QR Decomposition Algorithms

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1 QR Decomposition

The QR decomposition of an m-by-n matrix A with $m > n$, is the matrix product $A = QR$, where Q is an m-by-m unitary matrix, and R is upper triangular [2].

1.1 Matrix Q

The matrix Q is a transformation which preserves inner products of column vectors of R. If the inner product space is real, the matrix Q is equivalently orthogonal. One possibility of such a transformation is a rotation.

Another possibility of such an orthogonal transformation is a reflection. The matrix Q in general is a combination of rotations and reflections.

1.2 Matrix R

The matrix R is upper triangular, a form which has the following useful properties: (I) the determinant is equal to the product of the diagonal elements, (II) the eigenvalues are equal to the diagonal elements, (III) given the linear system $Rx = b$ it is easy to solve for x by back substitution.

2 Transformations

In order to compute the decomposition of A, the matrix is iteratively transformed by unitary matrices $\{U_i : 0 < i < k\}$ until the product is upper triangular. This upper triangular matrix is the matrix R in $A = QR$

$$R = U_k U_{k-i} \ldots U_1 A. \tag{1}$$

It follows, that the matrix Q is composed of the set of inverse transformations

$$Q = U_1^T U_2^T \ldots U_k^T. \tag{2}$$

The key to solving for R is to choose transformations U_i which produce zeros below the diagonal of the matrix product

$$A^{(i)} = U_i \ldots U_1 A, \tag{3}$$

and can iteratively be applied to achieve R. Two choices for U_i are Householder reflections, and Givens rotations.

2.1 Householder Reflections

The Householder reflection is a unitary transformation represented by a matrix $H \in \mathbb{R}^{N\times N}$ which reflects a vector $\mathbf{u} \in \mathbb{R}^N$ across a hyperplane defined by its unit normal vector $\{\mathbf{w} \in \mathbb{R}^N : \|\mathbf{w}\| = 1\}$. The transformation matrix is given by

$$H = I - 2\mathbf{w}\mathbf{w}^T \tag{4}$$

where $I \in \mathbb{R}^{N\times N}$ is the identity matrix. [3] [6]

To reflect a vector $\mathbf{u} \in \mathbb{R}^N$ such that it points in the direction of a target vector $\mathbf{v} \in \mathbb{R}^N$, the transformation matrix H can be computed by (4), where $\mathbf{w}$ is given by

$$\mathbf{w} = \mathbf{v} - \mathbf{u}, \tag{5}$$

such that,

$$H\mathbf{u} = \|\mathbf{u}\|\hat{\mathbf{v}}, \tag{6}$$

where $\hat{\mathbf{v}}$ is a unit vector in the direction of the target vector $\mathbf{v}$.

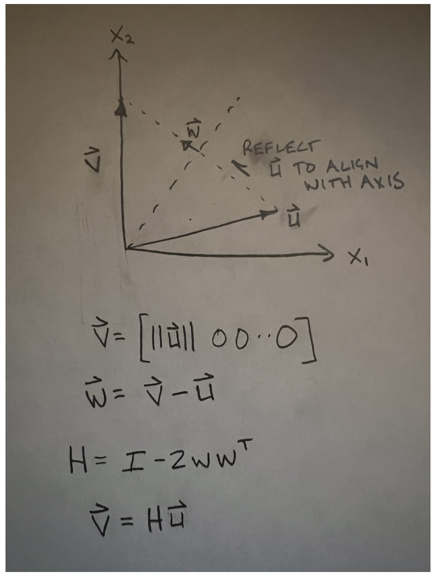

Figure 1: Geometric illustration of the reflection of a vector to an axis. The result of this transformation is that the vector now only has one non-zero component.

2.2 Givens Rotations

A Givens rotation is a unitary transformation which rotates a vector x counter-clockwise in a chosen plane. For example, possible Givens rotation matrices in $\mathbb{R}^4$ include

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & c & -s & 0 \\ 0 & s & c & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} c & -s & 0 & 0 \\ s & c & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, or \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c & -s \\ 0 & 0 & s & c \end{bmatrix}, \tag{7}$$

where $c = \cos\theta$ and $s = \sin\theta$. Each of these examples have the effect of rotating the vector in different planes.

