Lecture 9: QR algorithm

School of Mathematical Sciences, Xiamen University

1. Subspace iteration (SI)

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

Algorithm 1: Subspace iteration

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

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

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

If $n = 1$, then subspace iteration reduces to power iteration; see Lecture 8 for details.

Now we consider the case $n > 1$. Let

$$\mathbf{X}_n := \begin{bmatrix} \mathbf{I}_n & \mathbf{0} \end{bmatrix} \mathbf{S}^{-1}\mathbf{Q}_n^{(0)},$$

and

$$\mathbf{X}_\mathrm{c} := \begin{bmatrix} \mathbf{0} & \mathbf{I}_{m-n} \end{bmatrix} \mathbf{S}^{-1}\mathbf{Q}_n^{(0)}.$$

Assume that $\mathbf{X}_n$ has full rank (a generalization of the assumption $\alpha_1 \neq 0$ in power iteration). We have (the proof is left as an exercise)

$$\mathbf{Q}_n^{(k)} = \mathbf{A}^k\mathbf{Q}_n^{(0)}(\mathbf{R}_n^{(1)})^{-1}(\mathbf{R}_n^{(2)})^{-1}\cdots(\mathbf{R}_n^{(k)})^{-1}.$$

By $\mathbf{A} = \mathbf{S}\mathbf{\Lambda}\mathbf{S}^{-1}$, we have

$$\mathbf{Q}_n^{(k)} = \mathbf{S}\mathbf{\Lambda}^k\mathbf{S}^{-1}\mathbf{Q}_n^{(0)}(\mathbf{R}_n^{(1)})^{-1}(\mathbf{R}_n^{(2)})^{-1}\cdots(\mathbf{R}_n^{(k)})^{-1}.$$

Write $\mathbf{S} = \begin{bmatrix} \mathbf{S}_n & \mathbf{S}_{\rm c} \end{bmatrix}$ and $\mathbf{\Lambda} = \operatorname{diag}\{\mathbf{\Lambda}_n, \mathbf{\Lambda}_{\rm c}\}$. By $\mathbf{S}^{-1}\mathbf{Q}_n^{(0)} = \begin{bmatrix} \mathbf{X}_n \\ \mathbf{X}_{\rm c} \end{bmatrix}$, we have

$$
\begin{aligned}
\mathbf{Q}_n^{(k)} &= \begin{bmatrix} \mathbf{S}_n & \mathbf{S}_{\rm c} \end{bmatrix} \begin{bmatrix} \mathbf{\Lambda}_n^k & \\ & \mathbf{\Lambda}_{\rm c}^k \end{bmatrix} \begin{bmatrix} \mathbf{X}_n \\ \mathbf{X}_{\rm c} \end{bmatrix} (\mathbf{R}_n^{(1)})^{-1}(\mathbf{R}_n^{(2)})^{-1} \cdots (\mathbf{R}_n^{(k)})^{-1} \\
&= \begin{bmatrix} \mathbf{S}_n & \mathbf{S}_{\rm c} \end{bmatrix} \begin{bmatrix} \mathbf{\Lambda}_n^k \mathbf{X}_n (\mathbf{R}_n^{(1)})^{-1}(\mathbf{R}_n^{(2)})^{-1} \cdots (\mathbf{R}_n^{(k)})^{-1} \\ \mathbf{\Lambda}_{\rm c}^k \mathbf{X}_{\rm c} (\mathbf{R}_n^{(1)})^{-1}(\mathbf{R}_n^{(2)})^{-1} \cdots (\mathbf{R}_n^{(k)})^{-1} \end{bmatrix}.
\end{aligned}
$$

Exercise: Prove that

$$
\mathbf{S}_{\rm c} \mathbf{\Lambda}_{\rm c}^k \mathbf{X}_{\rm c} (\mathbf{R}_n^{(1)})^{-1}(\mathbf{R}_n^{(2)})^{-1} \cdots (\mathbf{R}_n^{(k)})^{-1} \to \mathbf{0}
$$

like $\left| \dfrac{\lambda_{n+1}}{\lambda_n} \right|^k$. Equivalently, we have the convergence result:

$$
\mathbf{Q}_n^{(k)} - \mathbf{S}_n \mathbf{\Lambda}_n^k \mathbf{X}_n (\mathbf{R}_n^{(1)})^{-1}(\mathbf{R}_n^{(2)})^{-1} \cdots (\mathbf{R}_n^{(k)})^{-1} \to \mathbf{0},
$$

which means that $\operatorname{span}\{\mathbf{Q}_n^{(k)}\}$ converges to $\operatorname{span}\{\mathbf{S}_n\}$.

