These notes correspond to Section 6.1 in the text.

Systems of Linear Equations

One of the most fundamental problems in computational mathematics is to solve a system of \( n \) linear equations

\[
\begin{align*}
    a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\
    a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\
    \vdots \\
    a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n &= b_n
\end{align*}
\]

for the \( n \) unknowns \( x_1, x_2, \ldots, x_n \). Many data fitting problems, including ones that we have previously discussed such as polynomial interpolation or least-squares approximation, involve the solution of such a system. Discretization of partial differential equations often yields systems of linear equations that must be solved. Systems of nonlinear equations are typically solved using iterative methods that solve a system of linear equations during each iteration. We will now study the solution of this type of problem in detail.

The basic idea behind methods for solving a system of linear equations is to reduce them to linear equations involving a single unknown, because such equations are trivial to solve. Such a reduction is achieved by manipulating the equations in the system in such a way that the solution does not change, but unknowns are eliminated from selected equations until, finally, we obtain an equation involving only a single unknown. These manipulations are called \textit{elementary row operations}, and they are defined as follows:

- Multiplying both sides of an equation by a scalar
- Reordering the equations by interchanging both sides of the \( i \)th and \( j \)th equation in the system
- Replacing equation \( i \) by the sum of equation \( i \) and a multiple of both sides of equation \( j \)

The third operation is by far the most useful. We will now demonstrate how it can be used to reduce a system of equations to a form in which it can easily be solved.
**Example** Consider the system of linear equations

\[
\begin{align*}
    x_1 + 2x_2 + x_3 &= 5, \\
    3x_1 + 2x_2 + 4x_3 &= 17, \\
    4x_1 + 4x_2 + 3x_3 &= 26.
\end{align*}
\]

First, we eliminate \(x_1\) from the second equation by subtracting 3 times the first equation from the second. This yields the equivalent system

\[
\begin{align*}
    x_1 + 2x_2 + x_3 &= 5, \\
    -4x_2 + x_3 &= 2, \\
    4x_1 + 4x_2 + 3x_3 &= 26.
\end{align*}
\]

Next, we subtract 4 times the first equation from the third, to eliminate \(x_1\) from the third equation as well:

\[
\begin{align*}
    x_2 + 2x_2 + x_3 &= 5, \\
    -4x_2 + x_3 &= 2, \\
    -4x_2 - x_3 &= 6.
\end{align*}
\]

Then, we eliminate \(x_2\) from the third equation by subtracting the second equation from it, which yields the system

\[
\begin{align*}
    x_1 + 2x_2 + x_3 &= 5, \\
    -4x_2 + x_3 &= 2, \\
    -2x_3 &= 4.
\end{align*}
\]

This system is in *upper-triangular form*, because the third equation depends only on \(x_3\), and the second equation depends on \(x_2\) and \(x_3\).

Because the third equation is a linear equation in \(x_3\), it can easily be solved to obtain \(x_3 = -2\). Then, we can substitute this value into the second equation, which yields \(-4x_2 = 4\). This equation only depends on \(x_2\), so we can easily solve it to obtain \(x_2 = -1\). Finally, we substitute the values of \(x_2\) and \(x_3\) into the first equation to obtain \(x_1 = 9\). This process of computing the unknowns from a system that is in upper-triangular form is called *back substitution*. □

In general, a system of \(n\) linear equations in \(n\) unknowns is in upper-triangular form if the \(i\)th equation depends only on the unknowns \(x_i, x_{i+1}, \ldots, x_n\), for \(i = 1, 2, \ldots, n\).

It can be seen from this example that continually rewriting a system of equations as it is reduced can be quite tedious. Therefore, we instead represent a system of linear equations using a *matrix*, which is an array of elements, or entries. We say that a matrix \(A\) is \(m \times n\) if it has \(m\) rows and \(n\)
columns, and we denote the element in row \(i\) and column \(j\) by \(a_{ij}\). We also denote the matrix \(A\) by \([a_{ij}]\).

