Numerical Analysis

10th ed

R L Burden, J D Faires, and A M Burden

Beamer Presentation Slides Prepared by Dr. Annette M. Burden Youngstown State University

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MOTIVATION

A system of nonlinear equations has the form

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

\n
$$
f_2(x_1, x_2, \ldots, x_n) = 0,
$$

\n
$$
\vdots \qquad \vdots
$$

\n
$$
f_n(x_1, x_2, \ldots, x_n) = 0,
$$

where each function *fi* can be thought of as mapping a vector $\mathbf{x} = (x_1, x_2, \dots, x_n)^t$ of the *n*-dimensional space \mathbb{R}^n into the real line R.

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MOTIVATION

This system of *n* nonlinear equations in *n* unknowns can also be represented by defining a function **F** mapping R*ⁿ* into R*ⁿ* as

$$
\mathbf{F}(x_1, x_2, \ldots, x_n) = (f_1(x_1, x_2, \ldots, x_n), f_2(x_1, x_2, \ldots, x_n))^{t}.
$$

 $\ldots, x_n), \ldots, f_n(x_1, x_2, \ldots, x_n))^{t}.$

If vector notation is used to represent the variables x_1, x_2, \ldots, x_n , then system from the previous slide assumes the form

$$
F(x)=0.
$$

The functions f_1, f_2, \ldots, f_n are called the **coordinate functions** of **F**.

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Definition (10.1)

et f be a function defined on a set $D \subset \mathbb{R}^n$ and mapping into \mathbb{R} . The function *f* is said to have the **limit** *L* at \mathbf{x}_0 , written

$$
\lim_{\mathbf{x}\to\mathbf{x}_0}f(\mathbf{x})=L,
$$

if, given any number $\varepsilon > 0$, a number $\delta > 0$ exists with

 $|f(\mathbf{X}) - L| < \varepsilon$,

whenever $x \in D$ and

$$
0<||\mathbf{x}-\mathbf{x}_0||<\delta.
$$

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Definition (10.2)

Let *f* be a function from a set $D \subset \mathbb{R}^n$ into \mathbb{R} . The function *f* is **continuous** at $\mathbf{x}_0 \in D$ provided $\lim_{\mathbf{x} \to \mathbf{x}_0} f(\mathbf{x})$ exists and

$$
\lim_{\mathbf{x}\to\mathbf{x}_0}f(\mathbf{x})=f(\mathbf{x}_0).
$$

Moreover, *f* is **continuous** on a set *D* if *f* is continuous at every point of D. This concept is expressed by writing $f \in C(D)$.

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Definition (10.3)

Let **F** be a function from $D \subset \mathbb{R}^n$ into \mathbb{R}^n of the form

$$
\mathbf{F}(\mathbf{x})=(f_1(\mathbf{x}),f_2(\mathbf{x}),\ldots,f_n(\mathbf{x}))^t,
$$

where f_i is a mapping from \mathbb{R}^n into $\mathbb R$ for each *i*. We define

$$
\lim_{\mathbf{x}\to\mathbf{x}_0} \mathbf{F}(\mathbf{x}) = \mathbf{L} = (L_1, L_2, \ldots, L_n)^t,
$$

if and only if $\lim_{\mathbf{x}\to\mathbf{x}_0} f_i(\mathbf{x}) = L_i$, for each $i = 1, 2, \ldots, n$.

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Theorem (10.4)

Let f be a function from D $\subset \mathbb{R}^n$ *into* \mathbb{R} *and* $\mathbf{x}_0 \in D$ *. Suppose that all the partial derivatives of f exist and constants* $\delta > 0$ *and K* > 0 *exist so that whenever* $\|\mathbf{x} - \mathbf{x}_0\| < \delta$ *and* $\mathbf{x} \in D$ *, we have*

$$
\left|\frac{\partial f(\bm{x})}{\partial x_j}\right|\leq K,\quad \text{for each }j=1,2,\ldots,n.
$$

Then f is continuous at \mathbf{x}_0 *.*

Definition (10.5)

A function G from $D \subset \mathbb{R}^n$ into \mathbb{R}^n has a fixed point at $p \in D$ if $G(p) = p$.