- Note that if we follow only the first $1 \le j \le n$ columns of $\mathbf{Q}_n^{(k)}$ through the iterations of the algorithm, they are *identical* to the iterates 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, subspace iteration is effectively running the algorithm for $j = 1, 2, \cdots, n$ all at the same time (simultaneous).

  So if *all* the first $n+1$ eigenvalues have distinct absolute values, i.e.,

$$|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n| > |\lambda_{n+1}|,$$

  and if *all* the leading principal submatrices of

$$\mathbf{X}_n = \begin{bmatrix} \mathbf{I}_n & \mathbf{0} \end{bmatrix} \mathbf{S}^{-1} \mathbf{Q}_n^{(0)}$$

  have full rank, the same convergence analysis as before implies that $\text{span}\{\mathbf{Q}_j^{(k)}\}$ with $\mathbf{Q}_j^{(k)} := \mathbf{Q}_n^{(k)} \begin{bmatrix} \mathbf{I}_j \\ \mathbf{0} \end{bmatrix}$ converges to $\text{span}\{\mathbf{S}_j\}$ with $\mathbf{S}_j := \mathbf{S} \begin{bmatrix} \mathbf{I}_j \\ \mathbf{0} \end{bmatrix}$ for each $j = 1, 2, \cdots, n$.

Theorem 1

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

$$\boldsymbol{\Lambda} = \mathrm{diag}\{\lambda_1, \lambda_2, \cdots, \lambda_m\}, \quad |\lambda_1| > |\lambda_2| > \cdots > |\lambda_m|,$$

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 a 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 $\mathbf{A}_{jj}^{(k)}$ converges to λ_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. "Pure" QR algorithm

Algorithm 2: "Pure" QR algorithm

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

for $k = 1, 2, 3, \ldots,$

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

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

end

Proposition 2

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

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

$$\begin{aligned}
\mathbf{A}^{(k)} &= \mathbf{R}^{(k)}\mathbf{Q}^{(k)} = (\mathbf{Q}^{(k)})^*\mathbf{A}^{(k-1)}\mathbf{Q}^{(k)} \\
&= (\mathbf{Q}^{(k)})^*(\mathbf{Q}^{(k-1)})^*\mathbf{A}^{(k-2)}\mathbf{Q}^{(k-1)}\mathbf{Q}^{(k)} \\
&= (\mathbf{Q}^{(k)})^*\cdots(\mathbf{Q}^{(1)})^*\mathbf{A}^{(0)}\mathbf{Q}^{(1)}\cdots\mathbf{Q}^{(k)} = (\underline{\mathbf{Q}}^{(k)})^*\mathbf{A}\underline{\mathbf{Q}}^{(k)}.
\end{aligned}$$ □

Proposition 3

We have (a QR *factorization of* $\mathbf{A}^k$*)*

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

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 $k=1$, $\mathbf{A} = \mathbf{A}^{(0)} = \mathbf{Q}^{(1)}\mathbf{R}^{(1)} = \underline{\mathbf{Q}}^{(1)}\underline{\mathbf{R}}^{(1)}$. Now we prove the case $k>1$ with the assumption $\mathbf{A}^{k-1} = \underline{\mathbf{Q}}^{(k-1)}\underline{\mathbf{R}}^{(k-1)}$. By Proposition 2, we have $\mathbf{A}^{(k-1)} = (\underline{\mathbf{Q}}^{(k-1)})^*\mathbf{A}\underline{\mathbf{Q}}^{(k-1)}$, which implies $\mathbf{A}\underline{\mathbf{Q}}^{(k-1)} = \underline{\mathbf{Q}}^{(k-1)}\mathbf{A}^{(k-1)}$. Then we have

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

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

$$\mathbf{\Lambda} = \operatorname{diag}\{\lambda_1, \lambda_2, \cdots, \lambda_m\}, \quad |\lambda_1| > |\lambda_2| > \cdots > |\lambda_m|,$$

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 a 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 to the matrix* $(\mathbf{Q}_n^{(k)})^*\mathbf{A}\mathbf{Q}_n^{(k)}$ *implicitly computed by running subspace iteration on matrix* $\mathbf{A} \in \mathbb{C}^{m\times m}$ *with* $n = m$ *and* $\mathbf{Q}_n^{(0)} = \mathbf{I}$. (*We need an assumption about* QR *factorizations used in subspace iteration.*)

