

## 7. LU factorization

- factor-solve method
- LU factorization
- solving  $Ax = b$  with  $A$  nonsingular
- the inverse of a nonsingular matrix
- LU factorization algorithm
- effect of rounding error
- sparse LU factorization

## Factor-solve approach

to solve  $Ax = b$ , first write  $A$  as a product of 'simple' matrices

$$A = A_1 A_2 \cdots A_k$$

then solve  $(A_1 A_2 \cdots A_k)x = b$  by solving  $k$  equations

$$A_1 z_1 = b, \quad A_2 z_2 = z_1, \quad \dots, \quad A_{k-1} z_{k-1} = z_{k-2}, \quad A_k x = z_{k-1}$$

### examples

- Cholesky factorization (for positive definite  $A$ )

$$k = 2, \quad A = LL^T$$

- sparse Cholesky factorization (for sparse positive definite  $A$ )

$$k = 4, \quad A = PLL^T P$$

# Complexity of factor-solve method

$$\#\text{flops} = f + s$$

- $f$  is cost of factoring  $A$  as  $A = A_1 A_2 \cdots A_k$  (factorization step)
- $s$  is cost of solving the  $k$  equations for  $z_1, z_2, \dots, z_{k-1}, x$  (solve step)
- usually  $f \gg s$

**example:** positive definite equations using the Cholesky factorization

$$f = (1/3)n^3, \quad s = 2n^2$$

## Multiple right-hand sides

two equations with the same matrix but different right-hand sides

$$Ax = b, \quad A\tilde{x} = \tilde{b}$$

- factor  $A$  once ( $f$  flops)
- solve with right-hand side  $b$  ( $s$  flops)
- solve with right-hand side  $\tilde{b}$  ( $s$  flops)

cost:  $f + 2s$  instead of  $2(f + s)$  if we solve second equation from scratch

**conclusion:** if  $f \gg s$ , we can solve the two equations at the cost of one

# LU factorization

## LU factorization without pivoting

$$A = LU$$

- $L$  unit lower triangular,  $U$  upper triangular
- does not always exist (even if  $A$  is nonsingular)

## LU factorization (with row pivoting)

$$A = PLU$$

- $P$  permutation matrix,  $L$  unit lower triangular,  $U$  upper triangular
- exists if and only if  $A$  is nonsingular (see later)

**cost:**  $(2/3)n^3$  if  $A$  has order  $n$

# Solving linear equations by LU factorization

solve  $Ax = b$  with  $A$  nonsingular of order  $n$

**factor-solve method** using LU factorization

1. factor  $A$  as  $A = PLU$  ( $(2/3)n^3$  flops)
2. solve  $(PLU)x = b$  in three steps
  - permutation:  $z_1 = P^T b$  (0 flops)
  - forward substitution: solve  $Lz_2 = z_1$  ( $n^2$  flops)
  - back substitution: solve  $Ux = z_2$  ( $n^2$  flops)

**total cost:**  $(2/3)n^3 + 2n^2$  flops, or roughly  $(2/3)n^3$

this is the standard method for solving  $Ax = b$

## Multiple right-hand sides

two equations with the same matrix  $A$  (nonsingular and  $n \times n$ ):

$$Ax = b, \quad A\tilde{x} = \tilde{b}$$

- factor  $A$  once
- forward/back substitution to get  $x$
- forward/back substitution to get  $\tilde{x}$

cost:  $(2/3)n^3 + 4n^2$  or roughly  $(2/3)n^3$

**exercise:** propose an efficient method for solving

$$Ax = b, \quad A^T \tilde{x} = \tilde{b}$$

## Inverse of a nonsingular matrix

suppose  $A$  is nonsingular of order  $n$ , with LU factorization

$$A = PLU$$

- inverse from LU factorization

$$A^{-1} = (PLU)^{-1} = U^{-1}L^{-1}P^T$$

- gives interpretation of solve step: evaluate

$$x = A^{-1}b = U^{-1}L^{-1}P^Tb$$

in three steps

$$z_1 = P^Tb, \quad z_2 = L^{-1}z_1, \quad x = U^{-1}z_2$$

# Computing the inverse

solve  $AX = I$  by solving  $n$  equations

$$AX_1 = e_1, \quad AX_2 = e_2, \quad \dots, \quad AX_n = e_n$$

$X_i$  is the  $i$ th column of  $X$ ;  $e_i$  is the  $i$ th unit vector of size  $n$

