2021 Spring MAS 365
Chapter 6: Direct Methods for Solving Linear Systems

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Mar/17, 2021

Introduction

- This chapter studies **direct methods** for solving a linear system of n equations in n variables.

$$
\begin{aligned}
E_1 &: a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1,\\
E_2 &: a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2,\\
&\qquad\qquad\qquad\qquad\vdots\\
E_n &: a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n.
\end{aligned}
$$

- Direct techniques are methods that theoretically give the exact solution to the system in a finite number of steps. In practice, it is affected by the round-off error, which we study in this chapter.

- Chapter 7 considers methods of approximating the solution to linear systems using iterative methods.

Elementary Operations

- Multiply E_i by $\lambda \neq 0$: $(\lambda E_i) \rightarrow (E_i)$
- Multiply E_j by λ and add to E_i: $(E_i + \lambda E_j) \rightarrow (E_i)$
- Interchange E_i and E_j: $(E_i) \leftrightarrow (E_j)$

- By a sequence of these operations, a linear system will be systematically transformed into a new linear system that is more easily solved and has the same solutions.

Gaussian Elimination with Backward Substitution

- Form the augmented matrix $\tilde{A}$

$$\tilde{A} = [A, \boldsymbol{b}] = \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & a_{1,n+1} \\ a_{21} & a_{22} & \cdots & a_{2n} & a_{2,n+1} \\ \vdots & \vdots & & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & a_{n,n+1} \end{array}\right]$$

- Provided $a_{11} \neq 0$, perform

$$(E_j - (a_{j1}/a_{11})E_1) \to (E_j) \quad \text{for each } j = 2, 3, \ldots, n$$

to eliminate the coefficient of x_1 in each of these rows.

- For simplicity, we will continue to use the notation a_{ij}, even though it is expected to change after the operations.

Gaussian Elimination with Backward Substitution (cont'd)

- Provided $a_{ii} \neq 0$ we perform the following operation sequentially

$$(E_j - (a_{ji}/a_{ii})E_i) \rightarrow (E_j) \quad \text{for each } j = i+1, i+2, \ldots, n.$$

- We then have

$$\tilde{\tilde{A}} = \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & a_{1,n+1} \\ 0 & a_{22} & \cdots & a_{2n} & a_{2,n+1} \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & a_{nn} & a_{n,n+1} \end{array}\right]$$

Gaussian Elimination with Backward Substitution (cont'd)

- The new linear system is triangular

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= a_{1,n+1}, \\ a_{22}x_2 + \cdots + a_{2n}x_n &= a_{2,n+1}, \\ &\vdots \\ a_{nn}x_n &= a_{n,n+1}. \end{aligned}$$

- Backward substitution

$$\begin{aligned} x_n &= \frac{a_{n,n+1}}{a_{nn}} \\ x_i &= \frac{a_{i,n+1} - \sum_{j=i+1}^{n} a_{ij}x_j}{a_{ii}}, \quad \text{for each } i = n-1, n-2, \ldots, 1. \end{aligned}$$

Gaussian Elimination with Backward Substitution (cont'd)

- Describe Gaussian elimination by forming a sequence of augmented matrices $\tilde{A}^{(1)} = \tilde{A}, \tilde{A}^{(2)}, \ldots, \tilde{A}^{(n)}$, where $\tilde{A}^{(k)}$ has entries $a_{ij}^{(k)}$:

$$a_{ij}^{(k)} = \begin{cases} a_{ij}^{(k-1)}, & i = 1, 2, \ldots, k-1, \text{ and } j = 1, 2, \ldots, n+1, \\ 0, & i = k, k+1, \ldots, n, \text{ and } j = 1, 2, \ldots, k-1, \\ a_{ij}^{(k-1)} - \dfrac{a_{i,k-1}^{(k-1)}}{a_{k-1,k-1}^{(k-1)}} a_{k-1,j}^{(k-1)}, & i = k, k+1, \ldots, n, \text{ and } j = k, k+1, \ldots, n+1. \end{cases}$$

