Ch06-2 Linear Systems of Equations, Pivoting Strategies

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Outline

1 Why Pivoting May be Necessary

2 Gaussian Elimination with Partial Pivoting

3 Gaussian Elimination with Scaled Partial (Scaled-Column) Pivoting

Pivoting Strategies: Motivation

When is Pivoting Required?

- In deriving the Gaussin Elimination with Backward Subsitition algorithm, we found that a row interchange was needed when one of the pivot elements $a_{kk}^{(k)}$ is 0.
- This row interchange has the form $(E_k) \leftrightarrow (E_p)$, where p is the smallest integer greater than k with $a_{pk}^{(k)} \neq 0$.
- To reduce round-off error, it is often necessary to perform row interchanges even when the pivot elements are not zero.

Pivoting Strategies: Motivation

When is Pivoting Required? (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 $a_{jl}^{(k+1)}$, which compounds the original error.

Pivoting Strategies: Motivation

When is Pivoting Required? (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 because of the division by $a_{kk}^{(k)}$.
- The following example will show that even for small systems, round-off error can dominate the calculations.

Pivoting Strategies: Motivation

Example

Apply Gaussian elimination to the system

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

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

Pivoting Strategies: Motivating Example

Solution (1/4)

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

$$m_{21} = \frac{5.291}{0.003000} = 1763.6\overline{6}$$

rounds to the large number 1764.

- Performing $(E_2 - m_{21}E_1) \to (E_2)$ and the appropriate rounding gives the system

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

Pivoting Strategies: Motivating Example

Solution (2/4)

We obtained

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

instead of the exact system, which is

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

The disparity in the magnitudes of $m_{21}a_{13}$ and a_{23} has introduced round-off error, but the round-off error has not yet been propagated.

Pivoting Strategies: Motivating Example

Solution (3/4)

Backward substitution yields

$$x_2 \approx 1.001$$

which is a close approximation to the actual value, $x_2 = 1.000$. However, because of the small pivot $a_{11} = 0.003000$,

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

contains the small error of 0.001 multiplied by

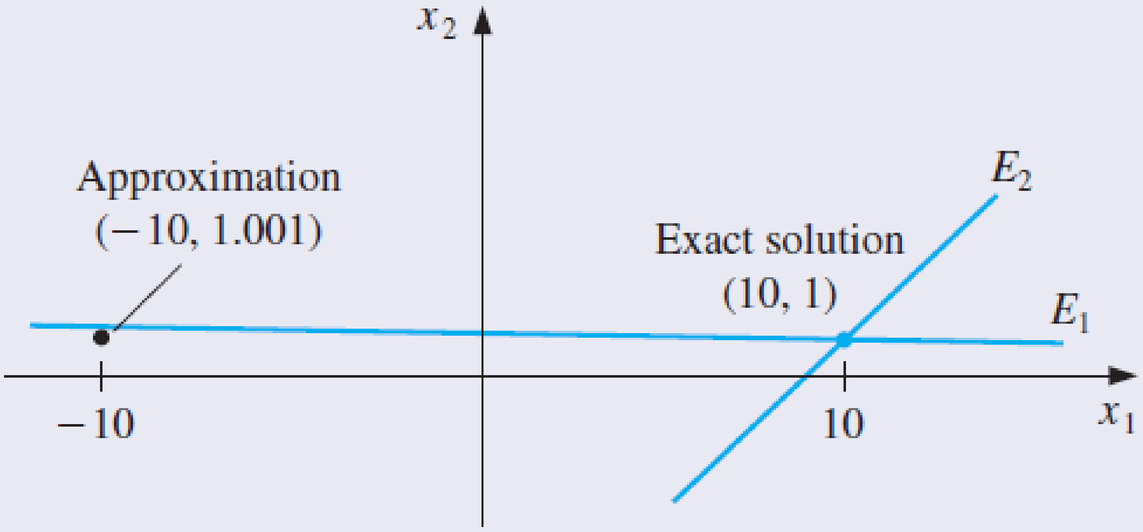
$$\frac{59.14}{0.003000} \approx 20000$$

This ruins the approximation to the actual value $x_1 = 10.00$.

Pivoting Strategies: Motivating Example

Solution (4/4)

This is clearly a contrived example and the graph shows why the error can so easily occur.



