Gauss Elimination and LU factorization

Standard Gauss Elimination: $A = [a_{k\ell}]_{1 \le k, \ell \le n}$

$$-\frac{a_{k1}}{a_{11}} \rightarrow \begin{pmatrix} & A & \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} a_{11} & a_{12} \cdots \\ 0 & \\ \vdots & A' \\ 0 & \end{pmatrix} = \begin{pmatrix} 1 & & & 0 \\ -\frac{a_{21}}{a_{11}} & 1 & & \\ \vdots & & \ddots & \\ -\frac{a_{n1}}{a_{11}} & 0 & & 1 \end{pmatrix} \cdot A$$

$$\downarrow$$

$$\begin{pmatrix} a_{11} & \cdots & \cdots \\ 0 & a'_{22} & \cdots \\ \vdots & 0 & \\ \vdots & \vdots & A'' \\ 0 & 0 & \end{pmatrix} = \begin{pmatrix} 1 & 0 & & \\ 0 & 1 & & 0 \\ \vdots & -\frac{a'_{32}}{a'_{22}} & 1 & \\ \vdots & \vdots & & \ddots \\ 0 & -\frac{a'_{n2}}{a'_{22}} & & & 1 \end{pmatrix} \begin{pmatrix} 1 & & & 0 \\ -\frac{a_{21}}{a_{11}} & 1 & & \\ \vdots & & \ddots & \\ -\frac{a_{n1}}{a_{11}} & 0 & & 1 \end{pmatrix} A$$

$$\vdots$$

$$\downarrow$$

$$U = \begin{pmatrix} \diagdown & \\ 0 & \diagdown \end{pmatrix} = \begin{pmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \\ & & x \;\; 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & & & 0 \\ x & 1 & & \\ \vdots & & \ddots & \\ x & 0 & & 1 \end{pmatrix} A$$

$$\Rightarrow A = \begin{pmatrix} 1 & & & \\ \frac{a_{21}}{a_{11}} & 1 & & \\ \vdots & & \ddots & \\ \frac{a_{n1}}{a_{11}} & & & 1 \end{pmatrix} \begin{pmatrix} 1 & & & \\ 0 & 1 & & 0 \\ \vdots & \frac{a'_{32}}{a'_{22}} & 1 & \\ \vdots & \vdots & 0 & \ddots \\ 0 & \frac{a'_{n2}}{a'_{22}} & & & 1 \end{pmatrix} \cdots \cdots \; U$$

$$= \underbrace{\begin{pmatrix} 1 & & & 0 \\ \frac{a_{21}}{a_{11}} & 1 & & \\ \vdots & \frac{a'_{32}}{a'_{22}} & 1 & \\ \vdots & \vdots & & \ddots \\ \frac{a_{n1}}{a_{11}} & \frac{a'_{n2}}{a'_{22}} & & & 1 \end{pmatrix}}_{L} \cdot U$$

Gauss-Elimination factors $A = LU$

L = lower triangular + diagonal elements = 1

U = upper triangular

Let $A = LU$. Then

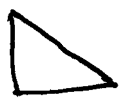
$$Ax = b \iff LUx = b$$

can be solved in 2 steps:

solve $Ly = b$

solve $Ux = y$

Cost:

$Ly = b \iff$  $\cdot y = b$

$$y_1 = b_1$$
$$y_2 = b_2 - l_{21} b_1 \qquad 2 \text{ flops}$$
$$y_3 = b_3 - l_{31} b_1 - l_{32} b_2 \qquad 4 \text{ flops}$$
$$\vdots$$

flops: $\sum_{i=1}^{n-1} 2i = n^2 + O(n)$

$Ux = y$: same flop count + n divisions

$\Rightarrow$ Given $A = LU$, $Ax = b$ can be solved in $2n^2 + O(n)$ flops

LU factorization: Algorithm

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for i = 1:n-1
    for j = i+1:n
        for k = i:n
            a_jk = a_jk - (a_ji / a_ii) a_ik
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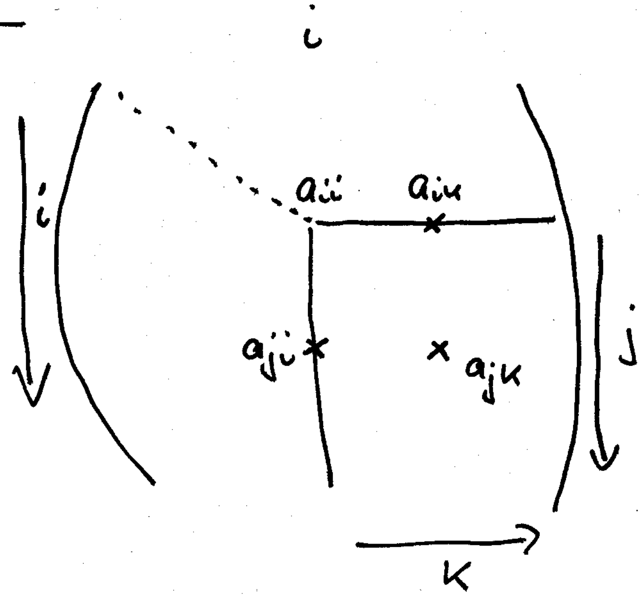