With this notation, a general system of \(n\) equations with \(n\) unknowns can be represented using a matrix \(A\) that contains the coefficients of the equations, a vectors \(\mathbf{x}\) that contains the unknowns, and a vector \(\mathbf{b}\) that contains the quantities on the right-hand sides of the equations. Specifically,

\[
A = \begin{bmatrix}
a_{11} & a_{12} & \cdots & a_{1n} \\
a_{21} & a_{22} & \cdots & a_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
a_{n1} & a_{n2} & \cdots & a_{nn}
\end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix}
x_1 \\
x_2 \\
\vdots \\
x_n
\end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix}
b_1 \\
b_2 \\
\vdots \\
b_n
\end{bmatrix}.
\]

Note that the vectors \(\mathbf{x}\) and \(\mathbf{b}\) are represented by column vectors.

Now, performing row operations on the system can be accomplished by performing them on the augmented matrix

\[
\begin{bmatrix}
A & \mathbf{b}
\end{bmatrix} = \begin{bmatrix}
a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\
a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
a_{n1} & a_{n2} & \cdots & a_{nn} & b_n
\end{bmatrix}.
\]

By working with the augmented matrix instead of the original system, there is no need to continually rewrite the unknowns or arithmetic operators. Once the augmented matrix is reduced to upper triangular form, the corresponding system of linear equations can be solved by back substitution, as before.

The process of eliminating variables from the equations, or, equivalently, zeroing entries of the corresponding matrix, in order to reduce the system to upper-triangular form is called Gaussian elimination. The algorithm is as follows:

\[
\textbf{for } j = 1, 2, \ldots, n - 1 \textbf{ do} \\
\quad \textbf{for } i = j + 1, j + 2, \ldots, n \textbf{ do} \\
\quad \quad m_{ij} = a_{ij}/a_{jj} \\
\quad \quad \textbf{for } k = j + 1, j + 2, \ldots, n \textbf{ do} \\
\quad \quad \quad a_{ik} = a_{ik} - m_{ij}a_{jk} \\
\quad \quad \textbf{end} \\
\quad \quad b_i = b_i - m_{ij}b_j \\
\quad \textbf{end} \\
\textbf{end}
\]

This algorithm requires approximately \(\frac{2}{3}n^3\) arithmetic operations, so it can be quite expensive if \(n\) is large. Later, we will discuss alternative approaches that are more efficient for certain kinds of systems, but Gaussian elimination remains the most generally applicable method of solving systems of linear equations.
The number \( m_{ij} \) is called a multiplier. It is the number by which row \( j \) is multiplied before adding it to row \( i \), in order to eliminate the unknown \( x_j \) from the \( i \)th equation. Note that this algorithm is applied to the augmented matrix, as the elements of the vector \( b \) are updated by the row operations as well.

It should be noted that in the above description of Gaussian elimination, each entry below the main diagonal is never explicitly zeroed, because that computation is unnecessary. It is only necessary to update entries of the matrix that are involved in subsequent row operations or the solution of the resulting upper triangular system. This system is solved by the following algorithm for back substitution. In the algorithm, we assume that \( U \) is the upper triangular matrix containing the coefficients of the system, and \( y \) is the vector containing the right-hand sides of the equations.

\[
\text{for } i = n, n-1, \ldots, 1 \text{ do}
\]
\[
x_i = y_i
\]
\[
\text{for } j = i + 1, i + 2, \ldots, n \text{ do}
\]
\[
x_i = x_i - u_{ij} x_j
\]
\[
\text{end}
\]
\[
x_i = x_i / u_{ii}
\]
\[
\text{end}
\]

This algorithm requires approximately \( n^2 \) arithmetic operations. We will see that when solving systems of equations in which the right-hand side vector \( b \) is changing, but the coefficient matrix \( A \) remains fixed, it is quite practical to apply Gaussian elimination to \( A \) only once, and then repeatedly apply it to each \( b \), along with back substitution, because the latter two steps are much less expensive.

We now illustrate the use of both these algorithms with an example.

