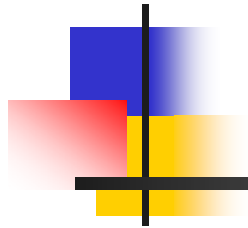


# Iterative Methods




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# Gauss-Seidel method

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix}$$

$$x_1^j = \frac{b_1 - a_{12}x_2^{j-1} - a_{13}x_3^{j-1}}{a_{11}}$$

$$x_2^j = \frac{b_2 - a_{21}x_1^j - a_{23}x_3^{j-1}}{a_{22}}$$

$$x_3^j = \frac{b_3 - a_{31}x_1^j - a_{32}x_2^j}{a_{33}}$$


Iterative until convergence

$$\varepsilon_{a,i} = \left| \frac{x_i^j - x_i^{j-1}}{x_i^j} \right| \times 100\% \leq \varepsilon_s$$

# An example using Gauss-Seidel method

$$\begin{aligned}3x_1 - 0.1x_2 - 0.2x_3 &= 7.85 \\0.1x_1 + 7x_2 - 0.3x_3 &= -19.3 \\0.3x_1 - 0.2x_2 + 10x_3 &= 71.4\end{aligned}$$

**True solution:**

$$x_1 = 3, x_2 = -2.5, x_3 = 7$$

**Iterative equations**

$$\begin{aligned}x_1 &= \frac{7.85 + 0.1x_2 + 0.2x_3}{3} \\x_2 &= \frac{-19.3 - 0.1x_1 + 0.3x_3}{7} \\x_3 &= \frac{71.4 - 0.3x_1 + 0.2x_2}{10}\end{aligned}$$

Error estimation

$$\varepsilon_{a,1} = \left| \frac{2.990557 - 2.616667}{2.990557} \right| \times 100\% = 12.5\% \quad \varepsilon_{a,2} = 11.8\% \quad \varepsilon_{a,3} = 0.076\%$$