Let's optimize

1.) $k = i$ yields zero elements (we know that)

for $i = 1:n-1$
  for $j = i+1:n$ ← change
    for $k = i+1:n$
      $a_{jk} = a_{jk} - \frac{a_{ji}}{a_{ii}} a_{ik}$

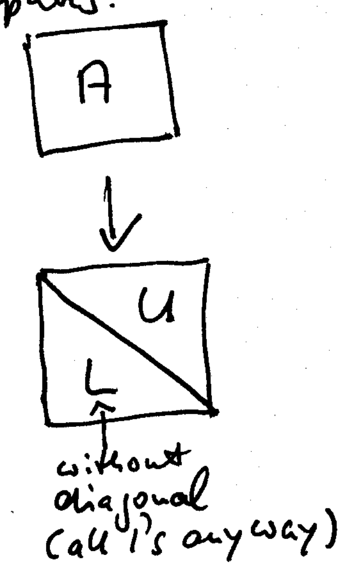
2.) $\frac{a_{ji}}{a_{ii}} = l_{ji}$ independent of k

for $i = 1:n-1$
  for $j = i+1:n$
    $l_{ji} = \frac{a_{ji}}{a_{ii}}$
    for $k = i+1:n$
      $a_{jk} = a_{jk} -$ ~~$\frac{a_{ji}}{a_{ii}}$~~ $l_{ji} \cdot a_{ik}$

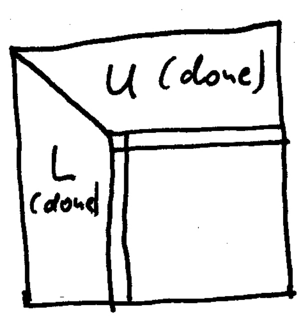
3.) Store l_{ji} in a_{ji}, since a_{ji} never touched again after zeroed out. Also, avoid division by a_{ii}

for $i = 1:n-1$
  $c = 1/a_{ii}$
  for $j = i+1:n$
    $a_{ji} = c \cdot a_{ji}$
    for $k = i+1:n$
      $a_{jk} = a_{jk} -$ ~~$\frac{a_{ji}}{a_{ii}}$~~ $a_{ji} \cdot a_{ik}$

computes:



intermediate step:



Cost analysis

- $(n-1)$ divisions
- flops: $$\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(1 + \sum_{k=i+1}^{n} 2\right) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(2(n-i)+1\right)$$
$$= \sum_{i=1}^{n-1} \left(2(n-i)^2 + (n-i)\right) = \sum_{i=1}^{n-1} \left(2i^2 + i\right)$$

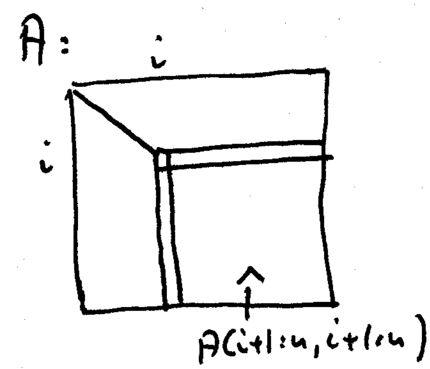
[Use: $\sum_{i=1}^{n-1} i^2 = \frac{(n-1)n(2n-1)}{6} = \frac{1}{3}n^3 + O(n^2)$]

$$= \frac{2}{3}n^3 + O(n^2)$$

Result: - $A = LU$ can be computed using $\frac{2}{3}n^3 + O(n^2)$ flops
- $Ax = b$ can be solved using $\frac{2}{3}n^3 + O(n^2)$ flops

(provided $A = LU$ exists, more later)

Vector form of LU factorization



for $i = 1:n-1$

[BLAS 1] $A(i+1:n, i) = A(i+1:n, i) / A(i,i)$

[BLAS 2] $A(i+1:n, i+1:n) = A(i+1:n, i+1:n) - A(i+1:n, i) \cdot A(i, i+1:n)$ } called "rank-1 update"

Pivoting:

Theorem: $A = LU$ exists if in each step of Gauss elimination $a_{ii} \neq 0$

$\Longleftrightarrow$ all matrices $A(1:j, 1:j)$ are invertible (non-singular)

