QR Algorithm for Dense Eigenvalue Problems

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Outline

QR Algorithm

Theorem (Schur Theorem)

There exists a unitary matrix U such that

$$AU = UR,$$

where R is upper triangular.

Iteration method (from Vojerodin)

$$\begin{array}{l} \text{Set } U_0 = I, \\ \text{For } i = 0, 1, 2, \cdots \\ \qquad AU_i = U_{i+1}R_{i+1}, \quad \text{(an QR factorization of } AU_i\text{.)} \\ \text{End} \end{array} \tag{1}$$

If U_i converges to U, then for $i \to \infty$

$$R_{i+1} = U_{i+1}^* A U_i \to U^* A U.$$

We now define

$$Q_i = U_{i-1}^* U_i, \; A_{i+1} = U_i^* A U_i. \tag{2}$$

Then from (1) we have

$$A_i = U_{i-1}^* A U_{i-1} = U_{i-1}^* U_i R_i = Q_i R_i.$$

On the other hand from (1) substituting i by $i-1$ we get

$$R_i U_{i-1}^* = U_i^* A$$

and thus

$$R_i Q_i = R_i U_{i-1}^* U_i = U_i^* A U_i = A_{i+1}.$$

So (1) for $U_0 = I$ and $A_1 = A$ is equivalent to:

QR Algorithm

For $i = 1, 2, 3, \cdots$

$$A_i = Q_i R_i \quad \text{(QR factorization of } A_i\text{)}, \tag{3}$$

$$A_{i+1} = R_i Q_i. \tag{4}$$

End

Equations (3)-(4) describe the basic form of QR algorithm.

Lemma

Let

$$P_i = Q_1 Q_2 \cdots Q_i, \quad S_i = R_i R_{i-1} \cdots R_1. \tag{5}$$

Then hold

$$A_{i+1} = P_i^* A P_i = S_i A S_i^{-1}, \quad i = 1, 2, \cdots \tag{6}$$

$$A^i = P_i S_i \quad i = 1, 2, \cdots . \tag{7}$$

Proof: (6) is evident. (7) can be proved by induction. For $i = 1, A_1 = Q_1 R_1,$ Suppose (7) holds for i. Then

$$\begin{aligned} A^{i+1} &= AP_iS_i = P_iA_{i+1}S_i \qquad \text{(from (6))} \\ &= P_iQ_{i+1}R_{i+1}S_i = P_{i+1}S_{i+1}. \end{aligned}$$

Theorem

Let $A \in \mathbb{C}^{n\times n}$ with eigenvalues λ_i under the following assumptions:

(a)
$$|\lambda_1| > |\lambda_2| > \cdots |\lambda_n| > 0; \tag{8}$$

(b) *The factorization*
$$A = X\Lambda X^{-1} \tag{9}$$
with $X^{-1} = Y$ and $\Lambda =$ diag$(\lambda_1, \cdots, \lambda_n)$ holds. Here Y has an LR factorization.

Then QR algorithm converges. Furthermore

(a) $\lim_{i\to\infty} a_{jk}^{(i)} = 0$, *for $j > k$, where $A_i = (a_{jk}^{(i)})$;*

(b) $\lim_{i\to\infty} a_{kk}^{(i)} = \lambda_k$, *for $k = 1, \cdots, n$.*

Proof: Let $X = QR$ be the QR factorization of X with $r_{ii} > 0$ and $Y = LU$ be the LR factorization of Y with $\ell_{ii} = 1$. Since $A = X\Lambda X^{-1} = QR\Lambda R^{-1}Q^*$, we have

$$Q^*AQ = R\Lambda R^{-1} \tag{10}$$

is an upper-triangular matrix with diagonal elements λ_i ordered in absolute value as in (8). Now

$$A^s = X\Lambda^s X^{-1} = QR\Lambda^s LU = QR\Lambda^s L\Lambda^{-s}\Lambda^s U$$

