QR Algorithm for Eigenvalue Problems

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Outline

- Basic QR algorithm
- Reduction to Hessenberg and tridiagonal forms
- Hessenberg QR algorithm

Eigenvalues via characteristic polynomial

Let $A \in \mathbb{C}^{n\times n}$ and $p(x) := \det(xI - A)$ be the characteristic polynomial of A. Then $\lambda \in \mathbb{C}$ is an eigenvalue of $A \iff p(\lambda) = 0$. Thus eigenvalues of A can be computed by finding the roots of $p(x)$. To see the efficacy of this method, consider $A := \mathrm{diag}(1, 2, \ldots, 22)$.

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```
>> A = diag(1:22) ; % eigenvalues 1,2,...,22
>> p = charpoly(A); % coefficents of the poly p(x)
>> rt = roots(p); % roots of p(x)
>> rt(6:9) % displays four roots
ans =
17.564435730130054 + 0.661474607910510i
17.564435730130054 - 0.661474607910510i
15.388471193084563 + 0.581348923952655i
15.388471193084563 - 0.581348923952655i
```

These roots do not have even a single correct digit! Never compute roots of $\det(\lambda I - A)$ for computing eigenvalues of A.

Computation of eigenvalues and eigenvectors

The MATLAB coammand `[V, D] = eig(A)` computes eigenvalues and eigenvectors of A. The diagonal matrix D contains the computed eigenvalues and the columns of V are the computed eigenvectors of A such that

$$\|AV - VD\|_2/\|A\|_2 = \mathcal{O}(\mathbf{u}).$$

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Then, when A is diagonalizable, setting $E := RV^{-1}$, we have

$$R = VD - AV \Longrightarrow (A + E)V = VD \text{ and } \|E\|_2/\|A\|_2 \leq \|R\|_2\|V^{-1}\|_2/\|A\|_2.$$

Hence computed eigenvalues and eigenvectors of A are exact eigenvalues and eigenvectors of $A + E$ and $\|E\|_2/\|A\|_2 = \mathcal{O}(\mathbf{u})\|V^{-1}\|_2$.

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Hence computed eigenvalues and eigenvectors of A are exact eigenvalues and eigenvectors of $A + E$ and $\|E\|_2/\|A\|_2 = \mathcal{O}(\mathbf{u})\|V^{-1}\|_2$. Note that the backward error $\|E\|_2/\|A\|_2 = \mathcal{O}(\mathbf{u})$ when $\|V^{-1}\|_2 = \mathcal{O}(1)$ and in such a case the algorithm is backward stable.

Example

The command `A = gallery(3)` generates a 3×3 test matrix in MATLAB with known eigenvalues and is given by

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$$V = \begin{bmatrix} 0.3162 & -0.4041 & -0.1391 \\ -0.9487 & 0.9091 & 0.9740 \\ -0.0000 & 0.1010 & -0.1789 \end{bmatrix}, \; D = \begin{bmatrix} 1.0000 & 0 & 0 \\ 0 & 2.0000 & 0 \\ 0 & 0 & 3.0000 \end{bmatrix}.$$

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$$\|R\|_2 \|V^{-1}\|_2 / \|A\|_2 = 1.4765 \times 10^{-13} \simeq \|E\|_2/\|A\|_2. \blacksquare$$

Perturbation of Jordan block

Let $\epsilon \geq 0$. Consider an $n \times n$ Jordan block A and its perturbation $A(\epsilon)$ given by

$$A := \begin{bmatrix} 2 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & 2 \end{bmatrix} \in \mathbb{C}^{n\times n} \quad \text{and} \quad A(\epsilon) := \begin{bmatrix} 2 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ \epsilon & & & 2 \end{bmatrix} \in \mathbb{C}^{n\times n}.$$

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Then $p_\epsilon(x) := \det(xI - A(\epsilon)) = (x-2)^n + \epsilon$ shows that $\lambda := 2$ is the eigenvalue of $A(0)$ of multiplicity n and $A(\epsilon)$ has n distinct eigenvalues

$$\lambda_j(\epsilon) := 2 + \epsilon^{1/n}\, e^{(2j-1)\pi i/n}, \;\; j = 1:n, \;\; \text{when } \epsilon > 0.$$

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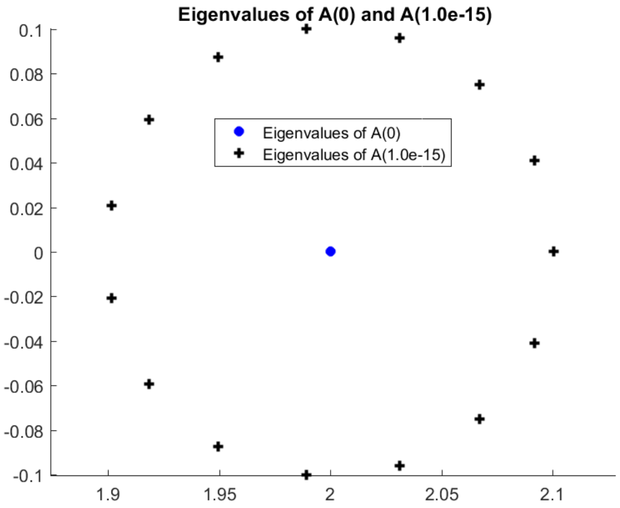
Perturbation of Jordan block



Computation of Schur triangular form

Let $A \in \mathbb{C}^{n\times n}$. Then by Schur theorem there is a unitary matrix $U \in \mathbb{C}^{n\times n}$ such that U^*AU is upper triangular, that is,

$$U^*AU = \begin{bmatrix} t_{11} & t_{12} & \cdots & t_{1n} \\ & t_{22} & \cdots & t_{2n} \\ & & \ddots & \vdots \\ & & & t_{nn} \end{bmatrix} =: T.$$

The diagonal entries of T are the eigenvalues of A and the eigenvectors of A can be obtained from those of T. Indeed, if (λ, v) is an eigenpair of T then (λ, Uv) is an eigenpair of A.

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The eigenvectors of T can be computed easily by solving the system $(T - \lambda I)v = 0$. Thus the problem of solving the eigenvalue problem $Av = \lambda v$ boils down to computing Schur decomposition of A.

Basic QR algorithm

The QR algorithm constructs a sequence of unitary matrices (Q_m) and performs the similarity transformations $A_m := Q_m^* A_{m-1} Q_m$ with $A_0 = A$ such that $A_m \longrightarrow T$ and $\prod_{j=1}^{m} Q_j \longrightarrow Q$ as $m \to \infty$, where T is upper triangular.

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Algorithm. (Basic QR algorithm)
Input: An $n \times n$ matrix A
Output: Upper triangular matrix $T = Q^* AQ$

$A_0 := A$
for $m = 1, 2, \ldots$
    $A_{m-1} = Q_m R_m$ % (QR factorization of A_{m-1})
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Note that $A_m = R_m Q_m = Q_m^* Q_m R_m Q_m = Q_m^* A_{m-1} Q_m$. The cost of computing QR factorization $A_{m-1} = Q_m R_m$ is $4n^3/3$ flops and the cost of computing $A_m = R_m Q_m$ is $2n^3$ flops. Hence the cost of a QR-step is $10n^3/3$ flops. (MATLAB demo)

Example

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$$A = \begin{bmatrix} -149 & -50 & -154 \\ 537 & 180 & 546 \\ -27 & -9 & -25 \end{bmatrix}.$$

The exact eigenvalues of A are $1, 2, 3$. We now apply basic QR algorithm to A and monitor converegence of strict lower triangular part of A_m to zero as the iteration progresses. We have the following results.

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>> A_{60} =

