

## Solving large scale eigenvalue problems <br> Lecture 4, March 14, 2018: The QR algorithm http://people.inf.ethz.ch/arbenz/ewp/

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## Survey of today's lecture

The QR algorithm is the most important algorithm to compute the Schur form of a dense matrix.

It is one of the 10 most important algorithms in CSE of the 20th century [1].

- Basic QR algorithm
- Hessenberg QR algorithm
- QR algorithm with shifts
- Double step QR algorithm for real matrices

The QZ algorithm is somewhat similar for solving $A \mathbf{x}=\lambda B \mathbf{x}$.

## Schur decomposition [reminder]

## Theorem

If $A \in \mathbb{C}^{n \times n}$ then there is a unitary matrix $U \in \mathbb{C}^{n \times n}$ such that

$$
\begin{equation*}
U^{*} A U=T \tag{1}
\end{equation*}
$$

is upper triangular. The diagonal elements of $T$ are the eigenvalues of $A$.
$U=\left[\mathbf{u}_{1}, \mathbf{u}_{2}, \ldots, \mathbf{u}_{n}\right]$ are called Schur vectors. They are in general not eigenvectors.

## Schur vectors

The $k$-th column of this equation is

$$
\begin{aligned}
A \mathbf{u}_{k} & =\lambda \mathbf{u}_{k}+\sum_{i=1}^{k-1} t_{i k} \mathbf{u}_{i}, \quad \lambda_{k}=t_{k k} \\
& \Longrightarrow A \mathbf{u}_{k} \in \operatorname{span}\left\{\mathbf{u}_{1}, \ldots, \mathbf{u}_{k}\right\}, \quad \forall k
\end{aligned}
$$

- The first Schur vector is an eigenvector of $A$.
- The first $k$ Schur vectors $\mathbf{u}_{1}, \ldots, \mathbf{u}_{k}$ form an invariant subspace for $A$.
- The Schur decomposition is not unique.


## Basic QR algorithm

1: Let $A \in \mathbb{C}^{n \times n}$. This algorithm computes an upper triangular matrix $T$ and a unitary matrix $U$ such that $A=U T U^{*}$ is the Schur decomposition of $A$.
2: Set $A_{0}:=A$ and $U_{0}=I$.
3: for $k=1,2, \ldots$ do
4: $\quad A_{k-1}=: Q_{k} R_{k} ;\{Q R$ factorization $\}$
5: $\quad A_{k}:=R_{k} Q_{k}$;
6: $\quad U_{k}:=U_{k-1} Q_{k} ;\{$ Update transformation matrix $\}$
7: end for
8: Set $T:=A_{\infty}$ and $U:=U_{\infty}$.

## Basic QR algorithm (cont.)

Notice first that

$$
\begin{equation*}
A_{k}=R_{k} Q_{k}=Q_{k}^{*} A_{k-1} Q_{k} \tag{2}
\end{equation*}
$$

and hence $A_{k}$ and $A_{k-1}$ are unitarily similar.
From (2) we see that

$$
\begin{aligned}
A_{k} & =Q_{k}^{*} A_{k-1} Q_{k} \\
& =Q_{k}^{*} Q_{k-1}^{*} A_{k-2} Q_{k-1} Q_{k} \\
& =\cdots \\
& =Q_{k}^{*} \cdots Q_{1}^{*} A_{0} \underbrace{Q_{1} \cdots Q_{k}}_{U_{k}}, \\
U_{k} & =U_{k-1} Q_{k} .
\end{aligned}
$$

## Basic QR algorithm (cont.)

Let us assume that the eigenvalues are mutually different in magnitude and we can therefore number the eigenvalues such that $\left|\lambda_{1}\right|>\left|\lambda_{2}\right|>\cdots>\left|\lambda_{n}\right|$. Then - as we will show later - the elements of $A_{k}$ below the diagonal converge to zero like

$$
\left|a_{i j}^{(k)}\right|=\mathcal{O}\left(\left|\lambda_{i} / \lambda_{j}\right|^{k}\right), \quad i>j
$$