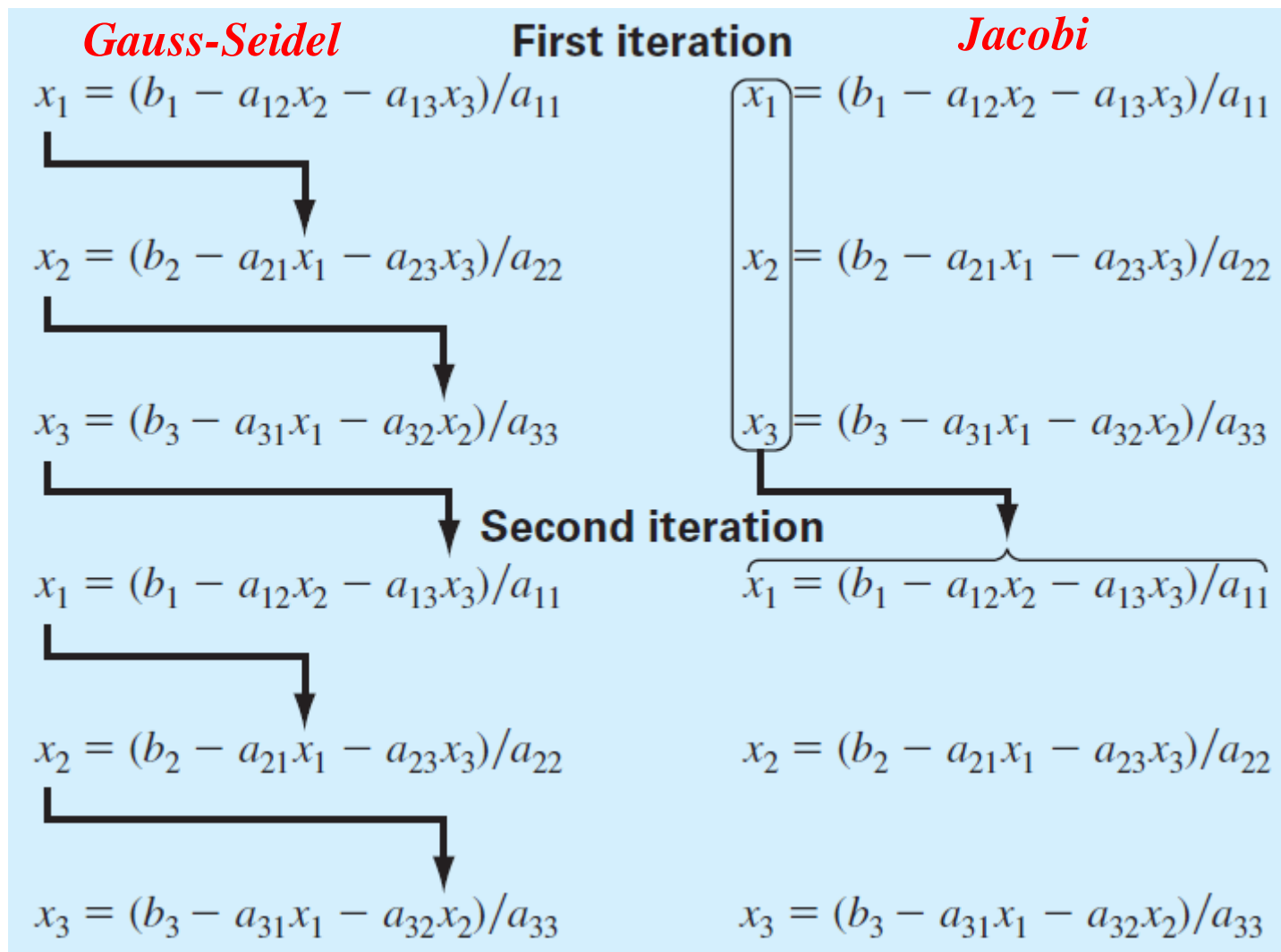
1<sup>st</sup> iteration

$$\begin{aligned}x_1 &= \frac{7.85 + 0.1(0) + 0.2(0)}{3} = 2.616667 \\x_2 &= \frac{-19.3 - 0.1(2.616667) + 0.3(0)}{7} = -2.794524 \\x_3 &= \frac{71.4 - 0.3(2.616667) + 0.2(-2.794524)}{10} = 7.005610\end{aligned}$$

2<sup>nd</sup> iteration

$$\begin{aligned}x_1 &= \frac{7.85 + 0.1(-2.794524) + 0.2(7.005610)}{3} = 2.990557 \\x_2 &= \frac{-19.3 - 0.1(2.990557) + 0.3(7.005610)}{7} = -2.499625 \\x_3 &= \frac{71.4 - 0.3(2.990557) + 0.2(-2.499625)}{10} = 7.000291\end{aligned}$$

# Gauss-Seidel vs. Jacobi iterative methods



# Diagonal dominance

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- The Gauss-Seidel method may diverge
- If the system is *diagonally dominant*, it will definitely converge.
- Diagonal dominance

$$|a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^n |a_{ij}|$$

## M-file to implement Gauss-Seidel

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$$x_1^{\text{new}} = \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}}x_2^{\text{old}} - \frac{a_{13}}{a_{11}}x_3^{\text{old}}$$

$$x_2^{\text{new}} = \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}}x_1^{\text{new}} - \frac{a_{23}}{a_{22}}x_3^{\text{old}}$$

$$x_3^{\text{new}} = \frac{b_3}{a_{33}} - \frac{a_{31}}{a_{33}}x_1^{\text{new}} - \frac{a_{32}}{a_{33}}x_2^{\text{new}}$$

Implemented by matrix operations

$$\{x\} = \{d\} - [C]\{x\}$$

where

$$\{d\} = \begin{Bmatrix} b_1/a_{11} \\ b_2/a_{22} \\ b_3/a_{33} \end{Bmatrix} \quad [C] = \begin{bmatrix} 0 & a_{12}/a_{11} & a_{13}/a_{11} \\ a_{21}/a_{22} & 0 & a_{23}/a_{22} \\ a_{31}/a_{33} & a_{32}/a_{33} & 0 \end{bmatrix}$$

