Gaussian Elimination with Partial Pivoting

Let's review: Gaussian Elimination

- An algorithm for solving a system of linear equations.

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1, \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2, \\ \vdots \qquad\qquad & \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= b_m \end{aligned}$$

- We want to know what $x_1, x_2, \ldots, x_n$ are.
- So we use our three matrix operations
  1. Add multiples of one equation onto another
  2. Interchange two equations
  3. Multiply an equation by a nonzero constant

Detail: Implementing Gaussian Elimination

1. Input Matrix

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 4 & 5 & -3 & 6 & 9 \\ -2 & 5 & -2 & 6 & 4 \\ 4 & 11 & -4 & 8 & 2 \end{array}\right)$$

2. We want to preserve the first a_{11} and eliminate everything else in that row
   1. i.e. make it zero

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 4 & 5 & -3 & 6 & 9 \\ -2 & 5 & -2 & 6 & 4 \\ 4 & 11 & -4 & 8 & 2 \end{array}\right)$$

Detail: Implementing Gaussian Elimination

3. To eliminate a_1 from the a_{i1} below it, we need to multiply equation 1 by a_{i1}/a_{11}:
   - For a_{21}, multiply by 2
     - Then subtract from eq 2
   - For a_{31}, multiply by -1
     - Then subtract from eq 3
   - For a_{41}, multiply by 2
     - Then subtract from eq 4

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 4 & 5 & -3 & 6 & 9 \\ -2 & 5 & -2 & 6 & 4 \\ 4 & 11 & -4 & 8 & 2 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ -2 & 5 & -2 & 6 & 4 \\ 4 & 11 & -4 & 8 & 2 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 6 & -3 & 8 & 9 \\ 4 & 11 & -4 & 8 & 2 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 6 & -3 & 8 & 9 \\ 0 & 9 & -2 & 4 & -8 \end{array}\right)$$

Detail: Implementing Gaussian Elimination

4. Now we've eliminated the coefficients of x1 for all equations except 1

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 6 & -3 & 8 & 9 \\ 0 & 9 & -2 & 4 & -8 \end{array}\right)$$

5. We will now use equation 2 to eliminate the coefficients a_{22} and a_{23}.
   - For a_{32}, multiply by 2
     - Then subtract from eq 3

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 0 & -1 & 4 & 11 \\ 0 & 9 & -2 & 4 & -8 \end{array}\right)$$

   - For a_{42}, multiply by 3
     - Then subtract from eq 4

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 0 & -1 & 4 & 11 \\ 0 & 0 & 1 & -2 & -5 \end{array}\right)$$

Note that we do NOT do equation 1

Detail: Implementing Gaussian Elimination

6. Finally, we want to eliminate the coefficient for x3 in equation 4, a_{43}.
    - For a_{43}, multiply by -1
        - Then subtract from eq 4

- We leave the upper triangular part of the matrix to be solved in back substitution.

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 0 & -1 & 4 & 11 \\ 0 & 0 & 1 & -2 & -5 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 0 & -1 & 4 & 11 \\ 0 & 0 & 0 & 2 & 6 \end{array}\right)$$

Detail: Implementing Gaussian Elimination

7. Back substitution is now easy on a triangular matrix.
   - We can see this in the equations
8. To perform back substitution, we start with the last row of the matrix,
   7. We have one coefficient times one variable equal to six. Thus:

$$X_4 = 6/2$$

$$\begin{aligned} 2x_1 + 1x_2 - 1x_3 + 2x_4 &= 5 \\ 3x_2 - 1x_3 + 2x_4 &= -1 \\ -1x_3 + 4x_4 &= 11 \\ 2x_4 &= 6 \end{aligned}$$

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 0 & -1 & 4 & 11 \\ 0 & 0 & 0 & \boxed{2} & \boxed{6} \end{array}\right)$$

The procedure is:
$X_4 = b_4/a_{44}$

Here, $x_4 = 3$

Detail: Implementing Gaussian Elimination

7. Now eliminate the fourth column by subtracting all x4 values:

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 0 & -1 & 4 & 11 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

