) for x_i $(i = 1, 2, 3) \Rightarrow$

$$\begin{aligned} \mathbf{x_1} &= \frac{1}{3}\cos(x_2x_3) + \frac{1}{6} \equiv g_1(x_1, x_2, x_3) \\ \mathbf{x_2} &= \frac{1}{9}\sqrt{x_1^2 + \sin x_3 + 1.06} - 0.1 \equiv g_2(x_1, x_2, x_3) \\ \mathbf{x_3} &= \frac{-1}{20}e^{-x_1x_2} - \frac{10\pi - 3}{60} \equiv g_3(x_1, x_2, x_3). \end{aligned} \qquad (5)$$

So, define a vectored-valued function $G : D \to \mathbb{R}^3$ by

$$G(x_1, x_2, x_3) = [g_1(x_1, x_2, x_3), g_2(x_1, x_2, x_3), g_3(x_1, x_2, x_3)]^T \in \mathbb{R}^3$$

for any $x = [x_1, x_2, x_3]^T \in D$. Now, consider the fixed-point form

$$x = G(x), \quad x \in D$$

obtained from the original nonlinear system (3).

Fist, we shall claim that $G(D) \subseteq D$. It is easily seen from (5) that for any $x \in D$, we have

$$
\begin{aligned}
|g_1(x)| &\le \frac{1}{3}|\cos(x_2x_3)| + \frac{1}{6} \le \mathbf{0.50},\\
|g_2(x)| &= \left|\frac{1}{9}\sqrt{x_1^2 + \sin x_3 + 1.06} - 0.1\right|\\
&\le \frac{1}{9}\sqrt{(1)^2 + \sin(1) + 1.06} - 0.1 < \mathbf{0.09}\\
|g_3(x)| &= \frac{1}{20}e^{-x_1x_2} + \frac{10\pi - 3}{60}\\
&\le \frac{1}{20}e + \frac{10\pi - 3}{60} < \mathbf{0.61}.
\end{aligned}
$$

Hence, we know that $G(D) \subseteq D$.

Next, simple manipulation from Calculus gives that

$$\frac{\partial g_1}{\partial x_2} = \frac{-x_3}{3}\sin(x_2x_3), \quad \frac{\partial g_1}{\partial x_3} = \frac{-x_2}{3}\sin(x_2x_3), \tag{6}$$

$$\frac{\partial g_2}{\partial x_1} = \frac{x_1}{9\sqrt{x_1^2 + \sin x_3 + 1.06}}, \quad \frac{\partial g_2}{\partial x_3} = \frac{\cos x_3}{18\sqrt{x_1^2 + \sin x_3 + 1.06}}, \tag{7}$$

$$\frac{\partial g_3}{\partial x_1} = \frac{-x_2}{20}e^{-x_1x_2}, \quad \frac{\partial g_3}{\partial x_2} = \frac{-x_1}{20}e^{-x_1x_2}, \quad \frac{\partial g_1}{\partial x_1} = \frac{\partial g_2}{\partial x_2} = \frac{\partial g_3}{\partial x_3} = 0. \tag{8}$$

$\Longrightarrow$ All first partial derivatives of g_1, g_2, g_3 are **conti.** on D!

Now, from (6) $\Longrightarrow$

$$\left|\frac{\partial g_1}{\partial x_2}\right| \leq \frac{|x_3|}{3} \cdot |\sin(x_2 x_3)| \leq \frac{\sin 1}{3} < \mathbf{0.281}, \quad \left|\frac{\partial g_1}{\partial x_3}\right| < \mathbf{0.281}.$$

From (7), we see that

$$\left|\frac{\partial g_2}{\partial x_1}\right| \leq \frac{1}{9\sqrt{\sin(-1)+1.06}} = \frac{1}{9\sqrt{0.218}} < \mathbf{0.238},$$

$$\left|\frac{\partial g_2}{\partial x_3}\right| \leq \frac{1}{18\sqrt{\sin(-1)+1.06}} = \frac{1}{18\sqrt{0.218}} < \mathbf{0.119},$$

and furthermore, from (8), we also have

$$\left|\frac{\partial g_3}{\partial x_1}\right| \leq \frac{e}{20} < \mathbf{0.14}, \quad \left|\frac{\partial g_3}{\partial x_2}\right| \leq \frac{e}{20} < \mathbf{0.14}.$$

Thus, the partial derivatives of g_1, g_2, g_3 are **bounded** on D. It follows from Thm 10.4 that G must be conti. on D and

$$\left|\frac{\partial g_i}{\partial x_j}\right| \leq \mathbf{0.281} = \frac{K}{n} = \frac{K}{3} \qquad \forall\, x \in D$$

for $i, j = 1.2.3$. So, the sufficient conditions of **Thm 10.6** are satisfied with the constant $K = (0.281)(3) = \mathbf{0.843} < 1$.

