# Lecture Notes 15: Direct Methods for Linear Systems

## CPSC 302: Numerical Computation for Algebraic Problems

Jessica Bosch
jbosch@cs.ubc.ca
http://www.cs.ubc.ca/~jbosch

University of British Columbia
Department of Computer Science

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# Goals of this Chapter

- Learn practical methods to handle the most common problem in numerical computation.
- Get familiar (again) with the ancient method of Gaussian elimination in its modern form of LU decomposition, and develop pivoting methods for its stable computation.
- Consider LU decomposition in the very important special cases of symmetric positive definite and sparse matrices.
- Study the expected quality of the computed solution, introducing as we go the fundamental concept of a condition number.

## Motivation

- Here and in Chapter 6 we consider the problem of finding $\mathbf{x}$ which solves

$$A\mathbf{x} = \mathbf{b},$$

  where $A$ is a given, real, nonsingular, $n \times n$ matrix, and $\mathbf{b}$ is a given, real vector.

- *Such problems are ubiquitous in applications*!

# Motivation (cont.)

Two solution approaches:

- *Direct methods*: yield exact solution in absence of roundoff error.
  - Variations of **Gaussian elimination**.
  - Considered in this chapter
- *Iterative methods*: iterate in a similar fashion to what we do for nonlinear problems.
  - Use only when direct methods are ineffective.
  - Considered in Chapter 6

## Chapter 4: Direct Methods for Linear Systems

- Gaussian Elimination and Backward Substitution
- LU Decomposition
- Pivoting Strategies
- Efficient Implementation
- Estimating Errors and Condition Number
- Cholesky Decomposition
- Sparse Matrices

# Outline

1. Review Gaussian Elimination

2. LU Decomposition

# Gaussian Elimination

$$(A|\mathbf{b}) = \left(\begin{array}{ccccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} & b_2 \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3n} & b_3 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{n(n-1)} & a_{nn} & b_n \end{array}\right)$$

$\Downarrow$ eliminate 1st column

$$(A^{(1)}|\mathbf{b}^{(1)}) = \left(\begin{array}{ccccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ 0 & a_{22}^{(1)} & a_{23}^{(1)} & \cdots & a_{2n}^{(1)} & b_2^{(1)} \\ \vdots & a_{32}^{(1)} & a_{33}^{(1)} & \cdots & a_{3n}^{(1)} & b_3^{(1)} \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{n(n-1)}^{(1)} & a_{nn}^{(1)} & b_n^{(1)} \end{array}\right)$$

$\Downarrow$ eliminate 2nd, . . . , (n-1)th column

$$(A^{(n-1)}|\mathbf{b}^{(n-1)}) = \left(\begin{array}{ccccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & b_1 \\ 0 & a_{22}^{(1)} & a_{23}^{(1)} & \cdots & a_{2n}^{(1)} & b_2^{(1)} \\ \vdots & 0 & a_{33}^{(2)} & \cdots & a_{3n}^{(2)} & b_3^{(2)} \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & a_{nn}^{(n-1)} & b_n^{(n-1)} \end{array}\right)$$

# Example

$$(A|\mathbf{b}) = \left(\begin{array}{rrr|r} 3 & -2 & 1 & 1 \\ 1 & 1 & 0 & 4 \\ 1 & -1 & 3 & 2 \end{array}\right)$$

$$\begin{aligned} l_{21} &= {}^{a_{21}}/_{a_{11}} = {}^{1}/_{3} \\ \mathbf{a}_{2:}^{(1)} &= \mathbf{a}_{2:} - l_{21}\,\mathbf{a}_{1:} \\ l_{31} &= {}^{a_{31}}/_{a_{11}} = {}^{1}/_{3} \\ \mathbf{a}_{3:}^{(1)} &= \mathbf{a}_{3:} - l_{31}\,\mathbf{a}_{1:} \end{aligned}$$