A Givens rotation can easily be computed to introduce zeros in the matrix P. The scalars c and s can be computed directly from elements in P in order to zero out targeted elements[5] [4]. For example, say we want to zero out element a_{21} in the matrix

$$P = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}. \tag{8}$$

We target the second dimension of the column vector, so we rotate on the plane spanned by the first two dimensions. The Givens rotation to rotate on

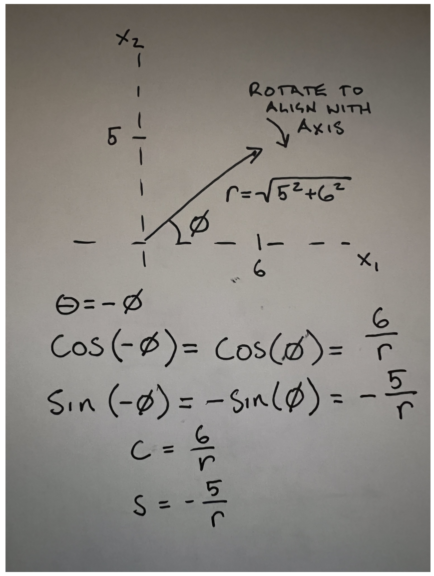

Figure 2: Geometric illustration of the rotation of a vector in $\mathbb{R}^3$ about the axis of basis vector $x3$ to align with the basis vector $x1$. The result of this transformation is that the component of the transformed vector in the direction of the basis vector $x2$ is zero, corresponding to a zero introduced in the transformed matrix.

this plane is of the form

$$G = \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{9}$$

which will leave the third row of P unmodified. We are aligning the column vector with the axis of the first dimension, making the component of the vector along the second dimension zero. Fig. 2 shows a geometric illustration of the rotation.

The scalars c and s of matrix G are computed directly from the values in matrix P by the equations

$$c = \frac{a_{11}}{r}, \tag{10}$$

$$s = -\frac{a_{21}}{r}, \tag{11}$$

where

$$r = \sqrt{a_{11}^2 + a_{21}^2} \tag{12}$$

The transformation to introduce the zero is then

$$P = GP_{prior} = \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \tag{13}$$

$$P = GP_{prior} = \begin{bmatrix} a_{11}/r & a_{21}/r & 0 \\ -a_{21}/r & a_{11}/r & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \tag{14}$$

$$P = GP_{prior} = \begin{bmatrix} a_{11}/r & a_{21}/r & 0 \\ -a_{21}/r & a_{11}/r & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \tag{15}$$

$$P = \begin{bmatrix} \frac{a_{11}a_{11}+a_{21}a_{21}}{r} & \frac{a_{11}a_{12}+a_{21}a_{22}}{r} & \frac{a_{11}a_{13}+a_{21}a_{23}}{r} \\ \frac{-a_{21}a_{11}+a_{11}a_{21}}{r} & \frac{-a_{21}a_{12}+a_{11}a_{22}}{r} & \frac{-a_{21}a_{13}+a_{11}a23}{r} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \tag{16}$$

$$P = \begin{bmatrix} \frac{a_{11}a_{11}+a_{21}a_{21}}{r} & \frac{a_{11}a_{12}+a_{21}a_{22}}{r} & \frac{a_{11}a_{13}+a_{21}a_{23}}{r} \\ 0 & \frac{-a_{21}a_{12}+a_{11}a_{22}}{r} & \frac{-a_{21}a_{13}+a_{11}a23}{r} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \tag{17}$$

the zero is introduced in the desired location.

3 Algorithms

3.1 Householder QR

In order to get the upper triangular matrix $R \in \mathbb{R}^{N \times N}$ given a matrix $A \in \mathbb{R}^{M \times N}$ using householder reflections, we can use (1), where the set of unitary transformations is a set of padded householder matrices $\{U_i \in \mathbb{R}^{M \times M} : 0 < i < N\}$, so that,

$$R = U_{N-1}U_{N-2} \dots U_1 A. \tag{18}$$

Let

$$A^{(i)} = U_i \dots U_1 A \tag{19}$$

represent the i-th update of matrix A, so $A^{(N)} = R$ and $A^{(0)} = A$. Then the calculation of U_i depends on the updated matrix $A^{(i-1)}$.

The householder QR algorithm procedure is to iteratively calculate each matrix U_i from $A^{(i-1)}$, then update the matrix $A^{(i)} = U_i A^{(i-1)}$ for the next iteration, until $A^{(N)} = R$ is achieved. At each iteration, U_i is determined such that the i-th column of $A^{(i-1)}$ is transformed so that all elements below the diagonal of the column are zero in the updated matrix $A^{(i)} = U_i A^{(i-1)}$ [5] [7].