Conclusions

- G has a unique fixed point $p \in D$ by Thm 10.6.
- This fixed point p is one of the solutions to the original nonlinear system (3).

Solution of (b)–Numerical Results

Finally, perform the FPI

$$x^{(k)} = G(x^{(k-1)}), \quad k = 1, 2, \ldots$$

with $x^{(0)} = [0.1, 0.1, -0.1]^T \in D$ and $\|x^{(k)} - x^{(k-1)}\|_\infty < 10^{-5}$.
Actual sol. $\mathbf{p} = [\mathbf{0.5}, \mathbf{0}, \frac{-\pi}{\mathbf{6}}]^{\mathbf{T}} \approx [\mathbf{0.5}, \mathbf{0}, -\mathbf{0.5235987757}]^{\mathbf{T}}$.

A Test for the Error Bound

- With the computed sol. $x^{(5)}$ and the actual fixed point $p \in D$,

$$\|x^{(5)} - p\|_\infty \leq \mathbf{2 \times 10^{-8}}.$$

- With $K = 0.843$, the theoretical error bound would become

$$\|x^{(5)} - p\|_\infty \leq \frac{(0.843)^5}{1 - 0.843}(0.423) < \mathbf{1.15}.$$

- **The error bound in Thm 10.6 might be much larger than the actual absolute error!**

Basic Ideas

- Use the latest estimates generated by the FPI

$$x_1^{(k)}, x_2^{(k)}, \cdots, x_{i-1}^{(k)}$$

instead of $x_1^{(k-1)}, x_2^{(k-1)}, \cdots, x_{i-1}^{(k-1)}$ to compute the ith component $x_i^{(k)}$.

- This is the same as the idea of Gauss-Seidel method for solving linear systems. (See Chapter 7)

Reformulation as Gauss-Seidel Method

Consider the following Gauss-Seidel form for Example 2

$$\begin{aligned} x_1^{(k)} &= \frac{1}{3}\cos(x_2^{(k-1)}x_3^{(k-1)}) + \frac{1}{6}, \\ x_2^{(k)} &= \frac{1}{9}\sqrt{(x_1^{(k)})^2 + \sin x_3^{(k-1)} + 1.06} - 0.1, \\ x_3^{(k)} &= \frac{-1}{20}e^{-x_1^{(k)}x_2^{(k)}} - \frac{10\pi - 3}{60}, \quad k = 1, 2, \ldots \end{aligned} \tag{9}$$

with $x^{(0)} = [0.1, 0.1, -0.1]^T \in \mathbb{R}^3$ and the same stopping criterion $\|x^{(k)} - x^{(k-1)}\|_\infty < 10^{-5}$.

Applying the iteration (9) with given initial vector $x^{(0)}$, the numerical results are shown in the following table.

Note: In general, this method does not always accelerate the convergence! (不一定每次都能加速固定點迭代法!)

Section 10.2
Newton's Method

Review of Newton's Method

- Newton's method for solving a nonlinear equation of one variable

$$f(x) = 0, \quad x \in \mathbb{R}$$

can be regarded as a **fixed-point iteration** with

$$g(x) = x - \frac{1}{f'(x)} \cdot f(x) \equiv x - \phi(x) \cdot f(x).$$

The **quadratic convergence** of Newton's method is always expected if the initial guess is **sufficiently close** to a zero of f.