and since

$$(\Lambda^s L\Lambda^{-s})_{ik} = \ell_{ik}\left(\frac{\lambda_i}{\lambda_k}\right)^s = \begin{cases} 0, & i < k, \\ 1, & i = k, \\ \to 0, & i > k \text{ as } s \to \infty, \end{cases}$$

where $\Lambda^s L\Lambda^{-s} = I + E_s$ with $\lim_{s\to\infty} E_s = 0$. Therefore

$$A^s = QR(I+E_s)\Lambda^s U = Q(I+RE_sR^{-1})R\Lambda^s U = Q(I+F_s)R\Lambda^s U$$

with $\lim_{s\to\infty} F_s = 0$. From the conclusion of QR factorization the matrices Q and R ($r_{ii} > 0$) depend continuously on A ($A = QR$). But $I = I \cdot I$ is the QR factorization of I, therefore it holds for the QR factorization:

$$I + F_s = \tilde{Q}_s \tilde{R}_s.$$

Thus for $F_s \to 0$, we have $\lim_{s\to\infty} \tilde{Q}_s = I$ and $\lim_{s\to\infty} \tilde{R}_s = I$. From (7) we have

$$A^s = (Q\tilde{Q}_s)(\tilde{R}_s R\Lambda^s U) = P_s R_s.$$

So from the "uniqueness" of QR factorization there exists a unitary diagonal matrix D_s with

$$P_s D_s = Q\tilde{Q}_s \to Q.$$

Thus from (6) we have

$$D_i^* A_{i+1} D_i = D_i^* P_i^* A P_i D_i \to Q^* A Q = R \Lambda R^{-1}. \qquad (11)$$

The assertions (a) and (b) are proved. $\square$

Remark

Assumption (9) *is not essential for convergence of the* QR *algorithm. If the assumption is not satisfied, the* QR *algorithm still converges, only the eigenvalues on the diagonal no longer necessary appear ordered in absolute values, i.e.* (b) *is replaced by* (b') $\lim_{i\to\infty} a_{kk}^{(i)} = \lambda_{\pi(k)}$, $k = 1, 2 \cdots, n$, *where* π *is a permutation of* $\{1, 2, \cdots, n\}$. *(See Wilkinson pp.519)*

Let A be diagonalizable and the eigenvalues λ_i satisfy

$$|\lambda_1| = \cdots = |\lambda_{\nu_1}| > |\lambda_{\nu_1+1}| = \cdots = |\lambda_{\nu_2}| > \cdots = |\lambda_{\nu s}| \qquad (12)$$

with $\nu_s = n$. We define a block partition of $n \times n$ matrix B in s^2 blocks $B_{k\ell}$ for $k, \ell = 1, 2, \cdots, s$

$$B = [B_{k\ell}]_{k,\ell=1}^{s}.$$

Theorem (Wilkinson)

Let A be diagonalizable and satisfy (12) *and* (9)*. Then it holds for the blocks $A_{jk}^{(i)}$ of A_i that*

(a) $\lim_{i\to\infty} A_{jk}^{(i)} = 0, \quad j > k$;

(b) *The eigenvalues of $A_{kk}^{(i)}$ converges to the eigenvalues $\lambda_{\nu_{k-1}+1}, \cdots, \lambda_{\nu_k}$.*

Special case: If A is real and all the eigenvalues have different absolute value except conjugate eigenvalues. Then

$$A_i \to \begin{bmatrix} \times & \times & + & + & + & + & + \\ \times & \times & + & + & + & + & + \\ & & \times & \times & + & + & + \\ & & \times & \times & + & + & + \\ & & & & \times & + & + \\ & & & & & \times & \times \\ 0 & & & & & \times & \times \end{bmatrix}.$$

Theorem

Let A be an upper Hessenberg matrix. Then the matrices Q_i and A_i in (3) *and* (4) *are also upper Hessenberg matrices.*