$$\rightsquigarrow \left(A^{(1)}\middle|\mathbf{b}^{(1)}\right) = \left(\begin{array}{rrr|r} 3 & -2 & 1 & 1 \\ 0 & {}^{5}/_{3} & -{}^{1}/_{3} & {}^{11}/_{3} \\ 0 & -{}^{1}/_{3} & {}^{8}/_{3} & {}^{5}/_{3} \end{array}\right)$$

$$\begin{aligned} l_{32} &= {}^{a_{32}^{(1)}}/_{a_{22}^{(1)}} = -{}^{1}/_{5} \\ \mathbf{a}_{3:}^{(2)} &= \mathbf{a}_{3:}^{(1)} - l_{32}\,\mathbf{a}_{2:}^{(1)} \end{aligned}$$

$$\rightsquigarrow \left(A^{(2)}\middle|\mathbf{b}^{(2)}\right) = \left(\begin{array}{rrr|r} \color{red}{3} & \color{red}{-2} & \color{red}{1} & 1 \\ \color{red}{0} & \color{red}{{}^{5}/_{3}} & \color{red}{-{}^{1}/_{3}} & {}^{11}/_{3} \\ \color{red}{0} & \color{red}{0} & \color{red}{{}^{13}/_{5}} & {}^{12}/_{5} \end{array}\right) = \left(\color{red}{U}\middle|\mathbf{b}^{(2)}\right)$$

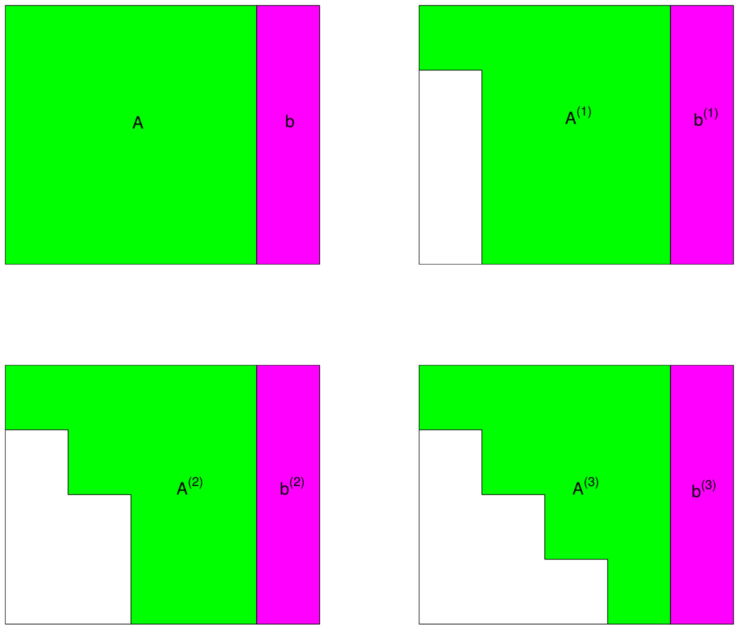
$$A^{(2)} = MA = \color{red}{U}$$

# Gaussian Elimination (cont.)

- Can multiply a row of $A\mathbf{x} = \mathbf{b}$ by a scalar and add to another row: **elementary transformation**.
- Use this to transform $A$ to upper triangular form:

$$MA\mathbf{x} = M\mathbf{b}, \quad U = MA.$$

- Apply backward substitution to solve $U\mathbf{x} = M\mathbf{b}$.



# Outline

# Outline

1. Review Gaussian Elimination

2. LU Decomposition
   - Elementary Transformation
   - Matrix Decomposition
   - Equivalence to Gaussian Elimination

# LU Decomposition

- What if we have many right hand side vectors, or we don't know $\mathbf{b}$ right away?
- Note that determining transformation $M$ such that $MA = U$ does not depend on $\mathbf{b}$.

