

# Lecture 9: QR algorithm



School of Mathematical Sciences, Xiamen University

## 1. Simultaneous iteration (SI)

- Sometimes also called *subspace iteration* or *orthogonal iteration* or *block power iteration*

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### Algorithm 1: Simultaneous iteration

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Pick  $\mathbf{Q}_n^{(0)} \in \mathbb{C}^{m \times n}$  with orthonormal columns  
for  $k = 1, 2, 3, \dots$ ,  
     $\mathbf{Z}^{(k)} = \mathbf{A}\mathbf{Q}_n^{(k-1)}$   
     $\mathbf{Q}_n^{(k)} \mathbf{R}_n^{(k)} = \mathbf{Z}^{(k)}$       (QR factorization)  
end

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- Here is an informal analysis of this method. Assume  $\mathbf{A} = \mathbf{S}\mathbf{\Lambda}\mathbf{S}^{-1}$  is diagonalizable with  $\mathbf{\Lambda} = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_m\}$  and

$$|\lambda_1| \geq \dots \geq |\lambda_n| > |\lambda_{n+1}| \geq \dots \geq |\lambda_m|.$$

We have

$$\mathbf{S}\mathbf{\Lambda}^k\mathbf{S}^{-1}\mathbf{Q}_n^{(0)} = \lambda_n^k \mathbf{S} \text{diag} \left\{ \left( \frac{\lambda_1}{\lambda_n} \right)^k, \dots, 1, \dots, \left( \frac{\lambda_m}{\lambda_n} \right)^k \right\} \mathbf{S}^{-1} \mathbf{Q}_n^{(0)}.$$

Let

$$\begin{bmatrix} \mathbf{X}_n^{(k)} \\ \mathbf{X}_c^{(k)} \end{bmatrix} := \text{diag} \left\{ \left( \frac{\lambda_1}{\lambda_n} \right)^k, \dots, 1, \dots, \left( \frac{\lambda_m}{\lambda_n} \right)^k \right\} \mathbf{S}^{-1} \mathbf{Q}_n^{(0)}.$$

Since  $\left| \frac{\lambda_i}{\lambda_n} \right| \geq 1$  if  $i \leq n$ , and  $\left| \frac{\lambda_i}{\lambda_n} \right| < 1$  if  $i > n$ , we get  $\mathbf{X}_c^{(k)}$

approaches zero like  $\left| \frac{\lambda_{n+1}}{\lambda_n} \right|^k$ , and  $\mathbf{X}_n^{(k)}$  does not approach zero.

Indeed, if  $\mathbf{X}_n^{(0)} := [\mathbf{I}_n \quad \mathbf{0}] \mathbf{S}^{-1} \mathbf{Q}_n^{(0)}$  has full rank (a generalization of the assumption  $\alpha_1 \neq 0$  in power iteration), then  $\mathbf{X}_n^{(k)}$  will have full rank too. We can prove (the proof is left as an exercise)

$$\text{span}\{\mathbf{Q}_n^{(k)}\} = \text{span}\{\mathbf{A}^k \mathbf{Q}_n^{(0)}\}.$$

Here,  $\text{span}\{\cdot\} = \text{range}(\cdot)$ . Write  $\mathbf{S} = [\mathbf{S}_n \quad \mathbf{S}_c]$ . Then

$$\mathbf{S} \mathbf{A}^k \mathbf{S}^{-1} \mathbf{Q}_n^{(0)} = \lambda_n^k (\mathbf{S}_n \mathbf{X}_n^{(k)} + \mathbf{S}_c \mathbf{X}_c^{(k)}).$$

Thus  $\text{span}\{\mathbf{Q}_n^{(k)}\}$  converges to

$$\begin{aligned} \text{span}\{\mathbf{Q}_n^{(k)}\} &= \text{span}\{\mathbf{A}^k \mathbf{Q}_n^{(0)}\} = \text{span}\{\mathbf{S} \mathbf{A}^k \mathbf{S}^{-1} \mathbf{Q}_n^{(0)}\} \\ &= \text{span}\{\mathbf{S}_n \mathbf{X}_n^{(k)} + \mathbf{S}_c \mathbf{X}_c^{(k)}\} \\ &\rightarrow \text{span}\{\mathbf{S}_n \mathbf{X}_n^{(k)}\} = \text{span}\{\mathbf{S}_n\}, \end{aligned}$$

the invariant subspace spanned by the first  $n$  eigenvectors.

- Note that if we follow only the first  $j < n$  columns of  $\mathbf{Q}_n^{(k)}$  through the iterations of the algorithm, they are *identical* to the columns that we would compute if we had started with only the first  $j$  columns of  $\mathbf{Q}_n^{(0)}$  instead of  $n$  columns.

In other words, **simultaneous** iteration is effectively running the algorithm for  $j = 1, 2, \dots, n$  **all at the same time**.

