Quick triangular orthogonal decomposition of matrices

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Abstract. A new algorithm for calculating the triangular orthogonal decomposition of matrices is proposed. It differs from previously known algorithms by the smallest asymptotic complexity.

Introduction

The problem of the orthogonal decomposition of matrices is still known as the QR-decomposition problem. It is one of the subtasks that are associated with spectral decomposition. Given the matrix A, it is required to represent it as a product of two factors, A=QR, where Q is a unitary matrix (orthogonal in the case of real numbers), R is an upper triangular matrix. The algorithm of the QR-decomposition should not be confused with the QR-algorithm, that is the algorithm for calculating the spectrum of the matrix (singular value decomposition). There are a large number of different approaches [1]-[4] to the problem of computing the orthogonal decomposition, including fast recursive algorithm [5]. However, the best-known algorithms in terms of the number of operations are algorithms that have cubic complexity. In this paper, we consider an algorithm of orthogonal decomposition, which has the complexity of matrix multiplication.

Let A be a matrix over a field. It is required to find the upper triangular matrix R and the orthogonal (unitary if the initial field is a field of complex numbers) Q matrix such that $A = QR$.

For definiteness, we will consider an algorithm applied to a square matrix A over a field of real numbers.

Consider the case of a 2×2 matrix. The desired decomposition $A = QR$ has the form:

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} = \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} a & b \\ 0 & d \end{pmatrix},$$

where the numbers s and c satisfy the equation $s^2 + c^2 = 1$.

After multiplying from the left of both sides of the equation by the inverse matrix $Q^{-1} = Q^T$, we get: $Q^T A = R$.

If $\gamma = 0$ then we can set $c = 1$, $s = 0$. If $\gamma \neq 0$, then $\Delta = \alpha^2 + \gamma^2 > 0$. Then we get $c\alpha + s\gamma = a$, $c\gamma - s\alpha = 0$ and $c = a\alpha/\Delta$, $s = a\gamma/\Delta$.

Therefore, $1 = s^2 + c^2 = a^2/\Delta$, hence $|a| = \sqrt{\Delta}$. $c = \alpha/\sqrt{\Delta}$, $s = \gamma/\sqrt{\Delta}$.

We denote such a matrix Q by $g_{\alpha,\gamma}$.

1. Sequential QR decomposition

Let the matrix A be given, its elements (i, j) and $(i+1, j)$ be α and γ, and all the elements to the left of them be zero: $\forall(s < j) : (a_{i,s} = 0)$ & $(a_{i+1,s} = 0)$.

Let $G_{i,j} = \mathbf{diag}(I_{i-1}, g_{\alpha,\gamma}, I_{n-i-1})$. Then the matrix $G_{i,j}A$ differs from A only in two rows i and $i+1$, but all the elements to the left of the column j remain zero, and in the column j in $i+1$ line will be 0.

This property of the Givens matrix allows us to formulate such an algorithm

Algorithm

(1). First we reset the elements under the diagonal in the left column:

$$A_1 = G_{1,1}G_{2,1}...G_{n-2,1}G_{n-1,1}A$$

(2). Then we reset the elements that are under the diagonal in the second column:

$$A_2 = G_{2,2}G_{3,2}...G_{n-2,2}G_{n-1,2}A_1$$

(k). Denote $G_{(k)} = G_{k,k}G_{k-1,k}...G_{n-2,k}G_{n-1,k}$, $k = 1, 2, .., n-1$. Then, to calculate the elements of the k th column, we need to obtain the product of matrices

$$A_k = G_{(k)}A_{k-1}.$$

(n-1). At the end of the calculation, the element in the $n-1$ column will be reseted: $A_{n-1} = G_{(n-1)}A_{n-2} = G_{n-1,n-1}A_{n-2}$.

You can find the number of operations. It is necessary to calculate the $(n^2 - n)/2$ turn matrices and for each of them 6 operations must be performed. when calculating A_1, the number of multiplications of the Givens matrices into columns of two elements (4 multiplications and 2 additions) is $(n-1)^2$. When calculating A_2, the number of such multiplications is $(n-2)^2$, and so on. As a result, we get

$$6(n^2 - n)/2 + 6 \sum_{i=1..n-1} i^2 = 3n^2 - 3n + 6(n-1)(2n-1)n/6 \approx 2n^3$$

Here we count the number of all arithmetic operations and the operations of extracting the square root.

2. QR_G decomposition

Let a matrix M of size $2n\times 2n$ be divided into four equal blocks: $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$. There are three steps in this algorithm.

Algorithm

(1). The first stage is the QR_G decomposition of the block C:

$$C = Q_1C_1,\ M_1 = \mathbf{diag}(I, Q_1)M = \begin{pmatrix} A & B \\ C_1 & D_1 \end{pmatrix}.$$

(2). The second stage is the cancellation of a parallelogram composed of two triangular blocks: the lower triangular part A^L of the block A and the upper triangular part C_1^U of the block C_1. Denote the upper triangular matrix A_1 and annihilating matrix Q_2:

$$\begin{pmatrix} A \\ C_1 \end{pmatrix} = \begin{pmatrix} A_1 \\ 0 \end{pmatrix},\ M_2 = Q_2M_1 = \begin{pmatrix} A_1 & B_1 \\ 0 & D_2 \end{pmatrix}.$$

(3). The third stage is the QR_G decomposition of the D_2 block: $D_2 = Q_3D_3$.

$$R = \mathbf{diag}(I, Q_3)M_2 = \begin{pmatrix} A_1 & B_1 \\ 0 & D_3 \end{pmatrix}.$$

As a result, we get:

$$M = Q^TR,\quad Q = \mathbf{diag}(I, Q_3)Q_2\,\mathbf{diag}(I, Q_1).$$

Since the first and third stages are recursive calls of the QR_G -procedures, it remains to describe the parallelogram cancellation procedure. Let's call it a QP decomposition.

