Dense LU factorization and its error analysis

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Plan

Basis of floating point arithmetic and stability analysis
- Notation, results, proofs taken from [N.J.Higham, 2002]

Direct methods of factorization
- LU factorization
  - Error analysis of LU factorization - main results
- Block LU factorization

Plan

Basis of floating point arithmetic and stability analysis

Notation, results, proofs taken from [N.J.Higham, 2002]

Direct methods of factorization

Norms and other notations

$$
\begin{aligned}
\|A\|_F &= \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{n}|a_{ij}|^2} \\
\|A\|_2 &= \sigma_{max}(A) \\
\|A\|_\infty &= \max_{1\le i\le n}\sum_{j=1}^{n}|a_{ij}| \\
\|A\|_1 &= \max_{1\le j\le n}\sum_{i=1}^{n}|a_{ij}|
\end{aligned}
$$

Inequalities $|x| \le |y|$ and $|A| \le |B|$ hold componentwise.

Floating point arithmetic

- The machine precision or unit roundoff is u
  - The maximum relative error for a given rounding procedure
  - u is of order 10^{-8} in single precision, $2^{-53} \approx 10^{-16}$ in double precision
  - Another definition: the smallest number that added to one gives a result different from one
- The evaluation involving basic arithmetic operations $+, -, *, /$ in floating point satisfies

$$fl(x\ op\ y) = (x\ op\ y)(1+\delta), \quad |\delta| \leq u$$

Relative error

- Given a real number x and its approximation $\hat{x}$, the absolute error and the relative errors are

$$E_{abs}(\hat{x}) = |x - \hat{x}|, \qquad E_{rel}(\hat{x}) = \frac{|x - \hat{x}|}{|x|} \tag{1}$$

- The relative error is scale independent
- Some examples, outline the difference with correct significant digits

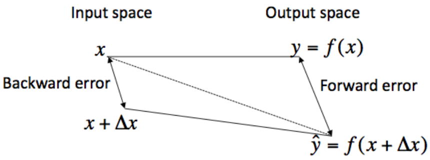
$$\begin{aligned} x &= 1.00000, \quad \hat{x} = 1.00499, \quad E_{rel}(\hat{x}) = 4.99 \times 10^{-3} \\ x &= 9.00000, \quad \hat{x} = 8.99899, \quad E_{rel}(\hat{x}) = 1.12 \times 10^{-4} \end{aligned}$$

- When x is a vector, the componentwise relative error is

$$\max_i \frac{|x_i - \hat{x}_i|}{|x_i|}$$

Backward and Forward errors

- Consider $y = f(x)$ a scalar function of a real scalar variable and $\hat{y}$ its approximation.
- Ideally we would like the forward error $E_{rel}(\hat{y}) \approx u$
- Instead we focus on the backward error, "For what set of data we have solved the problem?"
  that is we look for min $|\Delta x|$ such that $\hat{y} = f(x + \Delta x)$



Condition number

Assume f is twice continuously differentiable, then

$$\begin{aligned}\hat{y} - y &= f(x + \Delta x) - f(x) = f'(x)\Delta x + \frac{f''(x + \tau\Delta x)}{2!}(\Delta x)^2, \qquad \tau \in (0,1) \\ \frac{\hat{y} - y}{y} &= \left(\frac{xf'(x)}{f(x)}\right)\frac{\Delta x}{x} + O((\Delta x)^2)\end{aligned}$$

The condition number is

$$c(x) = \left|\frac{xf'(x)}{f(x)}\right|$$

Rule of thumb

When consistently defined, we have

$$\text{forward error} \leq \text{condition number} \times \text{backward error}$$

Preliminaries

Lemma (Lemma 3.1 in [N.J.Higham, 2002])

If $|\delta_i| \leq u$ *and* $\rho_i = \pm 1$ *for* $i = 1 : n$*, and* $nu < 1$*, then*

$$\prod_{i=1}^{n}(1+\delta_i)^{\rho_i} = 1 + \Theta_n, \qquad |\Theta_n| \leq \frac{nu}{1-nu} = \gamma_n$$