So if *all* the first  $n$  eigenvalues have distinct absolute values, i.e.,

$$|\lambda_1| > |\lambda_2| > \dots > |\lambda_n|,$$

and if *all* the leading principal submatrices of

$$\mathbf{X}_n^{(0)} := [\mathbf{I}_n \quad \mathbf{0}] \mathbf{S}^{-1} \mathbf{Q}_n^{(0)}$$

have full rank, the same convergence analysis as before implies that the first  $j \leq n$  columns of  $\mathbf{Q}_n^{(k)}$  converge to  $\text{span}\{\mathbf{S}_j\}$ .

## Theorem 1

Consider running simultaneous iteration on matrix  $\mathbf{A} \in \mathbb{C}^{m \times m}$  with  $n = m$  and  $\mathbf{Q}_n^{(0)} = \mathbf{I}$ . If  $\mathbf{A} = \mathbf{S}\mathbf{\Lambda}\mathbf{S}^{-1}$  is diagonalizable with

$$\mathbf{\Lambda} = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_m\}, \quad |\lambda_1| > |\lambda_2| > \dots > |\lambda_m|,$$

and if all the leading principal submatrices of  $\mathbf{S}^{-1}$  have full rank, then  $\mathbf{A}^{(k)} := (\mathbf{Q}_n^{(k)})^* \mathbf{A} \mathbf{Q}_n^{(k)}$  converges to the Schur form of  $\mathbf{A}$ . The eigenvalues will appear in decreasing order of absolute value.

Proof: See Demmel's book: Theorem 4.8, Page 158, **Applied numerical linear algebra**.

- The entry  $\mathbf{A}_{j,j}^{(k)}$  converges to  $\lambda_j$  like  $\max \left( \left| \frac{\lambda_{j+1}}{\lambda_j} \right|^k, \left| \frac{\lambda_j}{\lambda_{j-1}} \right|^k \right)$ .
- The block  $\mathbf{A}^{(k)}(j+1 : m, 1 : j)$  converges to zero like  $\left| \frac{\lambda_{j+1}}{\lambda_j} \right|^k$ .

## 2. QR algorithm without shifts

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### Algorithm 2: “Pure” QR algorithm

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$\mathbf{A}^{(0)} = \mathbf{A}$   
for  $k = 1, 2, 3, \dots$ ,  
     $\mathbf{Q}^{(k)} \mathbf{R}^{(k)} = \mathbf{A}^{(k-1)}$       (QR factorization)  
     $\mathbf{A}^{(k)} = \mathbf{R}^{(k)} \mathbf{Q}^{(k)}$   
end

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### Proposition 2

We have  $\mathbf{A}^{(k)} = (\underline{\mathbf{Q}}^{(k)})^* \mathbf{A} \underline{\mathbf{Q}}^{(k)}$ , where  $\underline{\mathbf{Q}}^{(k)} := \mathbf{Q}^{(1)} \mathbf{Q}^{(2)} \dots \mathbf{Q}^{(k)}$ .

### Proof.

Note that  $\mathbf{A}^{(k)} = (\mathbf{Q}^{(k)})^* \mathbf{A}^{(k-1)} \mathbf{Q}^{(k)}$ . □

### Proposition 3

The QR factorization of the  $k$ th power of  $\mathbf{A}$  is given by

$$\mathbf{A}^k = \underline{\mathbf{Q}}^{(k)} \underline{\mathbf{R}}^{(k)},$$

where  $\underline{\mathbf{Q}}^{(k)} := \mathbf{Q}^{(1)} \mathbf{Q}^{(2)} \dots \mathbf{Q}^{(k)}$ , and  $\underline{\mathbf{R}}^{(k)} := \mathbf{R}^{(k)} \mathbf{R}^{(k-1)} \dots \mathbf{R}^{(1)}$ .

### Proof.

We use induction. For  $k = 1$ ,  $\mathbf{A} = \mathbf{A}^{(0)} = \mathbf{Q}^{(1)} \mathbf{R}^{(1)} = \underline{\mathbf{Q}}^{(1)} \underline{\mathbf{R}}^{(1)}$ .

Assume  $\mathbf{A}^{k-1} = \underline{\mathbf{Q}}^{(k-1)} \underline{\mathbf{R}}^{(k-1)}$ . Then by  $\mathbf{A}^{(k-1)} = (\underline{\mathbf{Q}}^{(k-1)})^* \mathbf{A} \underline{\mathbf{Q}}^{(k-1)}$ , we have

$$\mathbf{A}^k = \mathbf{A} \underline{\mathbf{Q}}^{(k-1)} \underline{\mathbf{R}}^{(k-1)} = \underline{\mathbf{Q}}^{(k-1)} \mathbf{A}^{(k-1)} \underline{\mathbf{R}}^{(k-1)} = \underline{\mathbf{Q}}^{(k)} \underline{\mathbf{R}}^{(k)}.$$

This completes the proof. □



- Connection with power iteration: By  $\mathbf{A}^k = \underline{\mathbf{Q}}^{(k)} \underline{\mathbf{R}}^{(k)}$ , the first column of  $\underline{\mathbf{Q}}^{(k)}$  is the result of applying  $k$  steps of power iteration on  $\mathbf{A}$  to the vector  $\mathbf{e}_1$ .
- Connection with inverse iteration: By  $\underline{\mathbf{Q}}^{(k)} = (\mathbf{A}^*)^{-k} (\underline{\mathbf{R}}^{(k)})^*$ , the last column of  $\underline{\mathbf{Q}}^{(k)}$  is the result of applying  $k$  steps of inverse iteration on  $\mathbf{A}^*$  to the vector  $\mathbf{e}_m$ .