Proof: It is obvious from $A_{i+1} = R_i A_i R_i^{-1}$ and $Q_i = A_i R_i^{-1}$. $\square$

The Practical QR Algorithm

In the following paragraph we will develop an useful QR algorithm for real matrix A. We will concentrate on developing the iteration

$$
\begin{aligned}
&\text{Compute orthogonal } Q_0 \text{ such that} \\
&\qquad H_0 = Q_0^T A Q_0 \\
&\text{is upper Hessenberg.} \\
&\text{For } k = 1, 2, 3, \cdots \\
&\qquad \text{Compute QR factorization } H_k = Q_k R_k; \\
&\qquad \text{Set } H_{k+1} = R_k Q_k; \\
&\text{End}
\end{aligned}
\tag{13}
$$

Here $A \in \mathbb{R}^{n\times n}$, $Q_i \in \mathbb{R}^{n\times n}$ is orthogonal and $R_i \in \mathbb{R}^{n\times n}$ is upper triangular.

Theorem (Real Schur Decomposition)

If $A \in \mathbb{R}^{n\times n}$, then there exists an orthogonal $Q \in \mathbb{R}^{n\times n}$ such that

$$Q^T A Q = \begin{pmatrix} R_{11} & R_{12} & \cdots & R_{1m} \\ 0 & R_{21} & \cdots & R_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & R_{mm} \end{pmatrix} \tag{14}$$

where each R_{ii} is either 1×1 or 2×2 matrix having complex conjugate eigenvalues.

Proof: Let k be the number of complex conjugate pair in $\sigma(A)$. We prove the theorem by induction on k. The theorem holds if $k = 0$. Now suppose that $k \geq 1$. If $\lambda = \gamma + i\mu \in \sigma(A)$ and $\mu \neq 0$, then there exists vectors y and $z \in \mathbb{R}^n (z \neq 0)$ such that

$$A(y+iz) = (\gamma + i\mu)(y+iz) \Rightarrow A[y,z] = [y,z]\begin{bmatrix} \gamma & \mu \\ -\mu & \gamma \end{bmatrix}.$$

The assumption that $\mu \neq 0$ implies that y and z span a two dimensional, real invariant subspace for A. It then follows that

$$U^T A U = \left[\begin{array}{cc} T_{11} & T_{12} \\ 0 & T_{22} \end{array} \right] \text{ with } \sigma(T_{11}) = \{\lambda, \bar{\lambda}\}.$$

By induction, there exists an orthogonal $\tilde{U}$ so that $\tilde{U}^T T_{22} \tilde{U}$ has the require structure. The theorem follows by setting $Q = U diag(I_2, \tilde{U})$. $\square$

- Reduction to Hessenberg form

Take
$$A = \begin{pmatrix} \alpha_{11} & a_{12}^* \\ a_{21} & A_{22} \end{pmatrix}.$$
Let $\hat{H}_1$ be a Householder transformation such that
$$\hat{H}_1 a_{21} = v_1 e_1.$$
Set $H_1 = diag(1, \hat{H}_1)$. Then
$$H_1 A H_1 = \begin{pmatrix} \alpha_{11} & a_{12}^* \hat{H}_1 \\ \hat{H}_1 a_{21} & \hat{H}_1 A_{22} \hat{H}_1 \end{pmatrix} = \begin{pmatrix} \alpha_{11} & a_{12}^* \hat{H}_1 \\ v_1 e_1 & \hat{H}_1 A_{22} \hat{H}_1 \end{pmatrix}$$
For the general step, suppose $H_1, \cdots, H_{k-1}$ are Householder transformation such that
$$H_{k-1} \cdots H_1 A H_1 \cdots H_{k-1} = \begin{pmatrix} A_{11} & a_{1,k} & A_{1,k+1} \\ 0 & \alpha_{kk} & a_{k,k+1}^* \\ 0 & a_{k+1,k} & A_{k+1,k+1} \end{pmatrix},$$