For larger systems it is much more difficult to predict in advance when devastating round-off error might occur.

Gaussian Elimination with Partial Pivoting

Meeting a small pivot element

- The last example shows how 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 problem, pivoting is performed by selecting an element $a_{pq}^{(k)}$ with a larger magnitude as the pivot, and interchanging the kth and pth rows.
- This can be followed by the interchange of the kth and qth columns, if necessary.

Gaussian Elimination with Partial Pivoting

The Partial Pivoting Strategy

- The simplest strategy is to select an element in the same column that is below the diagonal and has the largest absolute value;
- specifically, we determine the smallest $p \geq k$ such that

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

  and perform $(E_k) \leftrightarrow (E_p)$.
- In this case no interchange of columns is used.

Gaussian Elimination with Partial Pivoting

Example

Apply Gaussian elimination to the system

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

using partial pivoting and 4-digit arithmetic with rounding, and compare the results to the exact solution $x_1 = 10.00$ and $x_2 = 1.000$.

Gaussian Elimination with Partial Pivoting

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

Solution (1/3)

The partial-pivoting procedure first requires finding

$$\max\left\{|a_{11}^{(1)}|, |a_{21}^{(1)}|\right\} = \max\{|0.003000|, |5.291|\} = |5.291| = |a_{21}^{(1)}|$$

This requires that the operation $(E_2) \leftrightarrow (E_1)$ be performed to produce the equivalent system

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

Gaussian Elimination with Partial Pivoting

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

Solution (2/3)

The multiplier for this system is

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

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

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

Gaussian Elimination with Partial Pivoting

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

Solution (3/3)

The 4-digit answers resulting from the backward substitution are the correct values

$$x_1 = 10.00 \qquad \text{and} \qquad x_2 = 1.000$$

Gaussian Elimination/Partial Pivoting Algorithm (1/4)

To solve the $n \times n$ linear system

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

INPUT number of unknowns and equations n; augmented matrix $A = [a_{ij}]$ where $1 \le i \le n$ and $1 \le j \le n+1$.

OUTPUT solution $x_1, \ldots, x_n$ or message that the linear system has no unique solution.

Gaussian Elimination/Partial Pivoting Algorithm (2/4)

Step 1 For $i = 1, \ldots, n$ set $NROW(i) = i$ (*Initialize row pointer*)

Step 2 For $i = 1, \ldots, n-1$ do Steps 3–6 (*Elimination process*)

Step 3 Let p be the smallest integer with $i \leq p \leq n$ and
$|a(NROW(p), i)| = \max_{i \leq j \leq n} |a(NROW(j), i)|$
(*Notation:* $a(NROW(i), j) \equiv a_{NROW_i, j}$)

Step 4 If $a(NROW(p), i) = 0$ then
OUTPUT('no unique solution exists')
STOP

Step 5 If $NROW(i) \neq NROW(p)$ then set $NCOPY = NROW(i)$
$NROW(i) = NROW(p)$
$NROW(p) = NCOPY$
(*Simulated row interchange*)

Gaussian Elimination/Partial Pivoting Algorithm (3/4)

Step 6 For $j = i + 1, \ldots, n$ do Steps 7 & 8

Step 7 Set

$$m(NROW(j), i) = a(NROW(j), i)/a(NROW(i), i)$$

Step 8 Perform

$$(E_{NROW(j)} - m(NROW(j), i) \cdot E_{NROW(i)}) \rightarrow (E_{NROW(j)})$$

Step 9 If $a(NROW(n), n) = 0$ then

OUTPUT('no unique solution exists')

STOP

Gaussian Elimination/Partial Pivoting Algorithm (4/4)

Step 10 Set $x_n = a(NROW(n), n+1)/a(NROW(n), n)$
(Start backward substitution)

Step 11 For $i = n-1, \ldots, 1$

$$\text{set } x_i = \frac{a(NROW(i), n+1) - \sum_{j=i+1}^{n} a(NROW(i), j) \cdot x_j}{a(NROW(i), i)}$$

Step 12 OUTPUT $(x_1, \ldots, x_n)$ *(Procedure completed successfully)*
STOP

Gaussian Elimination with Partial Pivoting

Can Partial Pivoting fail?