#### Theorem 4

If  $\mathbf{A} = \mathbf{S}\mathbf{\Lambda}\mathbf{S}^{-1}$  is diagonalizable with

$$\mathbf{\Lambda} = \text{diag}\{\lambda_1, \lambda_2, \dots, \lambda_m\}, \quad |\lambda_1| > |\lambda_2| > \dots > |\lambda_m|,$$

and if all the leading principal submatrices of  $\mathbf{S}^{-1}$  have full rank, then  $\mathbf{A}^{(k)}$  computed by “pure” QR algorithm converges to the Schur form of  $\mathbf{A}$ . The eigenvalues will appear in decreasing order of absolute value.

This theorem is a direct result of the following lemma.

## Lemma 5

The  $\mathbf{A}^{(k)}$  computed by “pure” QR algorithm is *identical* (we need an assumption about QR factorization here) to the matrix  $(\mathbf{Q}_n^{(k)})^* \mathbf{A} \mathbf{Q}_n^{(k)}$  implicitly computed by running simultaneous iteration on matrix  $\mathbf{A} \in \mathbb{C}^{m \times m}$  with  $n = m$  and  $\mathbf{Q}_n^{(0)} = \mathbf{I}$ .

## Proof.

We use induction. By  $\mathbf{Q}_n^{(1)} = \mathbf{Q}^{(1)}$ , we have  $\mathbf{A}^{(1)} = (\mathbf{Q}_n^{(1)})^* \mathbf{A} \mathbf{Q}_n^{(1)}$ . Assume  $\mathbf{A}^{(k-1)} = (\mathbf{Q}_n^{(k-1)})^* \mathbf{A} \mathbf{Q}_n^{(k-1)}$ . From simultaneous iteration, we can write  $\mathbf{A} \mathbf{Q}_n^{(k-1)} = \mathbf{Q}_n^{(k)} \mathbf{R}_n^{(k)}$ . Then  $\mathbf{R}_n^{(k)} = (\mathbf{Q}_n^{(k)})^* \mathbf{A} \mathbf{Q}_n^{(k-1)}$ , and

$$\mathbf{A}^{(k-1)} = (\mathbf{Q}_n^{(k-1)})^* \mathbf{A} \mathbf{Q}_n^{(k-1)} = (\mathbf{Q}_n^{(k-1)})^* \mathbf{Q}_n^{(k)} \mathbf{R}_n^{(k)} = \mathbf{Q}^{(k)} \mathbf{R}^{(k)}.$$

Thus

$$\mathbf{A}^{(k)} = \mathbf{R}^{(k)} \mathbf{Q}^{(k)} = (\mathbf{Q}_n^{(k)})^* \mathbf{A} \mathbf{Q}_n^{(k-1)} (\mathbf{Q}_n^{(k-1)})^* \mathbf{Q}_n^{(k)} = (\mathbf{Q}_n^{(k)})^* \mathbf{A} \mathbf{Q}_n^{(k)}.$$

This completes the proof. □

- From earlier analysis, we know that the convergence rate of “pure” QR algorithm depends on the ratios of eigenvalues. To speed convergence, we can use **shift and invert** techniques.

### 3. QR algorithm with shifts

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**Algorithm 3:** QR algorithm with shifts

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$$\mathbf{A}^{(0)} = \mathbf{A}$$

**for**  $k = 1, 2, 3, \dots$ ,

    Pick a shift  $\mu^{(k)}$  near an eigenvalue of  $\mathbf{A}$

$$\mathbf{Q}^{(k)} \mathbf{R}^{(k)} = \mathbf{A}^{(k-1)} - \mu^{(k)} \mathbf{I} \quad (\text{QR factorization})$$

$$\mathbf{A}^{(k)} = \mathbf{R}^{(k)} \mathbf{Q}^{(k)} + \mu^{(k)} \mathbf{I}$$

**end**

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#### Proposition 6

We have  $\mathbf{A}^{(k)} = (\underline{\mathbf{Q}}^{(k)})^* \mathbf{A} \underline{\mathbf{Q}}^{(k)}$ , where  $\underline{\mathbf{Q}}^{(k)} := \mathbf{Q}^{(1)} \mathbf{Q}^{(2)} \dots \mathbf{Q}^{(k)}$ .

## Proposition 7

We have the factorization (for  $k \geq 1$ )

$$(\mathbf{A} - \mu^{(k)}\mathbf{I})(\mathbf{A} - \mu^{(k-1)}\mathbf{I}) \cdots (\mathbf{A} - \mu^{(1)}\mathbf{I}) = \underline{\mathbf{Q}}^{(k)}\underline{\mathbf{R}}^{(k)},$$

where  $\underline{\mathbf{Q}}^{(k)} := \mathbf{Q}^{(1)}\mathbf{Q}^{(2)} \cdots \mathbf{Q}^{(k)}$ , and  $\underline{\mathbf{R}}^{(k)} := \mathbf{R}^{(k)}\mathbf{R}^{(k-1)} \cdots \mathbf{R}^{(1)}$ .