where A_{11} is a Hessenberg matrix of order $k-1$. Let $\hat{H}_k$ be a Householder transformation such that

$$\hat{H}_k a_{k+1,k} = v_k e_1.$$

Set $H_k = diag(I_k, \hat{H}_k)$, then

$$H_k H_{k-1} \cdots H_1 A H_1 \cdots H_{k-1} H_k = \begin{pmatrix} A_{11} & a_{1,k} & A_{1,k+1}\hat{H}_k \\ 0 & \alpha_{kk} & a_{k,k+1}^* \hat{H}_k \\ 0 & v_k e_1 & \hat{H}_k A_{k+1,k+1} \hat{H}_k \end{pmatrix}.$$

Reduce a matrix to Hessenberg form by QR factorization.

$$\begin{pmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{pmatrix} \xrightarrow{Q_1 A Q_1^*} \begin{pmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \end{pmatrix}$$

$$\xrightarrow{Q_2 A Q_2^*} \begin{pmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & \times \end{pmatrix}$$

$$\xrightarrow{Q_3 A Q_3^*} \begin{pmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{pmatrix}$$: upper He

Algorithm (Householder Reduction to Hessenberg Form)

Given $A \in \mathbb{R}^{n \times n}$. *The following algorithm overwrites* A *with* $H = Q_0^T A Q_0$, *where* H *is upper Hessenberg and* $Q_0 = P_1 \cdots P_{n-2}$ *is a product of Householder matrices.*

For $k = 1, \cdots, n-2$,

Determine a Householder matrix $\bar{P}_k$ *of order* $n-k$ *such that*

$$\bar{P}_k \begin{bmatrix} a_{k+1,k} \\ \vdots \\ \vdots \\ a_{n,k} \end{bmatrix} = \begin{bmatrix} * \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Compute $A \equiv P_k^T A P_k$ *where* $P_k = diag(I_k, \bar{P}_k)$.

End;

This algorithm requires $\frac{5}{3}n^3$ flops. Q_0 can be stored in factored form below the subdiagonal A. If Q_0 is explicitly formed, an additional $\frac{2}{3}n^3$ flops are required.

Theorem (Implicit Q Theorem)

Suppose $Q = [q_1, \cdots, q_n]$ *and* $V = [v_1, \cdots, v_n]$ *are orthogonal matrices with* $Q^T AQ = H$ *and* $V^T AV = G$ *are upper Hessenberg. Let* k *denote the smallest positive integer for which* $h_{k+1,k} = 0$ *with the convention that* $k = n$*, if* H *is unreduced. If* $v_1 = q_1$*, then* $v_i = \pm q_i$ *and* $|h_{i,i-1}| = |g_{i,i-1}|$*, for* $i = 2, \cdots, k$*. Moreover if* $k < n$ *then* $g_{k+1,k} = 0$*.*

Proof: Define $W = V^T Q = [w_1, \cdots, w_n]$ orthogonal, and observe $GW = WH$. For $i = 2, \cdots k$, we have

$$h_{i,i-1} w_i = G w_{i-1} - \sum_{j=1}^{i-1} h_{j,i-1} w_j.$$

Since $w_1 = e_1$, it follows that $[w_1, \cdots, w_k]$ is upper triangular and thus $w_i = \pm e_i$ for $i = 2, \cdots, k$.

Since $w_i = V^T q_i$ and $h_{i,i-1} = w_i^T G w_{i-1}$, it follows that $v_i = \pm q_i$ and $|h_{i,i-1}| = |g_{i,i-1}|$ for $i = 2, \cdots, k$. If $h_{k+1,k} = 0$, then ignoring signs we have

$$\begin{aligned} g_{k+1,k} &= e_{k+1}^T G e_k = e_{k+1}^T G W e_k = (e_{k+1}^T W)(H e_k) \\ &= e_{k+1}^T \sum_{i=1}^{k} h_{ik} W e_i = \sum_{i=1}^{k} h_{ik} e_{k+1}^T e_i = 0. \end{aligned}$$

$\square$

Remark

The gist of the implicit Q theorem is that if $Q^T A Q = H$ and $Z^T A Z = G$ are each unreduced upper Hessenberg matrices and Q and Z have the same first column, then G and H are "essentially equal" in the sense that $G = D^{-1} H D$, where $D = diag(\pm 1, \cdots, \pm 1)$.