Objectives

- For solving a nonlinear system

$$F(x) = [f_1(x), f_2(x), \cdots, f_n(x)]^T = \mathbf{0} \in \mathbb{R}^n, \quad x \in \mathbb{R}^n,$$

try to develop a FPI with the vector-valued function

$$\begin{aligned} G(x) &= x - A(x)^{-1} F(x) \\ &\equiv [g_1(x), g_2(x), \cdots, g_n(x)]^T \in \mathbb{R}^n, \quad x \in \mathbb{R}^n, \end{aligned} \tag{10}$$

assuming that $A(x) = [a_{ij}(x)] \in \mathbb{R}^{n \times n}$ is **nonsingular at the fixed point** p **of** G.

- Hopefully, the **quadratic convergence** can be achieved under reasonable conditions.

Thm 10.7 (FPI 二次收斂的充分條件)

Let $G(p) = p$. Suppose that $\exists\, \delta > 0$ with

(i) $\frac{\partial g_i}{\partial x_j}$ is **conti.** on $N_\delta(p)$ for $i, j = 1, 2, \ldots, n$;

(ii) $\frac{\partial^2 g_i}{\partial x_j \partial x_k}$ is **conti.** on $N_\delta(p)$, and $\exists\, M > 0$ s.t.

$$\left| \frac{\partial^2 g_i(x)}{\partial x_j \partial x_k} \right| \leq M \qquad \forall\, x \in N_\delta(p),$$

for $i, j, k = 1, 2, \ldots, n$;

(iii) $\frac{\partial g_i(p)}{\partial x_j} = 0$ for $i, j = 1, 2, \ldots, n$.

Then $\exists\, \hat{\delta} \leq \delta$ s.t. the seq. $\{x^{(k)}\}_{k=0}^{\infty}$ generated by FPI converges **quadratically** to p for any $x^{(0)} \in N_{\hat{\delta}}(p)$. Moreover,

$$\|x^{(k)} - p\|_\infty \leq \frac{n^2 M}{2} \|x^{(k-1)} - p\|_\infty^2 \qquad \forall\, k \geq 1.$$

- Write $A(x)^{-1} = [b_{ij}(x)] \in \mathbb{R}^{n\times n}$. From (10) $\Rightarrow$

$$g_i(x) = x_i - \sum_{k=1}^{n} b_{ik}(x) f_k(x), \quad i = 1, 2, \ldots, n.$$

- For each $i, j = 1, 2, \ldots, n$, the first partial derivatives of g_i are

$$\frac{\partial g_i(x)}{\partial x_j} = \begin{cases} 1 - \sum_{k=1}^{n} \left(\frac{\partial b_{ik}(x)}{\partial x_j} f_k(x) + b_{ik}(x) \frac{\partial f_k(x)}{\partial x_j} \right), & i = j, \\ - \sum_{k=1}^{n} \left(\frac{\partial b_{ik}(x)}{\partial x_j} f_k(x) + b_{ik}(x) \frac{\partial f_k(x)}{\partial x_j} \right), & i \neq j. \end{cases} \tag{11}$$

- From condition (iii) of Thm 10.7 and (11), we immediately obtain

$$0 = \frac{\partial g_i(p)}{\partial x_j} = \begin{cases} 1 - \sum_{k=1}^{n} b_{ik}(p) \frac{\partial f_k(p)}{\partial x_j}, & i = j, \\ -\sum_{k=1}^{n} b_{ik}(p) \frac{\partial f_k(p)}{\partial x_j}, & i \neq j. \end{cases} \quad (12)$$

- Define the **Jacobian matrix** $J(x) = [\frac{\partial f_i(x)}{\partial x_j}] \in \mathbb{R}^{n \times n}$ by

$$J(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x) & \frac{\partial f_1}{\partial x_2}(x) & \cdots & \frac{\partial f_1}{\partial x_n}(x) \\ \frac{\partial f_2}{\partial x_1}(x) & \frac{\partial f_2}{\partial x_2}(x) & \cdots & \frac{\partial f_2}{\partial x_n}(x) \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1}(x) & \frac{\partial f_n}{\partial x_2}(x) & \cdots & \frac{\partial f_n}{\partial x_n}(x) \end{bmatrix}, \quad x \in N_\delta(p).$$

It follows from (12) that $A(p)^{-1}J(p) = I$ or $A(p) = J(p)$.

