

# Numerical Analysis

Raphael Hauser  
with thanks to Endre Süli

Oxford Mathematical Institute

HT 2019

# The Symmetric QR Algorithm

We consider only the case where  $A$  is symmetric.

# The Symmetric QR Algorithm

We consider only the case where  $A$  is symmetric.

**Recall:** a symmetric matrix  $A$  is said to be *similar* to  $B$  if there is a nonsingular matrix  $P$  for which  $A = P^{-1}BP$ .

# The Symmetric QR Algorithm

We consider only the case where  $A$  is symmetric.

**Recall:** a symmetric matrix  $A$  is said to be *similar* to  $B$  if there is a nonsingular matrix  $P$  for which  $A = P^{-1}BP$ .

Similar matrices have the same eigenvalues.

# The Symmetric QR Algorithm

We consider only the case where  $A$  is symmetric.

**Recall:** a symmetric matrix  $A$  is said to be *similar* to  $B$  if there is a nonsingular matrix  $P$  for which  $A = P^{-1}BP$ .

Similar matrices have the same eigenvalues. Indeed: if  $A = P^{-1}BP$ ,

# The Symmetric QR Algorithm

We consider only the case where  $A$  is symmetric.

**Recall:** a symmetric matrix  $A$  is said to be *similar* to  $B$  if there is a nonsingular matrix  $P$  for which  $A = P^{-1}BP$ .

Similar matrices have the same eigenvalues. Indeed: if  $A = P^{-1}BP$ , then

$$0 = \det(A - \lambda I) = \det(P^{-1}(B - \lambda I)P) = \det(P^{-1}) \det(P) \det(B - \lambda I),$$

# The Symmetric QR Algorithm

We consider only the case where  $A$  is symmetric.

**Recall:** a symmetric matrix  $A$  is said to be *similar* to  $B$  if there is a nonsingular matrix  $P$  for which  $A = P^{-1}BP$ .

Similar matrices have the same eigenvalues. Indeed: if  $A = P^{-1}BP$ , then

$$0 = \det(A - \lambda I) = \det(P^{-1}(B - \lambda I)P) = \det(P^{-1}) \det(P) \det(B - \lambda I),$$

so

$$\det(A - \lambda I) = 0 \quad \text{if, and only if,} \quad \det(B - \lambda I) = 0.$$

The basic **QR algorithm** is:

```
Set  $A_1 = A$ .  
for  $k = 1, 2, \dots$   
    form the QR factorization  $A_k = Q_k R_k$   
    and set  $A_{k+1} = R_k Q_k$   
end
```



## Proposition

*The symmetric matrices  $A_1, A_2, \dots, A_k, \dots$  generated by the QR algorithm are all similar and thus have the same eigenvalues.*

## Proposition

*The symmetric matrices  $A_1, A_2, \dots, A_k, \dots$  generated by the QR algorithm are all similar and thus have the same eigenvalues.*

Proof. Since

$$A_{k+1} = R_k Q_k = (Q_k^{-1} Q_k) R_k Q_k = Q_k^{-1} (Q_k R_k) Q_k = Q_k^{-1} A_k Q_k,$$

$A_{k+1}$  is similar to  $A_k$ .

Furthermore, since  $Q_k^{-1} = Q_k^T$ , the matrix  $A_{k+1}$  is symmetric if  $A_k$  is.

By hypothesis,  $A_1 := A$  is symmetric; therefore each of the matrices  $A_k$ ,  $k = 1, 2, \dots$ , is symmetric. □

This basic QR algorithm works since  $A_k \rightarrow$  a diagonal matrix as  $k \rightarrow \infty$ , the diagonal entries of which are the eigenvalues.

This basic QR algorithm works since  $A_k \rightarrow$  a diagonal matrix as  $k \rightarrow \infty$ , the diagonal entries of which are the eigenvalues.

However, a really practical, fast algorithm is based on some refinements.

## Reduction to tridiagonal form:

the idea is to apply explicit similarity transformations  $QAQ^{-1} = QAQ^T$ , with  $Q$  orthogonal, so that  $QAQ^T$  is **tridiagonal**.

## Reduction to tridiagonal form:

the idea is to apply explicit similarity transformations  $QAQ^{-1} = QAQ^T$ , with  $Q$  orthogonal, so that  $QAQ^T$  is **tridiagonal**.

**Note:** direct reduction to triangular form would reveal the eigenvalues, but is not possible.

## Reduction to tridiagonal form:

the idea is to apply explicit similarity transformations  $QAQ^{-1} = QAQ^T$ , with  $Q$  orthogonal, so that  $QAQ^T$  is **tridiagonal**.