**Example** Consider the system of linear equations

\[
x_1 + 2x_2 + x_3 - x_4 = 5 \\
3x_1 + 2x_2 + 4x_3 + 4x_4 = 16 \\
4x_1 + 4x_2 + 3x_3 + 4x_4 = 22 \\
2x_1 + x_3 + 5x_4 = 15.
\]

This system can be represented by the coefficient matrix \( A \) and right-hand side vector \( b \), as follows:

\[
A = \begin{bmatrix}
1 & 2 & 1 & -1 \\
3 & 2 & 4 & 4 \\
4 & 4 & 3 & 4 \\
2 & 0 & 1 & 5
\end{bmatrix}, \quad b = \begin{bmatrix}
5 \\
16 \\
22 \\
15
\end{bmatrix}.
\]
To perform row operations to reduce this system to upper triangular form, we define the augmented matrix
\[
\tilde{A} = \begin{bmatrix} A & b \end{bmatrix} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
3 & 2 & 4 & 4 & 16 \\
4 & 4 & 3 & 4 & 22 \\
2 & 0 & 1 & 5 & 15
\end{bmatrix}.
\]

We first define \( \tilde{A}^{(1)} = \tilde{A} \) to be the original augmented matrix. Then, we denote by \( \tilde{A}^{(2)} \) the result of the first elementary row operation, which entails subtracting 3 times the first row from the second in order to eliminate \( x_1 \) from the second equation:
\[
\tilde{A}^{(2)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & -4 & 1 & 7 & 1 \\
4 & 4 & 3 & 4 & 22 \\
2 & 0 & 1 & 5 & 15
\end{bmatrix}.
\]

Next, we eliminate \( x_1 \) from the third equation by subtracting 4 times the first row from the third:
\[
\tilde{A}^{(3)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & -4 & 1 & 7 & 1 \\
0 & -4 & -1 & 8 & 2 \\
2 & 0 & 1 & 5 & 15
\end{bmatrix}.
\]

Then, we complete the elimination of \( x_1 \) by subtracting 2 times the first row from the fourth:
\[
\tilde{A}^{(4)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & -4 & 1 & 7 & 1 \\
0 & -4 & -1 & 8 & 2 \\
0 & -4 & -1 & 7 & 5
\end{bmatrix}.
\]

We now need to eliminate \( x_2 \) from the third and fourth equations. This is accomplished by subtracting the second row from the third, which yields
\[
\tilde{A}^{(5)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & -4 & 1 & 7 & 1 \\
0 & 0 & -2 & 1 & 1 \\
0 & -4 & -1 & 7 & 5
\end{bmatrix},
\]

and the fourth, which yields
\[
\tilde{A}^{(6)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & -4 & 1 & 7 & 1 \\
0 & 0 & -2 & 1 & 1 \\
0 & 0 & -2 & 0 & 4
\end{bmatrix}.
\]
Finally, we subtract the third row from the fourth to obtain the augmented matrix of an upper-
triangular system,

$$\tilde{A}^{(7)} = \begin{bmatrix}
1 & 2 & 1 & 1 & -1 & 5 \\
0 & -4 & 1 & 7 & 1 \\
0 & 0 & -2 & 1 & 1 \\
0 & 0 & 0 & -1 & 3 \\
\end{bmatrix}.$$ 

Note that in a matrix for such a system, all entries below the main diagonal (the entries where the row index is equal to the column index) are equal to zero. That is, $a_{ij} = 0$ for $i > j$.

Now, we can perform back substitution on the corresponding system,

$$x_1 + 2x_2 + x_3 - x_4 = 5,$$
$$-4x_2 + x_3 + 7x_4 = 1,$$
$$-2x_3 + x_4 = 1,$$
$$-x_4 = 3,$$

to obtain the solution, which yields $x_4 = -3$, $x_3 = -2$, $x_2 = -6$, and $x_1 = 16$. □

It can be seen from the above pseudocode that the algorithms for Gaussian elimination and back substitution can break down if a diagonal element of the matrix is equal to zero. In order to work around this potential pitfall, another elementary row operation can be used: a row interchange. If, when computing the multiplier $m_{ij}$ during Gaussian elimination, the entry $a_{jj}$ is equal to zero, then, to avoid breakdown of the algorithm, row $j$ of the augmented matrix can be interchanged with row $i$, for some $i > j$, where $a_{ij} \neq 0$, and then Gaussian elimination can continue.

