

## 7. Linear equations

- QR factorization method
- factor and solve
- LU factorization

# QR factorization and matrix inverse

## QR factorization of nonsingular matrix

every nonsingular  $A \in \mathbf{R}^{n \times n}$  has a QR factorization

$$A = QR$$

- $Q \in \mathbf{R}^{n \times n}$  is orthogonal ( $Q^T Q = QQ^T = I$ )
- $R \in \mathbf{R}^{n \times n}$  is upper triangular with positive diagonal elements

**Inverse from QR factorization:** the inverse  $A^{-1}$  can be written as

$$A^{-1} = (QR)^{-1} = R^{-1}Q^{-1} = R^{-1}Q^T$$

# Solving linear equations by QR factorization

**Algorithm:** to solve  $Ax = b$  with nonsingular  $A \in \mathbf{R}^{n \times n}$ ,

1. factor  $A$  as  $A = QR$
2. compute  $y = Q^T b$
3. solve  $Rx = y$  by back substitution

**Complexity:**  $2n^3 + 3n^2 \approx 2n^3$  flops

- QR factorization:  $2n^3$
- matrix-vector multiplication:  $2n^2$
- back substitution:  $n^2$

## Multiple right-hand sides

consider  $k$  sets of linear equations with the same coefficient matrix  $A$ :

$$Ax_1 = b_1, \quad Ax_2 = b_2, \quad \dots, \quad Ax_k = b_k$$

- can be solved in  $2n^3 + 3kn^2$  flops if we reuse the factorization  $A = QR$
- for  $k \ll n$ , cost is roughly equal to cost of solving one equation ( $2n^3$ )

**Application:** to compute  $A^{-1}$ , solve the matrix equation  $AX = I$

- equivalent to  $n$  equations

$$Rx_1 = Q^T e_1, \quad Rx_2 = Q^T e_2, \quad \dots, \quad Rx_n = Q^T e_n$$

( $x_i$  is column  $i$  of  $X$  and  $Q^T e_i$  is transpose of  $i$ th row of  $Q$ )

- complexity is  $2n^3 + n^3 = 3n^3$  (here the 2nd term  $n^3$  is not negligible)

# Outline

- QR factorization method
- **factor and solve**
- 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

- QR factorization:  $k = 2$ ,  $A = QR$
- LU factorization (this lecture)
- Cholesky factorization (later)

## Complexity of factor–solve method

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

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

**Example:** solving linear equations using the QR factorization

$$f = 2n^3, \quad s = 3n^2$$

# Outline

- QR factorization method
- factor and solve
- **LU factorization**



# 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)

**Complexity:**  $(2/3)n^3$  if  $A$  is  $n \times n$

# Solving linear equations by LU factorization

**Algorithm:** to solve  $Ax = b$  with nonsingular  $A$  of size  $n \times n$

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

**Complexity:**  $(2/3)n^3 + 2n^2 \approx (2/3)n^3$  flops

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  $\tilde{x}$

complexity:  $(2/3)n^3 + 4n^2 \approx (2/3)n^3$

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

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

# LU factorization and matrix inverse

suppose  $A$  is nonsingular and  $n \times n$ , with LU factorization

$$A = PLU$$

- inverse from LU factorization

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

- gives interpretation of solve step: we 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  $AX = I$  column by column

- one LU factorization of  $A$ :  $2n^3/3$  flops
- $n$  solve steps:  $2n^3$  flops
- total:  $(8/3)n^3$  flops

slightly faster methods exist that exploit structure in right-hand side  $I$

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

## LU factorization without pivoting

$$\begin{aligned} \begin{bmatrix} A_{11} & A_{1,2:n} \\ A_{2:n,1} & A_{2:n,2:n} \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ L_{2:n,1} & L_{2:n,2:n} \end{bmatrix} \begin{bmatrix} U_{11} & U_{1,2:n} \\ 0 & U_{2:n,2:n} \end{bmatrix} \\ &= \begin{bmatrix} U_{11} & U_{1,2:n} \\ U_{11}L_{2:n,1} & L_{2:n,1}U_{1,2:n} + L_{2:n,2:n}U_{2:n,2:n} \end{bmatrix} \end{aligned}$$

### Recursive algorithm

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

$$U_{11} = A_{11}, \quad U_{1,2:n} = A_{1,2:n}, \quad L_{2:n,1} = \frac{1}{A_{11}}A_{2:n,1}$$

- factor the  $(n-1) \times (n-1)$ -matrix  $A_{2:n,2:n} - L_{2:n,1}U_{1,2:n}$  as

$$A_{2:n,2:n} - L_{2:n,1}U_{1,2:n} = L_{2:n,2:n}U_{2:n,2:n}$$

this is an LU factorization (without pivoting) of size  $(n-1) \times (n-1)$

## 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

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

## Example

- 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)
- complexity:  $(2/3)n^3$  flops

we 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

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

solution:

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

- let us solve using LU factorization for the two possible permutations:

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

- we round intermediate results to four significant decimal digits

## First choice: $P = I$ (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 significant decimal 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

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

- back substitution

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

error in  $x_1$  is 100%

## Second choice: 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 significant decimal digits

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

- forward substitution

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

- backward substitution

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

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

## Conclusion: rounding error and LU factorization

- for some choices of  $P$ , small errors in the algorithm can cause very large errors in the solution
- this is called *numerical instability*: for the first choice of  $P$  in the example, 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 permutation (we skip the details, since we skipped the details of the factorization)

# 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  $U$ : several heuristic methods exist for selecting good permutations
- in practice: #flops  $\ll (2/3)n^3$ ; exact value depends on  $n$ , number of nonzero elements, sparsity pattern



# Conclusion

different levels of detail in understanding how linear equation solvers work

## Highest level

- $\mathbf{x} = \mathbf{A} \setminus \mathbf{b}$  costs  $(2/3)n^3$
- more efficient than  $\mathbf{x} = \text{inv}(\mathbf{A}) * \mathbf{b}$

**Intermediate level:** factorization step  $\mathbf{A} = \mathbf{PLU}$  followed by solve step

**Lowest level:** details of factorization  $\mathbf{A} = \mathbf{PLU}$

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