Other notations

$$\tilde{\gamma}_n = \frac{cnu}{1-cnu}$$

Inner product in floating point arithmetic

Consider computing $s_n = x^T y$, with an evaluation from left to right. We denote different errors as $1 + \delta_i \equiv 1 \pm \delta$

$$
\begin{aligned}
\hat{s}_1 &= fl(x_1 y_1) = x_1 y_1 (1 \pm \delta) \\
\hat{s}_2 &= fl(\hat{s}_1 + x_2 y_2) = (\hat{s}_1 + x_2 y_2 (1 \pm \delta))(1 \pm \delta) \\
&= x_1 y_1 (1 \pm \delta)^2 + x_2 y_2 (1 \pm \delta)^2 \\
&\vdots \\
\hat{s}_n &= x_1 y_1 (1 \pm \delta)^n + x_2 y_2 (1 \pm \delta)^n + x_3 y_3 (1 \pm \delta)^{n-1} + \ldots + x_n y_n (1 \pm \delta)^2
\end{aligned}
$$

After applying the previous lemma, we obtain

$$
\hat{s}_n = x_1 y_1 (1 + \Theta_n) + x_2 y_2 (1 + \Theta'_n) + \ldots + x_n y_n (1 + \Theta_2)
$$

Inner product in FP arithmetic - error bounds

We obtain the following backward and forward errors

$$\begin{aligned}
\hat{s}_n &= x_1 y_1 (1+\Theta_n) + x_2 y_2 (1+\Theta'_n) + \ldots + x_n y_n (1+\Theta_2) \\
fl(x^T y) &= (x+\Delta x)^T y = x^T (y+\Delta y), |\Delta x| \leq \gamma_n |x|, |\Delta y| \leq \gamma_n |y|, \\
|x^T y - fl(x^T y)| &\leq \gamma_n \sum_{i=1}^{n} |x_i y_i| = \gamma_n |x|^T |y|
\end{aligned}$$

- High relative accuracy is obtained when computing $x^T x$
- No guarantee of high accuracy when $|x^T y| << |x|^T |y|$

Plan

Basis of floating point arithmetic and stability analysis

Direct methods of factorization
- LU factorization
- Block LU factorization

LU factorization

Compute the factorization PA = LU

Example

Given the matrix

$$A = \begin{pmatrix} 3 & 1 & 3 \\ 6 & 7 & 3 \\ 9 & 12 & 3 \end{pmatrix}$$

Let

$$M_1 = \begin{pmatrix} 1 & & \\ -2 & 1 & \\ -3 & & 1 \end{pmatrix}, \quad M_1 A = \begin{pmatrix} 3 & 1 & 3 \\ 0 & 5 & -3 \\ 0 & 9 & -6 \end{pmatrix}$$

Algebra of the LU factorization

- In general

$$
\begin{aligned}
A^{(k+1)} &= M_k A^{(k)} := \begin{pmatrix} I_{k-1} & & & & \\ & 1 & & & \\ & -m_{k+1,k} & 1 & & \\ & \dots & & \ddots & \\ & -m_{n,k} & & & 1 \end{pmatrix} A^{(k)}, \text{where} \\
M_k &= I - m_k e_k^T, \quad M_k^{-1} = I + m_k e_k^T
\end{aligned}
$$

where e_k is the k-th unit vector, $e_i^T m_k = 0, \forall i \leq k$

- The factorization can be written as

$$M_{n-1} \dots M_1 A = A^{(n)} = U$$

Algebra of the LU factorization

- We obtain

$$\begin{aligned}
A &= M_1^{-1} \dots M_{n-1}^{-1} U \\
&= (I + m_1 e_1^T) \dots (I + m_{n-1} e_{n-1}^T) U \\
&= \left(I + \sum_{i=1}^{n-1} m_i e_i^T \right) U \\
&= \begin{pmatrix} 1 & & & \\ m_{21} & 1 & & \\ \vdots & \vdots & \ddots & \\ m_{n1} & m_{n2} & \dots & 1 \end{pmatrix} U = LU
\end{aligned}$$