- So, it is appropriate to choose $A(x) = J(x)$ for $x \in N_\delta(p)$.
- Basic form of Newton's method for nonlinear systems:

$$\begin{aligned} x^{(k)} &= G(x^{(k-1)}) = x^{(k-1)} - A(x^{(k-1)})^{-1} F(x^{(k-1)}) \\ &= x^{(k-1)} - J(x^{(k-1)})^{-1} F(x^{(k-1)}), \quad k = 1, 2, \ldots, \end{aligned} \tag{13}$$

  where $x^{(0)} \in N_{\hat{\delta}}(p)$ and $J(x)$ is **nonsingular** on $N_{\hat{\delta}}(p)$ with $0 < \hat{\delta} \leq \delta$.
- **Quadratic convergence** of Newton's method is guaranteed from Thm 10.7 if the initial guess is sufficiently close to p!

Some Comments on Newton's Method (13)

- We DO NOT compute $J(x^{(k-1)})^{-1}$ **explicitly** in practical computation.
- In order to save the operation counts, we first solve the linear system

$$J(x^{(k-1)})y = -F(x^{(k-1)})$$

  for the **correction vector** y using **Gaussian Elimination with Partial Pivoting**, and then compute the next iterate via

$$x^{(k)} = x^{(k-1)} + y.$$

- Floating-point operation counts $\approx \mathbf{O}(\frac{2}{3}\mathbf{n}^3)$ per iteration.

To approx. the sol. of the nonlinear system $F(x) = 0$, $x \in \mathbb{R}^n$.

Algorithm 10.1: Newton's Method for Systems

INPUT dim. n; initial $x \in \mathbb{R}^n$; tol. TOL; max. no. of iter. N_0.

OUTPUT an approx. sol. x to the nonlinear system.

Step 1 Set $k = 1$.

Step 2 While $(k \leq N_0)$ do **Steps 3–7**

- Step 3 Compute F(x) and the Jacobian matrix $J(x)$.
- Step 4 Solve the $n \times n$ linear system $J(x)y = -F(x)$.
- Step 5 Set $x = x + y$.
- Step 6 If $\|y\| < TOL$ then OUTPUT(x); **STOP**.
- Step 7 Set $k = k + 1$.

Step 8 OUTPUT('Maximum number of iterations exceeded'); **STOP**.

Example 1, p. 641 (See also Example 2 of Sec. 10.1)

Apply Newton's Method to solve the nonlinear system

$$\begin{cases} 3x_1 - \cos(x_2 x_3) - \frac{1}{2} = 0 \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 = 0 \\ e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3} = 0 \end{cases}$$

with $x^{(0)} = [0.1, 0.1, -0.1]^T$ and $\|x^{(k)} - x^{(k-1)}\|_\infty < 10^{-5}$.

The Jacobian matrix $J(x)$ is easily obtain from Calculus as

$$J(x_1, x_2, x_3) = \begin{bmatrix} 3 & x_3 \sim (x_2x_3) & x_3 \sin(x_2x_3) \\ 2x_1 & -162(x_2+0.1) & \cos x_3 \\ -x_2 e^{-x_1x_2} & -x_1 e^{-x_1x_2} & 20 \end{bmatrix}.$$

Actual sol. $\mathbf{p} = [\mathbf{0.5}, \mathbf{0}, \frac{-\pi}{\mathbf{6}}]^{\mathbf{T}} \approx [\mathbf{0.5}, \mathbf{0}, -\mathbf{0.5235987757}]^{\mathbf{T}}$.

Section 10.3
Quasi-Newton Methods
(擬牛頓法)

For Each Iterate of Newton's Method

- At least n^2 scalar functional evaluations for the Jacobian matrix $J(x^{(k)})$ and n scalar functional evaluations for $F(x^{(k)})$.
- Solving a linear system involving the Jacobian requires $O(n^3)$ operation counts.
- **Self-Correcting**: it will generally correct for roundoff error with the successive iterations.
- Quadratic convergence occurs if a good initial guess is given.

For Each Iterate of Broyden's Method

- Only n scalar functional evaluations are required!
- The amount of operation counts for solving the linear system is reduced to $O(n^2)$.
- It is **Not Self-Correcting** with the successive iterations.
- Only superlinear convergence occurs if a good initial guess is given, i.e., we have

$$\lim_{k\to\infty} \frac{\|x^{(k+1)} - p\|}{\|x^{(k)} - p\|} = 0,$$

where $p \in \mathbb{R}^n$ is a solution of the nonlinear system $F(x) = 0$.

