

DM554
Linear and Integer Programming

LU Factorization

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[Based on slides by Lieven Vandenberghe, UCLA]

Outline

1. Operation Count

2. LU Factorization

3. Other Topics

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1. Operation Count

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3. Other Topics

Complexity of matrix algorithms

- flop counts
- vector-vector operations
- matrix-vector product
- matrix-matrix product

Flop counts

floating-point operation (flop)

- one floating-point addition, subtraction, multiplication, or division
- other common definition: one multiplication followed by one addition

flop counts of matrix algorithm

- total number of flops is typically a polynomial of the problem dimensions
- usually simplified by ignoring lower-order terms

applications

- a simple, machine-independent measure of algorithm complexity
- not an accurate predictor of computation time on modern computers

Vector-vector operations

- inner product of two n -vectors

$$\mathbf{x}^T \mathbf{y} = x_1 y_1 + x_2 y_2 + \dots + x_n y_n$$

n multiplications and $n - 1$ additions = $2n$ flops ($2n$ if $n \gg 1$)

- addition or subtraction of n -vectors: n flops
- scalar multiplication of n -vector : n flops

Matrix-vector product

matrix-vector product with $m \times n$ -matrix A :

$$\mathbf{y} = A\mathbf{x}$$

m elements in \mathbf{y} ; each element requires an inner product of length n :

$$(2n - 1)m \text{ flops}$$

approximately $2mn$ for large n special cases

- $m = n$, A diagonal: n flops
- $m = n$, A lower triangular: $n(n + 1)$ flops
- A very sparse (lots of zero coefficients): $\#flops \ll 2mn$

Matrix-matrix product

product of $m \times n$ -matrix A and $n \times p$ -matrix B :

$$C = AB$$

mp elements in C ; each element requires an inner product of length n :

$$mp(2n - 1) \text{ flops}$$

approximately $2mnp$ for large n .

Outline

1. Operation Count

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3. Other Topics

- 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

Definitions

Definition (Triangular Matrices)

An $n \times n$ matrix is said to be **upper triangular** if $a_{ij} = 0$ for $i > j$ and **lower triangular** if $a_{ij} = 0$ for $i < j$. Also A is said to be **triangular** if it is either upper triangular or lower triangular.

Example:

$$\begin{bmatrix} 3 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & 4 & 3 \end{bmatrix} \quad \begin{bmatrix} 3 & 5 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 7 \end{bmatrix}$$

Definition (Diagonal Matrices)

An $n \times n$ matrix is **diagonal** if $a_{ij} = 0$ whenever $i \neq j$.

Example:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

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

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Numerical Solutions

- A matrix A is said to be **ill conditioned** if relatively small changes in the entries of A can cause relatively large changes in the solutions of $Ax = b$.
- A is said to be **well conditioned** if relatively small changes in the entries of A result in relatively small changes in the solutions of $Ax = b$.
- reaching RREF as in Gauss-Jordan requires more computation and more numerical instability hence disadvantageous.
- Gauss elimination is a **direct method**: the amount of operations can be specified in advance.
Indirect or **Iterative methods** work by iteratively improving approximate solutions until a desired accuracy is reached. Amount of operations depend on the accuracy required. (way to go if the matrix is sparse)

Gauss-Seidel Iterative Method

Example

$$\begin{aligned}x_1 - 0.25x_2 - 0.25x_3 &= 50 \\ -0.25x_1 + x_2 - 0.25x_4 &= 50 \\ -0.25x_1 + x_3 - 0.25x_4 &= 25 \\ -0.25x_2 - 0.25x_3 + x_4 &= 25\end{aligned}$$

$$\begin{aligned}x_1 &= 0.25x_2 + 0.25x_3 + 50 \\ x_2 &= 0.25x_1 + 0.25x_4 + 50 \\ x_3 &= 0.25x_1 + 0.25x_4 + 25 \\ x_4 &= 0.25x_2 + 0.25x_3 + 25\end{aligned}$$

We start from an approximation, eg, $x_1^{(0)} = 100, x_2^{(0)} = 100, x_3^{(0)} = 100, x_4^{(0)} = 100$, and use the equations above to find a perhaps better approximation:

$$\begin{aligned}x_1^{(1)} &= 0.25x_2^{(0)} + 0.25x_3^{(0)} + 50.00 = 100.00 \\ x_2^{(1)} &= 0.25x_1^{(1)} + 0.25x_4^{(0)} + 50.00 = 100.00 \\ x_3^{(1)} &= 0.25x_1^{(1)} + 0.25x_4^{(0)} + 25.00 = 75.00 \\ x_4^{(1)} &= 0.25x_2^{(1)} + 0.25x_3^{(1)} + 25.00 = 68.75\end{aligned}$$

$$\begin{aligned}
 x_1^{(2)} &= 0.25x_2^{(1)} + 0.25x_3^{(1)} + 50.00 = 93.750 \\
 x_2^{(2)} &= 0.25x_1^{(2)} + 0.25x_4^{(1)} + 50.00 = 90.625 \\
 x_3^{(2)} &= 0.25x_1^{(2)} + 0.25x_4^{(1)} + 25.00 = 65.625 \\
 x_4^{(2)} &= 0.25x_2^{(2)} + 0.25x_3^{(2)} + 25.00 = 64.062
 \end{aligned}$$