## Numerical experiment

$$
\begin{aligned}
& D=\operatorname{diag}\left(\left[\begin{array}{lll}
4 & 3 & 2 \\
1
\end{array}\right]\right) ; \\
& \text { rand }(' \operatorname{seed},, 0) ; \\
& \text { format short } e \\
& S=r a n d(4) ; S=(S-.5) * 2 ; \\
& A=S * D / S \quad \% A_{-} 0=A=S * D * S \sim\{-1\} \\
& \text { for } i=1: 20, \\
& \quad[Q, R]=\operatorname{qr}(A) ; A=R * Q \\
& \text { end }
\end{aligned}
$$

Same with

$$
\text { D = diag([5 } 2 \text { 2 } 2 \text { 1 } 1 \text { ) ; }
$$

## Hessenberg QR algorithm

Critique of QR algorithm

1. Slow convergence if eigenvalues close.
2. Expensive: $\mathcal{O}\left(n^{3}\right)$ flops per iteration step.

## Solution for point 2

- Hessenberg form (we have seen this earlier in Hyman's algo)
- Is the Hessenberg form preserved by the QR algorithm?
- Complexity: only $3 n^{2}$ flops/iteration step
- Still slow convergence.


## Transformation to Hessenberg form

- Givens rotations are designed to zero a single element in a vector.
- Householder reflectors are more efficient if multiple elements of a vector are to be zeroed at once.


## Definition

A matrix of the form

$$
P=I-2 \mathbf{u u}^{*}, \quad\|\mathbf{u}\|=1
$$

is called a Householder reflector.
Easy to verify:
$P$ is Hermitian, $P^{2}=I, P$ is unitary.

## Transformation to Hessenberg form (cont.)

Frequent task: find unitary transformation that maps a vector $\mathbf{x}$ into a multiple of $\mathbf{e}_{1}$,

$$
P \mathbf{x}=\mathbf{x}-\mathbf{u}\left(2 \mathbf{u}^{*} \mathbf{x}\right)=\alpha \mathbf{e}_{1}
$$

$P$ unitary $\quad \Longrightarrow \quad \alpha=\rho\|\mathbf{x}\|$, where $\rho \in \mathbb{C}$ with $|\rho|=1$

$$
\mathbf{u}=\frac{\mathbf{x}-\rho\|\mathbf{x}\| \mathbf{e}_{1}}{\|\mathbf{x}-\rho\| \mathbf{x}\left\|\mathbf{e}_{1}\right\|}=\frac{1}{\|\mathbf{x}-\rho\| \mathbf{x}\left\|\mathbf{e}_{1}\right\|}\left[\begin{array}{c}
x_{1}-\rho\|\mathbf{x}\| \\
x_{2} \\
\vdots \\
x_{n}
\end{array}\right]
$$

To avoid numerical cancellation we set $\rho=-e^{i \phi}$. If $\rho \in \mathbb{R}$ we set $\rho=-\operatorname{sign}\left(x_{1}\right)$. (If $x_{1}=0$ we can set $\rho$ in any way.)

## Reduction to Hessenberg form

1: This algorithm reduces a matrix $A \in \mathbb{C}^{n \times n}$ to Hessenberg form $H$ by a sequence of Householder reflections. $H$ overwrites $A$.
2: for $k=1$ to $n-2$ do
3: Generate the Householder reflector $P_{k}$;
4: $\quad A_{k+1: n, k: n}:=A_{k+1: n, k: n}-2 \mathbf{u}_{\mathbf{k}}\left(\mathbf{u}_{\mathbf{k}}{ }^{*} A_{k+1: n, k: n}\right)$;
5: $\quad A_{1: n, k+1: n}:=A_{1: n, k+1: n}-2\left(A_{1: n, k+1: n} \mathbf{u}_{\mathbf{k}}\right) \mathbf{u}_{\mathbf{k}}{ }^{*}$;
6: end for
7: if eigenvectors are desired form $U=P_{1} \ldots P_{n-2}$ then
8: $\quad U:=I_{n}$;
9: for $k=n-2$ downto 1 do
10: $\quad U_{k+1: n, k+1: n}:=U_{k+1: n, k+1: n}-2 \mathbf{u}_{\mathbf{k}}\left(\mathbf{u}_{\mathbf{k}}{ }^{*} U_{k+1: n, k+1: n}\right)$;
11: end for
12: end if

## Reduction to Hessenberg form (cont.)

The Householder vectors are stored at the locations of the zeros. The matrix $U=P_{1} \cdots P_{n-2}$ is computed after all Householder vectors have been generated, thus saving $(2 / 3) n^{3}$ flops.
Overall complexity of the reduction:

