GPU Teaching Kit

Accelerated Computing

Module 12 – Floating-Point Considerations

Lecture 12.2 - Numerical Stability

Objective

- Understand numerical stability in linear system solver algorithms
  - Cause of numerical instability
  - Pivoting for increased stability

Numerical Stability

- Linear system solvers may require different ordering of floating-point operations for different input values in order to find a solution
- An algorithm that can always find an appropriate operation order and thus a solution to the problem is a numerically stable algorithm
  - An algorithm that falls short is numerically unstable

Gaussian Elimination Example

Original

3X	+ 5Y	+2Z	= 19
2X	+ 3Y	+ Z	= 11
X	+ 2Y	+ 2Z	= 11

➡

X	+ 5/3Y	+ 2/3Z	= 19/3
X	+ 3/2Y	+ 1/2Z	= 11/2
X	+ 2Y	+ 2Z	= 11

Step 1: divide equation 1 by 3, equation 2 by 2

➡

X	+ 5/3Y	+2/3Z	= 19/3
	- 1/6Y	- 1/6Z	= -5/6
	1/3Y	+ 4/3Z	= 14/3

Step 2: subtract equation 1 from equation 2 and equation 3

Gaussian Elimination Example (Cont.)

$$\begin{array}{llll} X & +\ 5/3Y & +2/3Z & = 19/3 \\ & -\ 1/6Y & -\ 1/6Z & = -5/6 \\ & 1/3Y & +\ 4/3Z & = 14/3 \end{array} \Rightarrow \begin{array}{llll} X & +\ 5/3Y & +\ 2/3Z & = 19/3 \\ & Y & +\ Z & = 5 \\ & Y & +\ 4Z & = 14 \end{array}$$

Step 3: divide equation 2 by -1/6
and equation 3 by 1/3

$$\Rightarrow \begin{array}{llll} X & +\ 5/3Y & +\ 2/3Z & = 19/3 \\ & Y & +\ Z & = 5 \\ & & +\ 3Z & = 9 \end{array}$$

Step 4: subtract equation 2
from equation 3

Gaussian Elimination Example (Cont.)

$$\begin{aligned} X + \tfrac{5}{3}Y + \tfrac{2}{3}Z &= \tfrac{19}{3} \\ Y + Z &= 5 \\ 3Z &= 9 \end{aligned} \;\Rightarrow\; \begin{aligned} X + \tfrac{5}{3}Y + \tfrac{2}{3}Z &= \tfrac{19}{3} \\ Y + Z &= 5 \\ Z &= 3 \end{aligned}$$

Step 5: divide equation 3 by 3
We have solution for Z!

$$\Rightarrow\; \begin{aligned} X + \tfrac{5}{3}Y + \tfrac{2}{3}Z &= \tfrac{19}{3} \\ Y &= 2 \\ Z &= 3 \end{aligned}$$

Step 6: substitute Z solution into equation 2. Solution for Y!

$$\Rightarrow\; \begin{aligned} X &= 1 \\ Y &= 2 \\ Z &= 3 \end{aligned}$$

Step 7: substitute Y and Z into equation 1. Solution for X!

3	5	2	19
2	3	1	11
1	2	2	11

Original

1	5/3	2/3	19/3
1	3/2	1/2	11/2
1	2	2	11

Step 1: divide row 1 by 3, row 2 by 2

1	5/3	2/3	19/3
	- 1/6	- 1/6	-5/6
	1/3	4/3	14/3

Step 2: subtract row 1 from row 2 and row 3

1	5/3	2/3	19/3
	1	1	5
	1	4	14

Step 3: divide row 2 by -1/6 and row 3 by 1/3

1	5/3	2/3	19/3
	1	1	5
		3	9

Step 4: subtract row 2 from row 3

1	5/3	2/3	19/3
	1	1	5
		1	3

Step 5: divide equation 3 by 3
Solution for Z!

1	5/3	2/3	19/3
	1		2
		1	3

Step 6: substitute Z solution into equation 2. Solution for Y!