```
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-1.8461e-11 2.0000e+00 -1.5148e+02
3.0256e-20 -1.6389e-09 1.0000e+00
```

>> A_{85} =

```
3.0000e+00 -2.4098e+00 8.0360e+02
-7.3109e-16 2.0000e+00 1.5148e+02
-3.5709e-32 4.8844e-17 1.0000e+00
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Strategy

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Schematically

$$\underbrace{\begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{bmatrix}}_{\text{General matrix}} \to \underbrace{\begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times \end{bmatrix}}_{\text{Upper Hessenberg}} \to \underbrace{\begin{bmatrix} \times & \times & \times & \times \\ & \times & \times & \times \\ & & \times & \times \\ & & & \times \end{bmatrix}}_{\text{Upper triangular}}$$

Hessenberg/tridiagonal form

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The reduction of a matrix to Hessenberg/tridiagonal form is a finite process. A finite number of unitary similarity transformations can be used to reduce a matrix to Hessenberg/tridiagonal form.

Reduction to Hessenberg form

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Householder reflectors can be used to reduce A to Hessenberg/tridiagonal form in $n-2$ steps. Construct a Householder reflector Q_1 that does not alter the first row of A and creates zeros in the first column below the (2, 1) entry. Then perform the similarity transformation $Q_1^* A Q_1$. Schematically, we have

$$\underbrace{\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \end{bmatrix}}_{A} \rightarrow \underbrace{\begin{bmatrix} \times & \times & \times & \times & \times \\ * & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}}_{Q_1^* A} \rightarrow \underbrace{\begin{bmatrix} \times & * & * & * & * \\ \times & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \\ & * & * & * & * \end{bmatrix}}_{Q_1^* A Q_1}.$$

We now repeat this process in the second column and construct a reflector Q_2 that leaves the first 2 rows unchanged and creates zeros in second column below the (3, 2) entry.

