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

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

examples

- Cholesky factorization (for positive definite A)

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

- sparse Cholesky factorization (for sparse positive definite A)

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

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, . . . z_{k-1}, x (solve step)
- usually $f \gg s$

example: positive definite equations using the Cholesky factorization

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

Multiple right-hand sides

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

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

- 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 $n \times n$):

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

- 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

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

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

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

  in three steps

$$z_1 = P^T b, \qquad z_2 = L^{-1}z_1, \qquad x = U^{-1}z_2$$

Computing the inverse

solve $AX = I$ by solving n equations

$$AX_1 = e_1, \qquad AX_2 = e_2, \qquad \ldots, \qquad AX_n = e_n$$

X_i is the ith column of X; e_i is the ith 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:

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

- 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

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

- 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:

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

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

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

forward substitution

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

back substitution

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

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

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

forward substitution

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

backward substitution

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

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 $\tilde{A} = P_1^T A P_2^T$

$$\tilde{A} = LU$$

- 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\b` costs $(2/3)n^3$; more efficient than `x = 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