For example,

$$A^{(1)} = \begin{bmatrix} \times & \times & \cdots & \times & \times \\ 0 & \times & \cdots & \times & \times \\ 0 & \times & \cdots & \times & \times \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \times & \cdots & \times & \times \end{bmatrix} \tag{20}$$

$$A^{(2)} = \begin{bmatrix} \times & \times & \cdots & \times & \times \\ 0 & \times & \cdots & \times & \times \\ 0 & 0 & \cdots & \times & \times \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \times & \times \end{bmatrix} \tag{21}$$

$$A^{(N-1)} = R = \begin{bmatrix} \times & \times & \cdots & \times & \times \\ 0 & \times & \cdots & \times & \times \\ 0 & 0 & \cdots & \times & \times \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & \times \end{bmatrix} \tag{22}$$

Each padded householder transformation matrix $U_i \in \mathbb{R}^{M \times M}$ is created by padding a householder matrix $H_i \in \mathbb{R}^{(M-i)\times(M-i)}$ with ones along the upper diagonal.

$$U_i \in \mathbb{R}^{M \times M} = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & H_i \in \mathbb{R}^{(M-i)\times(M-i)} \end{bmatrix} \tag{23}$$

Let $A'^{(i)} \in \mathbb{R}^{(M-i)\times(M-i)}$ be the lower right submatrix of $A^{(i)}$, such that

$$A^{(i)} = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & A'^{(i)} \in \mathbb{R}^{(M-i)\times(M-i)} \end{bmatrix} \tag{24}$$

Each householder matrix H_i is calculated by obtaining $\mathbf{w}_i \in \mathbb{R}^{M-i}$ from the submatrix $A'^{(i-1)} \in \mathbb{R}^{(M-i+1)\times(M-i+1)}$, such that

$$A^{(i)} = \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & A'^{(i)} \in \mathbb{R}^{(M-i)\times(M-i)} \end{bmatrix} \tag{25}$$

and

$$A'^{(i)} = \begin{bmatrix} \mathbf{u_i} & \mathbf{c_2} & \cdots & \mathbf{c_j} & \cdots \mathbf{c}_{M-1} \end{bmatrix}. \tag{26}$$

where $\mathbf{c}_j$ is the j-th column of $A'^{(i)}$, and $\mathbf{u}_i \in \mathbb{R}^{M-i}$ is used as the vector $\mathbf{u}$ in (5) to calculate $\mathbf{w}_i$.

Let

$$\mathbf{v}_i \in \mathbb{R}^{M-i} = \begin{bmatrix} \|\mathbf{u_i}\| \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{27}$$

then $\mathbf{w}_i$ is obtained from $\mathbf{u}_i$ and $\mathbf{v}_i$ according to (5), H_i is determined by (4) from $\mathbf{w}_i$, U_i is obtained by padding H_i, $A^{(i+1)}$ is obtained by (3), and the iterations continue until R is achieved, as in (1).

Q can easily be computed by keeping a running matrix product according to (2) during the iterations of the algorithm.

The Householder algorithm can be written concisely using the notation in [**?**]. For the matrix A, the notation $A_{k:m,k}$ is defined as the submatrix of A formed by the k-th through m-th rows of the k-th column.

Algorithm 1 Calculate $A = QR$ using Householder reflections

```
1: for k = 1 to n do
2:     u = A_{k:m,k}
3:     v_k = sign(u_1)||u||_2 e_1 + u
4:     v_k = v_k/||v_k||_2
5:     A_{k:m,k:n} = A_{k:m,k:n} - 2v_k(v_k^T A_{k:m,k:n})
6: end for
```

In Algorithm 1, the householder vector $\mathbf{w}$ overwrites the vector $\mathbf{v}$. Recall, $U = H$ in (1) for the Householder QR algorithm. The transformation of A by the orthogonal Householder matrix U in (1) is implicit in the last line of the for loop, where A is distributed through (4).

3.1.1 FLOPS

We count the average FLOPS in 1 line-by-line in the inner loop, and multiply by N columns of the outer loop.

Line 2 The copy operation is realized by a for-loop iterating over the copied column. On average, the length of this column is $m/2$, so the contribution is $N * M/2$ FLOPs.

Line 3 The calculation of the magnitude of vector u takes an average M / 2 FLOPs, which is added to an additional M FLOPs for the multiply-accumulate into v_k for a total contribution of $3 * N * M/2$ FLOPs.

Line 4 Again, the magnitude of vector v_k requires an average M / 2 FLOPs, and the division adds another M / 2 FLOPs. The total contribution is $N * M$ FLOPs.

Line 5 The vector matrix product $(v_k^T A_{k:m,k:n})$ consists of a vector matrix product contributing

$$\frac{1}{N}\sum_{k=0}^{N}(M-k)(N-k)$$

FLOPs on average.

3.1.2 Parallelism

The dependence of U_i on $A^{(i-1)}$ limits the parallelism of the Householder QR algorithm, such that the outer loop of Algorithm 1 can't be parallelized, and we must repeat lines 2-5, for each of N columns.