Single-shift QR-iteration

Now we will investigate how the convergence (13) can be accelerated by incorporating "shifts". Let $\mu \in \mathbb{R}$ and consider the iteration

Algorithm (Single-shift QR-iteration)

1: *Give orthogonal Q_0 such that $H = Q_0^T A Q_0$ is upper Hessenberg.*
2: ***for** $k = 1, 2, \cdots$ **do***
3: $\quad H - \mu I = QR$, $\quad$ (*QR factorization*)
4: $\quad H = RQ + \mu I$,
5: ***end for***

- The scale μ is refereed to a shift.
- Each matrix H in Step 4 of Algorithm 2 is similar to A, since $RQ + \mu I = Q^T(QR + \mu I)Q = Q^T H Q$.

- If we order the eigenvalues λ_i of A so that $|\lambda_1 - \mu| \geq \cdots \geq |\lambda_n - \mu|$, then Theorem 6 says that the p-th subdiagonal entry in H converges to zero with rate $|\frac{\lambda_{p+1}-\mu}{\lambda_p-\mu}|^k$.
- Of course if $\lambda_p = \lambda_{p+1}$ then there is no convergence at all.
- But if μ is much closer to λ_n than to the other eigenvalues, the convergence is required.

Theorem

Let μ be an eigenvalues of an $n \times n$ unreduced Hessenberg matrix H. If $\bar{H} = RQ + \mu I$, where $(H - \mu I) = QR$ is the QR decomposition of $H - \mu I$, then $\bar{h}_{n,n-1} = 0$ and $\bar{h}_{nn} = \mu$.

Proof: If H is unreduced, then so is the upper Hessenberg matrix $H - \mu I$. Since $Q^T(H - \mu I) = R$ is singular and since it can be shown that

$$|r_{ii}| \geq |h_{i+1,i}|, \quad i = 1, 2, \cdots, n-1, \tag{15}$$

it follows that $r_m = 0$. Consequently, the bottom row of $\bar{H}$ is equal to $(0, \cdots, 0, \ \mu)$. □

Algorithm

1: *Give orthogonal* Q_0 *such that* $H = Q_0^T A Q_0$ *is upper Hessenberg.*
2: ***for*** $k = 1, 2, \cdots$ ***do***
3: $\quad H_i - h_{nn}I = Q_i R_i$, (*QR factorization*)
4: $\quad H_{i+1} := R_i Q_i + h_{nn} I$,
5: ***end for***

Quadratic convergence

If the $(n, n-1)$ entry converges to zero and let

$$H = \begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & \varepsilon & h_{nn} \end{bmatrix},$$

then one step of the single shift QR algorithm leads:

$$QR = H - h_{nn}I, \quad \bar{H} = RQ + h_{nn}I.$$

After $n-2$ steps in the reduction of $H - h_{nn}I$ to upper triangular we have

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & & \times & \times & \times \\ & & & a & b \\ & & & \varepsilon & 0 \end{bmatrix}.$$

And we have $(n, n-1)$ entry in $\bar{H}$ is given by

$$\bar{h}_{n,n-1} = \frac{\varepsilon^2 b}{\varepsilon^2 + a^2}\,.$$

If $\varepsilon \ll a$, then it is clear that $(n, n-1)$ entry has order ε^2.

Double Shift QR iteration

- If at some stage the eigenvalues α_1 and α_2 of

$$\begin{bmatrix} h_{n-1,n-1} & h_{n-1,n} \\ h_{n,n-1} & h_{nn} \end{bmatrix}$$

are complex, for then h_{nn} would tend to be a poor approximate eigenvalue.

