Dense LU and QR factorizations

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Plan

Direct methods of factorization

- LU factorization
- Block LU factorization
- QR factorization
- Block QR 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.

Plan

Direct methods of factorization

- LU factorization
- Block LU factorization
- QR factorization
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Algebra of the 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, $m_k = (0, \dots, 0, 1, m_{k+1,k}, \dots, m_{n,k})^T$, $e_i^T m_k = 0, \forall i \leq k$

- 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

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

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

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

- 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
```

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

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

where $\gamma_n = nu/(1 - nu)$, u is machine precision and assuming $nu < 1$.

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 $n \times n$

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

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:

$$P_1^T A = \begin{bmatrix} \bar{A}_{11} & \bar{A}_{12} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & \\ L_{21} & I_{n-b} \end{bmatrix} \cdot \begin{bmatrix} U_{11} & U_{12} \\ & A^1 \end{bmatrix}$$

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,

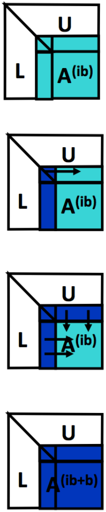
$$A^1 = \bar{A}_{22} - L_{21} U_{12}$$

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
$A(ib) = A(ib : n, ib : n)$

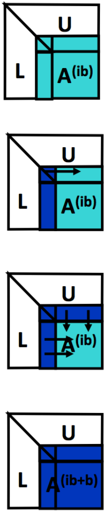
1. Compute panel factorization
   - find pivot in each column, swap rows
2. Apply all row permutations
   - broadcast pivot information along the rows
   - swap rows at left and right
3. Compute block row of U
   - broadcast right diagonal block of L of current panel
4. Update trailing matrix
   - broadcast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

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

The QR factorization

Given a matrix $A \in \mathbb{R}^{m \times n}$, $m \geq n$, its QR factorization is

$$A = QR = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 R_1$$

where $Q \in \mathbb{R}^{m \times m}$ is orthogonal and $R \in \mathbb{R}^{m \times n}$ is upper triangular.

If A has full rank, the factorization $Q_1 R_1$ is essentialy unique (modulo signs of diagonal elements of R).

- $A^T A = R_1^T R_1$ is a Cholesky factorization and $A = A R_1^{-1} R_1$ is a QR factorization.
- $A = Q_1 D \cdot D R_1$, $D = diag(\pm 1)$ is a QR factorization.

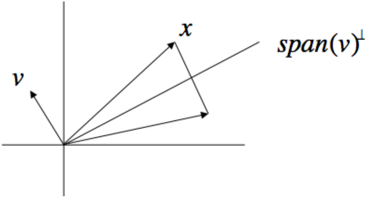
Householder transformation

The Householder matrix

$$P = I - \frac{2}{v^T v} v v^T$$

has the following properties:

- is symmetric and orthogonal, $P^2 = I$,
- is independent of the scaling of v,
- it reflects x about the hyperplane $span(v)^\perp$



$$Px = x - \frac{2v^T x}{v^T v} v = x - \alpha v$$

Presentation of Householder transformations and stability analysis from [N.J.Higham, 2002].

Householder for the QR factorization

We look for a Householder matrix that allows to annihilate the elements of a vector x, except first one.

$$Px = y, \quad \|x\|_2 = \|y\|_2, \quad y = \sigma e_1, \quad \sigma = \pm\|x\|_2$$

With the choice of sign made to avoid cancellation when computing $v_1 = x_1 - \sigma$ (where v_1, x_1 are the first elements of vectors v, x respectively), we have

$$\begin{aligned}
v &= x - y = x - \sigma e_1, \\
\sigma &= -sign(x_1)\|x\|_2, v = x - \sigma e_1, \\
P &= I - \beta v v^T, \beta = \frac{2}{v^T v}
\end{aligned}$$

Householder based QR factorization

$$A = \begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}$$

$$P_1 A = \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \end{pmatrix}, \begin{pmatrix} 1 & \\ & \tilde{P}_2 \end{pmatrix} P_1 = \begin{pmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \end{pmatrix} = R$$

So we have

$$\begin{aligned} Q^T A &= P_n P_{n-1} \ldots P_1 A = R, \\ Q &= (I - \beta_1 v_1 v_1^T) \ldots (I - \beta_{n-1} v_{n-1} v_{n-1}^T)(I - \beta_n v_n v_n^T) \end{aligned}$$

$\# flops = 2n^2(m - n/3)$

Error analysis of the QR factorization

The following result follows

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

Let $\hat{R} \in \mathbb{R}^{m\times n}$ be the computed factor of $A \in \mathbb{R}^{m\times n}$ obtained by using Householder transformations. Then there is an orthogonal $Q \in \mathbb{R}^{m\times m}$ such that

$$A + \Delta A = Q\hat{R}, \text{ where } \|\Delta a_j\|_2 \le \tilde{\gamma}_{mn}\|a_j\|_2, \quad j = 1 : n,$$

where $\tilde{\gamma}_{mn} = cmnu/(1 - cmnu)$, c is a constant, u is machine precision, $mnu < 1$, a_j denotes the j-th column of A.