- Application of $P_{k}$ from the left: $\sum_{k=1}^{n-2} 4(n-k-1)(n-k) \approx \frac{4}{3} n^{3}$
- Application of $P_{k}$ from the right: $\sum_{k=1}^{n-2} 4(n)(n-k) \approx 2 n^{3}$
- Form $U=P_{1} \ldots P_{n-2}: \sum_{k=1}^{n-2} 4(n-k)(n-k) \approx \frac{4}{3} n^{3}$
- In total $\frac{10}{3} n^{3}$ flops without $U, \frac{14}{3} n^{3}$ including $U$.


## Perfect shift QR algorithm

## Lemma

H Hessenberg matrix with $Q R$ factorization $H=Q R$.

$$
\begin{equation*}
\left|r_{k k}\right| \geq h_{k+1, k}, \quad 1 \leq k<n . \tag{3}
\end{equation*}
$$

## By consequence:

1. $H$ irreducible $\Longrightarrow\left|r_{k k}\right|>0$ for $1 \leq k<n$
2. $H$ irreducible and singular $\Longrightarrow r_{n n}=0$

## Perfect shift QR algorithm (cont.)

Let $\lambda$ be an eigenvalue of the irreducible Hessenberg matrix $H$.
What happens if we perform

$$
\begin{aligned}
& \text { 1: } H-\lambda I=Q R\{Q R \text { factorization }\} \\
& \text { 2: } \bar{H}=R Q+\lambda I
\end{aligned}
$$

First we notice that $\bar{H} \sim H$. In fact,

$$
\bar{H}=Q^{*}(H-\lambda I) Q+\lambda I=Q^{*} H Q
$$

Second, by the above Lemma we have

$$
H-\lambda I=Q R, \quad \text { with } \quad R=\left[\searrow_{0}\right]
$$

## Perfect shift QR algorithm (cont.)

Thus,

$$
R Q=\left[\begin{array}{l}
\ \\
00
\end{array}\right]
$$

and

$$
\bar{H}=R Q+\lambda I=\left[\begin{array}{l}
\vdots \\
0 \lambda
\end{array}\right]=\left[\begin{array}{cc}
\bar{H}_{1} & \mathbf{h}_{1} \\
\mathbf{0}^{T} & \lambda
\end{array}\right] .
$$

1. If we apply a QR step with a perfect shift to a Hessenberg matrix, the eigenvalue drops out.
2. Then we can deflate, i.e., proceed the algorithm with the smaller matrix $\bar{H}_{1}$.
3. However, we do not know the eigenvalues of H .

## Numerical example

```
D = diag([[4 3 2 1]); rand('seed',0);
S=rand(4); S = (S - .5)*2;
A = S*D/S;
format short e
H = hess(A)
    [Q,R] = qr(H - 2*eye(4))
H1 = R*Q + 2*eye(4)
format long
lam = eig(H1(1:3,1:3))
```


## QR algorithm with shifts

- It may be useful to introduce shifts into the QR algorithm.
- However, we cannot choose perfect shifts as we do not know the eigenvalues!
- Need heuristics to estimate eigenvalues.
- One such heuristic is the Rayleigh quotient shift: Set the shift $\sigma_{k}$ in the $k$-th step of the QR algorithm equal to the last diagonal element:

$$
\begin{equation*}
\sigma_{k}:=h_{n, n}^{(k-1)}=\mathbf{e}_{n}^{*} H^{(k-1)} \mathbf{e}_{n} \tag{4}
\end{equation*}
$$

## Hessenberg QR algorithm with Rayleigh quotient shift

1: Let $H_{0}=H \in \mathbb{C}^{n \times n}$ be an upper Hessenberg matrix. This algorithm computes its Schur normal form $H=U T U^{*}$.
2: $k:=0$;
3: for $m=n, n-1, \ldots, 2$ do
4: repeat

$$
\begin{array}{ll}
\text { 5: } & k:=k+1 ; \\
\text { 6: } & \sigma_{k}:=h_{m, m}^{(k-1) ;} \\
\text { 7: } & H_{k-1}-\sigma_{k} I=: Q_{k} R_{k} ; \\
\text { 8: } & H_{k}:=R_{k} Q_{k}+\sigma_{k} I ; \\
9: & U_{k}:=U_{k-1} Q_{k} ;
\end{array}
$$