The need for pivoting

- For stability, avoid division by small diagonal elements
- For example

$$A = \begin{pmatrix} 0 & 3 & 3 \\ 3 & 1 & 3 \\ 6 & 2 & 3 \end{pmatrix} \tag{2}$$

  has an LU factorization if we permute the rows of matrix A

$$PA = \begin{pmatrix} 6 & 2 & 3 \\ 0 & 3 & 3 \\ 3 & 1 & 3 \end{pmatrix} = \begin{pmatrix} 1 & & \\ & 1 & \\ 0.5 & & 1 \end{pmatrix} \cdot \begin{pmatrix} 6 & 2 & 3 \\ & 3 & 3 \\ & & 1.5 \end{pmatrix} \tag{3}$$

- Partial pivoting allows to bound the multipliers $m_{ik} \leq 1$ and hence $|L| \leq 1$

Existence of the LU factorization

Theorem

Given a full rank matrix A of size $m \times n$, $m \geq n$, the matrix A can be decomposed as $A = PLU$ where P is a permutation matrix of size $m \times m$, L is a unit lower triangular matrix of size $m \times n$ and U is a nonsingular upper triangular matrix of size $n \times n$.

Proof: simpler proof for the square case. Since A is full rank, there is a permutation P_1 such that $P_1 a_{11}$ is nonzero. Write the factorization as

$$P_1 A = \begin{pmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ A_{21}/a_{11} & I \end{pmatrix} \begin{pmatrix} a_{11} & A_{12} \\ 0 & A_{22} - a_{11}^{-1} A_{21} A_{12} \end{pmatrix},$$

where $S = A_{22} - a_{11}^{-1} A_{21} A_{12}$.
Since $det(A) \neq 0$, then $det(S) \neq 0$. Continue the proof by induction on S.

Solving $Ax = b$ by using Gaussian elimination

Composed of 4 steps

1. Factor $A = PLU$, $(2/3)n^3$) flops
2. Compute $P^T b$ to solve $LUx = P^T b$
3. Forward substitution: solve $Ly = P^T * b$, n^2 flops
4. Backward substitution: solve $Ux = y$, n^2 flops

Algorithm to compute the LU factorization

- Algorithm for computing the in place LU factorization of a matrix of size $n \times n$.
- $\#flops = 2n^3/3$

for k = 1:n-1 **do**
    Let a_{ik} be the element of maximum magnitude in $A(k : n, k)$
    Permute row i and row k
    $A(k+1 : n, k) = A(k+1 : n, k)/a_{kk}$
    for $i = k+1 : n$ **do**
        for $j = k+1 : n$ **do**
            $a_{ij} = a_{ij} - a_{ik}a_{kj}$
        end for
    end for
end for

Algorithm to compute the LU factorization

- Left looking approach, pivoting ignored, A of size $m \times n$
- $\#flops = n^2 m - n^3/3$

for k = 1:n **do**
    for j = k:n **do**
        $u_{kj} = a_{kj} - \sum_{i=1}^{k-1} l_{ki} u_{ij}$
    end for
    for i = k+1:m **do**
        $l_{ik} = (a_{ik} - \sum_{j=1}^{k-1} l_{ij} u_{jk}) / u_{kk}$
    end for
end for

Error analysis of the LU factorization

Given the first $k-1$ columns of L and $k-1$ rows of U were computed, we have

$$
\begin{aligned}
a_{kj} &= l_{k1}u_{1j} + \ldots + l_{k,k-1}u_{k-1,j} + u_{kj}, j = k : n \\
a_{ik} &= l_{i1}u_{1k} + \ldots + l_{ik}u_{kk}, i = k+1 : m
\end{aligned}
$$

The computed elements of $\hat{L}$ and $\hat{U}$ satisfy:

$$
\begin{aligned}
\left| a_{kj} - \sum_{i=1}^{k-1} \hat{l}_{ki}\hat{u}_{ij} - \hat{u}_{kj} \right| &\leq \gamma_k \sum_{i=1}^{k} |\hat{l}_{ki}||\hat{u}_{ij}|, \quad j \geq k, \\
\left| a_{ik} - \sum_{j=1}^{k} \hat{l}_{ij}\hat{u}_{jk} \right| &\leq \gamma_k \sum_{j=1}^{k} |\hat{l}_{ij}||\hat{u}_{jk}|, \quad i > k.
\end{aligned}
$$

Error analysis of the LU factorization (continued)

Theorem (Theorem 9.3 in [N.J.Higham, 2002])