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Theorem (10.6)

Let $D = \{ (x_1, x_2, \ldots, x_n)^t \mid a_i \le x_i \le b_i$, for each $i = 1, 2, \ldots, n \}$ for *some collection of constants* a_1, a_2, \ldots, a_n *and* b_1, b_2, \ldots, b_n *. Suppose* **G** *is a continuous function from* $D \subset \mathbb{R}^n$ *into* \mathbb{R}^n *with the property that* $G(x) \in D$ *whenever* $x \in D$ *. Then* G *has a fixed point in D. Suppose also that all the component functions of* **G** *have continuous partial derivatives and a constant K <* 1 *exists with*

> $\begin{array}{c} \hline \end{array}$ $\overline{}$ $\overline{}$ $\begin{array}{c} \end{array}$ $\partial g_i(\mathbf{x})$ ∂x_j $\begin{array}{c} \hline \end{array}$ $\overline{}$ $\overline{}$ $\begin{array}{c} \hline \end{array}$ \leq *K* $\frac{n}{n}$ *,* whenever $x \in D$ *,*

for each $j = 1, 2, \ldots, n$ *and each component function* g_j *. Then the fixed-point sequence* $\{x^{(k)}\}_{k=0}^{\infty}$ *defined by an arbitrarily selected* $x^{(0)}$ *in D and generated by* $\mathbf{x}^{(k)} = G(\mathbf{x}^{(k-1)}),$ *for each k* \geq 1 *converges to the unique fixed point* $p \in D$ *and* $\|\mathbf{x}^{(k)} - \mathbf{p}\|$ $\Big\|_{\infty} \leq \frac{K^k}{1-K}$ $\left\Vert \mathbf{x}^{(1)}-\mathbf{x}^{(0)}\right\Vert$ $\|_{\infty}$.

MOTIVATION

We will use an approach similar to the one used in the one-dimensional fixed-point method for the *n*-dimensional case. This involves a matrix

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$$
A(\mathbf{x}) = \begin{bmatrix} a_{11}(\mathbf{x}) & a_{12}(\mathbf{x}) & \cdots & a_{1n}(\mathbf{x}) \\ a_{21}(\mathbf{x}) & a_{22}(\mathbf{x}) & \cdots & a_{2n}(\mathbf{x}) \\ \vdots & \vdots & & \vdots \\ a_{n1}(\mathbf{x}) & a_{n2}(\mathbf{x}) & \cdots & a_{nn}(\mathbf{x}) \end{bmatrix}
$$

,

where each of the entries $a_{ij}(\mathbf{x})$ is a function from \mathbb{R}^n into \mathbb{R} . This requires that *A*(**x**) be found so that

$$
\mathbf{G}(\mathbf{x}) = \mathbf{x} - A(\mathbf{x})^{-1} \mathbf{F}(\mathbf{x})
$$

gives quadratic convergence to the solution of $F(x) = 0$, assuming that *A*(**x**) is nonsingular at the fixed point **p** of **G**.

Theorem (10.7)

Let **p** *be a solution of* $G(x) = x$ *. Suppose a number* $\delta > 0$ *exists with*

(i) $\partial g_i / \partial x_i$ *is continuous on* $N_\delta = \{ \mathbf{x} \mid ||\mathbf{x} - \mathbf{p}|| < \delta \}$, for each $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, n;$

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(ii) $\partial^2 g_i(\mathbf{x})/(\partial x_i \partial x_k)$ *is continuous, and* $|\partial^2 g_i(\mathbf{x})/(\partial x_i \partial x_k)| \leq M$ *for some constant M, whenever* $\mathbf{x} \in \mathbb{N}_{\delta}$ *, for each* $i = 1, 2, ..., n, j = 1, 2, ..., n,$ and $k = 1, 2, ..., n;$

(iii) $\partial g_i(\mathbf{p})/\partial x_k = 0$, for each $i = 1, 2, \ldots, n$ and $k = 1, 2, \ldots, n$.