10: until $\left|h_{m, m-1}^{(k)}\right|$ is sufficiently small

## 11: end for

12: $T:=H_{k}$;

## Convergence

What happens, if $h_{n, n}$ is a good approximation to an eigenvalue of $H$ ? Let us assume that we have an irreducible Hessenberg matrix

$$
\left[\begin{array}{ccccc}
\times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times \\
0 & \times & \times & \times & \times \\
0 & 0 & \times & \times & \times \\
0 & 0 & 0 & \varepsilon & h_{n, n}
\end{array}\right]
$$

where $\varepsilon$ is a small quantity.
If we perform a Hessenberg QR step with a Rayleigh quotient shift $h_{n, n}$, we first have to factor $H-h_{n, n} l, Q R=H-h_{n, n} l$.

## Convergence (cont.)

After $n-2$ steps the $R$-factor is almost upper triangular,

$$
\left[\begin{array}{ccccc}
+ & + & + & + & + \\
0 & + & + & + & + \\
0 & 0 & + & + & + \\
0 & 0 & 0 & \alpha & \beta \\
0 & 0 & 0 & \varepsilon & 0
\end{array}\right] .
$$

The last Givens rotation has the nontrivial elements

$$
c_{n-1}=\frac{\alpha}{\sqrt{|\alpha|^{2}+|\varepsilon|^{2}}}, \quad s_{n-1}=\frac{-\varepsilon}{\sqrt{|\alpha|^{2}+|\varepsilon|^{2}}}
$$

## Convergence (cont.)

Applying the Givens rotations from the right one sees that the last lower off-diagonal element of $\bar{H}=R Q+h_{n, n} I$ becomes

$$
\begin{equation*}
\bar{h}_{n, n-1}=\frac{\varepsilon^{2} \beta}{\alpha^{2}+\varepsilon^{2}} \tag{5}
\end{equation*}
$$

So, we have quadratic convergence unless $\alpha$ is also tiny.

## Convergence (cont.)

A second even more often used shift strategy is the Wilkinson shift:

$$
\sigma_{k}:=\text { eigenvalue of }\left[\begin{array}{cc}
h_{n-1, n-1}^{(k-1)} & h_{n-1, n}^{(k-1)} \\
h_{n, n-1}^{(k-1)} & h_{n, n}^{(k-1)}
\end{array}\right]
$$

that is closer to $h_{n, n}^{(k-1)}$.
Quadratic convergence can be proved.

## Numerical example

$$
\begin{aligned}
& D=\operatorname{diag}\left(\left[\begin{array}{lll}
4 & 3 & 2
\end{array}\right]\right) ; \\
& \text { rand }(\text { 'seed', } 0) ; \\
& S=r a n d(4) ; S=(S-.5) * 2 ; \\
& A=S * D / S ; \\
& H=\operatorname{hess}(A) \\
& \text { for } i=1: 8 \text {, } \\
& \quad[Q, R]=\operatorname{qr}(H-H(4,4) * \operatorname{eye}(4)) ; \\
& \quad H=R * Q+H(4,4) * \operatorname{eye}(4) ; \\
& \text { end }
\end{aligned}
$$

## The double-shift QR algorithm

Now we address the case when real Hessenberg matrices have complex eigenvalues.

- For reasonable convergence rates the shifts must be complex.
- If an eigenvalue $\lambda$ has been found we can execute a single perfect shift with $\bar{\lambda}$.
- It is (for rounding errors) unprobable however that we will get back to a real matrix.
- Since the eigenvalues come in complex conjugate pairs it is straightforward to search for a pair of eigenvalues right-away.
- This is done by collapsing two shifted QR steps in one double step with the two shifts being complex conjugates of each other.