Let $A \in \mathbb{R}^{m\times n}, m \geq n$ and let $\hat{L} \in \mathbb{R}^{m\times n}$ and $\hat{U} \in \mathbb{R}^{n\times n}$ be its computed LU factors obtained by Gaussian elimination (suppose there was no failure during GE). Then,

$$\hat{L}\hat{U} = A + \Delta A, \qquad |\Delta A| \leq \gamma_n |\hat{L}||\hat{U}|.$$

Theorem (Theorem 9.4 in [N.J.Higham, 2002])

Let $A \in \mathbb{R}^{m\times n}, m \geq n$ and let $\hat{x}$ be the computed solution to $Ax = b$ obtained by using the computed LU factors of A obtained by Gaussian elimination. Then

$$(A + \Delta A)\hat{x} = b, \qquad |\Delta A| \leq \gamma_{3n} |\hat{L}||\hat{U}|.$$

Error analysis of $Ax = b$

Theorem (Theorem 9.4 in [N.J.Higham, 2002] continued)

$$(A + \Delta A)\hat{x} = b, \qquad |\Delta A| \leq \gamma_{3n}|\hat{L}||\hat{U}|.$$

Proof.

We have the following:

$$\begin{aligned} \hat{L}\hat{U} &= A + \Delta A, \qquad |\Delta A| \leq \gamma_n |\hat{L}||\hat{U}|, \\ (\hat{L} + \Delta L)\hat{y} &= b, \qquad |\Delta L| \leq \gamma_n |\hat{L}|, \\ (\hat{U} + \Delta U)\hat{x} &= \hat{y}, \qquad |\Delta U| \leq \gamma_n |\hat{U}|. \end{aligned}$$

Thus

$$\begin{aligned} b &= (\hat{L} + \Delta L)(\hat{U} + \Delta U)\hat{x} = (A + \Delta A_1 + \hat{L}\Delta U + \Delta L \hat{U} + \Delta L \Delta U)\hat{x} \\ &= (A + \Delta A)\hat{x}, \textit{ where} \\ |\Delta A| &\leq (3\gamma_n + \gamma_n^2)|\hat{L}||\hat{U}| \leq \gamma_{3n}|\hat{L}||\hat{U}|. \end{aligned}$$

Wilkinson's backward error stability result

Growth factor g_W defined as

$$g_W = \frac{\max_{i,j,k} |a_{ij}^k|}{\max_{i,j} |a_{ij}|}$$

Note that

$$|u_{ij}| = |a_{ij}^i| \leq g_W \max_{i,j} |a_{ij}|$$

Theorem (Wilkinson's backward error stability result, see also [N.J.Higham, 2002] for more details)

Let $A \in \mathbb{R}^{n\times n}$ and let $\hat{x}$ be the computed solution of $Ax = b$ obtained by using GEPP. Then

$$(A + \Delta A)\hat{x} = b, \qquad \|\Delta A\|_\infty \leq n^2 \gamma_{3n} g_W(n) \|A\|_\infty.$$

The growth factor

- The LU factorization is backward stable if the growth factor is small (grows linearly with n).
- For partial pivoting, the growth factor $g(n) \leq 2^{n-1}$, and this bound is attainable.
- In practice it is on the order of $n^{2/3} - n^{1/2}$

Exponential growth factor for Wilkinson matrix

$$A = diag(\pm 1)\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 1 \\ -1 & 1 & 0 & \dots & 0 & 1 \\ -1 & -1 & 1 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 & 1 \\ -1 & -1 & \cdots & -1 & 1 & 1 \\ -1 & -1 & \cdots & -1 & -1 & 1 \end{bmatrix}$$

Experimental results for special matrices

Several errror bounds for GEPP, the normwise backward error η and the componentwise backward error w ($r = b - Ax$).