Then a number $\hat{\delta} \leq \delta$ exists such that the sequence generated by $\mathbf{x}^{(k)} = \mathbf{G}(\mathbf{x}^{(k-1)})$ converges quadratically to \mathbf{p} for any choice of $\mathbf{x}^{(0)}$, *provided that* $\|\mathbf{x}^{(0)} - \mathbf{p}\| < \hat{\delta}$. Moreover, $\|\mathbf{x}^{(k)} - \mathbf{p}\|_{\infty} \le \frac{n^2 M}{2} \|\mathbf{x}^{(k-1)} - \mathbf{p}\|_{\infty}^2$, for each $k \ge 1$.

The Jacobian Matrix

Define the matrix $J(x)$ by

$$
J(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(\mathbf{x}) & \frac{\partial f_1}{\partial x_2}(\mathbf{x}) & \cdots & \frac{\partial f_1}{\partial x_n}(\mathbf{x}) \\ \frac{\partial f_2}{\partial x_1}(\mathbf{x}) & \frac{\partial f_2}{\partial x_2}(\mathbf{x}) & \cdots & \frac{\partial f_2}{\partial x_n}(\mathbf{x}) \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_n}{\partial x_1}(\mathbf{x}) & \frac{\partial f_n}{\partial x_2}(\mathbf{x}) & \cdots & \frac{\partial f_n}{\partial x_n}(\mathbf{x}) \end{bmatrix}
$$

,

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It is required that

 $A(\mathbf{p})^{-1}J(\mathbf{p})=I$, the identity matrix, so $A(\mathbf{p})=J(\mathbf{p})$.

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The Jacobian Matrix

An appropriate choice for $A(x)$ is, consequently, $A(x) = J(x)$ since this satisfies condition (iii) in Theorem 10.7. The function **G** is defined by

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$$
\mathbf{G}(\mathbf{x}) = \mathbf{x} - J(\mathbf{x})^{-1} \mathbf{F}(\mathbf{x}),
$$

and the fixed-point iteration procedure evolves from selecting $\mathbf{x}^{(0)}$ and generating, for $k > 1$,

$$
\mathbf{x}^{(k)} = \mathbf{G}(\mathbf{x}^{(k-1)}) = \mathbf{x}^{(k-1)} - J(\mathbf{x}^{(k-1)})^{-1} \mathbf{F}(\mathbf{x}^{(k-1)}).
$$

This is called **Newton's method for nonlinear systems**, and it is generally expected to give quadratic convergence, provided that a sufficiently accurate starting value is known and that $J(p)^{-1}$ exists.

MOTIVATION

A generalization of the Secant method to systems of nonlinear equations is a technique known as **Broyden's method**

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The method requires only *n* scalar functional evaluations per iteration and also reduces the number of arithmetic calculations to $O(n^2)$. It belongs to a class of methods known as *least-change secant updates* that produce algorithms called **quasi-Newton**. These methods replace the Jacobian matrix in Newton's method with an approximation matrix that is easily updated at each iteration.

DISADVANTAGES OF QUASI-NEWTON METHODS

• Quadratic convergence of Newton's method is lost, being replaced, in general, by a convergence called **superlinear**. This implies that

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

where **p** denotes the solution to $F(x) = 0$ and $x^{(i)}$ and $x^{(i+1)}$ are consecutive approximations to **p**.

This is an acceptable trade-off for the decrease in the amount of computation.

► Unlike Newton's method, theyare not self-correcting. Newton's method will generally correct for roundoff error with successive iterations, but unless special safeguards are incorporated, Broyden's method will not.