About Broyden's Method . . .

- It belongs to a class of **least-change secant update methods** that produce algorithms called **quasi-Newton**.
- The quasi-Newton methods replace the Jacobian matrix in Newton's method with **an approximate matrix that is easily updated at each iteration**.

References (參考文獻)

[Broy] C G. Broyden, *A class of methods for solving nonlinear simultaneous equations*, Math. Comp., 19(92), 577-593, 1965.

[DM] J. E. Dennis, Jr. and J. J. Moré, *Quasi-Newton methods, motivation and theory*, SIAM Rev., 19(1), 46–89, 1977.

- For an initial approx. $x^{(0)} \in \mathbb{R}^n$, compute the Jacobian matrix $A_0 = J(x^{(0)}) \in \mathbb{R}^{n \times n}$ and the first iterate

$$x^{(1)} = x^{(0)} - A_0{}^{-1} F(x^{(0)})$$

as Newton's method.

- If we let

$$s_1 = x^{(1)} - x^{(0)} \quad \text{and} \quad y_1 = F(x^{(1)}) - F(x^{(0)}),$$

want to determine a matrix $A_1 \approx J(x^{(1)}) \in \mathbb{R}^{n \times n}$ satisfying the **quasi-Newton condition or secant condition**

$$A_1(x^{(1)} - x^{(0)}) = F(x^{(1)}) - F(x^{(0)}) \quad \text{or} \quad A_1 s_1 = y_1. \tag{14}$$

- To determine A_1 uniquely, Broyden [Broy] imposed

$$A_1 z = A_0 z \qquad \forall\, z \in \mathbb{R}^n \text{ with } s_1^T z = 0 \tag{15}$$

on the secant codition (14).So, it follows from (14) and (15) that [DM]

$$A_1 = A_0 + \frac{(y_1 - A_0 s_1)}{\|s_1\|_2^2} \cdot s_1^T$$

and hence $x^{(2)} = x^{(1)} - A_1{}^{-1} F(x^{(1)})$.

- In general, for $k \geq 2$, we have

$$A_k = A_{k-1} + \frac{(y_k - A_{k-1} s_k)}{\|s_k\|_2^2} \cdot s_k{}^T, \tag{16}$$

$$x^{(k+1)} = x^{(k)} - A_k{}^{-1} F(x^{(k)}),$$

where $s_k = x^{(k)} - x^{(k-1)} = -A_{k-1}^{-1} F(x^{(k-1)})$ and $y_k = F(x^{(k)}) - F(x^{(k-1)})$.

Remarks

- From (16), we see that A_k is obtained from the previous A_{k-1} plus an **rank-1 updating matrix**.
- This technique is called the **least-change secant updates**.
- In single-variable Newton's method, may write

$$f'(x_k) \approx \frac{f(x_k) - f(x_{k-1})}{x_k - x_{k-1}} \text{ or } f'(x_k)(x_k - x_{k-1}) \approx f(x_k) - f(x_{k-1});$$

while we try to determine uniquely $A_k \approx J(x^{(k)})$ s.t.

$$A_k(x^{(k)} - x^{(k-1)}) = F(x^{(k)}) - F(x^{(k-1)})$$

in the multidimensional case.

A Question

With the special structure of A_k, how to reduce the number of arithmetic calculations to $O(n^2)$ for solving the $n \times n$ linear system $A_k{}^{-1}F(X^{(k)})$?

Thm 10.8 (Sherman-Morrison Formula)