- A way around this difficulty is to perform two single shift QR steps in succession, using α_1 and α_2 as shifts:

$$\begin{aligned} H - \alpha_1 I &= Q_1 R_1, \\ H_1 &= R_1 Q_1 + \alpha_1 I, \\ H_1 - \alpha_2 I &= Q_2 R_2, \\ H_2 &= R_2 Q_2 + \alpha_2 I. \end{aligned} \tag{16}$$

We then have

$$\begin{aligned}
& (Q_1Q_2)(R_2R_1) \\
= \;& Q_1(H_1 - \alpha_2 I)R_1 = Q_1(R_1Q_1 + \alpha_1 I - \alpha_2 I)R_1 \\
= \;& (Q_1R_1)(Q_1R_1) + \alpha_1(Q_1R_1) - \alpha_2(Q_1R_1) \\
= \;& (H - \alpha_1 I)(H - \alpha_1 I) + \alpha_1(H - \alpha_1 I) - \alpha_2(H - \alpha_1 I) \\
= \;& (H - \alpha_1 I)(H - \alpha_2 I) = M, \qquad (17)
\end{aligned}$$

where

$$M = (H - \alpha_1 I)(H - \alpha_2 I). \qquad (18)$$

Note that M is a real matrix, since

$$M = H^2 - sH + tI,$$

where

$$\begin{aligned}
s &= \alpha_1 + \alpha_2 = h_{n-1,n-1} + h_{nn} \in \mathbb{R}, \\
t &= \alpha_1\alpha_2 = h_{n-1,n-1}h_{nn} - h_{n-1,n}h_{n,n-1} \in \mathbb{R}.
\end{aligned}$$

- Thus, (17) is the QR factorization of a real matrix, and we may choose Q_1 and Q_2 so that $Z = Q_1Q_2$ is real orthogonal.
- It follows that

$$H_2 = Q_2^* H_1 Q_2 = Q_2^*(Q_1^* H Q_1)Q_2 = (Q_1Q_2)^* H (Q_1Q_2) = Z^T H Z$$

is real.
- A real H_2 could be guaranteed if we
  (a) explicitly form the real matrix $M = H^2 - sH + tI$;
  (b) compute the real QR decomposition $M = ZR$ and
  (c) set $H_2 = Z^T H Z$.
- But since (a) requires $O(n^3)$ flops, this is not a practical course.

In light of the Implicit Q theorem, however, it is possible to effect the transition from H to H_2 in $O(n^2)$ flops if we

(a$'$) compute Me_1, the first column of M;

(b$'$) determine Householder matrix P_0 such that

$$P_0(Me_1) = \alpha e_1, \quad (\alpha \neq 0);$$

(c$'$) compute Householder matrices $P_1, \cdots, P_{n-2}$ such that if $Z_1 = P_0 P_1 \cdots P_{n-2}$ the $Z_1^T H Z_1$ is upper Hessenberg and the first column of Z and Z_1 are the same. If $Z^T H Z$ and $Z_1^T H Z_1$ are both unreduced upper Hessenberg, then they are essentially equal.

Since

$$Me_1 = (x, y, z, 0, \cdots, 0)^T,$$

where

$$\begin{aligned} x &= h_{11}^2 + h_{12}h_{21} - sh_{11} + t, \\ y &= h_{21}(h_{11} + h_{22} - s), \\ z &= h_{21}h_{32}. \end{aligned}$$