Theorem (10.8)

Suppose that A is a nonsingular matrix and that **x** *and* **y** *are vectors with* $y^tA^{-1}x \neq -1$. Then $A + xy^t$ is nonsingular and

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$$
(A + xyt)-1 = A-1 - \frac{A-1xytA-1}{1 + ytA-1x}.
$$

To approximate the solution of the nonlinear system $F(x) = 0$ given an initial approximation **x**:

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INPUT number *n* of equations and unknowns; initial approximation $\mathbf{x} = (x_1, \ldots, x_n)^t$; tolerance *TOL*; maximum number of iterations *N*. OUTPUT approximate solution $\mathbf{x} = (x_1, \ldots, x_n)^t$ or a message that the number of iterations was exceeded. Step 1 Set $A_0 = J(\mathbf{x})$ where $J(\mathbf{x})_{i,j} = \frac{\partial f_i}{\partial x_j}$ $\frac{\partial I_i}{\partial x_j}(\mathbf{x})$ for $1\leq i,j\leq n;$ ${\bf v} = {\bf F}({\bf x})$. (*Note:* ${\bf v} = {\bf F}({\bf x}^{(0)})$.) Step 2 Set $A = A_0^{-1}$. (*Use Gaussian elimination*.) Step 3 Set $s = -Av$; (*Note:* $s = s_1$.) **x** = **x** + **s**; (*Note:* **x** = **x**⁽¹⁾.) $k - 2$

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Algorithm 10.2: Broyden

Step 4 While $(k \leq N)$ do Steps 5–13. Step 5 Set $w = v$; (*Save* **v**.) **v** = **F**(**x**); (*Note:* **v** = **F**(**x**^(*k*)).) $y = v - w$. (*Note:* $y = y_k$.) Step 6 Set $z = -Ay$. (*Note:* $z = -A_{k-1}^{-1}y_k$.) Step 7 Set $p = -s^t z$. (*Note:* $p = s_k^t A_{k-1}^{-1} y_k$.) Step 8 Set $u^t = s^t A$. Step 9 Set $A = A + \frac{1}{\rho} (s + z) u^t$. (*Note:* $A = A_k^{-1}$.) Step 10 Set $s = -Av$. (*Note:* $s = -A_k^{-1}F(x^{(k)})$.) Step 11 Set $x = x + s$. (*Note:* $x = x^{(k+1)}$.) Step 12 If *||***s***|| < TOL* then OUTPUT (**x**); (*Procedure successful*.) STOP Step 13 Set $k = k + 1$. Step 14 OUTPUT ('Maximum number of iterations exceeded'); (*Procedure unsuccessful*.) STOP

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MOTIVATION

The method of Steepest Descent for finding a local minimum for an arbitrary function g from \mathbb{R}^n into $\mathbb R$ can be intuitively described as follows:

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- **1.** Evaluate *g* at an initial approximation $\mathbf{x}^{(0)}=$ $\left(x_1^{(0)}, x_2^{(0)}, \ldots, x_n^{(0)}\right)$ \setminus ^t .
- **2.** Determine a direction from $x^{(0)}$ that results in a decrease in the value of *g*.
- **3.** Move an appropriate amount in this direction and call the new value **x**(1) .
- **4.** Repeat steps 1 through 3 with $x^{(0)}$ replaced by $x^{(1)}$.

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MOTIVATION

For $g: \mathbb{R}^n \to \mathbb{R}$, the **gradient** of g at $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$ is denoted ∇ *g*(**x**) and defined by

$$
\nabla g(\mathbf{x}) = \left(\frac{\partial g}{\partial x_1}(\mathbf{x}), \frac{\partial g}{\partial x_2}(\mathbf{x}), \ldots, \frac{\partial g}{\partial x_n}(\mathbf{x})\right)^t.
$$

A differentiable multivariable function can have a relative minimum at **x** only when the gradient at **x** is the zero vector. Suppose that $\mathbf{v} = (v_1, v_2, \dots, v_n)^t$ is a unit vector in \mathbb{R}^n ; that is,