- a_{34} = 4, so from b_3, subtract $(a_{34}/a_{44})*b_4$ and set a_{34} to 0.
  - This eliminates a_{34}

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

- a_{24} = 2, so from b_2, subtract $(a_{24}/a_{44})*b_4$ and set a_{24} to 0
  - This eliminates a_{24}

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 0 & -7 \\ 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

- a_{14} = 2, so from b_2, subtract $(a_{14}/a_{44})*b_4$ and set a_{14} to 0
  - This eliminates a_{14}

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 0 & -1 \\ 0 & 3 & -1 & 0 & -7 \\ 0 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

Detail: Implementing Gaussian Elimination

7. Back substituting in column 4 enables us to solve for x_3: $x_3 = 1$.
   - $a_{23} = -1$, so from b_2, subtract $(a_{23}/a_{33})^*b_3$, and set a_{23} to 0
     - This eliminates a_{23}.
   - $a_{13} = -1$, so from b1, subtract $(a_{13}/a_{33})^*b_3$, and set a_{23} to 0
     - This eliminates a_{13}.

Now we can solve for x_2: -2

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 0 & -1 \\ 0 & 3 & -1 & 0 & -7 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 0 & -1 \\ \boxed{0} & \boxed{3} & \boxed{0} & \boxed{0} & \boxed{-6} \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} \boxed{2} & \boxed{1} & \boxed{0} & \boxed{0} & \boxed{0} \\ 0 & 3 & 0 & 0 & -6 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

Detail: Implementing Gaussian Elimination

7. Back substituting in column 3 enables us to solve for x_2: x_2 = -2.
   - a_{12} = -1, so from b_1, subtract $(a_{12}/a_{22})*b_2$, and set a_{12} to 0
     - This eliminates a_{12}.
8. Now we can solve for x1:
   - $x_1 = b_1/a_{11} = 1$
9. Our solutions are:

x1 = 1

x2 = -2

x3 = 1

x4 = 3

$$\left(\begin{array}{cccc|c} 2 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -2 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 2 & 0 & 0 & 0 & 2 \\ 0 & 1 & 0 & 0 & -2 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & -2 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right)$$

Solving and Inversion work the same

$$\left(\begin{array}{ccc|ccc} 1 & 2 & 1 & 1 & 0 & 0 \\ 2 & 6 & 1 & 0 & 1 & 0 \\ 1 & 1 & 4 & 0 & 0 & 1 \end{array}\right) \quad \left(\begin{array}{ccc|ccc} a_{11} & a_{12} & a_{13} & b_{11} & b_{12} & b_{13} \\ a_{21} & a_{22} & a_{23} & b_{21} & b_{22} & b_{23} \\ a_{31} & a_{32} & a_{33} & b_{31} & b_{32} & b_{33} \end{array}\right)$$

- Perform the same process with this matrix
- In the earlier example we only multiply and subtract b_1, b_2, b_3. Here we do it for all b's in the row
- When the left side is an identity matrix, then the right hand side is the inverse.

Partial Pivoting

- Each time we select the one of the coefficient values to isolate, that is a **pivot**.
- But several things (a_{11}-a_{14}) can be the in the pivoting position **because we can arbitrarily switch rows in this matrix**.
- In fixed pivoting there are **no alternatives**.

Pivot

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 4 & 5 & -3 & 6 & 9 \\ -2 & 5 & -2 & 6 & 4 \\ 4 & 11 & -4 & 8 & 2 \end{array}\right)$$

How do we pick the pivot?

- To solve for x1 we have four possibilities (a_{11} to b_{41}). In partial pivoting we always pick the largest value x_i as the new pivot

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 4 & 5 & -3 & 6 & 9 \\ -2 & 5 & -2 & 6 & 4 \\ 4 & 11 & -4 & 8 & 2 \end{array}\right)$$

- Why?
  - The largest value becomes a denominator in other operations, so it's size eliminates "small denominator" errors that propagate

Example: A system that requires pivoting

- Exact solutions:
  - $x_1 = 10.00$
  - $x_2 = 1.00$
- Use 4-digit accuracy
- Lets suppose that we do not do partial pivoting. So the first pivot is a_{11}.