# Example (cont.)

$$A = \begin{pmatrix} 3 & -2 & 1 \\ 1 & 1 & 0 \\ 1 & -1 & 3 \end{pmatrix}$$

$$M^{(1)}A = \begin{pmatrix} 1 & 0 & 0 \\ -l_{21} & 1 & 0 \\ -l_{31} & 0 & 1 \end{pmatrix} \begin{pmatrix} 3 & -2 & 1 \\ 1 & 1 & 0 \\ 1 & -1 & 3 \end{pmatrix} = A^{(1)}$$

$$M^{(2)}A^{(1)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -l_{32} & 1 \end{pmatrix} \begin{pmatrix} 3 & -2 & 1 \\ 0 & 5/3 & -1/3 \\ 0 & -1/3 & 8/3 \end{pmatrix} = A^{(2)}$$

$$U = A^{(2)} = M^{(2)}A^{(1)} = M^{(2)}M^{(1)}A = MA$$

# LU Decomposition (cont.)

$$MA = U$$

$M = M^{(n-1)} \dots M^{(2)} M^{(1)}$, where $M^{(k)}$ is the transformation of the $k$th outer loop step. These are elementary lower triangular matrices, e.g.,

$$M^{(2)} = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & -l_{32} & \ddots & & \\ & \vdots & & \ddots & \\ & -l_{n2} & & & 1 \end{pmatrix}.$$

# Outline

# Example (cont.) – Inverse of $M^{(1)}$, $M^{(2)}$

$$M^{(1)} = \begin{pmatrix} 1 & 0 & 0 \\ -1/3 & 1 & 0 \\ -1/3 & 0 & 1 \end{pmatrix}, \qquad \left[M^{(1)}\right]^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ 1/3 & 0 & 1 \end{pmatrix}$$

$$M^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/5 & 1 \end{pmatrix}, \qquad \left[M^{(2)}\right]^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1/5 & 1 \end{pmatrix}$$

# LU Decomposition (cont.)

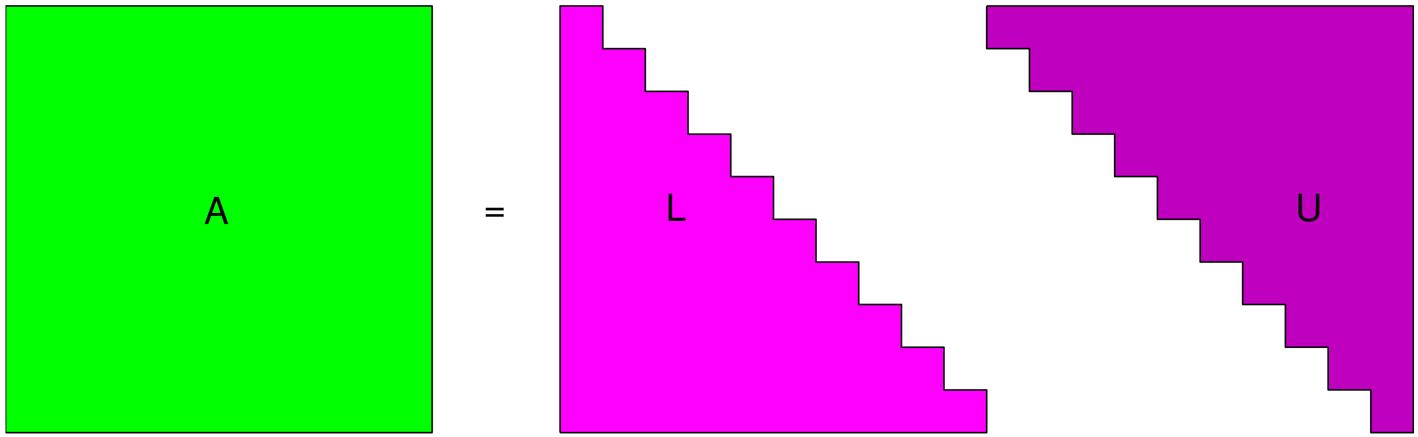
$$MA = U$$

- The matrix $M = M^{(n-1)} \cdots M^{(2)} M^{(1)}$ is unit lower triangular.
- The matrix $L = M^{-1}$ is also unit lower triangular:

$$A = LU, \quad L = \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ l_{31} & l_{32} & 1 & & \\ \vdots & \vdots & \ddots & \ddots & \\ l_{n1} & l_{n2} & \cdots & l_{n,n-1} & 1 \end{pmatrix}.$$

