MAT 222 Linear Algebra and Numerical Methods
Week 5
Lecture Notes 1

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Cofactor Expansion is Costly

- Cofactor expansion may seem easy for computation. One reason for this is that the signs of the cofactors follow a checker board pattern, e.g. in the 3×3 case

$$\begin{bmatrix} + & - & + \\ - & + & - \\ + & - & + \end{bmatrix}$$

- On the other hand, the number of multiplications required in a cofactor expansion is more than $n!$, which is unacceptably big.
- For example, for $n = 25$ we have $25! \approx 1.5 \times 10^{25}$. The world record (as of July 11, 2022) held by a supercomputer is 10^{18} operations per second, and even it takes approximately half a year to compute the determinant of a 25×25 matrix by cofactor expansion.
- In practice, the determinant has to be computed by a faster method.

Computing the Determinant

- Since cofactor expansion is costly, we should find other ways to compute determinants.
- Such a way is provided by properties (P5) and (P7). Let's restate them.

(P5) Adding a multiple of one row to another doesn't change the determinant.

(P7) The determinant of a triangular matrix is equal to the product of its diagonal entries.

- Since any invertible square matrix is row-equivalent to a triangular matrix, this gives a straightforward method to compute the determinant.
- Namely, row operations of type (3) (Add a multiple of one row to another) and row swaps (but NOT any operation of type (1)!) are used to reduce the matrix to echelon form, which is (upper) triangular. Then determinant $= \pm$(product of diagonal entries in echelon form)
- The plus or minus sign above depends on the number of row exchanges required to reduce the matrix to echelon form.
- Note that the above formula is also valid for singular matrices since the echelon form contains a zero in the diagonal in this case.

Computing the Determinant: Example

- Let us compute the determinant of $A = \begin{bmatrix} 3 & 2 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 7 & 5 & 2 \\ -1 & 4 & -6 & 3 \end{bmatrix}$.
- Let us start with a row exchange.
- $\begin{bmatrix} 3 & 2 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 7 & 5 & 2 \\ -1 & 4 & -6 & 3 \end{bmatrix} \xrightarrow{R_1 \leftrightarrow R_2} \begin{bmatrix} 1 & 2 & 4 & 2 \\ 3 & 2 & 2 & 1 \\ 2 & 7 & 5 & 2 \\ -1 & 4 & -6 & 3 \end{bmatrix}$
- Then we proceed as usual.
- $\begin{bmatrix} 1 & 2 & 4 & 2 \\ 3 & 2 & 2 & 1 \\ 2 & 7 & 5 & 2 \\ -1 & 4 & -6 & 3 \end{bmatrix} \xrightarrow{-3R_1+R_2,\,-2R_1+R_3,\,1R_1+R_4} \begin{bmatrix} 1 & 2 & 4 & 2 \\ 0 & -4 & -10 & -5 \\ 0 & 3 & -3 & -2 \\ 0 & 6 & -2 & 5 \end{bmatrix}$

$$\xrightarrow{\frac{3}{4}R_2+R_3,\,\frac{3}{2}R_2+R_4} \begin{bmatrix} 1 & 2 & 4 & 2 \\ 0 & -4 & -10 & -5 \\ 0 & 0 & -10.5 & -5.75 \\ 0 & 0 & -17 & -2.5 \end{bmatrix}$$

Computing the Determinant: Example

- $$\xrightarrow{-\frac{34}{21}R_3+R_4} \begin{bmatrix} 1 & 2 & 4 & 2 \\ 0 & -4 & -10 & -5 \\ 0 & 0 & -10.5 & -5.75 \\ 0 & 0 & 0 & 143/21 \end{bmatrix}$$
- We have performed only one row exchange. So we have

  $$\det(A) = -(\text{product of pivots}) = -(1\cdot(-4)\cdot(-10.5)\cdot(143/21)) = -286$$
- **Exercise:** Let $A = \begin{bmatrix} -2 & 3 & 0 \\ 3 & 1/2 & 1 \\ 5 & -1 & 4 \end{bmatrix}$ and $B = \begin{bmatrix} 1 & 4 & 2 & 3 \\ 0 & 1 & 4 & -4 \\ -1 & 0 & 1 & 0 \\ 2 & 0 & 4 & 1 \end{bmatrix}$.

  Calculate $\det(A)$ and $\det(B)$ by reducing the matrices to echelon form.