## M-file to implement Gauss-Seidel (cont.)

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```
function x = GaussSeidel(A,b,es,maxit)
    if nargin<4|isempty(maxit), maxit=50; end
    if nargin<3|isempty(es), es=0.00001; end
    C = A;
    n=length(A);
    for i = 1:n
        C(i,i) = 0;
        x(i) = 0;
    end
    x = x';
    for i = 1:n
        C(i,1:n) = C(i,1:n)/A(i,i);
    end
    for i = 1:n
        d(i) = b(i)/A(i,i);
    end
end
```

## M-file to implement Gauss-Seidel (cont.)

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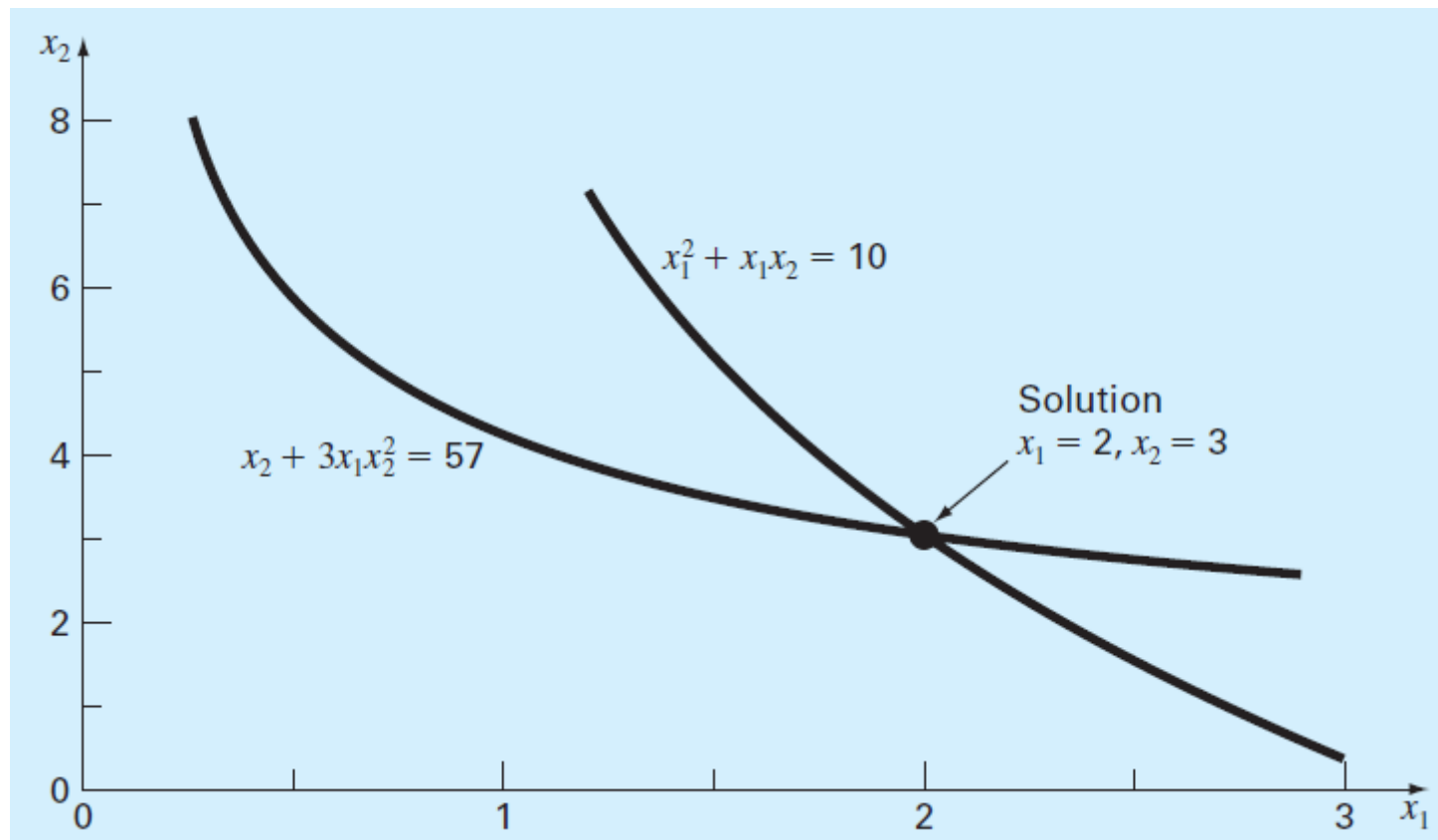
```
iter = 0;
while (1)
    xold = x;
    for i = 1:n
        x(i) = d(i)-C(i,:)*x;
        if x(i) ~= 0
            ea(i) = abs((x(i) - xold(i))/x(i)) * 100;
        end
    end
    iter = iter+1;
    if max(ea)<=es | iter >= maxit, break, end
end
```



# Nonlinear system

$$x_1^2 + x_1x_2 = 10$$

$$x_2 + 3x_1x_2^2 = 57$$



# Solving nonlinear systems by successive substitution, the same strategy as the Gauss-Seidel method

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$$x_1^2 + x_1x_2 = 10$$

$$x_2 + 3x_1x_2^2 = 57$$

Iterative equations

$$x_1 = \frac{10 - x_1^2}{x_2}$$

$$x_2 = 57 - 3x_1x_2^2$$

Initial guesses:  $x_1 = 1.5, x_2 = 3.5$

$$x_1 = \frac{10 - (1.5)^2}{3.5} = 2.21429$$

$$x_2 = 57 - 3(2.21429)(3.5)^2 = -24.37516$$

Next iteration

$$x_1 = \frac{10 - (2.21429)^2}{-24.37516} = -0.20910$$

$$x_2 = 57 - 3(-0.20910)(-24.37516)^2 = 429.709$$

**Diverging !!**

## Alternative format of iteration equation

$$x_1^2 + x_1x_2 = 10$$

$$x_2 + 3x_1x_2^2 = 57$$

Iterative equations

$$x_1 = \sqrt{10 - x_1x_2}$$

$$x_2 = \sqrt{\frac{57 - x_2}{3x_1}}$$

Initial guesses:  $x_1 = 1.5, x_2 = 3.5$

$$x_1 = \sqrt{10 - 1.5(3.5)} = 2.17945$$