## Proof.

We use induction. For  $k = 1$ ,  $\mathbf{A} - \mu^{(1)}\mathbf{I} = \mathbf{Q}^{(1)}\mathbf{R}^{(1)} = \underline{\mathbf{Q}}^{(1)}\underline{\mathbf{R}}^{(1)}$ .

Assume  $(\mathbf{A} - \mu^{(k-1)}\mathbf{I})(\mathbf{A} - \mu^{(k-2)}\mathbf{I}) \cdots (\mathbf{A} - \mu^{(1)}\mathbf{I}) = \underline{\mathbf{Q}}^{(k-1)}\underline{\mathbf{R}}^{(k-1)}$ .

Then by  $\mathbf{A}^{(k-1)} = (\underline{\mathbf{Q}}^{(k-1)})^* \mathbf{A} \underline{\mathbf{Q}}^{(k-1)}$ , we have

$$\begin{aligned} (\mathbf{A} - \mu^{(k)}\mathbf{I}) \cdots (\mathbf{A} - \mu^{(1)}\mathbf{I}) &= (\mathbf{A} \underline{\mathbf{Q}}^{(k-1)} - \mu^{(k)}\underline{\mathbf{Q}}^{(k-1)})\underline{\mathbf{R}}^{(k-1)} \\ &= (\underline{\mathbf{Q}}^{(k-1)}\mathbf{A}^{(k-1)} - \mu^{(k)}\underline{\mathbf{Q}}^{(k-1)})\underline{\mathbf{R}}^{(k-1)} \\ &= \underline{\mathbf{Q}}^{(k-1)}(\mathbf{A}^{(k-1)} - \mu^{(k)}\mathbf{I})\underline{\mathbf{R}}^{(k-1)} = \underline{\mathbf{Q}}^{(k)}\underline{\mathbf{R}}^{(k)}. \end{aligned}$$

This completes the proof. □

- Connection with shifted power iteration: By

$$(\mathbf{A} - \mu^{(k)}\mathbf{I})(\mathbf{A} - \mu^{(k-1)}\mathbf{I}) \cdots (\mathbf{A} - \mu^{(1)}\mathbf{I}) = \underline{\mathbf{Q}}^{(k)}\underline{\mathbf{R}}^{(k)},$$

the first column of  $\underline{\mathbf{Q}}^{(k)}$  is the result of applying  $k$  steps of shifted power iteration on  $\mathbf{A} - \mu^{(j)}\mathbf{I}$  to the vector  $\mathbf{e}_1$  using the shifts  $\mu^{(j)}$ ,  $j = 1 : k$ .

- Connection with shifted inverse iteration: By

$$\underline{\mathbf{Q}}^{(k)} = (\mathbf{A} - \mu^{(k)}\mathbf{I})^{-*}(\mathbf{A} - \mu^{(k-1)}\mathbf{I})^{-*} \cdots (\mathbf{A} - \mu^{(1)}\mathbf{I})^{-*}(\underline{\mathbf{R}}^{(k)})^*,$$

the last column of  $\underline{\mathbf{Q}}^{(k)}$  is the result of applying  $k$  steps of shifted inverse iteration on  $(\mathbf{A} - \mu^{(j)}\mathbf{I})^*$  to the vector  $\mathbf{e}_m$  using the shifts  $\mu^{(j)}$ ,  $j = 1 : k$ . If the shifts are good eigenvalue estimates, the last column of  $\underline{\mathbf{Q}}^{(k)}$ , i.e.,  $\underline{\mathbf{Q}}^{(k)}\mathbf{e}_m$ , converges quickly to a left eigenvector of  $\mathbf{A}$ .

- Connection with Rayleigh quotient iteration: Choose

$$\mu^{(1)} = r(\mathbf{e}_m), \quad \mu^{(k+1)} = r(\underline{\mathbf{Q}}^{(k)} \mathbf{e}_m),$$

as the shift at every step. The eigenvalue and eigenvector estimates  $\mu^{(k+1)}$  and  $\underline{\mathbf{Q}}^{(k)} \mathbf{e}_m$  are identical to those that are computed by the Rayleigh quotient iteration on  $\mathbf{A}^*$  starting with  $\mathbf{e}_m$ .