Reduction to Hessenberg form

Schematically,

$$\underbrace{\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix}}_{Q_1^* A Q_1} \rightarrow \underbrace{\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix}}_{Q_2^* Q_1^* A Q_1} \rightarrow \underbrace{\begin{bmatrix} \times & \times & * & * & * \\ \times & \times & * & * & * \\ & \times & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix}}_{Q_2^* Q_1^* A Q_1 Q_2}.$$

Reduction to Hessenberg form

Schematically,

$$\underbrace{\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix}}_{Q_1^* A Q_1} \rightarrow \underbrace{\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix}}_{Q_2^* Q_1^* A Q_1} \rightarrow \underbrace{\begin{bmatrix} \times & \times & * & * & * \\ \times & \times & * & * & * \\ & \times & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix}}_{Q_2^* Q_1^* A Q_1 Q_2}.$$

Again repeating the idea in the third column, we construct a reflector Q_3 that leaves the first 3 rows unchanged and creates zeros in third column below the $(4, 3)$ entry, and so on.

Reduction to Hessenberg form

Schematically,

$$\underbrace{\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix}}_{Q_1^* A Q_1} \rightarrow \underbrace{\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ & * & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix}}_{Q_2^* Q_1^* A Q_1} \rightarrow \underbrace{\begin{bmatrix} \times & \times & * & * & * \\ \times & \times & * & * & * \\ & \times & * & * & * \\ & & * & * & * \\ & & * & * & * \end{bmatrix}}_{Q_2^* Q_1^* A Q_1 Q_2}.$$

Again repeating the idea in the third column, we construct a reflector Q_3 that leaves the first 3 rows unchanged and creates zeros in third column below the (4, 3) entry, and so on. Repeating this process $n-2$ times, the matrix A is reduced to Hessenberg form

$$H = \underbrace{Q_{n-2}^* \cdots Q_2^* Q_1^*}_{Q^*} A \underbrace{Q_1 Q_2 \cdots Q_{n-2}}_{Q} = Q^* A Q.$$

Householder reduction to Hessenberg form

Step-1: Partition A as

$$A = \begin{bmatrix} a_{11} & c^\top \\ b & \widehat{A} \end{bmatrix}.$$

Choose a reflector $\widehat{Q}_1 \in \mathbb{C}^{(n-1)\times(n-1)}$ such that $\widehat{Q}_1^* b = [-\sigma_1, 0, \ldots, 0]^\top$. Set $Q_1 := \mathrm{diag}(1, \widehat{Q}_1)$. Then

$$Q_1^* A Q_1 = \left[\begin{array}{c|c} a_{11} & c^\top \widehat{Q}_1 \\ \hline -\sigma_1 & \\ 0 & \\ \vdots & \widehat{Q}_1^* \widehat{A} \widehat{Q}_1 \\ 0 & \end{array}\right] = \left[\begin{array}{c|ccc} a_{11} & * & \cdots & * \\ \hline -\sigma_1 & & & \\ 0 & & & \\ \vdots & & \widehat{A}_1 & \\ 0 & & & \end{array}\right].$$

Note that because of the form of Q_1, the zeros in the first column of $Q_1^* A$ remain unchanged when $Q_1^* A$ is transformed to $Q_1^* A Q_1$.

Householder reduction to Hessenberg form

Step-2: The second step creates zeros in the first column of $\widehat{A}_1$. Thus we choose a reflector $\widehat{Q}_2 \in \mathbb{C}^{(n-2)\times(n-2)}$ in just the same way as in the first step, except that A is replaced by $\widehat{A}_1$. Then

$$\underbrace{\left[\begin{array}{cc|ccc} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \hline 0 & 0 & & & \\ \vdots & \vdots & & \widehat{Q}_2 & \\ 0 & 0 & & & \end{array}\right]}_{Q_2} \text{ and } \underbrace{\left[\begin{array}{c|c|ccc} a_{11} & * & * & \cdots & * \\ \hline -\sigma_1 & * & * & \cdots & * \\ \hline 0 & -\sigma_2 & & & \\ \vdots & \vdots & & \widehat{Q}_2^* \widehat{A}_2 \widehat{Q}_2 & \\ 0 & 0 & & & \end{array}\right]}_{Q_2^* Q_1^* A Q_1 Q_2}.$$