**Example** Consider the system of linear equations

$$x_1 + 2x_2 + x_3 - x_4 = 5,$$
$$3x_1 + 6x_2 + 4x_3 + 4x_4 = 16,$$
$$4x_1 + 4x_2 + 3x_3 + 4x_4 = 22,$$
$$2x_1 + x_3 + 5x_4 = 15.$$ 

The coefficient matrix $A$ and the right-hand side vector $b$ for this system are

$$A = \begin{bmatrix}
1 & 2 & 1 & -1 \\
3 & 6 & 4 & 4 \\
4 & 4 & 3 & 4 \\
2 & 0 & 1 & 5
\end{bmatrix}, \quad b = \begin{bmatrix}
5 \\
16 \\
22 \\
15
\end{bmatrix}.$$ 

To perform Gaussian elimination on this system, we perform row operations on the augmented
matrix
\[ \tilde{A} = \begin{bmatrix} \lambda \\ \Lambda \end{bmatrix} = \begin{bmatrix} 1 & 2 & 1 & -1 & 5 \\ 3 & 6 & 4 & 4 & 16 \\ 4 & 4 & 3 & 4 & 22 \\ 2 & 0 & 1 & 5 & 15 \end{bmatrix}. \]

We first set \( \tilde{A}^{(1)} = \tilde{A} \), and then subtract 3 times the first row from the second row in \( A^{(1)} \) to obtain
\[ \tilde{A}^{(2)} = \begin{bmatrix} 1 & 2 & 1 & -1 & 5 \\ 0 & 0 & 1 & 7 & 1 \\ 4 & 4 & 3 & 4 & 22 \\ 2 & 0 & 1 & 5 & 15 \end{bmatrix}. \]

Then, we subtract 4 times the first row from the second to obtain
\[ \tilde{A}^{(3)} = \begin{bmatrix} 1 & 2 & 1 & -1 & 5 \\ 0 & 0 & 1 & 7 & 1 \\ 0 & -4 & -1 & 8 & 2 \\ 2 & 0 & 1 & 5 & 15 \end{bmatrix}. \]

We complete the elimination of \( x_1 \) by subtracting 2 times the first row from the fourth, which yields
\[ \tilde{A}^{(4)} = \begin{bmatrix} 1 & 2 & 1 & -1 & 5 \\ 0 & 0 & 1 & 7 & 1 \\ 0 & -4 & -1 & 8 & 2 \\ 0 & -4 & -1 & 7 & 5 \end{bmatrix}. \]

Normally, we would continue by subtracting multiples of the second row from the third and fourth, to eliminate \( x_2 \) from the third and fourth equations, but the computing the multiples requires dividing by \( [\tilde{A}^{(4)}]_{22} \), which is zero. Therefore, we interchange the second and third rows, which yields
\[ \tilde{A}^{(5)} = \begin{bmatrix} 1 & 2 & 1 & -1 & 5 \\ 0 & -4 & -1 & 8 & 2 \\ 0 & 0 & 1 & 7 & 1 \\ 0 & -4 & -1 & 7 & 5 \end{bmatrix}. \]

We then subtract the (new) second row from the fourth to obtain
\[ \tilde{A}^{(6)} = \begin{bmatrix} 1 & 2 & 1 & -1 & 5 \\ 0 & -4 & -1 & 8 & 2 \\ 0 & 0 & 1 & 7 & 1 \\ 0 & 0 & 0 & -1 & 3 \end{bmatrix}. \]

This matrix is already in upper-triangular form, so there is no need to subtract a multiple of the third row from the fourth, as Gaussian elimination would normally require. Now, we can perform
back substitution as usual to obtain the solution, which is \( x_1 = 4, x_2 = -12, x_3 = 22, \) and \( x_4 = -3. \)

\[ \square \]

Of course, it may happen that there is no suitable row \( i \) with which row \( j \) can be interchanged. In this case, Gaussian elimination fails, and it can be concluded that the system of equations does not have a unique solution. There are two possibilities that remain: either there is no solution, or there are infinitely many solutions. To determine which scenario applies, one can continue to apply Gaussian elimination with the remaining columns of the coefficient matrix. Because there is at least one column, column \( j \), for which all entries on or below the diagonal are equal to zero, it will follow that at least one equation in the system will have all coefficients equal to zero. If the corresponding element on the right-hand side of the equation is nonzero, then there is no solution, but if it is zero, then there are infinitely many solutions.