In the QR algorithm, the Rayleigh quotient  $r(\underline{\mathbf{Q}}^{(k)} \mathbf{e}_m)$  appears as the  $(m, m)$  entry of  $\mathbf{A}^{(k)}$ . So it comes for free! Actually, we have

$$\mathbf{A}_{mm}^{(k)} = \mathbf{e}_m^* \mathbf{A}^{(k)} \mathbf{e}_m = \mathbf{e}_m^* (\underline{\mathbf{Q}}^{(k)})^* \mathbf{A} \underline{\mathbf{Q}}^{(k)} \mathbf{e}_m = r(\underline{\mathbf{Q}}^{(k)} \mathbf{e}_m).$$

Then we can set  $\mu^{(k+1)} = \mathbf{A}_{mm}^{(k)}$ . This is known as the *Rayleigh quotient shift*. Assume the algorithm converges. Then  $\underline{\mathbf{Q}}^{(k)} \mathbf{e}_m$  converges quadratically or cubically to an eigenvector.

- Other issues: *Wilkinson shift* ...

## 4. Practical issues on QR algorithm

### Proposition 8

*Upper Hessenberg form is preserved by QR algorithm.*

### Proof.

For the upper Hessenberg matrix  $\mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I}$ , it is easy to show that there exists a QR factorization  $\mathbf{Q}^{(k)}\mathbf{R}^{(k)} = \mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I}$  such that  $\mathbf{Q}^{(k)}$  is upper Hessenberg. Then it is easy to confirm that  $\mathbf{R}^{(k)}\mathbf{Q}^{(k)}$  remains upper Hessenberg and adding  $\mu^{(k)}\mathbf{I}$  does not change this.  $\square$

### Proposition 9

*Hermitian tridiagonal form is preserved by QR algorithm (real shifts).*

### Proof.

Hermitian + tridiagonal = Hermitian + upper Hessenberg.  $\square$

- First phase: Reduction to Hessenberg or tridiagonal form

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \xrightarrow{\mathbf{Q}_1^*} \begin{bmatrix} \times & \times & \times & \times & \times \\ \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ 0 & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ 0 & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ 0 & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \end{bmatrix} \xrightarrow{\cdot \mathbf{Q}_1} \begin{bmatrix} \times & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ \times & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \end{bmatrix} \\
 \mathbf{A} & & \mathbf{Q}_1^* \mathbf{A} & & \mathbf{Q}_1^* \mathbf{A} \mathbf{Q}_1
 \end{math>$$

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} \xrightarrow{\mathbf{Q}_2^*} \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & 0 & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & 0 & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \end{bmatrix} \xrightarrow{\cdot \mathbf{Q}_2} \begin{bmatrix} \times & \times & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ \times & \times & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \times & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \end{bmatrix} \\
 \mathbf{Q}_1^* \mathbf{A} \mathbf{Q}_1 & & \mathbf{Q}_2^* \mathbf{Q}_1^* \mathbf{A} \mathbf{Q}_1 & & \mathbf{Q}_2^* \mathbf{Q}_1^* \mathbf{A} \mathbf{Q}_1 \mathbf{Q}_2
 \end{math>$$

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \end{bmatrix} \quad \underbrace{\mathbf{Q}_{m-2}^* \cdots \mathbf{Q}_2^* \mathbf{Q}_1^*}_{\mathbf{Q}^*} \mathbf{A} \underbrace{\mathbf{Q}_1 \mathbf{Q}_2 \cdots \mathbf{Q}_{m-2}}_{\mathbf{Q}} = \mathbf{H}.$$



- Second phase: generate a sequence of Hessenberg (or tridiagonal) matrices that converge to a triangular (or diagonal) form.

$$\begin{array}{ccccc}
 \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} & \xrightarrow{\text{Phase 1}} & \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \end{bmatrix} & \xrightarrow{\text{Phase 2}} & \begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \\ & & & & \times \end{bmatrix} \\
 \mathbf{A} \neq \mathbf{A}^* & & \mathbf{H} & & \mathbf{T}
 \end{array}$$

$$\begin{array}{ccccc}
 \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix} & \xrightarrow{\text{Phase 1}} & \begin{bmatrix} \times & \times \\ \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times & \times \\ & & & \times & \times \end{bmatrix} & \xrightarrow{\text{Phase 2}} & \begin{bmatrix} \times & & & & \\ & \times & & & \\ & & \times & & \\ & & & \times & \\ & & & & \times \end{bmatrix} \\
 \mathbf{A} = \mathbf{A}^* & & \mathbf{H} & & \mathbf{D}
 \end{array}$$

- ★ For simplicity, in the following we only consider the real case, i.e.,  $\mathbf{A} \in \mathbb{R}^{m \times m}$ .

## 4.1. Implicit Q theorem

### Definition 10

An upper Hessenberg matrix  $\mathbf{H}$  is unreduced if all  $(j+1, j)$  entries of  $\mathbf{H}$  are nonzero.

### Theorem 11 (Consider the real case. The complex case is similar.)

*Let  $\mathbf{A} \in \mathbb{R}^{m \times m}$ . Suppose that  $\mathbf{Q}^\top \mathbf{A} \mathbf{Q} = \mathbf{H}$  is unreduced upper Hessenberg and  $\mathbf{Q}$  is orthogonal. Then columns 2 to  $m$  of  $\mathbf{Q}$  are determined uniquely (up to signs) by the first column of  $\mathbf{Q}$ .*

- Implicit Q theorem implies that QR algorithm can be implemented cheaply on an upper Hessenberg matrix. The implementation will be *implicit* in the sense that we do not explicitly compute the QR factorization of an upper Hessenberg matrix each iteration but rather construct  $\mathbf{Q}$  implicitly as a product of Givens rotations and other simple orthogonal/unitary matrices.