**Note:** direct reduction to triangular form would reveal the eigenvalues, but is not possible.

Indeed, if

$$H(w)A = \begin{pmatrix} \times & \times & \cdots & \times \\ 0 & \times & \cdots & \times \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \times & \cdots & \times \end{pmatrix}$$

## Reduction to tridiagonal form:

the idea is to apply explicit similarity transformations  $QAQ^{-1} = QAQ^T$ , with  $Q$  orthogonal, so that  $QAQ^T$  is **tridiagonal**.

**Note:** direct reduction to triangular form would reveal the eigenvalues, but is not possible.

Indeed, if

$$H(w)A = \begin{pmatrix} \times & \times & \cdots & \times \\ 0 & \times & \cdots & \times \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \times & \cdots & \times \end{pmatrix}$$

then  $H(w)AH(w)^T$  is generally full, i.e., all zeros created by pre-multiplication are destroyed by the post-multiplication.



However, if

$$A = \begin{pmatrix} \gamma & u^T \\ u & C \end{pmatrix}$$

(as  $A = A^T$ )

However, if

$$A = \begin{pmatrix} \gamma & u^T \\ u & C \end{pmatrix}$$

(as  $A = A^T$ ) and

$$w = \begin{pmatrix} 0 \\ \hat{w} \end{pmatrix} \quad \text{where} \quad H(\hat{w})u = \begin{pmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

However, if

$$A = \begin{pmatrix} \gamma & u^T \\ u & C \end{pmatrix}$$

(as  $A = A^T$ ) and

$$w = \begin{pmatrix} 0 \\ \hat{w} \end{pmatrix} \text{ where } H(\hat{w})u = \begin{pmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{pmatrix},$$

it follows that

$$H(w)A = \begin{pmatrix} \gamma & & u^T & \\ \alpha & \times & \vdots & \times \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \times & \vdots & \times \end{pmatrix},$$

i.e., the  $u^T$  part of the first row of  $A$  is unchanged.

i.e., the  $u^T$  part of the first row of  $A$  is unchanged.

However, then

$$H(w)AH(w)^{-1} = H(w)AH(w)^T = H(w)AH(w)$$

i.e., the  $u^T$  part of the first row of  $A$  is unchanged.

However, then

$$H(w)AH(w)^{-1} = H(w)AH(w)^T = H(w)AH(w) = \left( \begin{array}{c|cccc} \gamma & \alpha & 0 & \cdots & 0 \\ \hline \alpha & & & & \\ 0 & & & & \\ \vdots & & & & \\ 0 & & & & \end{array} \right) B,$$

i.e., the  $u^T$  part of the first row of  $A$  is unchanged.

However, then

$$H(w)AH(w)^{-1} = H(w)AH(w)^T = H(w)AH(w) = \left( \begin{array}{c|cccc} \gamma & \alpha & 0 & \cdots & 0 \\ \alpha & & & & \\ 0 & & & & \\ \vdots & & & & \\ 0 & & & & \end{array} \right),$$

where  $B = H(\hat{w})CH^T(\hat{w})$ , as  $u^T H(\hat{w})^T = (\alpha, 0, \dots, 0)$ .

i.e., the  $u^T$  part of the first row of  $A$  is unchanged.

However, then

$$H(w)AH(w)^{-1} = H(w)AH(w)^T = H(w)AH(w) = \left( \begin{array}{c|cccc} \gamma & \alpha & 0 & \cdots & 0 \\ \alpha & & & & \\ 0 & & & & \\ \vdots & & & & \\ 0 & & & & \end{array} \right),$$

where  $B = H(\hat{w})CH^T(\hat{w})$ , as  $u^T H(\hat{w})^T = (\alpha, 0, \dots, 0)$ .

Note that  $H(w)AH(w)^T$  is symmetric as  $A$  is.



Now we inductively apply this to the smaller matrix  $B$ , as described for the QR factorization but using post- as well as pre-multiplications.

Now we inductively apply this to the smaller matrix  $B$ , as described for the QR factorization but using post- as well as pre-multiplications.

The result of  $n - 2$  such Householder similarity transformations is the matrix

$$H(w_{n-2}) \cdots H(w_2)H(w)AH(w)H(w_2) \cdots H(w_{n-2}),$$

which is tridiagonal.