Applications of Determinants

- The most straightforward (and the most important for us) application of determinants is to the problem of deciding if a matrix is invertible or not.
- For instance, the matrix $\begin{bmatrix} 3 & 2 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 7 & 5 & 2 \\ -1 & 4 & -6 & 3 \end{bmatrix}$ from the previous example is invertible since its determinant is nonzero, while the matrix $\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$ is noninvertible since its determinant is zero.
- Another application is to obtain the solutions of a linear system
- Let us see this in a 3×3 system $A\mathbf{x} = b$.
- Consider the product $A \begin{bmatrix} x_1 & 0 & 0 \\ x_2 & 1 & 0 \\ x_3 & 0 & 1 \end{bmatrix} = \begin{bmatrix} b_1 & a_{1,2} & a_{1,3} \\ b_2 & a_{2,2} & a_{2,3} \\ b_3 & a_{3,2} & a_{3,3} \end{bmatrix} := B_1$
- In view of (P9) we have $\det(B_1) = \det(A) \cdot \begin{vmatrix} x_1 & 0 & 0 \\ x_2 & 1 & 0 \\ x_3 & 0 & 1 \end{vmatrix} = \det(A) \cdot x_1$

Applications of Determinants: Cramer's Rule

- This implies that $x_1 = \dfrac{\det(B_1)}{\det(A)}$.
- By similar constructions we can define

$$B_2 := A \begin{bmatrix} 1 & x_1 & 0 \\ 0 & x_2 & 0 \\ 0 & x_3 & 1 \end{bmatrix} = \begin{bmatrix} a_{1,1} & b_1 & a_{1,3} \\ a_{2,1} & b_2 & a_{2,3} \\ a_{3,1} & b_3 & a_{3,3} \end{bmatrix} \text{ and}$$

$$B_3 := A \begin{bmatrix} 1 & 0 & x_1 \\ 0 & 1 & x_2 \\ 0 & 0 & x_3 \end{bmatrix} = \begin{bmatrix} a_{1,1} & a_{1,2} & b_1 \\ a_{2,1} & a_{2,2} & b_2 \\ a_{3,1} & a_{3,2} & b_3 \end{bmatrix}.$$

- From these constructions it follows that $x_2 = \dfrac{\det(B_2)}{\det(A)}$ and $x_3 = \dfrac{\det(B_3)}{\det(A)}$.
- This procedure can be generalized to square systems of any size.

Cramer's rule

Let a be an $n \times n$ matrix and consider the system $A\mathbf{x} = \mathbf{b}$, where the unknowns are $x_1, x_2, \ldots, x_n$. For $i = 1, 2, \ldots, n$ define the matrix B_i to be the $n \times n$ matrix whose i-th column is $\mathbf{b}$ and the other columns are the same as the columns of A, in the same order. Then we have

$$x_1 = \frac{\det(B_1)}{\det(A)}, x_2 = \frac{\det(B_2)}{\det(A)}, \ldots, x_n = \frac{\det(B_n)}{\det(A)}.$$

Cramer's Rule: Example

- Let us use Cramer's rule to solve the system $\begin{aligned} 2x + y &= 1 \\ x + 2y + z &= 70 \\ y + 2z &= 0 \end{aligned}$
- We have $A = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}$ and

$$B_1 = \begin{bmatrix} 1 & 1 & 0 \\ 70 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix}, \; B_2 = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 70 & 1 \\ 0 & 0 & 2 \end{bmatrix}, \; B_3 = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 70 \\ 0 & 1 & 0 \end{bmatrix}.$$

- For the determinants we have
  $\det(A) = 4, \det(B_1) = -137, \det(B_2) = 278, \det(B_3) = -139.$
- So the solutions are

$$x = \frac{\det(B_1)}{\det(A)} = -\frac{137}{4}, \; y = \frac{\det(B_2)}{\det(A)} = \frac{278}{4} = 69.5, \; z = \frac{\det(B_1)}{\det(A)} = -\frac{139}{4}.$$

Gaussian Elimination and Roundoff Error

- Theoretically, Gaussian elimination gives the exact solution of a linear system, but in practice, what we find is actually an approximate solution due to roundoff error.
- As an example, consider the following 2×2 system.

$$\begin{aligned} 0.003x + 59.14y &= 59.17 \\ 5.291x - 6.13y &= 46.78 \end{aligned}$$

- The exact solution is $x = 10$, $y = 1$.
- In order to illustrate the point, let us assume that our computer system uses four-digit arithmetic with rounding.
- In order to eliminate the entry 5.291, Gaussian elimination uses the value 0.003 as pivot and adds $-\dfrac{5.291}{0.003} = -1763.\bar{6} \approx -1764$ times the first row to the second row.
- This row operation gives the system

$$\begin{aligned} 0.003x + 59.14y &= 59.17 \\ -104300y &= -104400 \end{aligned} .$$

(Don't forget that we are using 4-digit rounding arithmetic.)