### Proof. (Implicit Q theorem).

Suppose that  $\mathbf{Q}^\top \mathbf{A} \mathbf{Q} = \mathbf{H}$  and  $\mathbf{V}^\top \mathbf{A} \mathbf{V} = \mathbf{G}$  are unreduced upper Hessenberg,  $\mathbf{Q}$  and  $\mathbf{V}$  are orthogonal, and the first columns of  $\mathbf{Q}$  and  $\mathbf{V}$  are equal. Let  $(\mathbf{X})_i$  denote the  $i$ th column of  $\mathbf{X}$ . Let  $\mathbf{W} \equiv \mathbf{V}^\top \mathbf{Q}$ . By  $\mathbf{G} \mathbf{W} = \mathbf{G} \mathbf{V}^\top \mathbf{Q} = \mathbf{V}^\top \mathbf{A} \mathbf{Q} = \mathbf{V}^\top \mathbf{Q} \mathbf{H} = \mathbf{W} \mathbf{H}$ , we have

$$\mathbf{G}(\mathbf{W})_i = \mathbf{W}(\mathbf{H})_i = \sum_{j=1}^{i+1} h_{ji}(\mathbf{W})_j.$$

Thus,  $h_{i+1,i}(\mathbf{W})_{i+1} = \mathbf{G}(\mathbf{W})_i - \sum_{j=1}^i h_{ji}(\mathbf{W})_j$ . Since  $(\mathbf{W})_1 = \mathbf{e}_1$  and  $\mathbf{G}$  is upper Hessenberg, we can use induction on  $i$  to show that  $(\mathbf{W})_i$  is nonzero in entries 1 to  $i$  only; i.e.,  $\mathbf{W}$  is upper triangular. Since  $\mathbf{W}$  is also orthogonal, then  $\mathbf{W}$  is diagonal:  $\mathbf{W} = \text{diag}\{1, \pm 1, \dots, \pm 1\}$ , which implies

$$\mathbf{V} \text{diag}\{1, \pm 1, \dots, \pm 1\} = \mathbf{Q}.$$



## 4.2. Implicit single shift QR algorithm

- To compute  $\mathbf{H}^{(k)} = (\mathbf{Q}^{(k)})^\top \mathbf{H}^{(k-1)} \mathbf{Q}^{(k)}$  from  $\mathbf{H}^{(k-1)}$  in the QR algorithm, we will need only to
  - (1) compute the first column of  $\mathbf{Q}^{(k)}$  (which is parallel to the first column of  $\mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I}$  and so can be gotten just by normalizing this column vector).
  - (2) choose other columns of  $\mathbf{Q}^{(k)}$  so  $\mathbf{Q}^{(k)}$  is orthogonal and  $\mathbf{H}^{(k)}$  is unreduced upper Hessenberg.
- By the implicit Q theorem, we know that we will have computed  $\mathbf{H}^{(k)}$  correctly because  $\mathbf{Q}^{(k)}$  is unique up to signs, which do not matter. (Signs do not matter because changing the signs of the columns of  $\mathbf{Q}^{(k)}$  is the same as changing  $\mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I} = \mathbf{Q}^{(k)}\mathbf{R}^{(k)}$  to  $(\mathbf{Q}^{(k)}\mathbf{S}^{(k)})(\mathbf{S}^{(k)}\mathbf{R}^{(k)})$ , where  $\mathbf{S}^{(k)} = \text{diag}\{\pm 1, \pm 1, \dots, \pm 1\}$ . Then  $\mathbf{H}^{(k)} = (\mathbf{S}^{(k)}\mathbf{R}^{(k)})(\mathbf{Q}^{(k)}\mathbf{S}^{(k)}) + \mu^{(k)}\mathbf{I} = \mathbf{S}^{(k)}(\mathbf{R}^{(k)}\mathbf{Q}^{(k)} + \mu^{(k)}\mathbf{I})\mathbf{S}^{(k)}$ , which is an orthogonal similarity that just changes the signs of some columns and rows of  $\mathbf{H}^{(k)}$ .)

- To see how to use the implicit Q theorem to compute  $\mathbf{H}^{(1)}$  from  $\mathbf{H}^{(0)} = \mathbf{H}$ , we use a  $5 \times 5$  example.