- Thus

$$\tilde{A}^{(k)} = \left[\begin{array}{cccccccc:c} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1,k-1}^{(1)} & a_{1k}^{(1)} & \cdots & a_{1n}^{(1)} & a_{1,n+1}^{(1)} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} & \cdots & a_{2,k-1}^{(2)} & a_{2k}^{(2)} & \cdots & a_{2n}^{(2)} & a_{2,n+1}^{(2)} \\ \vdots & \ddots & \ddots & & \vdots & \vdots & & \vdots & \vdots \\ \vdots & & \ddots & \ddots & a_{k-1,k-1}^{(k-1)} & a_{k-1,k}^{(k-1)} & \cdots & a_{k-1,n}^{(k-1)} & a_{k-1,n+1}^{(k-1)} \\ \vdots & & & \ddots & 0 & a_{kk}^{(k)} & \cdots & a_{kn}^{(k)} & a_{k,n+1}^{(k)} \\ \vdots & & & & \vdots & \vdots & & \vdots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & a_{nk}^{(k)} & \cdots & a_{nn}^{(k)} & a_{n,n+1}^{(k)} \end{array}\right]$$

Gaussian Elimination with Backward Substitution (cont'd)

- This will fail if one of the elements $a_{11}^{(1)}, a_{22}^{(2)}, \ldots, a_{nn}^{(n)}$ is zero because the step

$$\left(E_i - \frac{a_{i,k}^{(k)}}{a_{kk}^{(k)}}(E_k)\right) \to E_i$$

  either cannot be performed (if one of $a_{11}^{(1)}, a_{22}^{(2)}, \ldots, a_{n-1,n-1}^{(n-1)}$ is zero) or the backward substitution cannot be accomplished (if $a_{nn}^{(n)} = 0$).

- We need some change in the method.

Gaussian Elimination with Backward Substitution (cont'd)

Ex. Represent the linear system

$$\begin{aligned} E_1 &: x_1 - x_2 + 2x_3 - x_4 = -8, \\ E_2 &: 2x_1 - 2x_2 + 3x_3 - 3x_4 = -20, \\ E_3 &: x_1 + x_2 + x_3 = -2, \\ E_4 &: x_1 - x_2 + 4x_3 + 3x_4 = 4, \end{aligned}$$

as an augmented matrix and use Gaussian Elimination to find its solution.

Sol. The first two augmented matrices are

$$\tilde{A}^{(1)} = \left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 2 & -2 & 3 & -3 & -20 \\ 1 & 1 & 1 & 0 & -2 \\ 1 & -1 & 4 & 3 & 4 \end{array}\right] \quad \text{and} \quad \tilde{A}^{(2)} = \left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 0 & 0 & -1 & -1 & -4 \\ 0 & 2 & -1 & 1 & 6 \\ 0 & 0 & 2 & 4 & 12 \end{array}\right]$$

- $a_{22}^{(2)}$, called the **pivot element**, is 0.
  The pivot element for a specific column is the entry that is used to place zeros in the other entries in that column.

Gaussian Elimination with Backward Substitution (cont'd)

Sol. Since $a_{32}^{(2)} \neq 0$, we perform $(E_2) \leftrightarrow (E_3)$, which yields

$$\tilde{A}^{(2)'} = \left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 0 & 2 & -1 & 1 & 6 \\ 0 & 0 & -1 & -1 & -4 \\ 0 & 0 & 2 & 4 & 12 \end{array}\right]$$

- We now already have $\tilde{A}^{(3)} = \tilde{A}^{(2)'}$, the next step gives

$$\tilde{A}^{(4)} = \left[\begin{array}{cccc|c} 1 & -1 & 2 & -1 & -8 \\ 0 & 2 & -1 & 1 & 6 \\ 0 & 0 & -1 & -1 & -4 \\ 0 & 0 & 0 & 2 & 4 \end{array}\right]$$

and the backward substitution provides the solution.

Gaussian Elimination with Backward Substitution (cont'd)

- When $a_{kk}^{(k)} = 0$, search the first nonzero entry of the kth column of $\tilde{A}^{(k)}$ from the kth row to the nth row.