$$\left(\begin{array}{cc|c} .003 & 59.14 & 59.17 \\ 5.2 & -6.13 & 46.78 \end{array}\right)$$

$$\left(\begin{array}{cc|c} .003 & 59.14 & 59.17 \\ 0 & 1024000 & 1025000 \end{array}\right)$$

  - So scale equation 1 by $(a_{21}/a_{11}) \approx 17330$ and subtract from equation 2.
  - So x2 = 1.001

Example from Wikipedia

Example: A system that requires pivoting

- We have found that x_2=1.001
- Backsolve for x_1:
  - $(a_{12}/a_1)*b_2 = 59.19$
  - Set $a_{12} = 0$ and $b_2 = .02$
  - Then $x_1 = a_{11}/b_1 = .02/.003 = 6.667$

Large Propagation

$$\left(\begin{array}{cc|c} .003 & 59.14 & 59.17 \\ 0 & 1 & 1.001 \end{array}\right)$$

$$\left(\begin{array}{cc|c} 1 & 0 & 6.667 \\ 0 & 1 & 1.001 \end{array}\right)$$

- But the actual solutions are:
  - $x_1 = 10.00$
  - $x_2 = 1.00$

Example from Wikipedia

Lets redo the example with partial pivoting

- So we want to solve for x_1. But we observe that a_{12} is larger than a_{11}.
  - No problem! Swap rows with row 1.
  - Next, find the multiple of equation 1 and subtract from equation 2:
    - (x_{21}/x_{11}) = .0005769
    - Here we get x_2 = 1.000
    - Now backsolve for x_1

$$\left(\begin{array}{cc|c} .003 & 59.14 & 59.17 \\ 5.2 & -6.13 & 46.78 \end{array}\right)$$

$$\left(\begin{array}{cc|c} 5.2 & -6.13 & 46.78 \\ .003 & 59.14 & 59.17 \end{array}\right)$$

$$\left(\begin{array}{cc|c} 5.2 & -6.13 & 46.78 \\ 0 & 59.14 & 59.14 \end{array}\right)$$

Lets redo the example with partial pivoting

- We found $x_2 = 1.000$
  - To backsolve, we subtract $(a_{12}/a_{22})*b_2$ from b_1, getting:
  - $b_1 = 52.91$
  - This leaves $x_1 = 10.175$
- This is much much closer than the 6.667 we had earlier

$$\left(\begin{array}{cc|c} 5.2 & -6.13 & 46.78 \\ 0 & 1 & 1 \end{array}\right)$$

$$\left(\begin{array}{cc|c} 1 & 0 & 10.175 \\ 0 & 1 & 1 \end{array}\right)$$

So how do we do partial pivoting?

- When we have to select a pivot, pick the pivot with the largest absolute magnitude
- Swap the largest pivot with the default pivot
- This happens each time you start working on a new column

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 4 & 5 & -3 & 6 & 9 \\ -2 & 5 & -2 & 6 & 4 \\ 4 & 11 & -4 & 8 & 2 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 6 & -3 & 8 & 9 \\ 0 & 9 & -2 & 4 & -8 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 2 & 1 & -1 & 2 & 5 \\ 0 & 3 & -1 & 2 & -1 \\ 0 & 0 & -1 & 4 & 11 \\ 0 & 0 & 1 & -2 & -5 \end{array}\right)$$

What did we see here?

- Partial pivoting is one way we can reorder our computations to reduce error without sacrificing anything else in the method
  - It changes the computation time because you must now scan the column each time you select a pivot
- Partial pivoting does not escape from all kinds of numerical problems
  - We could still be dividing by very small numbers and commiting other errors
- People have gone through a lot of effort to find other (complicated) ways to reduce error

Homework

- You will implement gaussian elimination for matrix inversion, as well as GE with partial pivoting
  - Find a matrix that has no errors on both approaches
  - Find a matrix that creates numerical errors on simple GE but is more accurate on partial pivoting
  - How large can you make the magnitude of the error?
    - If you are careful you can design a matrix that still propagates error viciously and is hard to invert.