The QR factorization of a tridiagonal matrix can now easily be achieved with  $n - 1$  Givens rotations:

The QR factorization of a tridiagonal matrix can now easily be achieved with  $n - 1$  Givens rotations: if  $A$  is tridiagonal

$$\underbrace{J(n-1, n) \cdots J(2, 3) J(1, 2)}_{Q^T} A = R, \quad \text{upper triangular.}$$

The QR factorization of a tridiagonal matrix can now easily be achieved with  $n - 1$  Givens rotations: if  $A$  is tridiagonal

$$\underbrace{J(n-1, n) \cdots J(2, 3) J(1, 2)}_{Q^T} A = R, \quad \text{upper triangular.}$$

Precisely,  $R$  has a diagonal and 2 super-diagonals,

$$R = \begin{pmatrix} \times & \times & \times & 0 & 0 & 0 & \cdots & 0 \\ 0 & \times & \times & \times & 0 & 0 & \cdots & 0 \\ 0 & 0 & \times & \times & \times & 0 & \cdots & 0 \\ \vdots & \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & \times & \times & \times & 0 \\ 0 & 0 & 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \times \end{pmatrix}$$

(exercise: check!).

The QR factorization of a tridiagonal matrix can now easily be achieved with  $n - 1$  Givens rotations: if  $A$  is tridiagonal

$$\underbrace{J(n-1, n) \cdots J(2, 3) J(1, 2)}_{Q^T} A = R, \quad \text{upper triangular.}$$

Precisely,  $R$  has a diagonal and 2 super-diagonals,

$$R = \begin{pmatrix} \times & \times & \times & 0 & 0 & 0 & \cdots & 0 \\ 0 & \times & \times & \times & 0 & 0 & \cdots & 0 \\ 0 & 0 & \times & \times & \times & 0 & \cdots & 0 \\ \vdots & \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & \times & \times & \times & 0 \\ 0 & 0 & 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & 0 & 0 & \times & \times \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \times \end{pmatrix}$$

(exercise: check!).

In the QR algorithm, the next matrix in the sequence is  $RQ$ .

## Lemma

*In the QR algorithm applied to a tridiagonal matrix, the tridiagonal form is preserved when Givens rotations are used.*

## Lemma

*In the QR algorithm applied to a tridiagonal matrix, the tridiagonal form is preserved when Givens rotations are used.*

Proof. If

$$A_k = QR = J(1, 2)^T J(2, 3)^T \cdots J(n-1, n)^T R$$

is tridiagonal,



## Lemma

*In the QR algorithm applied to a tridiagonal matrix, the tridiagonal form is preserved when Givens rotations are used.*

Proof. If

$$A_k = QR = J(1, 2)^T J(2, 3)^T \cdots J(n-1, n)^T R$$

is tridiagonal, then

$$A_{k+1} = RQ = RJ(1, 2)^T J(2, 3)^T \cdots J(n-1, n)^T.$$

## Lemma

*In the QR algorithm applied to a tridiagonal matrix, the tridiagonal form is preserved when Givens rotations are used.*

Proof. If

$$A_k = QR = J(1, 2)^T J(2, 3)^T \cdots J(n-1, n)^T R$$

is tridiagonal, then

$$A_{k+1} = RQ = RJ(1, 2)^T J(2, 3)^T \cdots J(n-1, n)^T.$$

Recall that:

post-multiplication of a matrix by  $J(i, i+1)^T$  replaces columns  $i$  and  $i+1$  by linear combinations of the pair of columns, while leaving columns  $j \neq i, i+1$  alone.

Thus, since  $R$  is upper triangular, the only subdiagonal entry in  $RJ(1, 2)^T$  is in position  $(2, 1)$ .

Thus, since  $R$  is upper triangular, the only subdiagonal entry in  $RJ(1, 2)^T$  is in position  $(2, 1)$ .

Similarly, the only subdiagonal entries in

$$RJ(1, 2)^T J(2, 3)^T = (RJ(1, 2)^T) J(2, 3)^T$$

are in positions  $(2, 1)$  and  $(3, 2)$ .

Thus, since  $R$  is upper triangular, the only subdiagonal entry in  $RJ(1, 2)^T$  is in position  $(2, 1)$ .

Similarly, the only subdiagonal entries in

$$RJ(1, 2)^T J(2, 3)^T = (RJ(1, 2)^T) J(2, 3)^T$$

are in positions  $(2, 1)$  and  $(3, 2)$ .

Inductively, the only subdiagonal entries in

$$\begin{aligned} & RJ(1, 2)^T J(2, 3)^T \cdots J(i-2, i-1)^T J(i-1, i)^T \\ &= (RJ(1, 2)^T J(2, 3)^T \cdots J(i-2, i-1)^T) J(i-1, i)^T \end{aligned}$$

are in positions  $(j, j-1)$ ,  $j = 2, \dots, i$ .

So, the lower triangular part of  $A_{k+1}$  only has nonzeros on its first subdiagonal.

