Lecture 6

Gaussian Elimination

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Gaussian Elimination

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- Elementary Elimination Matrices And LU Factorization

Gaussian Elimination

Gaussian elimination is a mostly general method for solving square systems.

We will work with systems in their matrix form, such as

$$\begin{aligned} x_1 + 3x_2 + 5x_3 &= 4 \\ 9x_1 + 7x_2 + 8x_3 &= 6 \\ 3x_1 + 2x_2 + 7x_3 &= 1, \end{aligned}$$

in its equivalent matrix form,

$$\begin{bmatrix} 1 & 3 & 5 \\ 9 & 7 & 8 \\ 3 & 2 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 6 \\ 1 \end{bmatrix}.$$

Triangular Systems

The generic lower and upper triangular matrices are

$$L = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & & 0 \\ \vdots & & \ddots & \vdots \\ l_{n1} & & \cdots & l_{nn} \end{bmatrix}$$

and

$$U = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & & u_{2n} \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & u_{nn} \end{bmatrix}$$

The triangular systems

$$Ly = b \qquad Ux = c$$

are easily solved by **forward substitution** and **backward substitution**, respectively

Solving Triangular Systems

Solving for $x_1, x_2, \ldots, x_n$ for an upper triangular system is called **backward substitution**.

Listing 1: backward substitution (page 252)

```
given A (upper △), b
x_n = b_n/a_nn
for i = n-1...1
   s = b_i
   for j = i+1...n
      s = s - a_{i,j} x_j
   end
   x_i = s/a_{i,i}
end
```

Solving Triangular Systems

Solving for $x_1, x_2, \ldots, x_n$ for an upper triangular system is called **backward substitution**.

Listing 2: backward substitution (page 252)

```
given A (upper △), b
x_n = b_n/a_nn
for i = n-1...1
   s = b_i
   for j = i+1...n
      s = s - a_{i,j} x_j
   end
   x_i = s/a_{i,i}
end
```

Using forward or backward substitution is sometimes referred to as performing a **triangular solve**.

Operations?

cheap!

- begin in the bottom corner: 1 div
- row -2: 1 mult, 1 add, 1 div, or 3 FLOPS
- row -3: 2 mult, 2 add, 1 div, or 5 FLOPS
- row -4: 3 mult, 3 add, 1 div, or 7 FLOPS
- $\vdots$
- row -j: about $2j - 1$ FLOPS

Total FLOPS? $\sum_{j=1}^{n} 2j - 1 = 2\frac{n(n+1)}{2} - n$ or $\mathcal{O}(n^2)$ FLOPS

Gaussian Elimination

- Triangular systems are easy to solve in $\mathcal{O}(n^2)$ FLOPS
- Goal is to transform an arbitrary, square system into an equivalent upper triangular system
- Then easily solve with backward substitution

This process is equivalent to the *formal solution* of $Ax = b$, where A is an $n \times n$ matrix.

$$x = A^{-1}b$$

Gaussian Elimination — Hand Calculations

Solve

$$\begin{aligned} x_1 + 3x_2 &= 5 \\ 2x_1 + 4x_2 &= 6 \end{aligned}$$

Subtract 2 times the first equation from the second equation

$$\begin{aligned} x_1 + 3x_2 &= 5 \\ -2x_2 &= -4 \end{aligned}$$

This equation is now in triangular form, and can be solved by backward substitution.

Gaussian Elimination — Hand Calculations

The elimination phase transforms the matrix and right hand side to an equivalent system

$$\begin{aligned} x_1 + 3x_2 &= 5 \\ 2x_1 + 4x_2 &= 6 \end{aligned} \qquad \longrightarrow \qquad \begin{aligned} x_1 + 3x_2 &= 5 \\ -2x_2 &= -4 \end{aligned}$$

The two systems have the same solution. The right hand system is upper triangular.
Solve the second equation for x_2

$$x_2 = \frac{-4}{-2} = 2$$

Substitute the newly found value of x_2 into the first equation and solve for x_1.

$$x_1 = 5 - (3)(2) = -1$$

Gaussian Elimination — Hand Calculations

When performing Gaussian Elimination by hand, we can avoid copying the x_i by using a shorthand notation.
For example, to solve:

$$A = \begin{bmatrix} -3 & 2 & -1 \\ 6 & -6 & 7 \\ 3 & -4 & 4 \end{bmatrix} \qquad b = \begin{bmatrix} -1 \\ -7 \\ -6 \end{bmatrix}$$

Form the *augmented* system

$$\tilde{A} = [A \;\; b] = \left[\begin{array}{ccc|c} -3 & 2 & -1 & -1 \\ 6 & -6 & 7 & -7 \\ 3 & -4 & 4 & -6 \end{array}\right]$$

The vertical bar inside the augmented matrix is just a reminder that the last column is the b vector.