1			1
	1		2
		1	3

Step 7: substitute Y and Z into equation 1. Solution for X!

Basic Gaussian Elimination is Easy to Parallelize

- Have each thread to perform all calculations for a row
  - All divisions in a division step can be done in parallel
  - All subtractions in a subtraction step can be done in parallel
  - Will need barrier synchronization after each step

- However, there is a problem with numerical stability

Pivoting

	5	2	16
2	3	1	11
1	2	2	11

➡

2	3	1	11
	5	2	16
1	2	2	11

Pivoting: Swap row 1 (Equation 1) with row 2 (Equation 2)

➡

1	3/2	1/2	11/2
	5	2	16
1	2	2	11

Step 1: divide row 1 by 3, no need to divide row 2 or row 3

Pivoting (Cont.)

1	3/2	1/2	11/2
	5	2	16
1	2	2	11

⇒

1	3/2	1/2	11/2
	5	2	16
	1/2	3/2	11/2

Step 2: subtract row 1 from row 3 (column 1 of row 2 is already 0)

⇒

1	3/2	1/2	11/2
	1	2/5	16/5
	1	3	11

Step 3: divide row 2 by 5 and row 3 by 1/2

Pivoting (Cont.)

$$\begin{array}{cccc} 1 & 3/2 & 1/2 & 11/2 \\ & 1 & 2/5 & 16/5 \\ & 1 & 3 & 11 \end{array} \Rightarrow \begin{array}{cccc} 1 & 3/2 & 1/2 & 11/2 \\ & 1 & 2/5 & 16/5 \\ & & 13/5 & 39/5 \end{array}$$

Step 4: subtract row 2 from row 3

$$\Rightarrow \begin{array}{cccc} 1 & 5/3 & 2/3 & 19/3 \\ & 1 & 2/5 & 16/5 \\ & & 1 & 3 \end{array}$$

Step 5: divide row 3 by 13/5
Solution for Z!

Pivoting (Cont.)

$$\begin{array}{cccc} 1 & 5/3 & 2/3 & 19/3 \\ & 1 & 2/5 & 16/5 \\ & & 1 & 3 \end{array} \Rightarrow \begin{array}{cccc} 1 & 5/3 & 2/3 & 19/3 \\ & 1 & & 2 \\ & & 1 & 3 \end{array}$$

Step 6: substitute Z solution into equation 2. Solution for Y!

$$\Rightarrow \begin{array}{cccc} 1 & & & 1 \\ & 1 & & 2 \\ & & 1 & 3 \end{array}$$

Step 7: substitute Y and Z into equation 1. Solution for X!

	5	2	16
2	3	1	11
1	2	2	11

Original

2	3	1	11
	5	2	16
1	2	2	11

Pivoting: Swap row 1 (Equation 1) with row 2 (Equation 2)

1	3/2	1/2	11/2
	5	2	16
1	2	2	11

Step 1: divide row 1 by 3, no need to divide row 2 or row 3

1	3/2	1/2	11/2
	5	2	16
	1/2	3/2	11/2

Step 2: subtract row 1 from row 3 (column 1 of row 2 is already 0)

1	3/2	1/2	11/2
	1	2/5	16/5
	1	3	11

Step 3: divide row 2 by 5 and row 3 by 1/2

1	3/2	1/2	11/2
	1	2/5	16/5
		13/5	39/5

Step 4: subtract row 2 from row 3

1	5/3	2/3	19/3
	1	2/5	16/5
		1	3

Step 5: divide row 3 by 13/5
Solution for Z!

1	5/3	2/3	19/3
	1		2
		1	3

Step 6: substitute Z solution into equation 2. Solution for Y!

1			1
	1		2
		1	3

Step 7: substitute Y and Z into equation 1. Solution for X!

Figure 7.11

Why is Pivoting Hard to Parallelize?

- Need to scan through all rows (in fact columns in general) to find the best pivoting candidate
  - A major disruption to the parallel computation steps
  - Most parallel algorithms avoid full pivoting
  - Thus most parallel algorithms have some level of numerical instability

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