Dense QR factorization and its error analysis

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Plan

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Direct methods of factorization

- QR factorization
- Block QR factorization

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 $A = AR_1^{-1} R_1$ is a QR factorization.
- $A = Q_1 D \cdot DR_1$, $D = diag(\pm 1)$ is a QR factorization.

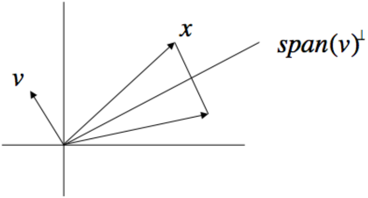
Householder transformation

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 $v_1 = x_1 - \sigma$, 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

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

So we have

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

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

Error analysis of Householder transformations

Lemma (Lemma 19.1 in [N.J.Higham, 2002])

Consider the computation of $P = I - \beta vv^T$, where $Px = \sigma e_1$, $v \in \mathbb{R}^m$, as

1: $v = x$

2: $s = sign(x_1)\|x\|_2, \quad \%\sigma = -s$

3: $v_1 = v_1 + s$

4: $\beta = 1/(sv_1)$

Then we have

$$\begin{aligned} \hat{v}(2:n) &= v(2:n) \\ \hat{\beta} &= \beta(1+\tilde{\theta}_m), \quad \hat{v}_1 = v_1(1+\tilde{\theta}_m), \ \textit{where } |\tilde{\theta}_m| \le \tilde{\gamma}_m \end{aligned}$$

Proof based on the fact that $fl(x^T x) = (1+\theta_m)x^T x$. The result can be re-written as

$$\hat{v} = v + \Delta v, \quad |\Delta v| \le \tilde{\gamma}_m |v|$$

In the following results, the Householder matrix is $I - vv^T$, hence $v = \sqrt{\beta} v$, $\beta = 1$, and so $\|v\|_2 = \sqrt{2}$.

Error analysis of Householder transformations

Lemma (Lemma 19.2 in [N.J.Higham, 2002])

Consider the computation $y = \hat{P}b = (I - \hat{v}\hat{v}^T)b$*, where* $b, \hat{v} \in \mathbb{R}^m$*. Then*

$$\hat{y} = (P + \Delta P)b, \quad \|\Delta P\|_F \leq \tilde{\gamma}_m. \tag{1}$$

Proof.

$$\begin{aligned} \hat{w} &= fl(\hat{v}(\hat{v}^T b)) = (\hat{v} + \Delta\hat{v})(\hat{v}^T(b + \Delta b)), \quad |\Delta\hat{v}| \leq u|\hat{v}| \text{ and } |\Delta b| \leq \gamma_m|b| \\ &= (v + \Delta v + \Delta\hat{v})(v + \Delta v)^T(b + \Delta b) \end{aligned}$$

Hence

$$\hat{w} = v(v^T b) + \Delta w, \quad \text{where } |\Delta w| \leq \tilde{\gamma}_m|v||v^T||b|$$

□

Error analysis of Householder transformations

Continued proof of the previos lemma. We obtain

$$\hat{y} = fl(b - \hat{w}) = b - v(v^T b) - \Delta w + \Delta y_1, \qquad |\Delta y_1| \leq u|b - \hat{w}|$$

Since

$$|-\Delta w + \Delta y_1| \leq u|b| + \tilde{\gamma}_m |v||v^T||b|$$

we obtain

$$\hat{y} = Pb + \Delta y, \qquad \|\Delta y\|_2 \leq \tilde{\gamma}_m \|b\|_2$$

Finally, with $\Delta P = \Delta y b^T / b^T b$, we have

$$\hat{y} = (P + \Delta P)b, \qquad \|\Delta P\|_F = \|\Delta y\|_2 / \|b\|_2 \leq \tilde{\gamma}_m$$

Error analysis of a sequence of transformations

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

Let $Q = P_r P_{r-1} \dots P_1$ and let $A_{r+1} = Q^T A$, $A \in \mathbb{R}^{m \times n}$. We have

$$\hat{A}_{r+1} = Q^T(A + \Delta A), \quad \|\Delta a_j\|_2 \leq r\tilde{\gamma}_m \|a_j\|_2, \; j = 1 : n$$

Sketch of the proof: Let a_j be the j-th column of A.

$$\hat{a}_j^{(r+1)} = (P_r + \Delta P_r) \dots (P_1 + \Delta P_1) a_j, \quad \|\Delta P_k\|_F \leq \tilde{\gamma}_m, \; k = 1 : r$$

We obtain

$$\begin{aligned} \hat{a}_j^{(r+1)} &= Q^T(a_j + \Delta a_j), \\ \|\Delta a_j\|_2 &\leq ((1 + \tilde{\gamma}_m)^r - 1)\|a_j\|_2 \leq \frac{r\tilde{\gamma}_m}{1 - r\tilde{\gamma}_m}\|a_j\|_2 = r\tilde{\gamma}_m^{'}\|a_j\|_2 \end{aligned}$$

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

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

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**

$\triangleright$ 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 $\mathcal{T}(k)$

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

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

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

$\triangleright$ 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

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

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

$$(A_{12}^1; A_{22}^1) = (A_{12}; A_{22}) - (A_{12}; A_{22}) * W'$$

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

$$A = QR = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} \tag{2}$$

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

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

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