

How to Write Fast Numerical Code

Spring 2011
Lecture 13

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Miscellaneous

- No class next Monday, April 11th (Sechseläuten)
- Midterm exam: Friday, April 15th

Today

- Solving linear systems
- Matrix inversion
- PLU factorization
- Determinant

Linear system solving

Matrix inversion

Singular value decomposition

... and more

LAPACK

BLAS

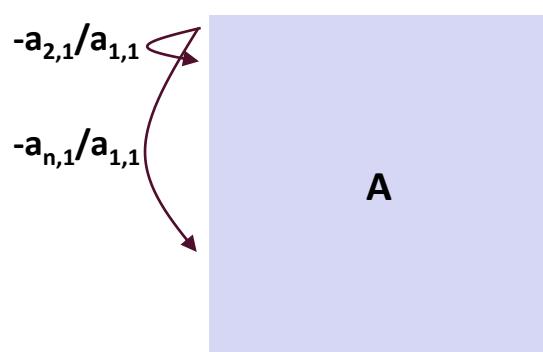
BLAS 1: vector-vector ops

BLAS 2: matrix-vector ops

BLAS 3: matrix-matrix ops

Chapter 2 in James W. Demmel, Applied Numerical Linear Algebra, SIAM, 1997

Gauss Elimination and LU Factorization

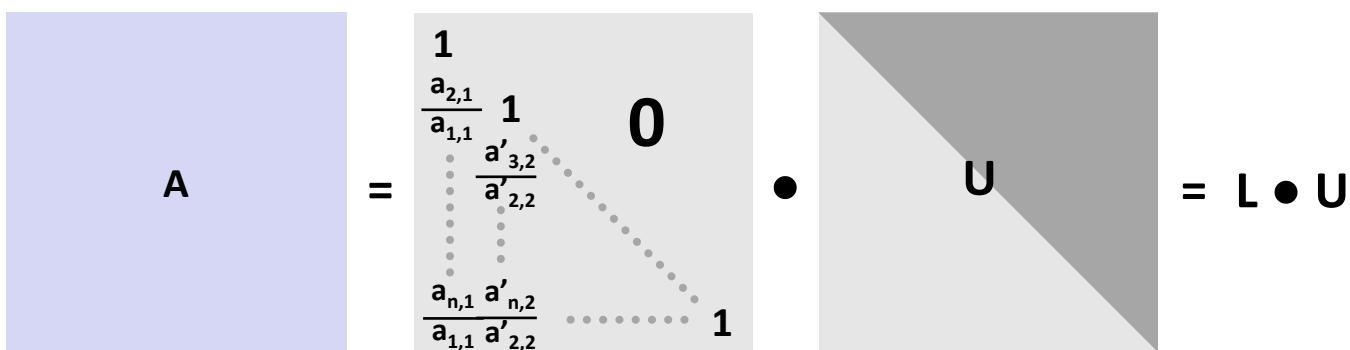
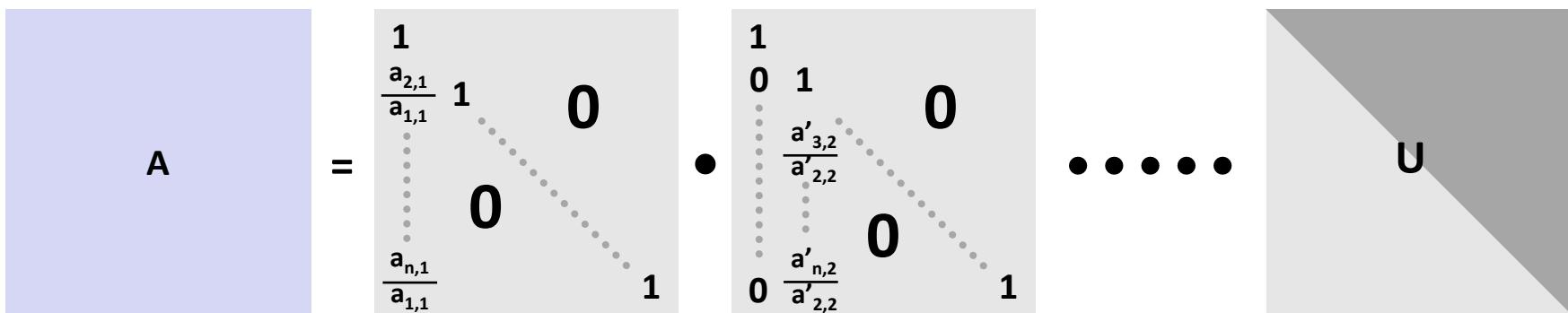
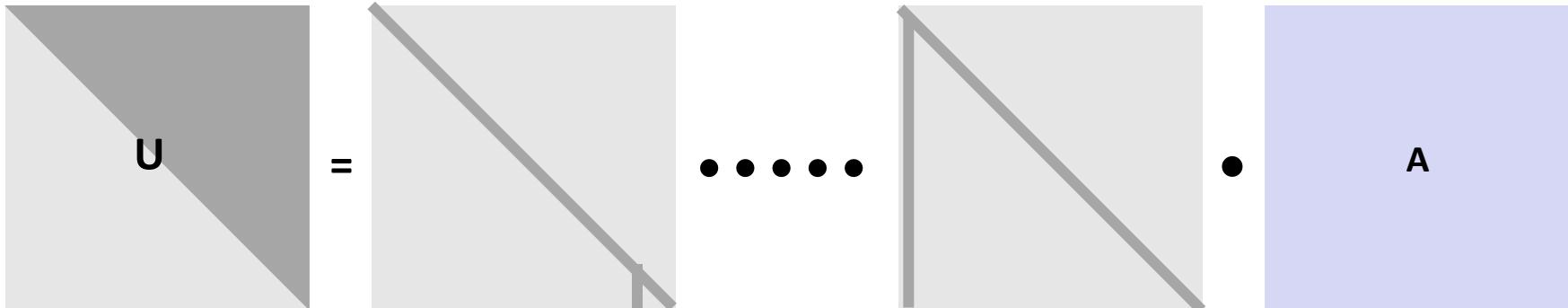