- one LU factorization of  $A$ :  $2n^3/3$  flops
- $n$  solve steps:  $2n^3$  flops

**total:**  $(8/3)n^3$  flops

**conclusion:** do not solve  $Ax = b$  by multiplying  $A^{-1}$  with  $b$

## LU factorization without pivoting

partition  $A$ ,  $L$ ,  $U$  as block matrices:

$$A = \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \quad L = \begin{bmatrix} 1 & 0 \\ L_{21} & L_{22} \end{bmatrix}, \quad U = \begin{bmatrix} u_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}$$

- $a_{11}$  and  $u_{11}$  are scalars
- $L_{22}$  unit lower-triangular,  $U_{22}$  upper triangular of order  $n - 1$

determine  $L$  and  $U$  from  $A = LU$ , *i.e.*,

$$\begin{aligned} \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} u_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix} \\ &= \begin{bmatrix} u_{11} & U_{12} \\ u_{11}L_{21} & L_{21}U_{12} + L_{22}U_{22} \end{bmatrix} \end{aligned}$$

## recursive algorithm:

- determine first row of  $U$  and first column of  $L$

$$u_{11} = a_{11}, \quad U_{12} = A_{12}, \quad L_{21} = (1/a_{11})A_{21}$$

- factor the  $(n - 1) \times (n - 1)$ -matrix  $A_{22} - L_{21}U_{12}$  as

$$A_{22} - L_{21}U_{12} = L_{22}U_{22}$$

this is an LU factorization (without pivoting) of order  $n - 1$

**cost:**  $(2/3)n^3$  flops (no proof)

## Example

LU factorization (without pivoting) of

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

write as  $A = LU$  with  $L$  unit lower triangular,  $U$  upper triangular

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- first row of  $U$ , first column of  $L$ :

$$\begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/4 & l_{32} & 1 \end{bmatrix} \begin{bmatrix} 8 & 2 & 9 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- second row of  $U$ , second column of  $L$ :

$$\begin{bmatrix} 9 & 4 \\ 7 & 9 \end{bmatrix} - \begin{bmatrix} 1/2 \\ 3/4 \end{bmatrix} \begin{bmatrix} 2 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{22} & u_{23} \\ 0 & u_{33} \end{bmatrix}$$

$$\begin{bmatrix} 8 & -1/2 \\ 11/2 & 9/4 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 11/16 & 1 \end{bmatrix} \begin{bmatrix} 8 & -1/2 \\ 0 & u_{33} \end{bmatrix}$$

- third row of  $U$ :  $u_{33} = 9/4 + 11/32 = 83/32$

conclusion:

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/4 & 11/16 & 1 \end{bmatrix} \begin{bmatrix} 8 & 2 & 9 \\ 0 & 8 & -1/2 \\ 0 & 0 & 83/32 \end{bmatrix}$$

## Not every nonsingular $A$ can be factored as $A = LU$

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- first row of  $U$ , first column of  $L$ :

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & l_{32} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- second row of  $U$ , second column of  $L$ :

$$\begin{bmatrix} 0 & 2 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{22} & u_{23} \\ 0 & u_{33} \end{bmatrix}$$

$$u_{22} = 0, u_{23} = 2, l_{32} \cdot 0 = 1 ?$$

# LU factorization (with row pivoting)

if  $A$  is  $n \times n$  and nonsingular, then it can be factored as

$$A = PLU$$

$P$  is a permutation matrix,  $L$  is unit lower triangular,  $U$  is upper triangular