## Two single steps

Let $\sigma_{1}$ and $\sigma_{2}$ be two eigenvalues of the real matrix

$$
G=\left[\begin{array}{cc}
h_{n-1, n-1}^{(k-1)} & h_{n-1, n}^{(k-1)} \\
h_{n, n-1}^{(k-1)} & h_{n, n}^{(k-1)}
\end{array}\right] \in \mathbb{R}^{2 \times 2} .
$$

If $\sigma_{1} \in \mathbb{C} \backslash \mathbb{R}$ then $\sigma_{2}=\bar{\sigma}_{1}$.
Let us perform two QR steps using $\sigma_{1}$ and $\sigma_{2}$ as shifts. Setting $k=1$ for convenience we get

$$
\begin{align*}
H_{0}-\sigma_{1} I & =Q_{1} R_{1} \\
H_{1} & =R_{1} Q_{1}+\sigma_{1} I  \tag{6}\\
H_{1}-\sigma_{2} I & =Q_{2} R_{2} \\
H_{2} & =R_{2} Q_{2}+\sigma_{2} I
\end{align*}
$$

## Two single steps (cont.)

From the second and third equation in (6) we obtain

$$
R_{1} Q_{1}+\left(\sigma_{1}-\sigma_{2}\right) I=Q_{2} R_{2}
$$

Multiplying with $Q_{1}$ from the left and $R_{1}$ from the right we get

$$
\begin{aligned}
Q_{1} R_{1} Q_{1} R_{1}+\left(\sigma_{1}-\sigma_{2}\right) Q_{1} R_{1} & =Q_{1} R_{1}\left(Q_{1} R_{1}+\left(\sigma_{1}-\sigma_{2}\right) I\right) \\
& =\left(H_{0}-\sigma_{1} I\right)\left(H_{0}-\sigma_{2} I\right)=Q_{1} Q_{2} R_{2} R_{1}
\end{aligned}
$$

Because $\sigma_{2}=\bar{\sigma}_{1}$ we have

$$
M:=\left(H_{0}-\sigma_{1} I\right)\left(H_{0}-\bar{\sigma}_{1} I\right)=H_{0}^{2}-2 \operatorname{Re}\left(\sigma_{1}\right) H_{0}+\left|\sigma_{1}\right|^{2} I=Q_{1} Q_{2} R_{2} R_{1}
$$

So, $\left(Q_{1} Q_{2}\right)\left(R_{2} R_{1}\right)$ is $Q R$ factorization of a real matrix.
We can choose $Q_{1}, Q_{2}$ s.t. $Z:=Q_{1} Q_{2}$ is real orthogonal. Thus,

$$
H_{2}=\left(Q_{1} Q_{2}\right)^{*} H_{0}\left(Q_{1} Q_{2}\right)=Z^{T} H_{0} Z \in \mathbb{R}^{n \times n}
$$

## Two single steps (cont.)

A procedure to compute $\mathrm{H}_{2}$ by avoiding complex arithmetic could consist of three steps:
(1) Form the real matrix $M=H_{0}^{2}-s H_{0}+t l$ with

$$
\begin{aligned}
& s=2 \operatorname{Re}(\sigma)=\operatorname{trace}(G)=h_{n-1, n-1}^{(k-1)}+h_{n, n}^{(k-1)} \text { and } \\
& t=|\sigma|^{2}=\operatorname{det}(G)=h_{n-1, n-1}^{(k-1)} h_{n, n}^{(k-1)}-h_{n-1, n}^{(k-1)} h_{n, n-1}^{(k-1)}
\end{aligned}
$$

Notice that $M$ has two lower off-diagonals,

$$
M=[\sqrt{W}]
$$

(2) Compute the $Q R$ factorization $M=Z R$,
(3) Set $H_{2}=Z^{T} H_{0} Z$.

This procedure is however too expensive since item (1),
i.e. forming $H^{2}$, requires $\mathcal{O}\left(n^{3}\right)$ flops.

## The implicit Q theorem

> Theorem
> Let $A \in \mathbb{R}^{n \times n}$. Let $Q=\left[\mathbf{q}_{1}, \ldots, \mathbf{q}_{n}\right]$ and $V=\left[\mathbf{v}_{1}, \ldots, \mathbf{v}_{n}\right]$ be orthogonal matrices that both similarly transform $A$ to Hessenberg form, $H=Q^{T} A Q$ and $G=V^{T} A V$. Let $k$ denote the smallest positive integer for which $h_{k+1, k}=0$, with $k=n$ if $H$ is irreducible. If $\mathbf{q}_{1}=\mathbf{v}_{1}$ then $\mathbf{q}_{i}= \pm \mathbf{v}_{i}$ and $\left|h_{i, i-1}\right|=\left|g_{i, i-1}\right|$ for $i=2, \ldots, k$. If $k<n$, then $g_{k+1, k}=0$.