Gaussian Elimination and Roundoff Error

- Now let us solve the system $\begin{aligned} 0.003x + 59.14y &= 59.17 \\ -104300y &= -104400 \end{aligned}$.
- We have $y = \dfrac{-104400}{-104300} \approx 1.001$. Not far from the exact solution $y = 1$.
- As for x we have $x = \dfrac{59.17 - (59.14)\cdot(1.001)}{0.003} \approx -10.00$. The exact solution was $x = 10$.
- This unacceptable deviation resulted from the fact that the pivot 0.003 was too small with respect to the value 5.291 which it was used to eliminate, thus producing a big multiplier -1764.
- Thus, an absolute error of 0.001 in the value of y gave rise to an error of

$$\frac{59.14}{0.003}\cdot(0.001) \approx 20$$

  in the value of x.
- As a remedy, it may be a good idea to change the pivot entry that we use.

Pivoting Strategies: Partial Pivoting

- We consider the same system $\begin{aligned} 0.003x + 59.14y &= 59.17 \\ 5.291x - 6.13y &= 46.78 \end{aligned}$.
- This time let us use the value 5.291 as the pivot. For this purpose first we should swap the rows. The result is the following:

$$\begin{aligned} 5.291x - 6.13y &= 46.78 \\ 0.003x + 59.14y &= 59.17 \end{aligned}$$

- This time the multiplier is calculated as $-\dfrac{0.003}{5.291} \approx -0.0005670$.
- Adding -0.0005670 times the first row to the second yields the system

$$\begin{aligned} 5.291x - 6.13y &= 46.78 \\ 59.14y &= 59.14 \end{aligned}.$$

- Backward-substitution gives $y = 1.000$ and $x = 10.00$, which are the exact solutions.
- This pivoting strategy is known to be partial pivoting. In each step of Gaussian elimination, partial pivoting uses the entry with the greatest absolute value as the pivot.

A Pitfall of Partial Pivoting

- Partial pivoting doesn't always give good results as the following example shows.
- Let us consider the same system one more time, but this time let us multiply the first equation by 10000. The resulting system is

$$\begin{aligned} 30.00x + 591400y &= 591700 \\ 5.291x - 6.13y &= 46.78 \end{aligned}.$$

- According to partial pivoting, the value 30.00 must be used as the pivot since it is the (absolutely) greatest value in the first column.
- This produces the multiplier $-\dfrac{5.291}{30.00} \approx -0.1764$. The row operation $-0.1764R_1 + R_2$ results in the following:

$$\begin{aligned} 30.00x + 591400y &= 591700 \\ -104300y &= -104400 \end{aligned}$$

- The solution is $y = 1.001, x = \dfrac{591700 - 591400 \cdot (1.001)}{30.00} \approx -10.00$.
- This time partial pivoting hasn't worked.

Scaled Partial Pivoting

- This time the problem has been brought about by the division $\dfrac{591400 \cdot (1.001)}{30.00}$. This shows that the pivot should not be relatively small to other entries in its row.
- For that reason, in each step of elimination, we should compare the pivot candidates with the other entries in their rows.
- In the system $\begin{aligned} 30.00x + 591400y &= 591700 \\ 5.291x - 6.13y &= 46.78 \end{aligned}$, the pivot candidates are $a_{1,1} = 30.00$ and $a_{2,1} = 5.291$. We compare them to the greatest (in absolute value) among the other numbers in their row (In this case there is actually only one other entry).
- So we have $\dfrac{|a_{1,1}|}{|a_{1,2}|} = \dfrac{30.00}{591400} = 0.00005073$ and $\dfrac{|a_{2,1}|}{|a_{2,2}|} = \dfrac{5.291}{6.13} = 0.8631$.
- Since $0.00005073 < 0.8631$ we should choose the value 5.291 as the pivot.
- This requires a row exchange, giving the system
$$\begin{aligned} 5.291x - 6.13y &= 46.78 \\ 30.00x + 591400y &= 591700 \end{aligned}.$$
- Gaussian elimination now gives $x = 10.00$, $y = 1.000$, which are the exact solutions.
- When choosing a pivot for column p, scaled partial pivoting computes a scale factor $s_i = \max_{p<k\leq n} |a_{i,k}|$ for each row $i \geq p$ and computes a score $\dfrac{|a_{i,p}|}{s_i}$ for each pivot candidate. The candidate with the biggest score is chosen as the pivot.

Other Pivoting Strategies

- There are cases where scaled partial pivoting cannot prevent significant roundoff errors.
- A strategy may be to search for the greatest value in the entire matrix and to use that value as the pivot. This is known as complete pivoting and requires columns exchanges in addition to row exchanges.
- Searching the entire matrix brings a substantial amount of extra work, so such algorithms are implemented only when extreme accuracy is essential.
- **Exercise:**
$$\begin{aligned} 58.9x + 0.03y &= 59.2 \\ -6.10x + 5.31y &= 47.0 \end{aligned}$$
Exact solution: $x = 1, y = 10$.

  Solve the above system first using Gaussian elimination without pivoting, then with partial pivoting, and lastly with scaled partial pivoting. In each case, compare your solution to the exact solution. Use 3-digit rounding arithmetic.