$$x_2 = \sqrt{\frac{57 - 3.5}{3(2.17945)}} = 2.86051$$

Next iteration

$$x_1 = \sqrt{10 - 2.17945(2.86051)} = 1.94053$$

$$x_2 = \sqrt{\frac{57 - 2.86051}{3(1.94053)}} = 3.04955$$

Converging !!

**Shortcoming of successive substitution: convergence often depends on the format of iteration equations.**

# Reform of nonlinear equation solving by root finding of nonlinear equations

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

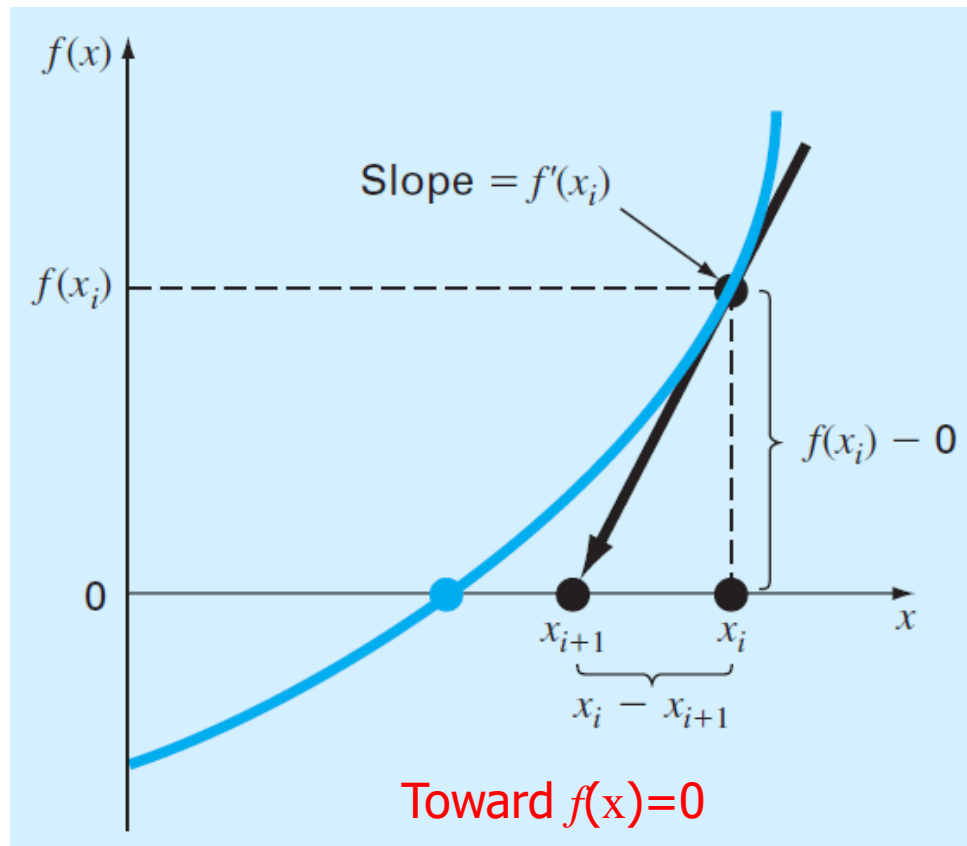
$$f_2(x_1, x_2, \dots, x_n) = 0$$

$$\vdots$$

$$f_n(x_1, x_2, \dots, x_n) = 0$$

# Recall of Newton-Raphson method for finding a root

$$f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i)f'(x_i)$$



$$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}}$$

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

# Solving nonlinear systems by Newton-Raphson

- A first-order Taylor series

$$f_{1,i+1} = f_{1,i} + (x_{1,i+1} - x_{1,i}) \frac{\partial f_{1,i}}{\partial x_1} + (x_{2,i+1} - x_{2,i}) \frac{\partial f_{1,i}}{\partial x_2}$$

$$f_{2,i+1} = f_{2,i} + (x_{1,i+1} - x_{1,i}) \frac{\partial f_{2,i}}{\partial x_1} + (x_{2,i+1} - x_{2,i}) \frac{\partial f_{2,i}}{\partial x_2}$$

$f_{1,i+1}$  and  $f_{2,i+1}$  equal zero



$$\frac{\partial f_{1,i}}{\partial x_1} x_{1,i+1} + \frac{\partial f_{1,i}}{\partial x_2} x_{2,i+1} = -f_{1,i} + x_{1,i} \frac{\partial f_{1,i}}{\partial x_1} + x_{2,i} \frac{\partial f_{1,i}}{\partial x_2}$$

$$\frac{\partial f_{2,i}}{\partial x_1} x_{1,i+1} + \frac{\partial f_{2,i}}{\partial x_2} x_{2,i+1} = -f_{2,i} + x_{1,i} \frac{\partial f_{2,i}}{\partial x_1} + x_{2,i} \frac{\partial f_{2,i}}{\partial x_2}$$

$J$ , Jacobian matrix

Solution

$$[J]\{x_{i+1}\} = -\{f\} + [J]\{x_i\}$$