Golub \& van Loan [2, p.347] write "The gist of the implicit $Q$ theorem is that if $Q^{T} A Q=H$ and $Z^{T} A Z=G$ are both irreducible Hessenberg matrices and $Q$ and $Z$ have the same first column, then $G$ and $H$ are "essentially equal" in the sense that $G=D H D$ with $D=\operatorname{diag}( \pm 1, \ldots, \pm 1)$."

## Application of the implicit Q Theorem

- We want to compute Hessenberg matrix $H_{k+1}=Z^{T} H_{k-1} Z$ where $Z R$ is QR factorization of $M=H_{k-1}^{2}-s H_{k-1}+t l$.
- The Implicit Q Theorem tells us that we essentially get $H_{k+1}$ by any orthogonal similarity transformation $H_{k-1} \rightarrow Z_{1}^{*} H_{k-1} Z_{1}$ provided that $Z_{1}^{*} H Z_{1}$ is Hessenberg and $Z_{1} \mathbf{e}_{1}=Z \mathbf{e}_{1}$.
- Let $P_{0}$ be the Householder reflector with

$$
P_{0}^{T} M \mathbf{e}_{1}=P_{0}^{T}\left(H_{k-1}^{2}-2 \operatorname{Re}(\sigma) H_{k-1}+|\sigma|^{2} I\right) \mathbf{e}_{1}=\alpha \mathbf{e}_{1} .
$$

## Application of the implicit Q Theorem (cont.)

- Since only the first three elements of the first column $M \mathbf{e}_{1}$ of $M$ are nonzero, $P_{0}$ has the structure

$$
P_{0}=\left[\begin{array}{cccccc}
\times & \times & \times & & & \\
\times & \times & \times & & & \\
\times & \times & \times & & & \\
& & & 1 & & \\
& & & & \ddots & \\
& & & & & 1
\end{array}\right]
$$

## Application of the implicit Q Theorem (cont.)

- So,

$$
H_{k-1}^{\prime}:=P_{0}^{T} H_{k-1} P_{0}=\left[\begin{array}{ccc|cccc}
\times & \times & \times & \times & \times & \times & \times \\
\times & \times & \times & \times & \times & \times & \times \\
+ & \times & \times & \times & \times & \times & \times \\
\hline+ & + & \times & \times & \times & \times & \times \\
& & & \times & \times & \times & \times \\
& & & & \times & \times & \times \\
& & & & \times & \times
\end{array}\right] .
$$

- Recover the Hessenberg form by applying a sequence of similarity transformations with Householder reflectors. (Chase the bulge down the diagonal until it drops out of the matrix.)


## Application of the implicit Q Theorem (cont.)

- We need $n-1$ additional Householder reflectors

$$
P_{i}=I-2 \mathbf{p}_{i} \mathbf{p}_{i}^{*}, \quad i=1, \ldots, n-1
$$

to achieve this. Notice that
(1) the $\mathbf{p}_{i}$ have just 3 nonzero elements, and that
(2) the first entry of $\mathbf{p}_{i}$ is zero.

Therefore,

$$
P_{0} P_{1} \cdots P_{n-1} \mathbf{e}_{1}=P_{0} \mathbf{e}_{1}=\frac{1}{\alpha}\left(H_{k-1}^{2}+s H_{k-1}+t /\right) \mathbf{e}_{1}=Z \mathbf{e}_{1} .
$$

## The Francis double step QR algorithm

1: Let $H_{0}=H \in \mathbb{R}^{n \times n}$ be an upper Hessenberg matrix. This algorithm computes its real Schur form $H=U T U^{T}$ using the Francis double step QR algorithm. $T$ is a quasi upper triangular matrix.
2: $p:=n ;\{p$ indicates the 'active' matrix size. $\}$
3: while $p>2$ do
4: $\quad q:=p-1$;
5: $\quad s:=H_{q, q}+H_{p, p} ; \quad t:=H_{q, q} H_{p, p}-H_{q, p} H_{p, q}$;
6: $\quad\{$ Compute first 3 elements of first column of $M$ \}
7: $\quad x:=H_{1,1}^{2}+H_{1,2} H_{2,1}-s H_{1,1}+t$;
8: $\quad y:=H_{2,1}\left(H_{1,1}+H_{2,2}-s\right)$;
9: $\quad z:=H_{2,1} H_{3,2}$;