$$\eta = \frac{||r||_1}{||A||_1 \; ||x||_1 + ||b||_1},$$
$$w = \max_i \frac{|r_i|}{(|A| \; |x| + |b|)_i}.$$

matrix	cond(A,2)	g_W	$\|\|L\|\|_1$	cond(U,1)	$\frac{\|\|PA-LU\|\|_F}{\|\|A\|\|_F}$	η	w_b
hadamard	1.0E+0	4.1E+3	4.1E+3	5.3E+5	0.0E+0	3.3E-16	4.6E-15
randsvd	6.7E+7	4.7E+0	9.9E+2	1.4E+10	5.6E-15	3.4E-16	2.0E-15
chebvand	3.8E+19	2.0E+2	2.2E+3	4.8E+22	5.1E-14	3.3E-17	2.6E-16
frank	1.7E+20	1.0E+0	2.0E+0	1.9E+30	2.2E-18	4.9E-27	1.2E-23
hilb	8.0E+21	1.0E+0	3.1E+3	2.2E+22	2.2E-16	5.5E-19	2.0E-17

Block formulation of the LU factorization

Partitioning of matrix A of size $n \times n$

$$A = \left[\begin{array}{cc} A_{11} & A_{12} \\ A_{21} & A_{22} \end{array} \right]$$

where A_{11} is of size $b \times b$, A_{21} is of size $(m-b) \times b$, A_{12} is of size $b \times (n-b)$ and A_{22} is of size $(m-b) \times (n-b)$.

Block LU algebra

The first iteration computes the factorization:

$$P_1^T A = \left[\begin{array}{cc} L_{11} & \\ L_{21} & I_{n-b} \end{array} \right] \cdot \left[\begin{array}{cc} I_b & \\ & A^1 \end{array} \right] \cdot \left[\begin{array}{cc} U_{11} & U_{12} \\ & I_{n-b} \end{array} \right]$$

The algorithm continues recursively on the trailing matrix A^1.

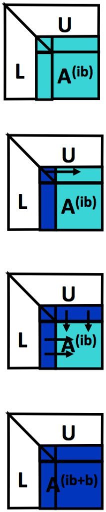
Block LU factorization - the algorithm

1. Compute the LU factorization with partial pivoting of the first block column
$$P_1 \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} = \begin{pmatrix} L_{11} \\ L_{21} \end{pmatrix} U_{11}$$
2. Pivot by applying the permutation matrix P_1^T on the entire matrix,
$$\bar{A} = P_1^T A.$$
3. Solve the triangular system
$$L_{11} U_{12} = \bar{A}_{12}$$
4. Update the trailing matrix,
$$A^1 = \bar{A}_{22} - L_{21} U_{12}$$
5. Compute recursively the block LU factorization of A^1.

LU Factorization as in ScaLAPACK

LU factorization on a P = Pr x Pc grid of processors
For ib = 1 to n-1 step b
$A(ib) = A(ib : n, ib : n)$

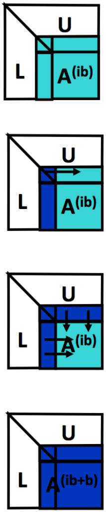
1. Compute panel factorization
   - find pivot in each column, swap rows
2. Apply all row permutations
   - broadcast pivot information along the rows
   - swap rows at left and right
3. Compute block row of U
   - broadcast right diagonal block of L of current panel
4. Update trailing matrix
   - broadcast right block column of L
   - broadcast down block row of U



Cost of LU Factorization in ScaLAPACK

LU factorization on a P = Pr x Pc grid of processors
For ib = 1 to n-1 step b
$A(ib) = A(ib : n, ib : n)$

1. Compute panel factorization
   - $\#messages = O(n \log_2 P_r)$
2. Apply all row permutations
   - $\#messages = O(n/b(\log_2 P_r + \log_2 P_c))$
3. Compute block row of U
   - $\#messages = O(n/b \log_2 P_c)$
4. Update trailing matrix
   - $\#messages = O(n/b(\log_2 P_r + \log_2 P_c)$



Cost of parallel block LU

Consider that we have a $\sqrt{P} \times \sqrt{P}$ grid, block size b

$$\gamma \cdot \left(\frac{2/3 n^3}{P} + \frac{n^2 b}{\sqrt{P}} \right) + \beta \cdot \frac{n^2 \log P}{\sqrt{P}} + \alpha \cdot \left(1.5 n \log P + \frac{3.5 n}{b} \log P \right).$$

Acknowledgement

- Stability analysis results presented from [N.J.Higham, 2002]
- Some of the examples taken from [Golub and Van Loan, 1996]

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