$$\rightarrow \{x_{i+1}\} = \{x_i\} - [J]^{-1}\{f\}$$

# Nonlinear systems by Newton-Raphson (cont.)

Extending to  $n$  nonlinear equations

$$\frac{\partial f_{k,i}}{\partial x_1} x_{1,i+1} + \frac{\partial f_{k,i}}{\partial x_2} x_{2,i+1} + \cdots + \frac{\partial f_{k,i}}{\partial x_n} x_{n,i+1} = -f_{k,i} + x_{1,i} \frac{\partial f_{k,i}}{\partial x_1} + x_{2,i} \frac{\partial f_{k,i}}{\partial x_2} + \cdots + x_{n,i} \frac{\partial f_{k,i}}{\partial x_n}$$

Jacobian matrix

$$[J] = \begin{bmatrix} \frac{\partial f_{1,i}}{\partial x_1} & \frac{\partial f_{1,i}}{\partial x_2} & \cdots & \frac{\partial f_{1,i}}{\partial x_n} \\ \frac{\partial f_{2,i}}{\partial x_1} & \frac{\partial f_{2,i}}{\partial x_2} & \cdots & \frac{\partial f_{2,i}}{\partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_{n,i}}{\partial x_1} & \frac{\partial f_{n,i}}{\partial x_2} & \cdots & \frac{\partial f_{n,i}}{\partial x_n} \end{bmatrix} \quad \begin{aligned} \{x_i\}^T &= [x_{1,i} \quad x_{2,i} \quad \cdots \quad x_{n,i}] \\ \{x_{i+1}\}^T &= [x_{1,i+1} \quad x_{2,i+1} \quad \cdots \quad x_{n,i+1}] \\ \{f\}^T &= [f_{1,i} \quad f_{2,i} \quad \cdots \quad f_{n,i}] \end{aligned}$$

$$[J]\{x_{i+1}\} = -\{f\} + [J]\{x_i\} \quad \Rightarrow \quad \{x_{i+1}\} = \{x_i\} - [J]^{-1}\{f\}$$

## M-file to implement Newton-Raphson method for nonlinear systems of equations

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```
function [x,f,ea,iter]=newtmult(func,x0,es,maxit)
    if nargin<3|isempty(es), es=0.0001; end
    if nargin<4|isempty(maxit), maxit=50; end
    iter = 0;
    x=x0;
    while (1)
        [J,f]=func(x);
        dx=J\f;
        x=x-dx;
        iter = iter + 1;
        ea=100*max(abs(dx./x));
        if iter>=maxit|ea<=es, break, end
    end
```