Householder-QR factorization

Require: $A \in \mathbb{R}^{m \times n}$

Let $R \in \mathbb{R}^{n \times n}$ be initialized with zero matrix

for k = 1 to n **do**

  ▷ Compute Householder matrix $P_k = I - \beta_k v_k v_k^T$ s.t. $P_k A(k:m,k) = \pm\|A(k:m,k)\|_2 e_1$. Store v_k in $Y()$ and β_k in $\mathcal{T}(k)$

  $R(k,k) = -sgn(A(k,k)) \cdot \|A(k:m,k)\|_2$

  $\mathcal{T}(k) = \frac{R(k,k)-A(k,k)}{R(k,k)}$

  $Y(k+1:m,k) = \frac{1}{R(k,k)-A(k,k)} \cdot A(k+1:m,k)$

  ▷ Update trailing matrix

  $A(k:m,k+1:n) = (I - Y(k+1:m,k)\mathcal{T}(k)Y(k+1:m,k)^T) \cdot A(k:m,k+1:n)$

  $R(k,k+1:n) = A(k,k+1:n)$

end for

Assert: $A = QR$, where $Q = P_1 \dots P_n = (I - \beta_1 v_1 v_1^T) \dots (I - \beta_n v_n v_n^T)$, the Householder vectors v_k are stored in Y and $\mathcal{T}$ is an array of size n.

Computational complexity

- Flops per iterations
  - Dot product $w = v_k^T A(k:m, k+1:n)$: $2(m-k)(n-k)$
  - Outer product $v_k w$: $(m-k)(n-k)$
  - Subtraction $A(k:m, k+1:n) - \dots$: $(m-k)(n-k)$
- Flops of Householder-QR

$$
\begin{aligned}
&\sum_{k=1}^{n} 4(m-k)(n-k) = 4\sum_{k=1}^{n}(mn - k(m+n) + k^2) \\
&\approx 4mn^2 - 4(m+n)n^2/2 + 4n^3/3 = 2mn^2 - 2n^3/3
\end{aligned}
$$

Algebra of block QR

Storage efficient representation for Q [Schreiber and Loan, 1989]

$$Q = Q_1 Q_2 \dots Q_k = (I - \beta_1 v_1 v_1^T) \dots (I - \beta_k v_k v_k^T) = I - YTY^T$$

Example for $k = 2$

$$Y = (v_1 | v_2), \quad T = \begin{pmatrix} \beta_1 & -\beta_1 v_1^T v_2 \beta_2 \\ 0 & \beta_2 \end{pmatrix}$$

Example for combining two compact representations

$$\begin{aligned} Q &= (I - Y_1 T_1 Y_1^T)(I - Y_2 T_2 Y_2^T) \\ T &= \begin{pmatrix} T_1 & -T_1 Y_1^T Y_2 T_2 \\ 0 & T_2 \end{pmatrix} \end{aligned}$$

Block algorithm for computing the QR factorization

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

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

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 QR algebra

The first step of the block QR factorization algorithm computes:

$$Q_1^T A = \begin{pmatrix} R_{11} & R_{12} \\ & A^1 \end{pmatrix}$$

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

Algebra of block QR factorization

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = Q_1 \begin{pmatrix} R_{11} & R_{12} \\ & A^1 \end{pmatrix}$$

Block QR algebra

1. Compute the factorization

$$\begin{pmatrix} A_{11} \\ A_{12} \end{pmatrix} = Q_1 R_{11}$$

2. Compute the compact representation $Q_1 = I - YTY^T$
3. Apply Q_1^T on the trailing matrix

$$(I - YT^T Y^T) \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} = \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} - Y \left(T^T \left(Y^T \begin{pmatrix} A_{12} \\ A_{22} \end{pmatrix} \right) \right)$$

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

Parallel implementation of the QR factorization

QR factorization on a $P = P_r \times P_c$ grid of processors

For ib = 1 to n-1 step b

1. Compute panel factorization on P_r processors
$$\begin{pmatrix} A_{11} \\ A_{12} \end{pmatrix} = Q_1 R_{11} = (I - YTY^T) R_{11}$$
2. The P_r processors broadcast along the rows their parts of Y and T
3. Apply Q_1^T on the trailing matrix:
   - All processors compute their local part of
   $$W_l = Y_l^T (A_{12l}; A_{22l})$$
   - The processors owning block row *ib* compute the sum over W_l, that is
   $$W = Y^T (A_{12}; A_{22})$$
   and then compute $W' = T^T W$
   - The processors owning block row *ib* broadcast along the columns their part of W'
4. All processors compute
$$(A_{12}^1; A_{22}^1) = (A_{12}; A_{22}) - Y * W'$$

Cost of parallel QR factorization

$$
\begin{aligned}
& \gamma \cdot \left(\frac{6mnb - 3n^2 b}{2p_r} + \frac{n^2 b}{2p_c} + \frac{2mn^2 - 2n^3/3}{p} \right) \\
+ \quad & \beta \cdot \left(nb \log p_r + \frac{2mn - n^2}{p_r} + \frac{n^2}{p_c} \right) \\
+ \quad & \alpha \cdot \left(2n \log p_r + \frac{2n}{b} \log p_c \right).
\end{aligned}
$$

Solving least squares problems

Given matrix $A \in \mathbb{R}^{m\times n}$, $rank(A) = n$, vector $b \in \mathbb{R}^{m\times 1}$, the unique solution to $\min_x \|Ax - b\|_2$ is

$$x = A^+ b, \qquad A^+ = (A^T A)^{-1} A^T$$

Using the QR factorization of A

$$A = QR = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \tag{3}$$

We obtain

$$\begin{aligned} ||r||_2^2 &= ||b - Ax||_2^2 = ||b - \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} x||_2^2 \\ &= || \begin{pmatrix} Q_1^T \\ Q_2^T \end{pmatrix} b - \begin{pmatrix} R_1 \\ 0 \end{pmatrix} x||_2^2 = || \begin{pmatrix} Q_1^T b - R_1 x \\ Q_2^T b \end{pmatrix} ||_2^2 \\ &= ||Q_1^T b - R_1 x||_2^2 + ||Q_2^T b||_2^2 \end{aligned}$$

Solve $R_1 x = Q_1^T b$ to minimize $||r||_2$.

Acknowledgement

- Some of the examples taken from [Golub and Van Loan, 1996]

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