## The Francis double step QR algorithm (cont.)

## 10: $\quad$ for $k=0$ to $p-3$ do

11: $\quad$ Determine the Householder reflector $P$ with $P^{T}[x ; y ; z]^{T}=\alpha \mathbf{e}_{1}$;
12: $\quad r:=\max \{1, k\}$;
13:
14: $\quad r:=\min \{k+4, p\}$;
15: $\quad H_{1: r, k+1: k+3}:=H_{1: r, k+1: k+3} P$;
16: $\quad x:=H_{k+2, k+1} ; \quad y:=H_{k+3, k+1}$;
17: $\quad$ if $k<p-3$ then
18: $\quad z:=H_{k+4, k+1}$;
19: end if
20: end for

## The Francis double step QR algorithm (cont.)

21: $\quad$ Determine the Givens rotation $P$ with $P^{T}[x ; y]^{T}=\alpha \mathbf{e}_{1}$;
22: $\quad H_{q: p, p-2: n}:=P^{T} H_{q: p, p-2: n}$;
23: $\quad H_{1: p, p-1: p}:=H_{1: p, p-1: p} P$;
24: $\quad$ \{check for convergence $\}$
25: if $\left|H_{p, q}\right|<\varepsilon\left(\left|H_{q, q}\right|+\left|H_{p, p}\right|\right)$ then
26: $\quad H_{p, q}:=0 ; \quad p:=p-1 ; \quad q:=p-1$;
27: else if $\left|H_{p-1, q-1}\right|<\varepsilon\left(\left|H_{q-1, q-1}\right|+\left|H_{q, q}\right|\right)$ then
28: $\quad H_{p-1, q-1}:=0 ; \quad p:=p-2 ; \quad q:=p-1$;
29: end if
30: end while

Solving large scale eigenvalue problems
LThe double-shift QR algorithm

## Numerical example

$$
A=\left[\begin{array}{rrrrrr}
7 & 3 & 4 & -11 & -9 & -2 \\
-6 & 4 & -5 & 7 & 1 & 12 \\
-1 & -9 & 2 & 2 & 9 & 1 \\
-8 & 0 & -1 & 5 & 0 & 8 \\
-4 & 3 & -5 & 7 & 2 & 10 \\
6 & 1 & 4 & -11 & -7 & -1
\end{array}\right]
$$

has the spectrum

$$
\sigma(A)=\{1 \pm 2 i, 3,4,5 \pm 6 i\} .
$$

## Complexity

Most expensive operations: applications of $3 \times 3$ Householder reflectors,

$$
\mathbf{x}:=\left(I-2 \mathbf{u} \mathbf{u}^{T}\right) \mathbf{x}=\mathbf{x}-\mathbf{u}\left(2 \mathbf{u}^{T} \mathbf{x}\right)
$$

which costs 12 flops.
In $k$-th step of the loop: $n-k$ reflections from the left and $k+4$ from the right. Thus about $12 n+\mathcal{O}(1)$ flops.
$k$ runs from 1 to $p-3$ : $12 p n$ flops/step.
$p$ runs from $n$ down to $2: 6 n^{3}$ flops.
Assuming two steps per eigenvalue: the flop count for Francis' double step QR algorithm to compute all eigenvalues of a real Hessenberg matrix is $12 n^{3}$.

## Complexity (cont.)

If also the eigenvector matrix is accumulated two additional statements have to be inserted into the algorithm. After steps 15 and 23 we have

$$
\text { 1: } Q_{1: n, k+1: k+3}:=Q_{1: n, k+1: k+3} P
$$

1: $Q_{1: n, p-1: p}:=Q_{1: n, p-1: p} P$;
which costs another $12 n^{3}$ flops.

## Complexity (cont.)

The single step Hessenberg $Q R$ algorithm costs $6 n^{3}$ flops. If the latter has to be spent in complex arithmetic then the single shift Hessenberg QR algorithm is more expensive than the double shift Hessenberg QR algorithm that is executed in real arithmetic.

Remember that the reduction to Hessenberg form costs $\frac{10}{3} n^{3}$ flops without forming the transformation matrix and $\frac{14}{3} n^{3}$ if this matrix is formed.

## References

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