

Lecture 9: QR algorithm



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1. Simultaneous iteration (SI)

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

Algorithm 1: Simultaneous iteration

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

- Here is an informal analysis of this method. Assume $\mathbf{A} = \mathbf{S}\mathbf{\Lambda}\mathbf{S}^{-1}$ 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

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

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 $\text{span}\{\mathbf{S}_n\}$:

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

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 $\mathbf{A} = \mathbf{S}\mathbf{\Lambda}\mathbf{S}^{-1}$ 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 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. QR algorithm without shifts

Algorithm 2: “Pure” QR algorithm

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

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

Algorithm 3: QR algorithm with shifts

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

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

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

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

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

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

- 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 5×5 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 6×6 example. Assume \mathbf{H} is upper Hessenberg and the shifts are μ 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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