So, the lower triangular part of  $A_{k+1}$  only has nonzeros on its first subdiagonal.

However, then since  $A_{k+1}$  is symmetric, it must be tridiagonal. □

## Using shifts.

One further and final step in making an efficient algorithm is the use of **shifts**:

for  $k = 1, 2, \dots$

    form the QR factorization of  $A_k - \mu_k I = Q_k R_k$

    and set  $A_{k+1} = R_k Q_k + \mu_k I$

end



For any chosen sequence of values of  $\mu_k \in \mathbb{R}$ ,  $\{A_k\}_{k=1}^{\infty}$  are symmetric and tridiagonal if  $A_1$  has these properties, and similar to  $A_1$ :

For any chosen sequence of values of  $\mu_k \in \mathbb{R}$ ,  $\{A_k\}_{k=1}^{\infty}$  are symmetric and tridiagonal if  $A_1$  has these properties, and similar to  $A_1$ :

$$\begin{aligned}A_2 &= R_1 Q_1 + \mu_1 I \\&= Q_1^T (Q_1 R_1) Q_1 + \mu_1 Q_1^T Q_1 \\&= Q_1^T (A_1 - \mu_1 I) Q_1 + \mu_1 Q_1^T Q_1 \\&= Q_1^T A_1 Q_1,\end{aligned}$$

For any chosen sequence of values of  $\mu_k \in \mathbb{R}$ ,  $\{A_k\}_{k=1}^{\infty}$  are symmetric and tridiagonal if  $A_1$  has these properties, and similar to  $A_1$ :

$$\begin{aligned}A_2 &= R_1 Q_1 + \mu_1 I \\&= Q_1^T (Q_1 R_1) Q_1 + \mu_1 Q_1^T Q_1 \\&= Q_1^T (A_1 - \mu_1 I) Q_1 + \mu_1 Q_1^T Q_1 \\&= Q_1^T A_1 Q_1,\end{aligned}$$

$$\begin{aligned}A_3 &= R_2 Q_2 + \mu_2 I \\&= Q_2^T (Q_2 R_2) Q_2 + \mu_2 Q_2^T Q_2 \\&= Q_2^T A_2 Q_2 = Q_2^T Q_1^T A_1 Q_1 Q_2,\end{aligned}$$

and similarly for  $A_4, A_5, \dots$

The simplest shift to use is  $\mu_k = a_{n,n}$  for all  $k$ , which leads rapidly in almost all cases to

$$A_k = \left( \begin{array}{c|c} T_k & 0 \\ \hline 0^T & \lambda \end{array} \right),$$

where  $T_k$  is  $n - 1$  by  $n - 1$  and tridiagonal, and  $\lambda$  is an eigenvalue of  $A_1$ .

The simplest shift to use is  $\mu_k = a_{n,n}$  for all  $k$ , which leads rapidly in almost all cases to

$$A_k = \left( \begin{array}{c|c} T_k & 0 \\ \hline 0^T & \lambda \end{array} \right),$$

where  $T_k$  is  $n - 1$  by  $n - 1$  and tridiagonal, and  $\lambda$  is an eigenvalue of  $A_1$ .

Inductively, once this form has been found, the QR algorithm with shift  $a_{n-1,n-1}$  can be concentrated only on the  $(n - 1) \times (n - 1)$  leading submatrix  $T_k$ .

The simplest shift to use is  $\mu_k = a_{n,n}$  for all  $k$ , which leads rapidly in almost all cases to

$$A_k = \left( \begin{array}{c|c} T_k & 0 \\ \hline 0^T & \lambda \end{array} \right),$$

where  $T_k$  is  $n - 1$  by  $n - 1$  and tridiagonal, and  $\lambda$  is an eigenvalue of  $A_1$ .

Inductively, once this form has been found, the QR algorithm with shift  $a_{n-1,n-1}$  can be concentrated only on the  $(n - 1) \times (n - 1)$  leading submatrix  $T_k$ .

This process is called **deflation**.

## The overall algorithm

for calculating the eigenvalues of an  $n$  by  $n$  symmetric matrix:

reduce  $A$  to tridiagonal form by orthogonal (Householder) similarity transformations.

for  $m = n, n - 1, \dots, 2$

  while  $a_{m-1,m} > \text{tol}$

$[Q, R] = \text{qr}(A - a_{m,m} * I)$

$A = R * Q + a_{m,m} * I$

  end while

  record eigenvalue  $\lambda_m = a_{m,m}$

$A \leftarrow$  leading  $m - 1$  by  $m - 1$  submatrix of  $A$

end

record eigenvalue  $\lambda_1 = a_{1,1}$