Proof. We use induction. For $k = 1$, let $\mathbf{Q}_n^{(1)} = \mathbf{Q}^{(1)}$ and $\mathbf{R}_n^{(1)} = \mathbf{R}^{(1)}$. We have $\mathbf{A}^{(1)} = (\mathbf{Q}_n^{(1)})^*\mathbf{A}\mathbf{Q}_n^{(1)}$. Assume $\mathbf{A}^{(k-1)} = (\mathbf{Q}_n^{(k-1)})^*\mathbf{A}\mathbf{Q}_n^{(k-1)}$. Then from the "pure" QR algorithm and the induction hypothesis,

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

Let $\mathbf{Q}_n^{(k)} = \mathbf{Q}_n^{(k-1)}\mathbf{Q}^{(k)}$ and $\mathbf{R}_n^{(k)} = \mathbf{R}^{(k)}$ be the QR factorization of $\mathbf{A}\mathbf{Q}_n^{(k-1)}$ used in subspace iteration. By $\mathbf{R}_n^{(k)} = (\mathbf{Q}_n^{(k)})^*\mathbf{A}\mathbf{Q}_n^{(k-1)}$, $\mathbf{R}^{(k)} = \mathbf{R}_n^{(k)}$, and $\mathbf{Q}^{(k)} = (\mathbf{Q}_n^{(k-1)})^*\mathbf{Q}_n^{(k)}$, we have

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

This completes the proof. $\square$

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

3. QR algorithm with shifts

Algorithm 3: QR algorithm with shifts

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

for $k = 1, 2, 3, \ldots,$

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

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

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

end

Proposition 6

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

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 $(\mathbf{A} - \mu^{(k-1)}\mathbf{I})(\mathbf{A} - \mu^{(k-2)}\mathbf{I}) \cdots (\mathbf{A} - \mu^{(1)}\mathbf{I}) = \underline{\mathbf{Q}}^{(k-1)}\underline{\mathbf{R}}^{(k-1)}$. By Proposition 6, we have $\mathbf{A}^{(k-1)} = (\underline{\mathbf{Q}}^{(k-1)})^*\mathbf{A}\underline{\mathbf{Q}}^{(k-1)}$. Then

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

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 the matrix $\mathbf{A}$ using the starting vector $\mathbf{e}_1$ and the shifts $\mu^{(j)}$, $j=1:k$.

- Connection with shifted inverse iteration: By

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

  the last column of $\underline{\mathbf{Q}}^{(k)}$ is the result of applying k steps of shifted inverse iteration on the matrix $\mathbf{A}^*$ using the starting vector $\mathbf{e}_m$ and the shifts $\overline{\mu^{(j)}}$, $j=1:k$.

  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 an eigenvector of $\mathbf{A}^*$.

- Connection with Rayleigh quotient iteration: Choose

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

as the shifts. Then $\overline{\mu^{(k+1)}}$ and $\underline{\mathbf{Q}}^{(k)} \mathbf{e}_m$ are identical to those computed by the Rayleigh quotient iteration on $\mathbf{A}^*$ starting with $\mathbf{e}_m$. Assume the algorithm converges. Then $\underline{\mathbf{Q}}^{(k)} \mathbf{e}_m$ converges quadratically or cubically to an eigenvector of $\mathbf{A}^*$.

- *Rayleigh quotient shift* $\mu^{(k+1)} = \mathbf{A}_{mm}^{(k)}$: In the QR algorithm, we have

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

which means that 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!

- Other issues: *Wilkinson shift ...*

4. Upper Hessenberg structure in QR algorithm

Proposition 8

Upper Hessenberg structure 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 structure is preserved by QR *algorithm if real shifts are used.*

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

For simplicity, in subsections 4.1 – 4.3, we only consider the real case.

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 (Implicit Q theorem)

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 $\mathbf{Q}$.

Remark 12

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. See subsections 4.2 – 4.3.

Proof of 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 both 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 ith column of $\mathbf{X}$. Let $\mathbf{W} := \mathbf{V}^\top \mathbf{Q}$. 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

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

Thus,

$$h_{i+1,i}(\mathbf{W})_{i+1} = \mathbf{G}(\mathbf{W})_i - \sum\nolimits_{j=1}^{i} h_{ji}(\mathbf{W})_j.$$

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 and

$$\mathbf{W} = \mathrm{diag}\{1, \pm 1, \cdots, \pm 1\},$$

which implies

$$\mathbf{V}\mathrm{diag}\{1, \pm 1, \cdots, \pm 1\} = \mathbf{Q}. \quad \square$$

4.2. Implicit single shift QR algorithm ($\mu^{(k)} \in \mathbb{R}$)

- 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 (assume that $\mathbf{H}^{(k)}$ is unreduced), 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 $\mathbf{Q}^{(k)}$ such that $\mathbf{Q}^{(k)}$ is orthogonal and $(\mathbf{Q}^{(k)})^\top \mathbf{H}^{(k-1)} \mathbf{Q}^{(k)}$ 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 $\mathbf{Q}^{(k)}\mathbf{R}^{(k)} = \mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I}$ to

$$(\mathbf{Q}^{(k)}\mathbf{S}^{(k)})(\mathbf{S}^{(k)}\mathbf{R}^{(k)}) = \mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I},$$

  where $\mathbf{S}^{(k)} = \mathrm{diag}\{1, \pm 1, \cdots, \pm 1\}$.