1. If $a_{pk}^{(k)} \neq 0$ for some p, with $k+1 \leq p \leq n$, then $(E_k) \leftrightarrow (E_p)$ is performed to obtain $\tilde{A}^{(k)'}$.

2. If $a_{pk}^{(k)} = 0$ for each p, with $k \leq p \leq n$, it can be shown that the linear system does not have a unique solution and the procedure stops.

Pivoting

- To reduce round-off error, it is often necessary to perform row interchanges even when the pivot elements are not zero. When and why?

Pivoting (cont'd)

- If $a_{kk}^{(k)}$ is small in magnitude compared to $a_{jk}^{(k)}$, then the magnitude of the multiplier

$$m_{jk} = \frac{a_{jk}^{(k)}}{a_{kk}^{(k)}}$$

will be much larger than 1. Round-off error introduced in the computation of one of the terms $a_{kl}^{(k)}$ is multiplied by m_{jk} when computing $a_{jl}^{(k+1)}$.

Pivoting (cont'd)

- Also, when performing the backward substitution for

$$x_k = \frac{a_{k,n+1}^{(k)} - \sum_{j=k+1}^{n} a_{kj}^{(k)}}{a_{kk}^{(k)}}$$

with a small value of $a_{kk}^{(k)}$, any error in the numerator can be dramatically increased.

Pivoting (cont'd)

Ex. Apply Gaussian elimination to the system

$$E_1 \;:\; 0.003000x_1 + 59.14x_2 = 59.17,$$
$$E_2 \;:\; 5.291x_1 - 6.130x_2 = 46.78,$$

using four-digit arithmetic with rounding, and compare the results to the exact solution $x_1 = 10.00$ and $x_2 = 1.000$.

Pivoting (cont'd)

Sol. The first pivot element, $a_{11}^{(1)} = 0.003000$, is small, and its associated multiplier,

$$m_{21} = \frac{5.291}{0.003000} = 1763.\overline{6} \approx 1764.$$

Performing $(E_2 - m_{21}E_1) \to (E_2)$ with appropriate round gives

$$\begin{aligned} 0.003000x_1 + 59.14x_2 &\approx 59.17, \\ -104300x_2 &= -104400, \end{aligned}$$

instead of the exact system

$$\begin{aligned} 0.003000x_1 + 59.14x_2 &= 59.17, \\ -104309.37\overline{6}x_2 &= -104309.37\overline{6}. \end{aligned}$$

Pivoting (cont'd)

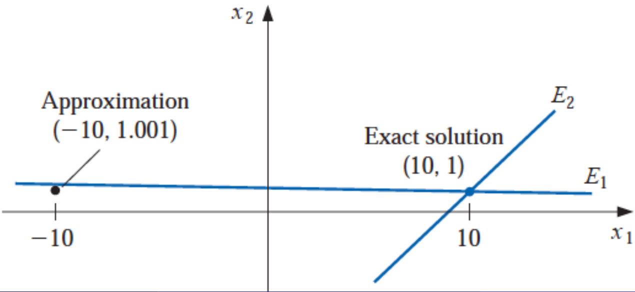
Sol. Backward substitution yields

$$x_2 \approx 1.001,$$

which is close to the actual value $x_2 = 1.000$. However, we have

$$x_1 \approx \frac{59.17 - (59.14)(1.001)}{0.003000} = -10.00,$$

where the the small error 0.001 is multiplied by $\frac{59.14}{0.003000} \approx 20000$. The actual value is $x_1 = 10.00$.



Pivoting (cont'd)

- Difficulties can arise when the pivot element $a_{kk}^{(k)}$ is small relative to the entries $a_{ij}^{(k)}$ for $k \leq i \leq n$ and $k \leq j \leq n$.
- To avoid this, pivoting is performed by selecting an element $a_{pq}^{(k)}$ with a larger magnitude as the pivot. Then we interchange the kth and pth rows, followed by the interchange of the kth and qth columns, if necessary.

- Partial pivoting (maximal column pivoting)
- Scaled partial pivoting (scaled column pivoting)
- Complete pivoting (maximal pivoting)

Partial Pivoting

- Partial pivoting (maximal column pivoting):

  Determine the smallest $p \geq k$ such that

  $$|a_{pk}^{(k)}| = \max_{k \leq i \leq n} |a_{ik}^{(k)}|$$

  and perform $(E_k) \leftrightarrow (E_p)$.