$$A = [a_{k,l}]_{1 \leq k, l \leq n}$$

$$\begin{matrix} a_{1,1} & \dots & a_{1,n} \\ 0 & & \\ \vdots & & \\ 0 & & \end{matrix} \begin{matrix} A' \\ \bullet \\ A \end{matrix} = \begin{matrix} 1 & & & \\ -\frac{a_{2,1}}{a_{1,1}} & 1 & & \\ \vdots & \vdots & & \\ -\frac{a_{n,1}}{a_{1,1}} & & 1 & \\ & & & 1 \end{matrix} \bullet \begin{matrix} A \\ \bullet \\ A \end{matrix}$$

$$\begin{matrix} a_{1,1} & \dots & a_{1,n} \\ 0 & a'_{2,2} & \dots & a'_{1,n} \\ \vdots & \vdots & & \\ 0 & 0 & & \end{matrix} \begin{matrix} A' \\ \bullet \\ \bullet \\ A \end{matrix} = \begin{matrix} 1 & & & \\ 0 & 1 & & \\ \vdots & \vdots & & \\ 0 & -\frac{a'_{3,2}}{a'_{2,2}} & 1 & \\ & \vdots & \vdots & \\ 0 & -\frac{a'_{n,2}}{a'_{2,2}} & & 1 \end{matrix} \bullet \begin{matrix} A \\ \bullet \\ \bullet \\ A \end{matrix}$$

after n-1 steps



Summary

■ Gauss elimination is LU factorization

- We assume that the occurring diagonal elements $a_{1,1}, a'_{2,2}, \dots$ are all $\neq 0$ (otherwise the LU factorization does not exist)
- U = upper triangular
- L = lower triangular (1's on diagonal)
- L contains the multipliers occurring in Gauss elimination

■ Now $Ax = b$ is $LUX = b$ and can be solved in two steps:

- Solve $Ly = b$
- Solve $Ux = y$
- Cost: $n^2 + O(n)$ for each step = $2n^2 + O(n)$

LU Factorization: Algorithm

- From straightforward algorithm to optimized BLAS 3 based one (blackboard)

Chapter 2 in James W. Demmel, Applied Numerical Linear Algebra, SIAM, 1997