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

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MOTIVATION

The **directional derivative** of *g* at **x** in the direction of **v** measures the change in the value of the function *g* relative to the change in the variable in the direction of **v**. It is defined by

$$
D_{\mathbf{v}}g(\mathbf{x})=\lim_{h\to 0}\frac{1}{h}[g(\mathbf{x}+h\mathbf{v})-g(\mathbf{x})]=\mathbf{v}^t\cdot\nabla g(\mathbf{x}).
$$

When *g* is differentiable, the direction that produces the maximum value for the directional derivative occurs when **v** is chosen to be parallel to $\nabla g(\mathbf{x})$, provided that $\nabla g(\mathbf{x}) \neq \mathbf{0}$. As a consequence, the direction of greatest decrease in the value of *g* at **x** is the direction given by $-\nabla g(\mathbf{x})$.

Algorithm 10.3 STEEPEST DESCENT

To approximate a solution **p** to the minimization problem

$$
g(\mathbf{p}) = \min_{\mathbf{x} \in \mathbb{R}^n} g(\mathbf{x})
$$

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given an initial approximation **x**:

INPUT number *n* of variables; initial approximation $\mathbf{x} = (x_1, \ldots, x_n)^t$ *TOL*; maximum number of iterations *N*. OUTPUT approximate solution $\mathbf{x} = (x_1, \ldots, x_n)^t$ or message of failure. Step 1 Set $k = 1$. Step 2 While $(k \leq N)$ do Steps 3–15. Step 3 Set $g_1 = g(x_1, ..., x_n);$ (*Note:* $g_1 = g(\mathbf{x}^{(k)})$.) $\mathbf{z} = \nabla g(x_1, \ldots, x_n); \quad (\text{Note: } \mathbf{z} = \nabla g(\mathbf{x}^{(k)})).$ $z_0 = ||z||_2.$

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Algorithm 10.3 STEEPEST DESCENT

Step 4 If $z_0 = 0$ then OUTPUT ('Zero gradient'); OUTPUT (*x*1*,..., xn, g*1); (*The procedure completed, may have a minimum*.) STOP. Step 5 Set $z = z/z_0$; (*Make* z *a unit vector.*) $\alpha_1 = 0$: $\alpha_3 = 1$; $g_3 = g(\mathbf{x} - \alpha_3 \mathbf{z}).$ Step 6 While $(g_3 \geq g_1)$ do Steps 7 and 8. Step 7 Set $\alpha_3 = \alpha_3/2$; $g_3 = g(\mathbf{x} - \alpha_3 \mathbf{z})$. Step 8 If $\alpha_3 < \text{TOL}/2$ then OUTPUT ('No likely improvement'); OUTPUT (*x*1*,..., xn, g*1); STOP (*Procedure completed, may have a minimum*.)

Algorithm 10.3 STEEPEST DESCENT

Step 9 Set $\alpha_2 = \alpha_3/2$; $g_2 = g(\mathbf{x} - \alpha_2 \mathbf{z})$. Step 10 Set $h_1 = (g_2 - g_1)/\alpha_2$; $h_2 = (g_3 - g_2)/(\alpha_3 - \alpha_2);$ $h_3 = (h_2 - h_1)/\alpha_3$. (*Note: Newton's forward divided-difference formula* used to find *the quadratic* $P(\alpha) = g_1 + h_1 \alpha + h_3 \alpha (\alpha - \alpha_2)$ that interpolates *h*(α) *at* $\alpha = 0, \alpha = \alpha_2, \alpha = \alpha_3$.) Step 11 Set $\alpha_0 = 0.5(\alpha_2 - h_1/h_3)$; (*Critical point of P at* α_0 .) $g_0 = g(\mathbf{x} - \alpha_0 \mathbf{z}).$ Step 12 Find α from $\{\alpha_0, \alpha_3\}$ so $g = g(\mathbf{x} - \alpha \mathbf{z}) = \min\{g_0, g_3\}.$ Step 13 Set $\mathbf{x} = \mathbf{x} - \alpha \mathbf{z}$.