Partial Pivoting (cont'd)

Ex. Apply Gaussian elimination to the system

$$\begin{aligned} E_1 &: 0.003000x_1 + 59.14x_2 = 59.17, \\ E_2 &: 5.291x_1 - 6.130x_2 = 46.78, \end{aligned}$$

using partial pivoting and four-digit arithmetic with rounding, and compare the results to the exact solution $x_1 = 10.00$ and $x_2 = 1.000$.

Partial Pivoting (cont'd)

Sol. The multiplier for this system is

$$m_{21} = \frac{a_{21}^{(1)}}{a_{11}^{(1)}} = 0.0005670,$$

and the operation $(E_2 - m_{21}E_1) \to (E_2)$ yields

$$\begin{aligned} 5.291x_1 - 6.130x_2 &\approx 46.78, \\ 59.14x_2 &\approx 59.14, \end{aligned}$$

which gives the correct values.

Partial Pivoting (cont'd)

Ex. Apply Gaussian elimination to the system

$$\begin{aligned} E_1 &: 30.00x_1 + 591400x_2 = 591700, \\ E_2 &: 5.291x_1 - 6.130x_2 = 46.78, \end{aligned}$$

using partial pivoting and four-digit arithmetic with rounding.

Sol. The maximal value in the first column is 30.00 and the multiplier

$$m_{21} = \frac{5.291}{30.00} = 0.1764$$

yields

$$\begin{aligned} 30.00x_1 + 591400x_2 &\approx 591700, \\ -104300x_2 &\approx -104400, \end{aligned}$$

which has the inaccurate solution $x_1 = -10.00$ and $x_2 = 1.001$.

Scaled Partial Pivoting

- Scaled partial pivoting (scaled column pivoting): place the element in the pivot position that is largest relative to the entries in its row.

1. Define a scale factor s_i for each row as

$$s_i = \max_{1 \le j \le n} |a_{ij}|.$$

Let $s_i \neq 0$ for all i. Otherwise, the system has no unique solution.

2. Choose the least integer p with

$$\frac{|a_{p1}|}{s_p} = \max_{1 \le k \le n} \frac{|a_{k1}|}{s_k}$$

and perform $(E_k) \leftrightarrow (E_p)$. This ensures that the largest element in each row has a relative magnitude of 1 before the comparison for row interchange is performed.

Scaled Partial Pivoting (cont'd)

3. Similarly, before eliminating the variable x_i using $E_k - m_{ki}E_i$, we select the smallest integer $p \geq i$ with

$$\frac{|a_{pi}|}{s_p} = \max_{1 \leq k \leq n} \frac{|a_{ki}|}{s_k}$$

and perform $(E_i) \leftrightarrow (E_p)$ if $i \neq p$.

Scaled Partial Pivoting (cont'd)

Ex. Apply Gaussian elimination to the system

$$\begin{aligned} E_1 &: 30.00x_1 + 591400x_2 = 591700, \\ E_2 &: 5.291x_1 - 6.130x_2 = 46.78, \end{aligned}$$

using scaled partial pivoting and four-digit arithmetic with rounding.

Complete Pivoting

- Complete (or maximal) pivoting: at the kth step searches all the entries a_{ij}, for $i = k, k+1, \ldots, n$ and $j = k, k+1, \ldots, n$, to find the entry with the largest magnitude. Both row and column interchanges are performed to bring this entry to the pivot position.

- The total time required to incorporate complete pivoting is

$$\sum_{k=2}^{n}(k^2 - 1) = \frac{n(n-1)(2n+5)}{6} \text{ comparisons.}$$

- Scaled partial pivoting requires a total of

$$n(n-1) + \sum_{k=1}^{n-1} k = \frac{3}{2}n(n-1) \text{ comparisons, and}$$

$$\sum_{k=2}^{n} k = \frac{1}{2}(n-1)(n+2) \text{ divisions.}$$