Gaussian Elimination — Hand Calculations

Add 2 times row 1 to row 2, and add (1 times) row 1 to row 3

$$\tilde{A}_{(1)} = \left[\begin{array}{rrr|r} -3 & 2 & -1 & -1 \\ 0 & -2 & 5 & -9 \\ 0 & -2 & 3 & -7 \end{array}\right]$$

Subtract (1 times) row 2 from row 3

$$\tilde{A}_{(2)} = \left[\begin{array}{rrr|r} -3 & 2 & -1 & -1 \\ 0 & -2 & 5 & -9 \\ 0 & 0 & -2 & 2 \end{array}\right]$$

Gaussian Elimination — Hand Calculations

The transformed system is now in upper triangular form

$$\tilde{A}_{(2)} = \left[\begin{array}{ccc|c} -3 & 2 & -1 & -1 \\ 0 & -2 & 5 & -9 \\ 0 & 0 & -2 & 2 \end{array}\right]$$

Solve by back substitution to get

$$x_3 = \frac{2}{-2} = -1$$

$$x_2 = \frac{1}{-2}\left(-9 - 5x_3\right) = 2$$

$$x_1 = \frac{1}{-3}\left(-1 - 2x_2 + x_3\right) = 2$$

Gaussian Elimination — Cartoon Version

Start with the augmented system

$$\begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix}$$

The x's represent numbers, they are generally *not* the same values.

Begin elimination using the first row as the *pivot row* and the first element of the first row as the pivot element

$$\begin{bmatrix} \boxed{x} & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix}$$

Gaussian Elimination — Cartoon Version

- Eliminate elements under the pivot element in the first column.
- x' indicates a value that has been changed once.

$$\begin{bmatrix} \boxed{x} & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix} \longrightarrow \begin{bmatrix} \boxed{x} & x & x & x & x \\ 0 & x' & x' & x' & x' \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix}$$

$$\longrightarrow \begin{bmatrix} \boxed{x} & x & x & x & x \\ 0 & x' & x' & x' & x' \\ 0 & x' & x' & x' & x' \\ x & x & x & x & x \end{bmatrix}$$

$$\longrightarrow \begin{bmatrix} \boxed{x} & x & x & x & x \\ 0 & x' & x' & x' & x' \\ 0 & x' & x' & x' & x' \\ 0 & x' & x' & x' & x' \end{bmatrix}$$

Gaussian Elimination — Cartoon Version

- The pivot element is now the diagonal element in the second row.
- Eliminate elements under the pivot element in the second column.
- x'' indicates a value that has been changed twice.

$$\begin{bmatrix} x & x & x & x & x \\ 0 & \boxed{x'} & x' & x' & x' \\ 0 & x' & x' & x' & x' \\ 0 & x' & x' & x' & x' \end{bmatrix} \longrightarrow \begin{bmatrix} x & x & x & x & x \\ 0 & \boxed{x'} & x' & x' & x' \\ 0 & 0 & x'' & x'' & x'' \\ 0 & x' & x' & x' & x' \end{bmatrix}$$

$$\longrightarrow \begin{bmatrix} x & x & x & x & x \\ 0 & \boxed{x'} & x' & x' & x' \\ 0 & 0 & x'' & x'' & x'' \\ 0 & 0 & x'' & x'' & x'' \end{bmatrix}$$

Gaussian Elimination — Cartoon Version

- The pivot element is now the diagonal element in the third row.
- Eliminate elements under the pivot element in the third column.
- x''' indicates a value that has been changed three times.