$$1. \mathbf{Q}_1^\top = \begin{bmatrix} c_1 & s_1 & & & \\ -s_1 & c_1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}, \quad \mathbf{H}_1 = \mathbf{Q}_1^\top \mathbf{H} \mathbf{Q}_1 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ + & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

$$2. \mathbf{Q}_2^\top = \begin{bmatrix} 1 & & & & \\ & c_2 & s_2 & & \\ & -s_2 & c_2 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}, \quad \mathbf{Q}_2^\top \mathbf{H}_1 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

$$\mathbf{H}_2 = \mathbf{Q}_2^\top \mathbf{H}_1 \mathbf{Q}_2 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & + & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

$$3. \mathbf{Q}_3^\top = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & c_3 & s_3 & \\ & & -s_3 & c_3 & \\ & & & & 1 \end{bmatrix}, \quad \mathbf{Q}_3^\top \mathbf{H}_2 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

$$\mathbf{H}_3 = \mathbf{Q}_3^\top \mathbf{H}_2 \mathbf{Q}_3 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & + & \times & \times \end{bmatrix}$$

$$4. \mathbf{Q}_4^\top = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & c_4 & s_4 \\ & & & -s_4 & c_4 \end{bmatrix}, \quad \mathbf{Q}_4^\top \mathbf{H}_3 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

$$\mathbf{H}_4 = \mathbf{Q}_4^\top \mathbf{H}_3 \mathbf{Q}_4 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

Altogether  $\mathbf{Q}^\top \mathbf{H} \mathbf{Q} = \mathbf{H}_4$  is upper Hessenberg, where

$$\mathbf{Q} = \mathbf{Q}_1 \mathbf{Q}_2 \mathbf{Q}_3 \mathbf{Q}_4 = \begin{bmatrix} c_1 & \times & \times & \times & \times \\ s_1 & \times & \times & \times & \times \\ & s_2 & \times & \times & \times \\ & & s_3 & \times & \times \\ & & & s_4 & c_4 \end{bmatrix},$$

so the first column of  $\mathbf{Q}$  is  $[c_1 \ s_1 \ 0 \ \cdots \ 0]^\top$ , which by the implicit Q theorem has uniquely determined the other columns of  $\mathbf{Q}$  (up to signs). We now choose the first column of  $\mathbf{Q}$  to be proportional to the first column of  $\mathbf{H}^{(0)} - \mu^{(1)}\mathbf{I}$ . This means  $\mathbf{Q}$  is the same (up to signs) as in the QR factorization of  $\mathbf{H}^{(0)} - \mu^{(1)}\mathbf{I}$ .

### 4.3. Implicit double shift QR algorithm

- We describe how to maintain real arithmetic by shifting  $\mu^{(k)}$  and  $\overline{\mu^{(k)}}$  in succession:

$$\begin{aligned}\mathbf{Q}^{(k-1/2)}\mathbf{R}^{(k-1/2)} &= \mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I} \\ \mathbf{H}^{(k-1/2)} &= \mathbf{R}^{(k-1/2)}\mathbf{Q}^{(k-1/2)} + \mu^{(k)}\mathbf{I} \\ &= (\mathbf{Q}^{(k-1/2)})^*\mathbf{H}^{(k-1)}\mathbf{Q}^{(k-1/2)}\end{aligned}$$

$$\begin{aligned}\mathbf{Q}^{(k)}\mathbf{R}^{(k)} &= \mathbf{H}^{(k-1/2)} - \overline{\mu^{(k)}}\mathbf{I} \\ \mathbf{H}^{(k)} &= \mathbf{R}^{(k)}\mathbf{Q}^{(k)} + \overline{\mu^{(k)}}\mathbf{I} = (\mathbf{Q}^{(k)})^*\mathbf{H}^{(k-1/2)}\mathbf{Q}^{(k)} \\ &= (\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)})^*\mathbf{H}^{(k-1)}\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}\end{aligned}$$



## Lemma 12

We can choose  $\mathbf{Q}^{(k-1/2)}$  and  $\mathbf{Q}^{(k)}$  such that

- (1)  $\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}$  is real,
- (2)  $\mathbf{H}^{(k)}$  is therefore real,
- (3) the first column of  $\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}$  is easy to compute.

Proof. Since

$$\mathbf{Q}^{(k)}\mathbf{R}^{(k)} = \mathbf{H}^{(k-1/2)} - \overline{\mu^{(k)}}\mathbf{I} = \mathbf{R}^{(k-1/2)}\mathbf{Q}^{(k-1/2)} + (\mu^{(k)} - \overline{\mu^{(k)}})\mathbf{I},$$

we get

$$\begin{aligned} & \mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}\mathbf{R}^{(k)}\mathbf{R}^{(k-1/2)} \\ &= \mathbf{Q}^{(k-1/2)}(\mathbf{R}^{(k-1/2)}\mathbf{Q}^{(k-1/2)} + (\mu^{(k)} - \overline{\mu^{(k)}})\mathbf{I})\mathbf{R}^{(k-1/2)} \\ &= \mathbf{Q}^{(k-1/2)}\mathbf{R}^{(k-1/2)}\mathbf{Q}^{(k-1/2)}\mathbf{R}^{(k-1/2)} + (\mu^{(k)} - \overline{\mu^{(k)}})\mathbf{Q}^{(k-1/2)}\mathbf{R}^{(k-1/2)} \\ &= (\mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I})^2 + (\mu^{(k)} - \overline{\mu^{(k)}})(\mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I}) \\ &= (\mathbf{H}^{(k-1)})^2 - 2\operatorname{Re}(\mu^{(k)})\mathbf{H}^{(k-1)} + |\mu^{(k)}|^2\mathbf{I} \equiv \mathbf{M}. \end{aligned}$$