## Example of nonlinear equations

- Determining the roots of two nonlinear equations:

$$f_1(x_1, x_2) = \frac{5 + x_1 + x_2}{(50 - 2x_1 - x_2)^2(20 - x_1)} - 4 \times 10^{-4}$$
$$f_2(x_1, x_2) = \frac{(5 + x_1 + x_2)}{(50 - 2x_1 - x_2)(10 - x_2)} - 3.7 \times 10^{-2}$$

The partial derivatives comprising the Jacobian

$$\frac{\partial f_1}{\partial x_1} = \frac{f_1(x_1 + \delta x_1, x_2) - f_1(x_1, x_2)}{\delta x_1} \quad \frac{\partial f_1}{\partial x_2} = \frac{f_1(x_1, x_2 + \delta x_2) - f_1(x_1, x_2)}{\delta x_2}$$
$$\frac{\partial f_2}{\partial x_1} = \frac{f_2(x_1 + \delta x_1, x_2) - f_2(x_1, x_2)}{\delta x_1} \quad \frac{\partial f_2}{\partial x_2} = \frac{f_2(x_1, x_2 + \delta x_2) - f_2(x_1, x_2)}{\delta x_2}$$

## M-file to compute function values and Jacobian

---

```
function [J,f]=jf_2eq(x)
del=0.000001;
df1dx1=(u(x(1)+del*x(1),x(2))-u(x(1),x(2)))/(del*x(1));
df1dx2=(u(x(1),x(2)+del*x(2))-u(x(1),x(2)))/(del*x(2));
df2dx1=(v(x(1)+del*x(1),x(2))-v(x(1),x(2)))/(del*x(1));
df2dx2=(v(x(1),x(2)+del*x(2))-v(x(1),x(2)))/(del*x(2));
J=[df1dx1 df1dx2;df2dx1 df2dx2];
f1=u(x(1),x(2));
f2=v(x(1),x(2));
f=[f1;f2];
```

```
function f=u(x,y)
f = (5 + x + y) / (50 - 2 * x - y) ^ 2 / (20 - x) - 0.0004;
```

```
function f=v(x,y)
f = (5 + x + y) / (50 - 2 * x - y) / (10 - y) - 0.037;
```

## Example of nonlinear equations (cont.)

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Employ the Newton-Raphson method to derive the  $x_1$  and  $x_2$

```
format short e
```

```
x0=[3; 3];
```

```
[x,f,ea,iter]=newtmult(@jf_2eq,x0)
```

After 4 iterations, a solution of  $x_1=3.3366$  and  $x_2=2.6772$  is obtained.

## Reference

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- Steven C. Chapra "Applied Numerical Methods with MATLAB", 3rd ed., McGraw Hill, 2012.