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The third step creates zeros in the third column, and so on. After $n-2$ steps, we have the unitary matrix $Q := Q_1 Q_2 \cdots Q_{n-2}$ and the Hessenberg matrix

$$H = \underbrace{Q_{n-2}^* \cdots Q_2^* Q_1^*}_{Q^*} A \underbrace{Q_1 Q_2 \cdots Q_{n-2}}_{Q} = Q^* A Q.$$

Algorithm for reduction to Hessenberg form

Algorithm: Householder reduction to Hessenberg form
Input: An $n \times n$ matrix $\mathtt{A}$
Output: Hessenberg matix $\mathtt{A} \leftarrow \mathtt{Q}^*\mathtt{AQ}$

$$
\begin{array}{l}
\mathtt{for}\ \mathtt{k} = 1\colon \mathtt{n}-2 \\
\quad \mathtt{x} := \mathtt{A}(\mathtt{k}+1\colon\mathtt{n}, \mathtt{k}) \qquad \text{\% choose } k\text{-th column of } A \\
\quad \mathtt{u} := \mathrm{sign}(\mathtt{x}_1)\|\mathtt{x}\|_2\mathtt{e}_1 + \mathtt{x} \qquad \text{\% Householder vector for reflector } Q_k \\
\quad \mathtt{u} := \mathtt{u}/\|\mathtt{u}\|_2 \\
\quad \mathtt{A}(\mathtt{k}+1\colon\mathtt{n}, \mathtt{k}\colon\mathtt{n}) := \mathtt{A}(\mathtt{k}+1\colon\mathtt{n}, \mathtt{k}\colon\mathtt{n}) - 2\mathtt{u}(\mathtt{u}^*\mathtt{A}(\mathtt{k}+1\colon\mathtt{n}, \mathtt{k}\colon\mathtt{n})) \\
\quad \mathtt{A}(1\colon\mathtt{n}, \mathtt{k}+1\colon\mathtt{n}) := \mathtt{A}(1\colon\mathtt{n}, \mathtt{k}+1\colon\mathtt{n}) - 2(\mathtt{A}(1\colon\mathtt{n}, \mathtt{k}+1\colon\mathtt{n})\mathtt{u})\mathtt{u}^* \\
\mathtt{end}
\end{array}
$$

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$\mathtt{for}\ \mathtt{k} = 1{:}\,\mathtt{n} - 2$

$\quad \mathtt{x} := \mathtt{A}(\mathtt{k}+1{:}\,\mathtt{n}, \mathtt{k})$ % choose k-th column of A

$\quad \mathtt{u} := \mathrm{sign}(\mathtt{x}_1)\|\mathtt{x}\|_2\mathtt{e}_1 + \mathtt{x}$ % Householder vector for reflector Q_k

$\quad \mathtt{u} := \mathtt{u}/\|\mathtt{u}\|_2$

$\quad \mathtt{A}(\mathtt{k}+1{:}\,\mathtt{n}, \mathtt{k}{:}\,\mathtt{n}) := \mathtt{A}(\mathtt{k}+1{:}\,\mathtt{n}, \mathtt{k}{:}\,\mathtt{n}) - 2\mathtt{u}(\mathtt{u}^*\mathtt{A}(\mathtt{k}+1{:}\,\mathtt{n}, \mathtt{k}{:}\,\mathtt{n}))$

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$\mathtt{end}$

The above algorithm can be modified to store the Householder vectors in each step, which can be used to assemble the unitary matrix Q.