- Each multiplier m_{ji} in the partial pivoting algorithm has magnitude less than or equal to 1.
- Although this strategy is sufficient for many linear systems, situations do arise when it is inadequate.
- The following (contrived) example illusrates the point.

Gaussian Elimination with Partial Pivoting

Example: When Partial Pivoting Fails

The linear system

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

is the same as that in the two previous examples except that all the entries in the first equation have been multiplied by 10^4.

The partial pivoting procedure described in the algorithm with 4-digit arithmetic leads to the same incorrect results as obtained in the first example (Gaussian elimination without pivoting).

Gaussian Elimination with Partial Pivoting

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

Apply Partial Pivoting

The maximal value in the first column is 30.00, and the multiplier

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

leads to the system

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

which has the same inaccurate solutions as in the first example: $x_2 \approx 1.001$ and $x_1 \approx -10.00$.

Gaussian Elimination with Scaled Partial Pivoting

Scaled Partial Pivoting

- Scaled partial pivoting places the element in the pivot position that is largest relative to the entries in its row.
- The first step in this procedure is to define a scale factor s_i for each row as
$$s_i = \max_{1 \le j \le n} |a_{ij}|$$
- If we have $s_i = 0$ for some i, then the system has no unique solution since all entries in the ith row are 0.

Gaussian Elimination with Scaled Partial Pivoting

Scaled Partial Pivoting (Cont'd)

- Assuming that this is not the case, the appropriate row interchange to place zeros in the first column is determined by choosing the least integer p with

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

  and performing $(E_1) \leftrightarrow (E_p)$.
- The effect of scaling is to ensure that the largest element in each row has a relative magnitude of 1 before the comparison for row interchange is performed.

Gaussian Elimination with Scaled Partial Pivoting

Scaled Partial Pivoting (Cont'd)

- In a similar manner, before eliminating the variable x_i using the operations
$$E_k - m_{ki}E_i, \quad \text{for } k = i+1, \ldots, n,$$
we select the smallest integer $p \geq i$ with
$$\frac{|a_{pi}|}{s_p} = \max_{i \leq k \leq n} \frac{|a_{ki}|}{s_k}$$
and perform the row interchange $(E_i) \leftrightarrow (E_p)$ if $i \neq p$.
- The scale factors $s_1, \ldots, s_n$ are computed only once, at the start of the procedure.
- They are row dependent, so they must also be interchanged when row interchanges are performed.

Gaussian Elimination with Scaled Partial Pivoting

Example

Returning to the previous ewxample, we will appl scaled partial pivoting for the linear system:

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

Gaussian Elimination with Scaled Partial Pivoting

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

Solution (1/2)

We compute

$$\begin{aligned} s_1 &= \max\{|30.00|, |591400|\} = 591400 \\ \text{and} \qquad s_2 &= \max\{|5.291|, |-6.130|\} = 6.130 \end{aligned}$$

so that

$$\frac{|a_{11}|}{s_1} = \frac{30.00}{591400} = 0.5073 \times 10^{-4}, \qquad \frac{|a_{21}|}{s_2} = \frac{5.291}{6.130} = 0.8631,$$

and the interchange $(E_1) \leftrightarrow (E_2)$ is made.

Gaussian Elimination with Scaled Partial Pivoting

Solution (2/2)

Applying Gaussian elimination to the new system

$$5.291x_1 - 6.130x_2 = 46.78$$
$$30.00x_1 + 591400x_2 = 591700$$

produces the correct results: $x_1 = 10.00$ and $x_2 = 1.000$.

Gaussian Elimination/Scaled Partial Pivoting Algorithm

The only steps in this algorithm that differ from those of the Gaussian Elimination with Scaled Partial Pivoting Algorithm are:

Step 1 For $i = 1, \ldots, n$ set $s_i = \max_{1 \leq j \leq n} |a_{ij}|$
if $s_i = 0$ then OUTPUT ('no unique solution exists')
STOP
else set $NROW(i) = i$

Step 2 For $i = 1, \ldots, n-1$ do Steps 3–6 (*Elimination process*)

Step 3 Let p be the smallest integer with $i \leq p \leq n$ and

$$\frac{|a(NROW(p), i)|}{s(NROW(p))} = \max_{i \leq j \leq n} \frac{|a(NROW(j), i)|}{s(NROW(j))}$$