If $A \in \mathbb{R}^{n\times n}$ is nonsingular and $x, y \in \mathbb{R}^n$ are nonzero vectors with $y^TA^{-1}x \neq -1$, then $A+xy^T$ is **nonsingular** and

$$(A+xy^T)^{-1} = A^{-1} - \frac{A^{-1}xy^TA^{-1}}{1+y^TA^{-1}x}.$$

Reformulation of A_k^{-1}

For each $k \geq 1$, from (16) and Sherman-Morrison formula $\Longrightarrow$

$$
\begin{aligned}
A_k^{-1} &= \left(A_{k-1} + \frac{(y_k - A_{k-1}s_k)}{\|s_k\|_2^2} \cdot s_k^T\right)^{-1} \\
&= A_{k-1}^{-1} - \frac{A_{k-1}^{-1}\left(\frac{y_k - A_{k-1}s_k}{\|s_k\|_2^2}\right)s_k^T A_{k-1}^{-1}}{1 + s_k^T A_{k-1}^{-1}\left(\frac{y_k - A_{k-1}s_k}{\|s_k\|_2^2}\right)} \\
&= A_{k-1}^{-1} - \frac{(A_{k-1}^{-1}y_k - s_k)(s_k^T A_{k-1}^{-1})}{\|s_k\|_2^2 + s_k^T A_{k-1}^{-1}y_k - \|s_k\|_2^2} \\
&= A_{k-1}^{-1} + \frac{(s_k - A_{k-1}^{-1}y_k)(s_k^T A_{k-1}^{-1})}{s_k^T A_{k-1}^{-1}y_k} \\
&= A_{k-1}^{-1} + \frac{(s_k - A_{k-1}^{-1}y_k)(s_k^T A_{k-1}^{-1})}{-s_k^T \cdot (-A_{k-1}^{-1}y_k)}.
\end{aligned}
\tag{17}
$$

INPUT dim. n; initial $x \in \mathbb{R}^n$; tol. TOL; max. no. of iter. N_0.

OUTPUT an approx. sol. x of nonlinear system $F(x) = 0$.

Step 1 Set $A_0 = J(x)$: the Jacobian matrix evaluated at x.
$v = F(x)$. (Note: $\mathbf{v} = \mathbf{F}(\mathbf{x}^{(0)})$.)

Step 2 Set $A = A_0^{-1}$. (Use Gaussian elimination.)

Step 3 Set $s = -Av$; $x = x + s$; $k = 1$. (Note: $\mathbf{s} = \mathbf{s_1}$, $\mathbf{x} = \mathbf{x}^{(1)}$.)

Step 4 While ($k \leq N_0$) do **Steps 5–11**.

- Step 5 Set $w = v$; $v = F(x)$; $y = v - w$. (Note: $\mathbf{y} = \mathbf{y_k}$.)
- Step 6 Set $z = -Ay$. (Note: $\mathbf{z} = -\mathbf{A}_{\mathbf{k-1}}^{-1}\mathbf{y_k}$.)
- Step 7 Set $p = -s^T z$. (Note: $\mathbf{p} = \mathbf{s}_{\mathbf{k}}^{\mathbf{T}}\mathbf{A}_{\mathbf{k-1}}^{-1}\mathbf{y_k}$.)
- Step 8 Set $u^T = s^T A$; $A = A + \frac{1}{p}(s + z)u^T$. (Note: $\mathbf{A} = \mathbf{A}_{\mathbf{k}}^{-1}$.)
- Step 9 Set $s = -Av$; $x = x + s$. (Note: $\mathbf{s} = -\mathbf{A}_{\mathbf{k}}^{-1}\mathbf{F}(\mathbf{x}^{(\mathbf{k})})$ and $\mathbf{x} = \mathbf{x}^{(\mathbf{k+1})}$.)
- Step 10 If $\|s\| < TOL$ then OUTPUT(x); **STOP**.
- Step 11 Set $k = k + 1$.

Step 12 OUTPUT('Maximum number of iterations exceeded'); **STOP**.

Example 1, p. 651 (See also Example 2 of Sec. 10.1)

Use Broyden's Method to solve the nonlinear system

$$\begin{cases} 3x_1 - \cos(x_2 x_3) - \frac{1}{2} = 0 \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 = 0 \\ e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3} = 0 \end{cases}$$

with $x^{(0)} = [0.1, 0.1, -0.1]^T$ and $\|x^{(k)} - x^{(k-1)}\|_2 < 10^{-5}$.

Numerical Results for Example 1

The **superlinear convergence** of Broyden's method for Example 1 is demonstrated in the following table and the computed solutions are **less accurate** than those computed by Newton's method.

Actual sol. $\mathbf{p} = [0.5, 0, -\frac{\pi}{6}]^T \approx [0.5, 0, -0.5235987757]^T$.

Thank you for your attention!