**Example** Consider the system of linear equations

\[
\begin{align*}
-x_1 + 2x_2 + x_3 - x_4 &= 5 \\
3x_1 + 6x_2 + 4x_3 + 4x_4 &= 16 \\
4x_1 + 8x_2 + 3x_3 + 4x_4 &= 22 \\
2x_1 + 4x_2 + x_3 + 5x_4 &= 15.
\end{align*}
\]

The coefficient matrix \( A \) and the right-hand side vector \( b \) for this system are

\[
A = \begin{bmatrix}
1 & 2 & 1 & -1 \\
3 & 6 & 4 & 4 \\
4 & 8 & 3 & 4 \\
2 & 4 & 1 & 5
\end{bmatrix}, \quad b = \begin{bmatrix}
5 \\
16 \\
22 \\
15
\end{bmatrix}.
\]

To perform Gaussian elimination on this system, we perform row operations on the augmented matrix

\[
\tilde{A} = [A \ b] = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
3 & 6 & 4 & 4 & 16 \\
4 & 8 & 3 & 4 & 22 \\
2 & 4 & 1 & 5 & 15
\end{bmatrix}.
\]

We first set \( \tilde{A}^{(1)} = \tilde{A} \), and then subtract 3 times the first row from the second row in \( A^{(1)} \) to obtain

\[
\tilde{A}^{(2)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & 0 & 1 & 7 & 1 \\
4 & 8 & 3 & 4 & 22 \\
2 & 4 & 1 & 5 & 15
\end{bmatrix}.
\]
Then, we subtract 4 times the first row from the second to obtain

\[ \tilde{A}^{(3)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & 0 & 1 & 7 & 1 \\
0 & 0 & -1 & 8 & 2 \\
2 & 4 & 1 & 5 & 15
\end{bmatrix}. \]

We complete the elimination of \( x_1 \) by subtracting 2 times the first row from the fourth, which yields

\[ \tilde{A}^{(4)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & 0 & 1 & 7 & 1 \\
0 & 0 & -1 & 8 & 2 \\
0 & 0 & -1 & 7 & 5
\end{bmatrix}. \]

Normally, we would continue by subtracting multiples of the second row from the third and fourth, to eliminate \( x_2 \) from the third and fourth equations, but the computing the multiples requires dividing by \( [\tilde{A}^{(4)}]_{22} \), which is zero. However, we cannot solve this problem by interchanging the second row with either the third or fourth row, because the elements in those rows, and the second column, are also zero. Therefore, this system does not have a unique solution.

To determine whether there is a solution at all, we continue the elimination process with \( x_3 \), in order to zero elements in the third column. We first add the second row to the third, which yields

\[ \tilde{A}^{(5)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & 0 & 1 & 7 & 1 \\
0 & 0 & 0 & 15 & 3 \\
0 & 0 & -1 & 7 & 5
\end{bmatrix}. \]

We also add the second row to the fourth to obtain

\[ \tilde{A}^{(6)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & 0 & 1 & 7 & 1 \\
0 & 0 & 0 & 15 & 3 \\
0 & 0 & 0 & 14 & 6
\end{bmatrix}. \]

Finally, we subtract 14/15 times the third row from the fourth to complete the elimination:

\[ \tilde{A}^{(7)} = \begin{bmatrix}
1 & 2 & 1 & -1 & 5 \\
0 & 0 & 1 & 7 & 1 \\
0 & 0 & 0 & 15 & 3 \\
0 & 0 & 0 & 0 & 16/5
\end{bmatrix}. \]

The fourth row corresponds to the equation \( 0 = 16/5 \), which is a contradiction. Therefore, we conclude that the original system of linear equations has no solution. If the value on the right-hand side of this equation had been zero, then the original system would have infinitely many solutions. \( \square \)