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for k = 1:n − 2
    x: = A(k + 1:n, k)            % choose k-th column of A
    u: = sign(x_1)||x||_2 e_1 + x     % Householder vector for reflector Q_k
    u: = u/||u||_2
    A(k + 1:n, k:n): = A(k + 1:n, k:n) − 2u(u* A(k + 1:n, k:n))
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end
```

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Cost: The update $A \leftarrow Q_k A$ requires $4(n-k)^2$ flops as it operates on $A(k+1:n, k:n)$. Total cost $\sum_{k=1}^{n-2} 4(n-k)^2 \sim 4n^3/3$ flops.

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  $\mathtt{u}\colon= \mathtt{u}/\|\mathtt{u}\|_2$
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Example

The matlab command `[Q, H] = hess(A)` computes a unitary matrix $\mathtt{Q}$ and a Hessenberg matrix $\mathtt{H}$ such that $\mathtt{H} = \mathtt{Q}^*\mathtt{A}\mathtt{Q}$. For the matrix

$$A = \begin{bmatrix} -149 & -50 & -154 \\ 537 & 180 & 546 \\ -27 & -9 & -25 \end{bmatrix},$$

`[Q, H] = hess(A)` yields

$$\mathtt{Q} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.9987 & 0.0502 \\ 0 & 0.0502 & 0.9987 \end{bmatrix}, \ \mathtt{H} = \begin{bmatrix} -149.0000 & 42.2037 & -156.3165 \\ -537.6783 & 152.5511 & -554.9272 \\ 0 & 0.0728 & 2.4489 \end{bmatrix}.$$

Reduction to tridiagonal form

Suppose that A is Hermitian. Then the Hessenberg matrix $H = Q^*AQ$ is Hermitian $\Rightarrow H$ is tridiagonal. Consequently, the Householder reduction of A to Hessenberg form reduces A to tridiagonal form.

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The symmetry of A allows an efficient implementation of Householder reduction to tridiagonal form and brings down the cost of the reduction algorithm to $4n^3/3$ flops.

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Indeed, in the k-th step, we compute the update $A \leftarrow Q_k A Q_k$, where $Q_k := I + \gamma uu^*$ with $\gamma := -2/u^*u$ is a reflector. Now

$$
\begin{aligned}
Q_k A Q_k &= (I + \gamma uu^*)A(I + \gamma uu^*) \\
&= A + \gamma uu^*A + \gamma Auu^* + \gamma^2 uu^*Auu^* \\
&= A + uv^* + vu^* + 2\delta uu^* \\
&= A + u(v + \delta u)^* + (v + \delta u)u^* \\
&= A + uw^* + wu^*
\end{aligned}
$$

where $v := \gamma Au, \delta := \dfrac{1}{2}\gamma u^* v$ and $w := v + \delta u$.

Reduction to tridiagonal form

Note that $A \leftarrow A + uw^* + wu^*$ is a Hermitian rank-2 update. By symmetry, the update operates on $A(k:n, k:n)$ and requires $2(n-k)^2$ flops

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The 4×4 Hilbert matrix is given by

$A = \begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix}$. The command `[Q, T] = hess(A)` gives

$$Q = \begin{bmatrix} -0.1589 & 0.7036 & -0.6926 & 0 \\ 0.7417 & -0.3780 & -0.5541 & 0 \\ -0.6516 & -0.6018 & -0.4618 & 0 \\ 0 & 0 & 0 & 1.0000 \end{bmatrix} \text{ and}$$

$$T = \begin{bmatrix} 0.0031 & -0.0068 & 0 & 0 \\ -0.0068 & 0.1806 & -0.2683 & 0 \\ 0 & -0.2683 & 1.3497 & -0.3609 \\ 0 & 0 & -0.3609 & 0.1429 \end{bmatrix}.$$

Hessenberg QR algorithm

Let $A \in \mathbb{C}^{n \times n}$ be a Hessenberg matrix. Suppose we perform a QR step on A to obtain $A = QR$ and $A_1 := RQ = Q^*AQ$.

Question: Is the matrix A_1 Hessenberg? In other words, does the QR step preserve the Hessenberg structure of A?

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If the answer is NO then the reduction to Hessenberg form is of no use as far as QR algorithm is concerned.

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Theorem: Let A be a nonsingular Hessenberg matrix. Let A_1 be the result of a QR step on A, that is, $A = QR$ and $A_1 := RQ$. Then A_1 is a Hessenberg matrix.

Proof. Note that R is nonsingular and $A = QR \Longrightarrow Q = AR^{-1}$. Since R^{-1} is upper triangular and A is Hessenberg, it is easy to see that AR^{-1} is Hessenberg. Hence Q is Hessenberg. Consequently, $A_1 = RQ$ is Hessenberg. ■

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A QR step applied to a nonsingular Hessenberg matrix A preserves the Hessenberg structure.

Hessenberg QR algorithm

However, a QR step applied to a singular Hessenberg matrix A may not preserve the Hessenberg structure. Consider

$$\underbrace{\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}}_{Q} \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{R}$$

$$\underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}}_{A_1} = \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{R} \underbrace{\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}}_{Q}.$$

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Note that A is singular and Hessenberg but A_1 is not Hessenberg. The QR factorization of a singular matrix is not unique. Among many QR factorization, some may not preserve the Hessenberg structure when they are used in a QR step.

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Note that A is singular and Hessenberg but A_1 is not Hessenberg. The QR factorization of a singular matrix is not unique. Among many QR factorization, some may not preserve the Hessenberg structure when they are used in a QR step. However, one can choose a QR factorization that preserves the Hessenberg structure.