$$\begin{bmatrix} x & x & x & x & x \\ 0 & x' & x' & x' & x' \\ 0 & 0 & \boxed{x''} & x'' & x'' \\ 0 & 0 & x'' & x'' & x'' \end{bmatrix} \longrightarrow \begin{bmatrix} x & x & x & x & x \\ 0 & x' & x' & x' & x' \\ 0 & 0 & \boxed{x''} & x'' & x'' \\ 0 & 0 & 0 & x''' & x''' \end{bmatrix}$$

Gaussian Elimination — Cartoon Version

Summary

- Gaussian Elimination is an orderly process for transforming an augmented matrix into an equivalent upper triangular form.
- The elimination operation at the k^{th} step is

$$\tilde{a}_{ij} = \tilde{a}_{ij} - (\tilde{a}_{ik}/\tilde{a}_{kk})\tilde{a}_{kj}, \quad i > k, \quad j \geqslant k$$

- Elimination requires three nested loops.
- The result of the elimination phase is represented by the image below.

$$\begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix} \longrightarrow \begin{bmatrix} x & x & x & x & x \\ 0 & x' & x' & x' & x' \\ 0 & 0 & x'' & x'' & x'' \\ 0 & 0 & 0 & x''' & x''' \end{bmatrix}$$

Summary

- Transform a linear system into (upper) triangular form. i.e. transform lower triangular part to zero
- Transformation is done by taking linear combinations of rows
- Example: $a = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$
- If $a_1 \neq 0$, then

$$\begin{bmatrix} 1 & 0 \\ -a_2/a_1 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} a_1 \\ 0 \end{bmatrix}$$

Gaussian Elimination Algorithm

Listing 3: Forward Elimination beta

```
given A, b

for k = 1...n-1
   for i = k+1...n
      for j = k...n
         a_ij = a_ij - (a_ik/a_kk) a_kj
      end
      b_i = b_i - (a_ik/a_kk) b_k
   end
end
```

- the multiplier can be moved outside the j-loop
- no reason to actually compute 0

Challenge: The loops over i and j may be exchanged—why would one be preferable?

Gaussian Elimination Algorithm

Listing 4: Forward Elimination

```
given A, b

for k = 1...n-1
   for i = k+1...n
      xmult = a_ik / a_kk
      a_ik = xmult
      for j = k+1...n
         a_ij = a_ij - (xmult) a_kj
      end
      b_i = b_i - (xmult) b_k
   end
end
```

Naive Gaussian Elimination Algorithm

- Forward Elimination
- + Backward substitution
- = Naive Gaussian Elimination

Forward Elimination Cost?

What is the cost in converting from A to U?

Step	Add	Multiply	Divide
1	$(n-1)^2$	$(n-1)^2$	$n-1$
2	$(n-2)^2$	$(n-2)^2$	$n-2$
$\vdots$			
n-1	1	1	1

or

add	$\sum_{j=1}^{n-1} j^2$
multiply	$\sum_{j=1}^{n-1} j^2$
divide	$\sum_{j=1}^{n-1} j$

Forward Elimination Cost?

add	$\sum_{j=1}^{n-1} j^2$
multiply	$\sum_{j=1}^{n-1} j^2$
divide	$\sum_{j=1}^{n-1} j$

We know $\sum_{j=1}^{p} j = \frac{p(p+1)}{2}$ and $\sum_{j=1}^{p} j^2 = \frac{p(p+1)(2p+1)}{6}$, so

add-subtracts	$\frac{n(n-1)(2n-1)}{6}$
multiply-divides	$\frac{n(n-1)(2n-1)}{6} + \frac{n(n-1)}{2} = \frac{n(n^2-1)}{3}$

Forward Elimination Cost?

add-subtracts	$\frac{n(n-1)(2n-1)}{6}$
multiply-divides	$\frac{n(n^2-1)}{3}$
add-subtract for b	$\frac{n(n-1)}{2}$
multipply-divides for b	$\frac{n(n-1)}{2}$