- To see how to use the implicit Q theorem, we use a 5×5 example.

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

   Here c_1 and s_1 are unknown, and $\mathbf{H} = \mathbf{H}^{(k-1)}$.

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 $\mathbf{Q}^\top \mathbf{H}^{(k-1)} \mathbf{Q} = \mathbf{H}_4$ is upper Hessenberg, where

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

The first column of $\mathbf{Q}$ is $\begin{bmatrix} c_1 & s_1 & 0 & \cdots & 0 \end{bmatrix}^\top$, 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 $\mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I}$. Then we have $\mathbf{Q} = \mathbf{Q}^{(k)}\mathrm{diag}\{1, \pm 1, \cdots, \pm 1\}$, which means $\mathbf{Q}$ is the Q-factor of a QR factorization of $\mathbf{H}^{(k-1)} - \mu^{(k)}\mathbf{I}$.

4.3. Implicit double shift QR algorithm ($\mu^{(k)} \in \mathbb{C}$)

- 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 13

Assume $\mathbf{H}^{(0)} = \mathbf{H}$ *is real. 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

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

Note that

$$\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}\mathbf{R}^{(k)}\mathbf{R}^{(k-1/2)} = \mathbf{M}$$

is a QR factorization of the real matrix $\mathbf{M}$. Therefore, $\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}$ and $\mathbf{R}^{(k)}\mathbf{R}^{(k-1/2)}$ 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

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

whose sparsity pattern is $\begin{bmatrix}\times & \times & \times & 0 & \cdots & 0\end{bmatrix}^\top$. Obviously, the first column of $\mathbf{Q}^{(k-1/2)}\mathbf{Q}^{(k)}$ is easy to compute since $\mathbf{H}^{(k-1)}$ is upper Hessenberg. $\square$

The implicit Q theorem and the last lemma can be used to compute $\mathbf{H}^{(k)}$ from $\mathbf{H}^{(k-1)}$.

- We provide a 6×6 example. Let $\mathbf{H} = \mathbf{H}^{(k-1)}$.

1. Choose an orthogonal matrix

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

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

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

so

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

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

$$\mathbf{Q}_2^\top = \begin{bmatrix} 1 & & & & & \\ & \times & \times & \times & & \\ & \times & \times & \times & & \\ & \times & \times & \times & & \\ & & & & 1 & \\ & & & & & 1 \end{bmatrix}, \quad \mathbf{Q}_2^\top \mathbf{H}_1 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & + & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix},$$

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

3. Choose a Householder reflector $\mathbf{Q}_3^\top$, which affects only rows 3,4, and 5 of $\mathbf{H}_2$, 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):

$$\mathbf{Q}_3^\top = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & \times & \times & \times & \\ & & \times & \times & \times & \\ & & \times & \times & \times & \\ & & & & & 1 \end{bmatrix}, \quad \mathbf{Q}_3^\top \mathbf{H}_2 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & + & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix},$$

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

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

$$\mathbf{Q}_4^\top = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & \times & \times & \times \\ & & & \times & \times & \times \\ & & & \times & \times & \times \end{bmatrix}, \quad \mathbf{Q}_4^\top \mathbf{H}_3 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & + & \times & \times \end{bmatrix},$$

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

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 $\mathbf{Q}^\top \mathbf{H}^{(k-1)} \mathbf{Q} = \mathbf{H}_5$ is upper Hessenberg, where

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

4.4. Two phases of QR algorithm

- First phase: reduce to an upper Hessenberg matrix

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

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

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

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

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

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

5. Further reading

- J. L. Aurentz, T. Mach, L. Robol, R. Vandebril, and D. S. Watkins
  Core-Chasing Algorithms for the Eigenvalue Problem
  Society for Industrial and Applied Mathematics (SIAM), 2018

- A. Casulli and L. Robol
  Rank-structured QR for Chebyshev rootfinding
  SIAM J. Matrix Anal. Appl., 42, 1148–1171, 2021.

- D. S. Watkins
  Understanding the QR algorithm
  SIAM Review, 24, 427–440, 1982.
  The QR algorithm revisited
  SIAM Review, 50, 133–145, 2008.