- not unique; there may be several possible choices for  $P$ ,  $L$ ,  $U$
- interpretation: permute the rows of  $A$  and factor  $P^T A$  as  $P^T A = LU$
- also known as *Gaussian elimination with partial pivoting* (GEPP)
- cost:  $(2/3)n^3$  flops

we will skip the details of calculating  $P$ ,  $L$ ,  $U$

## Example

$$\begin{bmatrix} 0 & 5 & 5 \\ 2 & 9 & 0 \\ 6 & 8 & 8 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ 0 & 15/19 & 1 \end{bmatrix} \begin{bmatrix} 6 & 8 & 8 \\ 0 & 19/3 & -8/3 \\ 0 & 0 & 135/19 \end{bmatrix}$$

the factorization is not unique; the same matrix can be factored as

$$\begin{bmatrix} 0 & 5 & 5 \\ 2 & 9 & 0 \\ 6 & 8 & 8 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & -19/5 & 1 \end{bmatrix} \begin{bmatrix} 2 & 9 & 0 \\ 0 & 5 & 5 \\ 0 & 0 & 27 \end{bmatrix}$$

## Effect of rounding error

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

exact solution:

$$x_1 = \frac{-1}{1 - 10^{-5}}, \quad x_2 = \frac{1}{1 - 10^{-5}}$$

let us solve the equations using LU factorization, rounding intermediate results to 4 significant decimal digits

we will do this for the two possible permutation matrices:

$$P = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{or} \quad P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

**first choice of  $P$ :  $P = I$  (no pivoting)**

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix} \begin{bmatrix} 10^{-5} & 1 \\ 0 & 1 - 10^5 \end{bmatrix}$$

$L, U$  rounded to 4 decimal significant digits

$$L = \begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix}, \quad U = \begin{bmatrix} 10^{-5} & 1 \\ 0 & -10^5 \end{bmatrix}$$

forward substitution

$$\begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \Longrightarrow \quad z_1 = 1, \quad z_2 = -10^5$$

back substitution

$$\begin{bmatrix} 10^{-5} & 1 \\ 0 & -10^5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -10^5 \end{bmatrix} \quad \Longrightarrow \quad x_1 = 0, \quad x_2 = 1$$

error in  $x_1$  is 100%

**second choice of  $P$ :** interchange rows

$$\begin{bmatrix} 1 & 1 \\ 10^{-5} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 - 10^{-5} \end{bmatrix}$$

$L, U$  rounded to 4 decimal significant digits

$$L = \begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix}, \quad U = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

forward substitution

$$\begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \implies z_1 = 0, \quad z_2 = 1$$

backward substitution

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \implies x_1 = -1, \quad x_2 = 1$$

error in  $x_1, x_2$  is about  $10^{-5}$

## conclusion:

- for some choices of  $P$ , small rounding errors in the algorithm cause very large errors in the solution
- this is called **numerical instability**: for the first choice of  $P$ , the algorithm is unstable; for the second choice of  $P$ , it is stable
- from numerical analysis: there is a simple rule for selecting a good (stable) permutation (we'll skip the details, since we skipped the details of the factorization algorithm)
- in the example, the second permutation is better because it permutes the largest element (in absolute value) of the first column of  $A$  to the 1,1-position

# Sparse linear equations

if  $A$  is sparse, it is usually factored as

$$A = P_1 L U P_2$$

$P_1$  and  $P_2$  are permutation matrices

- interpretation: permute rows and columns of  $A$  and factor  $\tilde{A} = P_1^T A P_2^T$

$$\tilde{A} = L U$$

- choice of  $P_1$  and  $P_2$  greatly affects the sparsity of  $L$  and  $U$ : many heuristic methods exist for selecting good permutations
- in practice: #flops  $\ll (2/3)n^3$ ; exact value is a complicated function of  $n$ , number of nonzero elements, sparsity pattern

# Conclusion

different levels of understanding how linear equation solvers work:

**highest level:**  $x = A \setminus b$  costs  $(2/3)n^3$ ; more efficient than  $x = \text{inv}(A)*b$

**intermediate level:** factorization step  $A = PLU$  followed by solve step

**lowest level:** details of factorization  $A = PLU$

- for most applications, level 1 is sufficient
- in some situations (*e.g.*, multiple right-hand sides) level 2 is useful
- level 3 is important only for experts who write numerical libraries