Back Substitution Cost

As before

add-subtract	$\frac{n(n-1)}{2}$
multipply-divides	$\frac{n(n+1)}{2}$

Naive Gaussian Elimination Cost

Combining the cost of forward elimination and backward substitution gives

add-subtracts	$\frac{n(n-1)(2n-1)}{6} + \frac{n(n-1)}{2} + \frac{n(n-1)}{2}$ $= \frac{n(n-1)(2n+5)}{6}$
multiply-divides	$\frac{n(n^2-1)}{3} + \frac{n(n-1)}{2} + \frac{n(n+1)}{2}$ $= \frac{n(n^2+3n-1)}{3}$

So the total cost of add-subtract-multiply-divide is about

$$\frac{2}{3}n^3$$

$\Rightarrow$ double n results in a cost increase of a factor of 8

Elimination Matrices

- Another way to zero out entries in a column of A
- Annihilate entries below k^{th} element in a with matrix, M_k:

$$M_k a = \begin{bmatrix} 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 1 & 0 & \dots & 0 \\ 0 & \dots & -m_{k+1} & 1 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & -m_n & 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

  where $m_i = a_i / a_k$, $i = k+1, \dots, n$.
- The divisor a_k is the "pivot" (and needs to be nonzero)

Elimination Matrices

- Matrix M_k is an "elementary elimination matrix"
  - Adds a multiple of row k to each subsequent row, with "multipliers" m_i
  - Result is zeros in the k^{th} column for rows $i > k$.
- M_k is unit lower triangular and nonsingular
- $M_k = I - m_k e_k^T$ where $m_k = [0, \ldots, 0, m_{k+1}, \ldots, m_n]^T$ and e_k is the k^{th} column of the identity matrix I.
- $M_k^{-1} = I + m_k e_k^T$, which means M_k^{-1} is also lower triangular, and we will denote $M_k^{-1} = L_k$.

Can you prove $M_k^{-1} = I + m_k e_k^T$?

Elimination Matrices

- Suppose M_j and M_k are elementary elimination matrices with $j > k$, then

$$\begin{aligned} M_k M_j &= I - m_k e_k^T - m_j e_j^T + m_k e_k^T m_j e_j^T \\ &= I - m_k e_k^T - m_j e_j^T + m_k (e_k^T m_j) e_j^T \\ &= I - m_k e_k^T - m_j e_j^T \end{aligned}$$

  because the k^{th} entry of vector m_j is zero (since $j > k$)
- Thus $M_k M_j$ is essentially a union of their columns.
- Note this is also true for $M_k^{-1} M_j^{-1}$.

Example

Let $a = \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix}$.

$$M_1 a = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$$

and

$$M_2 a = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 0 \end{bmatrix}$$

Example

So

$$L_1 = M_1^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}, \; L_2 = M_2^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1/2 & 1 \end{bmatrix}$$

which means

$$M_1 M_2 = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 1/2 & 1 \end{bmatrix}, \; L_1 L_2 = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -1/2 & 1 \end{bmatrix}$$

Gaussian Elimination

- To reduce $Ax = b$ to upper triangular form, first construct M_1 with a_{11} as the pivot (eliminating the first column of A below the diagonal.)
- Then $M_1Ax = M_1b$ still has the same solution.
- Next construct M_2 with pivot a_{22} to eliminate the second column below the diagonal.
- Then $M_2M_1Ax = M_2M_1b$ still has the same solution
- $M_{n-1} \dots M_1Ax = M_{n-1} \dots M_1b$
- Let $M = M_nM_{n-1} \dots M_1$. Then $MAx = Mb$, with MA upper triangular.
- Do back substitution on $MAx = Mb$.

Another Way to Look at A

We've mentioned L and U today. Why?
Consider this

$$
\begin{aligned}
A &= A \\
A &= (M^{-1}M)A \\
A &= (M_1^{-1}M_2^{-1}\dots M_n^{-1})(M_nM_{n-1}\dots M_1)A \\
A &= (M_1^{-1}M_2^{-1}\dots M_n^{-1})((M_nM_{n-1}\dots M_1)A) \\
A &= \qquad\quad L \qquad\qquad\qquad\qquad U
\end{aligned}
$$

But MA is upper triangular, and we've seen that $M_1^{-1}\dots M_n^{-1}$ is lower triangular. Thus, we have an algorithm that factors A into two matrices L and U.

Why is this "naive"?

Example

$$A = \begin{bmatrix} 0 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

Example

$$A = \begin{bmatrix} 1e-10 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$