The matrix update portion $A_{k:m,k:n} = A_{k:m,k:n} - 2v_k(v_k^T A_{k:m,k:n})$ can be computed by parallel matrix multiply algorithms, however these operations are interspersed with the computation of the padded householder matrix U_i, which is highly sequential. If the parallel portions of this algorithm are implemented on a GPU, and the sequential portions on the host CPU, memory bandwidth and latency become a significant speed and efficiency bottleneck, as the data is passed back and forth between CPU memory and GPU memory [7] [1].

3.2 WY-representation

For the factored form of $Q \in \mathbb{R}^{M\times M} = Q_1 Q_2 \ldots Q_i \ldots Q_n$ where $Q_i = I_m - \beta_i v_i {v_i}^T$ and the factors v_i, β_i are stored as

$$V \in \mathbb{R}^{M\times n} = \begin{bmatrix}\mathbf{w}_1 & \mathbf{w}_2 & \cdots & \mathbf{w}_n\end{bmatrix} \tag{28}$$

$$B \in \mathbb{R}^{n} = \begin{bmatrix}\beta_1 & \beta_2 & \cdots & \beta_n\end{bmatrix} \tag{29}$$

the W and Y factors such that $Q = I_m - WY^T$ can be calculated from V, and B [5] [7].

The algorithm is as follows.

3.3 Block QR

The Block QR algorithm reduces the memory workload by combining multiple householder transformations into a single matrix via the WY-representation of matrix products, before doing the matrix update [1].

Algorithm 2 Calculate W, Y from the factored form of Q: V and B

$Y = v^{(1)}$
$W = \beta_1 v^{(1)}$
for $j = 2$ to r **do**
  $z = \beta_j (I_m - WY^T) v^{(j)}$
  $W = [W|z]$
  $Y = [Y|v^{(j)}]$
end for

Returning to equation (1), the Block QR algorithm splits the matrix $A \in \mathbb{R}^{M \times N}$ into $b = ceil(\frac{N}{n_b})$ panels $\{P_j \in \mathbb{R}^{M \times n_b} : 0 < j <= b\}$ of width n_b [7].

$$A = \begin{bmatrix} P_1 & P_2 & \cdots & P_b \end{bmatrix} \tag{30}$$

For each panel, n_b householder vectors $\{\mathbf{w}_k \in \mathbb{R}^M : 0 < k <= n_b\}$ are determined by performing the Householder QR decomposition on the panel, and saving the vectors $\mathbf{w}_k$ at each iteration to form a transformation $U_j \in \mathbb{R}^{M \times M} = I - W_j Y_j^T$ using the WY transformation, such that the set $\{U_j : 0 < j <= b\}$ satisfies (1).

W_j and Y_j are computed using the Householder factors $\mathbf{w}_k$ and β in the general householder equation $H = I - \beta \mathbf{w}\mathbf{w}^T$, where in our case $\beta = 2$ as in (4).

$$W_j, Y_j = wy\_representation(V_j, B_j) \tag{31}$$

where

$$V_j \in \mathbb{R}^{M \times n_b} = \begin{bmatrix} \mathbf{w}_1 & \mathbf{w}_2 & \cdots & \mathbf{w}_{n_b} \end{bmatrix} \tag{32}$$

and

$$B_j \in \mathbb{R}^{n_b} = \begin{bmatrix} \beta_1 & \beta_2 & \cdots & \beta_{n_b} \end{bmatrix} \tag{33}$$

At each iteration j of the block QR algorithm, U_j is computed by the W-Y representation, then the sub-matrix $A'^{(j)} \in \mathbb{R}^{(m-(j*n_b)) \times (n-(j*n_b))}$ is updated by $A'^{(j)} = U_j A'^{(j-1)}$ [7] [5].

When $j = b$ then $(j * n_b) = N$, the width of sub-matrix $A'^{(j)}$ is zero, the matrix $A^{(j)} = A^{(n_b)} = R$, and the decomposition is complete.

Using the same notation as in Algorithm 1, the Block Householder QR algorithm can be written concisely as

References

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Algorithm 3 Block Householder QR Decomposition

$Q = I_m$
$\lambda = 1$
$k = 0$
while $\lambda \leq n$ **do**
  $\tau \leftarrow min(\lambda + r - 1, n)$
  $k = k + 1$
  $A_{\lambda:m,\lambda:\tau} \leftarrow Householder\_qr(A_{\lambda:m,\lambda:\tau})$
end while

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[7] L. Minah Yang, Alyson Fox, and Geoffrey Sanders. Rounding error analysis of mixed precision block householder qr algorithms. *SIAM Journal on Scientific Computing*, 43(3):A1723–A1753, 2021.