So, a similarity transformation with P_0 only changes rows and columns 1, 2 and 3. Since $P_0^T H P_0$ has the form

$$\begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix},$$

it follows that

$$\begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix} \xrightarrow{P_1} \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}$$

$$\xrightarrow{P_2} \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \end{bmatrix} \xrightarrow{P_3} \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \end{bmatrix}$$

$$\xrightarrow{P_4} \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}.$$

- $P_k = \text{diag}(I_k, \bar{P}_k, I_{n-k-3})$, $\bar{P}_k$ is 3×3-Householder matrix. The applicability of Implicit Q-Theorem follows from that $P_k e_1 = e_1$, for $k = 1, \cdots, n-2$, and that P_0 and Z have the same first column. Hence $Z_1 e_1 = Z e_1$.
- Deflation:
  1. If the eigenvalues of $\begin{pmatrix} h_{n-1,n-1} & h_{n-1,n} \\ h_{n,n-1} & h_{n,n} \end{pmatrix}$ are complex and nondefective, then $h_{n-1,n-2}$ converges quadratically to zero.
  2. If the eigenvalues are real and nondefective, both the $h_{n-1,n-2}$ converge quadratically to zero. The subdiagonal elements other than $h_{n-1,n-2}$ and $h_{n,n-1}$ may show a slow convergent to zero.
  3. Deflate matrix to a middle size of matrix.
  4. Converge to a block upper triangular with order one or two diagonal blocks. $i, e.$ converge to real Schur form.

Algorithm (Francis QR step)

Set $m := n-1$;

$s := h_{mm} + h_{nn}, \quad t := h_{mm}h_{nn} - h_{mn}h_{nm}$;

$x := h_n^2 + h_{12}h_{21} - sh_{11} + t,\ y := h_{21}(h_{11} + h_{22} - s),\ z := h_{21}h_{32}$;

For $k = 0, \cdots, n-2$,

If $k < n-2$, *then*

Determine a Householder matrix $\bar{P}_k \in \mathbb{R}^{3\times 3}$ *such that*

$$\bar{P}_k \begin{bmatrix} x & y & z \end{bmatrix}^T = \begin{bmatrix} * & 0 & 0 \end{bmatrix}^T;$$

Set

$$H := P_k H P_k^T,\ P_k = \text{diag}\left(I_k, \bar{P}_k, I_{n-k-3}\right);$$

else determine a Householder matrix $\bar{P}_{n-2} \in \mathbb{R}^{2\times 2}$ *such that*

$$\bar{P}_{n-2} \begin{bmatrix} x & y \end{bmatrix}^T = \begin{bmatrix} * & 0 \end{bmatrix}^T;$$

Set

$$H := P_{n-2} H P_{n-2}^T,\ P_{n-2} = \text{diag}\left(I_{n-2}, \bar{P}_{n-2}\right);$$

End if

$x := h_{k+2,k+1}, \quad y := h_{k+3,k+1}$;

If $k < n-3$, *then* $z := h_{k+4,k+1}$;

End for;

Algorithm (QR Algorithm)

Using Algorithm 1 to compute the Hessenberg decomposition
$Q^TAQ = H$, where $Q = P_1 \cdots P_{n-2}$ and H is Hessenberg;
Repeat: Set to zero all subdiagonal elements that satisfy
$$|h_{i,i-1}| \leq \varepsilon\left(|h_{ii}| + |h_{i-1,i-1}|\right);$$
Find the largest non-negative q and the smallest non-negative p s.t.

$$H = \begin{array}{cc} \begin{bmatrix} H_{11} & H_{12} & H_{13} \\ 0 & H_{22} & H_{23} \\ 0 & 0 & H_{33} \end{bmatrix} & \begin{array}{c} p \\ n-p-q \\ q \end{array} \\ \begin{array}{ccc} p & n-p-q & q \end{array} & \end{array},$$

where H_{33} is upper quasi-triangular and H_{22} is unreduced.
If $q = n$, then upper triangularize all 2×2 diagonal blocks in H that have real eigenvalues, accumulate the orthogonal transformations if necessary, and quit.
Apply a Francis QR-step to H_{22}: $H_{22} := Z^T H_{22} Z$;
If Q and T are desired, then $Q := Q$ diag(I_p, Z, I_q);
Set $H_{12} := H_{12}Z$ and $H_{23} := Z^T H_{23}$;
Go To Repeat.