Thus,  $\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}\mathbf{R}^{(k)}\mathbf{R}^{(k-1/2)}$  is the QR factorization of the real matrix  $\mathbf{M}$ , and therefore,  $\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}$ , as well as  $\mathbf{R}^{(k)}\mathbf{R}^{(k-1/2)}$ , can be chosen real. This means that

$$\mathbf{H}^{(k)} = (\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)})^* \mathbf{H}^{(k-1)} \mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}$$

also is real if  $\mathbf{H}^{(k-1)}$  is real. The first column of  $\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}$  is proportional to the first column of

$$(\mathbf{H}^{(k-1)})^2 - 2\operatorname{Re}(\mu^{(k)})\mathbf{H}^{(k-1)} + |\mu^{(k)}|^2\mathbf{I},$$

whose sparsity pattern is  $\begin{bmatrix} \times & \times & \times & 0 & \cdots & 0 \end{bmatrix}^\top$ .

□

- We provide a  $6 \times 6$  example. Assume  $\mathbf{H}$  is upper Hessenberg and the shifts are  $\mu$  and  $\bar{\mu}$ .

1. Choose an orthogonal matrix

$$\mathbf{Q}_1^\top = \begin{bmatrix} \tilde{\mathbf{Q}}^\top & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \quad \tilde{\mathbf{Q}}^\top \tilde{\mathbf{Q}} = \mathbf{I}_3,$$

where the first column of  $\mathbf{Q}_1$  is proportional to the first column of

$$\mathbf{H}^2 - 2\operatorname{Re}(\mu)\mathbf{H} + |\mu|^2\mathbf{I},$$

so

$$\mathbf{Q}_1^\top \mathbf{H} = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ + & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}, \quad \mathbf{Q}_1^\top \mathbf{H} \mathbf{Q}_1 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ + & \times & \times & \times & \times & \times \\ + & + & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}$$

2. Choose a Householder reflector  $\mathbf{Q}_2^\top$ , which affects only rows 2,3, and 4 of  $\mathbf{Q}_2^\top \mathbf{H}_1$ , zeroing out entries (3,1) and (4,1) of  $\mathbf{H}_1 = \mathbf{Q}_1^\top \mathbf{H} \mathbf{Q}_1$  (this means that  $\mathbf{Q}_2^\top$  is the identity matrix outside rows and columns 2 through 4):

$$\mathbf{Q}_2^\top \mathbf{H}_1 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & + & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix},$$

$$\mathbf{H}_2 = \mathbf{Q}_2^\top \mathbf{H}_1 \mathbf{Q}_2 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & + & \times & \times & \times & \times \\ 0 & + & + & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}$$

3. Choose a Householder reflector  $\mathbf{Q}_3^\top$ , which affects only rows 3,4, and 5 of  $\mathbf{Q}_3^\top \mathbf{H}_2$ , zeroing out entries (4,2) and (5,2) of  $\mathbf{H}_2$  (this means that  $\mathbf{Q}_3^\top$  is the identity matrix outside rows and columns 3 through 5):

$$\mathbf{Q}_3^\top \mathbf{H}_2 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & + & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}$$

$$\mathbf{H}_3 = \mathbf{Q}_3^\top \mathbf{H}_2 \mathbf{Q}_3 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & + & \times & \times & \times \\ 0 & 0 & + & + & \times & \times \end{bmatrix}$$

4. Choose a Householder reflector  $\mathbf{Q}_4^\top$ , which affects only rows 4,5, and 6 of  $\mathbf{Q}_4^\top \mathbf{H}_3$ , zeroing out entries (5,3) and (6,3) of  $\mathbf{H}_2$  (this means that  $\mathbf{Q}_4^\top$  is the identity matrix outside rows and columns 4 through 6):

$$\mathbf{Q}_4^\top \mathbf{H}_3 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & + & \times & \times \end{bmatrix}$$

$$\mathbf{H}_4 = \mathbf{Q}_4^\top \mathbf{H}_3 \mathbf{Q}_4 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & + & \times & \times \end{bmatrix}$$

5. Choose a Givens rotation  $\mathbf{Q}_5^\top$

$$\mathbf{Q}_5^\top = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & c & s \\ & & & & -s & c \end{bmatrix}, \quad \mathbf{Q}_5^\top \mathbf{H}_4 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}$$

$$\mathbf{H}_5 = \mathbf{Q}_5^\top \mathbf{H}_4 \mathbf{Q}_5 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}.$$

Altogether  $\mathbf{Q}^\top \mathbf{H} \mathbf{Q}$  is upper Hessenberg, where

$$\mathbf{Q} = \mathbf{Q}_1 \mathbf{Q}_2 \mathbf{Q}_3 \mathbf{Q}_4 \mathbf{Q}_5 \quad \text{with} \quad \mathbf{Q} \mathbf{e}_1 = \mathbf{Q}_1 \mathbf{e}_1.$$

## 5. Further reading

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