# Outline

# LU Decomposition (cont.)




So, the Gaussian elimination method is equivalent to:

1. decompose $A = LU$. *Now, for a given* $\mathbf{b}$ *we have to solve* $L(U\mathbf{x}) = \mathbf{b}$ :
2. use forward substitution to solve $L\mathbf{y} = \mathbf{b}$;
3. use backward substitution to solve $U\mathbf{x} = \mathbf{y}$.

# Examples where the LU Decomposition is Useful

- When we have multiple right-hand sides, form *once* the LU decomposition (which costs $\mathcal{O}(n^3)$ flops); then for each right-hand side only apply forward/backward substitutions (which are computationally cheap at $\mathcal{O}(n^2)$ flops each).

- Can compute $A^{-1}$ by decomposing $A = LU$ once, and then solving $LU\mathbf{x} = \mathbf{e}_k$ for each column $\mathbf{e}_k$ of the unit matrix. These are $n$ right hand sides, so the cost is approximately $\frac{2}{3}n^3 + n \cdot 2n^2 = \frac{8}{3}n^3$ flops. (However, typically we try to avoid computing the inverse $A^{-1}$; the need to compute it *explicitly* is rare.)

- Compute determinant of $A$ by

$$\det(A) = \det(L)\det(U) = \Pi_{k=1}^{n} u_{kk}.$$

# Another Example (1/3) – Home

$$A = \begin{pmatrix} 1 & -4 & 3 \\ 1 & 1 & 0 \\ 3 & -2 & 1 \end{pmatrix}.$$

Obtain

1. $l_{21} = \frac{1}{1} = 1, \ l_{31} = \frac{3}{1} = 3$, so

$$M^{(1)} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -3 & 0 & 1 \end{pmatrix}, \quad A^{(1)} = M^{(1)}A = \begin{pmatrix} 1 & -4 & 3 \\ 0 & 5 & -3 \\ 0 & 10 & -8 \end{pmatrix}.$$

2. $l_{32} = \frac{10}{5} = 2$, so

$$M^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{pmatrix}, \quad A^{(2)} = M^{(2)}A^{(1)} = \begin{pmatrix} 1 & -4 & 3 \\ 0 & 5 & -3 \\ 0 & 0 & -2 \end{pmatrix}.$$

## Example (2/3)

- We thus obtain

$$U = A^{(2)} = M^{(2)}A^{(1)} = \begin{pmatrix} 1 & -4 & 3 \\ 0 & 5 & -3 \\ 0 & 0 & -2 \end{pmatrix}.$$

- Note that since $U = M^{(2)}M^{(1)}A$, we have $A = [M^{(1)}]^{-1}[M^{(2)}]^{-1}U$.
- Verify directly that

$$[M^{(1)}]^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & 0 & 1 \end{pmatrix}, \quad [M^{(2)}]^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 2 & 1 \end{pmatrix},$$

and hence that

$$L = [M^{(1)}]^{-1}[M^{(2)}]^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & 2 & 1 \end{pmatrix}.$$

# Example (3/3)

- To get the matrix $L$ we therefore collect the multipliers $l_{21}$, $l_{31}$ and $l_{32}$ into the unit lower triangular matrix

$$L = \begin{pmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & 2 & 1 \end{pmatrix}.$$

- Indeed, $A = LU$:

$$\begin{pmatrix} 1 & -4 & 3 \\ 1 & 1 & 0 \\ 3 & -2 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & -4 & 3 \\ 0 & 5 & -3 \\ 0 & 0 & -2 \end{pmatrix}.$$