Example: $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ has no LU factorization

Modify Gauss elimination:

GEPP (Gauss elimination with partial pivoting):

for $i = 1:n-1$
  permute rows s.t. $a_{ii} \neq 0$ and $|a_{ii}|$ largest in column (for numerical stability)
  [as before

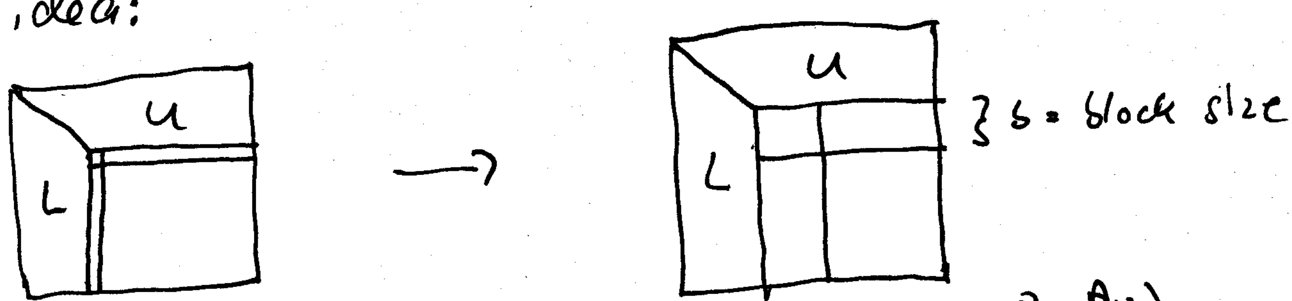
- computes $A = PLU$, P a permutation matrix
- adds $O(n^2)$ comparisons

Blocking (as implemented in LAPACK)

Reminder: Why blocking?

		memory ops	flops	ratio
BLAS 1	$y = x_1^T x_2$	$3n$	$2n-1$	$\sim \frac{2}{3}$
BLAS 2	$y = Ax$	n^2+2n	$2n^2-n$	~ 2
BLAS 3	$A = B \cdot C$	$3n^2$	$2n^3-n^3$	$\sim \frac{2}{3}n$
[FFT		$2n(3n)$	$\sim 4n\log n$	$O(\log n)$]

Basic idea:



standard

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

step 1: LU factorization of

$$\begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} = \begin{pmatrix} L_{11} \\ L_{21} \end{pmatrix} \cdot U_{11}$$

using standard algorithm

then: $A = \begin{pmatrix} L_{11}U_{11} & A_{12} \\ L_{21}U_{11} & A_{22} \end{pmatrix}$

$$= \begin{pmatrix} L_{11} & 0 \\ L_{21} & I \end{pmatrix} \begin{pmatrix} U_{11} & L_{11}^{-1}A_{12} \\ 0 & A_{22} - L_{21}L_{11}^{-1}A_{12} \end{pmatrix} \qquad U_{12} = L_{11}^{-1}A_{12}$$

$$= \begin{pmatrix} L_{11} & 0 \\ L_{21} & I \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} \\ 0 & A_{22} - L_{21}U_{12} \end{pmatrix} \qquad U_{22} = A_{22} - L_{12}U_{12}$$

thus:

step 2: $U_{12} = L_{11}^{-1}A_{12}$

step 3: $U_{22} = A_{22} - L_{21}U_{12}$

final algorithm:

for $i = 1 : b : n-1$

use standard algorithm to factorize $A(i:n, i:i+b-1) = \begin{pmatrix} L_{11} \\ L_{21} \end{pmatrix} U_{22}$

BLAS 3 $\quad A(i:i+b-1, i+b:n) = L_{11}^{-1} A(i:i+b-1, i+b:n)$

$A(i+b:n, i+b:n) = A(i+b:n, i+b:n) - A(i+b:n, i:i+b-1) \cdot A(i:i+b-1, i+b:n)$

BLAS3 (mm)

Matrix inversion

Given A, find M: $AM = I_n \iff$ solving n systems of linear equations $A m_i = e_i$

(m_i ↑ ith column of M)

step 1: compute $A = PLU$ $\left(\frac{2}{3}n^3 + O(n^2)\right)$

step 2: solve n systems of l.e. $(2n^2 + O(n)$ each$)$

$\Rightarrow$ cost $\frac{8}{3}n^3 + O(n^2)$

Determinant

step 1: compute $A = PLU$

step 2: $\det(A) = \prod_{i=1}^{n} u_{ii} \cdot \underbrace{\det(P)}_{\pm 1}$

$\Rightarrow$ cost $\frac{2}{3}n^3 + O(n^2)$