3. QP-decomposition

Let the matrix $M = \begin{pmatrix} A \\ B^U \end{pmatrix}$ have dimensions $2n \times n$ and, at the same time, the lower unit B^U of size $n \times n$, n -countable, has an upper triangular shape - all elements under its main diagonal are zero. We are looking for the factorization of the matrix $M = QP = Q\begin{pmatrix} A^U \\ 0 \end{pmatrix}$, with the orthogonal matrix Q.

It is required to annul all elements between the upper and lower diagonals of the M matrix, including the lower diagonal. It is easy to see that this can be done with Givens matrices. We will consistently perform column invalidation by traversing column elements from bottom to top and traversing columns from left to right.

But we are interested in the block procedure. Since n is even, we can break the parallelogram formed by the diagonals into 4 parts using its two middle lines. We get 4 equal parallelograms. To cancel each of them, we will simply call the parallelogram cancellation procedure 4 times. We will perform the calculations in this order: the bottom left (P_{ld}), then we simultaneously cancel the top left (P_{lu}) and the bottom right (P_{rd}), and last we will cancel the top right (P_{en}). The corresponding orthogonal Givens matrices of size $n \times n$ are denoted Q_{ld}. Q_{lu}. Q_{rd} and Q_{ru}. Let

$$\bar{Q}_{ld} = \mathbf{diag}(I_{n/2}, Q_{ld}, I_{n/2}), \quad \bar{Q}_{ru} = \mathbf{diag}(I_{n/2}, Q_{ru}, I_{n/2}),$$

As a result, we get:

$$Q = \bar{Q}_{ru}\,\mathbf{diag}(Q_{lu}, Q_{rd})\bar{Q}_{ld}$$

The number of multiplications of matrix blocks of size $n/2 \times n/2$ is 24. Hence the total number of operations: $Cp(2n) = 4Cp(n) + 24M(n/2)$.. Suppose that for multiplication of two matrices of size $n \times n$ you need γn^{β} operations and $n = 2^k$, then we get: $Cp(2^{k+1}) = 4Cp(2^k) + 24M(2^{k-1}) = 4^k Cp(2^1) + 24\gamma \sum_{i=0}^{k-1} 4^{k-i-1} 2^{i\beta} = 24\gamma(n^2/4)\frac{2^{k(\beta-2)}-1}{2^{(\beta-2)}-1} + 6n^2 = 6\gamma\frac{n^{\beta}-n^2}{2^{\beta}-4} + 6n^2$

$$Cp(n) = \frac{6\gamma n^{\beta}}{2^{\beta}(2^{\beta}-4)} + \frac{3n^2}{2}(1 - \frac{\gamma}{2^{\beta}-4})$$

4. The complexity of QR_G decomposition

Let us estimate the number of operations $C(n)$ in this block-recursive decomposition algorithm, assuming that the complexity of the matrix multiplication is $M(n) = \gamma n^{\beta}$, the complexity of canceling the parallelogram is $Cp(n) = \alpha n^{\beta}$, where α, β, γ are constants, $\alpha = \frac{6\gamma}{2^{\beta}(2^{\beta}-4)}$ and $n = 2^k$:

$$C(n) = 2C(n/2) + Cp(n) + 6M(n/2) = 2C(2^{k-1}) + Cp(2^k) + 6M(2^{k-1}) =$$

$$C(2^0)2^k + \sum_{i=0}^{k} 2^{k-i}Cp(2^i) + 6\sum_{i=0}^{k} 2^{k-i}M(2^{i-1}) = \alpha\sum_{i=0}^{k} 2^{k-i}2^{i\beta} + 6\gamma\sum_{i=0}^{k} 2^{k-i}2^{(i-1)\beta} =$$

$$(\alpha 2^k + 6\gamma 2^{k-\beta})\sum_{i=0}^{k} 2^{i(\beta-1)} = (\alpha + 6\gamma 2^{-\beta})\frac{2^{\beta}n^{\beta} - 2n}{2^{\beta}-2} = \frac{\gamma 6(2^{\beta}-3)(n^{\beta} - \frac{2n}{2^{\beta}})}{(2^{\beta}-4)(2^{\beta}-2)}$$

Conclusion

Thus, presented algorithm has the complexity of matrix multiplication. If we apply the standard matrix multiplication ($2n^3$ operations for the matrix $n \times n$), then we need only $\approx 2.5n^3$ operations.

References

[1] Golub, Gene H.; Van Loan, Charles F. (1996), Matrix Computations (3rd ed.), Johns Hopkins, ISBN 978-0-8018-5414-9

[2] [10] Nicholas J. Higham. Accuracy and Stability of Numerical Algorithms. Second edition, Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2002.

[3] Press, WH; Teukolsky, SA; Vetterling, WT; Flannery, BP (2007), "Section 2.10. QR Decomposition", Numerical Recipes: The Art of Scientific Computing (3rd ed.), New York: Cambridge University Press, ISBN 978-0-521-88068-8

[4] Stoer, Josef; Bulirsch, Roland (2002), Introduction to Numerical Analysis (3rd ed.), Springer, ISBN 0-387-95452-X.

[5] Daniel Kressner, Ana Susnjara. Fast QR decomposition of HODLR matrices (Submitted on 27 Sep 2018) arXiv:1809.10585v1

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