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Algorithm 10.3 STEEPEST DESCENT

```
Step 14 If |g - g_1| < TOL then
               OUTPUT (x1,..., xn, g);
               (The procedure was successful.)
               STOP.
     Step 15 Set k = k + 1.
Step 16 OUTPUT ('Maximum iterations exceeded');
        (The procedure was unsuccessful.)
        STOP.
```
Chapter 10.5: Homotopy; Continuation Methog

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Homotopy, or *continuation*, methods for nonlinear systems embed the problem to be solved within a collection of problems. Specifically, to solve a problem of the form

$$
\boldsymbol{F}(\boldsymbol{x})=\boldsymbol{0},
$$

which has the unknown solution **x**^{*}, we consider a family of problems described using a parameter λ that assumes values in [0*,* 1]. A problem with a known solution **x**(0) corresponds to the situation when $\lambda = 0$, and the problem with the unknown solution $x(1) \equiv x^*$ corresponds to $\lambda = 1$.

Chapter 10.5: Homotopy; Continuation Method

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CONTINUATION PROBLEM

The **continuation** problem is to: Determine a way to proceed from the known solution $\mathbf{x}(0)$ of $\mathbf{G}(0,\mathbf{x}) = \mathbf{zero}$ to the unknown solution $\mathbf{x}(1) = \mathbf{x}^*$ of $\mathbf{G}(1, \mathbf{x}) = \mathbf{0}$, that is, the solution to $\mathbf{F}(\mathbf{x}) = \mathbf{0}$.

Theorem (10.10)

Let $F(x)$ *be continuously differentiable for* $x \in \mathbb{R}^n$ *. Suppose that the Jacobian matrix* $J(x)$ *is nonsingular for all* $x \in \mathbb{R}^n$ *and that a constant M* exists with $||J(\mathbf{x})^{-1}|| \leq M$, for all $\mathbf{x} \in \mathbb{R}^n$. Then, for any $\mathbf{x}(0)$ in \mathbb{R}^n , *there exists a unique function* $\mathbf{x}(\lambda)$ *, such that*

 $G(\lambda, \mathbf{x}(\lambda)) = \mathbf{0}$

for all λ *in* [0, 1]*. Moreover,* $\mathbf{x}(\lambda)$ *is continuously differentiable and* $\mathbf{x}'(\lambda) = -J(\mathbf{x}(\lambda))^{-1}\mathbf{F}(\mathbf{x}(0)), \text{ for each } \lambda \in [0, 1].$

Chapter 10.5: Homotopy; Continuation Methog

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Algorithm 10.4 CONTINUATION

To approximate the solution of the nonlinear system $F(x) = 0$ given an initial approximation **x**: INPUT number *n* of equations and unknowns; integer *N >* 0; initial approximation $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$. OUTPUT approximate solution $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$.

Step 1 Set
$$
h = 1/N
$$
;
\n $\mathbf{b} = -h\mathbf{F}(\mathbf{x})$.
\nStep 2 For $i = 1, 2, ..., N$ do Steps 3–7.
\nStep 3 Set $A = J(\mathbf{x})$; Solve the linear system $A\mathbf{k}_1 = \mathbf{b}$.
\nStep 4 Set $A = J(\mathbf{x} + \frac{1}{2}\mathbf{k}_1)$; Solve the linear system $A\mathbf{k}_2 = \mathbf{b}$.
\nStep 5 Set $A = J(\mathbf{x} + \frac{1}{2}\mathbf{k}_2)$; Solve the linear system $A\mathbf{k}_3 = \mathbf{b}$.
\nStep 6 Set $A = J(\mathbf{x} + \mathbf{k}_3)$; Solve the linear system $A\mathbf{k}_3 = \mathbf{b}$.
\nStep 7 Set $\mathbf{x} = \mathbf{x} + (\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4)/6$.
\nStep 8 OUTPUT $(x_1, x_2, ..., x_n)$; STOP.