

Solving large scale eigenvalue problems Lecture 5, March 23, 2016: The QR algorithm II 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.

- Basic QR algorithm
- Hessenberg QR algorithm
- QR algorithm with shifts
- Double step QR algorithm for real matrices
- The symmetric QR algorithm
- The QZ algorithm for solving $A\mathbf{x} = \lambda B\mathbf{x}$.

Spectral decomposition

Theorem

Let $A \in \mathbb{C}^{n \times n}$ be hermitian, $A^* = A$. Then there is a unitary matrix $U \in \mathbb{C}^{n \times n}$ such that

$$U^*AU = \Lambda = diag(\lambda_1, \dots, \lambda_n)$$
(1)

is diagonal. The diagonal elements λ_i of Λ are the eigenvalues of A.

Let $U = [\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n]$. Then $A\mathbf{u}_i = \lambda_i \mathbf{u}_i, \qquad 1 \leq i \leq n.$

 \mathbf{u}_i is the eigenvector associated with the eigenvalue λ_i .

- The symmetric QR algorithm

The symmetric QR algorithm

- The QR algorithm can be applied straight to Hermitian or symmetric matrices.
- The QR algorithm generates a sequence {A_k} of symmetric matrices.
- Taking into account the symmetry, the performance of the algorithm can be improved considerably.
- Hermitian matrices have a real spectrum. Therefore, we can restrict ourselves to single shifts.

The symmetric QR algorithm

Reduction to tridiagonal form

Apply a sequence of Householder transformations to arrive at tridiagonal (= symmetric Hessenberg) form. First step: Let

$$P_1 = \begin{bmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & I_{n-1} - 2\mathbf{u}_1\mathbf{u}_1^* \end{bmatrix}, \qquad \mathbf{u}_1 \in \mathbb{C}^n, \quad \|\mathbf{u}_1\| = 1.$$

Then,

$$A_{1} := P_{1}^{*}AP_{1} = (I - 2\mathbf{u}_{1}\mathbf{u}_{1}^{*})A(I - 2\mathbf{u}_{1}\mathbf{u}_{1}^{*})$$

= $A - \mathbf{u}_{1}(\underbrace{2\mathbf{u}_{1}^{*}A - 2(\mathbf{u}_{1}^{*}A\mathbf{u}_{1})\mathbf{u}_{1}^{*}}_{\mathbf{v}_{1}^{*}}) - \underbrace{(2A\mathbf{u}_{1} - 2\mathbf{u}_{1}(\mathbf{u}_{1}^{*}A\mathbf{u}_{1}))}_{\mathbf{v}_{1}}\mathbf{u}_{1}^{*}$
= $A - \mathbf{u}_{1}\mathbf{v}_{1}^{*} - \mathbf{v}_{1}\mathbf{u}_{1}^{*}.$

The symmetric QR algorithm

Reduction to tridiagonal form (cont.)

In the k-th step of the reduction we similarly have

$$A_k = P_k^* A_{k-1} P_k = A_{k-1} - \mathbf{u}_{k-1} \mathbf{v}_{k-1}^* - \mathbf{v}_{k-1} \mathbf{u}_{k-1}^*,$$

where the last n - k elements of \mathbf{u}_{k-1} and \mathbf{v}_{k-1} are nonzero. Essential computation in the *k*th step:

$$\mathbf{v}_{k-1} = 2A_{k-1}\mathbf{u}_{k-1} - 2\mathbf{u}_{k-1}(\mathbf{u}_{k-1}^*A_{k-1}\mathbf{u}_{k-1})$$

which costs $2(n-k)^2 + O(n-k)$ flops.

Altogether, the reduction to tridiagonal form costs

$$\sum_{k=1}^{n-1} (4(n-k)^2 + \mathcal{O}(n-k)) = \frac{4}{3}n^3 + \mathcal{O}(n^2) \text{ flops.}$$

- The symmetric QR algorithm

The explicit tridiagonal QR algorithm

In the explicit form, a QR step is essentially

- 1: Choose a shift μ
- 2: Compute the QR factorization $A \mu I = QR$
- 3: Update A by $A = RQ + \mu I$.

Of course, this is done by means of plane rotations and by respecting the symmetric tridiagonal structure of A.

Shifting strategies: Rayleigh quotient shifts, Wilkinson shifts

The symmetric QR algorithm

The implicit tridiagonal QR algorithm

In the more elegant implicit form of the algorithm we first compute the first Givens rotation $G_0 = G(1, 2, \vartheta)$ of the QR factorization that zeros the (2, 1) element of $A - \mu I$,

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a_{11} - \mu \\ a_{21} \end{bmatrix} = \begin{bmatrix} * \\ 0 \end{bmatrix}, \qquad c = \cos(\vartheta_0), \quad s = \sin(\vartheta_0).$$
(2)

Performing a similarity transformation with G_0 we have (n = 5)

The symmetric QR algorithm

The implicit tridiagonal QR algorithm (cont.)

Similarly as with the double step Hessenberg QR algorithm we chase the bulge down the diagonal.

The symmetric QR algorithm

The implicit tridiagonal QR algorithm (cont.)

The full step is given by

$$\overline{A} = Q^* A Q, \qquad Q = G_0 G_1 \cdots G_{n-2}.$$

Because $G_k \mathbf{e}_1 = \mathbf{e}_1$ for k > 0 we have

$$Q \mathbf{e}_1 = G_0 G_1 \cdots G_{n-2} \mathbf{e}_1 = G_0 \mathbf{e}_1.$$

Both explicit and implicit QR step form the same first plane rotation G_0 . By referring to the Implicit Q Theorem we see that explicit and implicit QR step compute *essentially* the same \overline{A} .

The symmetric QR algorithm

Symm. tridiag. QR algo with Wilkinson shifts

- Let T ∈ ℝ^{n×n} be a symmetric tridiagonal matrix with diagonal entries a₁,..., a_n and off-diagonal entries b₂,..., b_n. This algorithm computes the eigenvalues λ₁,..., λ_n of T and corresponding eigenvectors q₁,..., q_n. The eigenvalues are stored in a₁,..., a_n. The eigenvectors are stored in the matrix Q, such that TQ = Q diag(a₁,..., a_n).
- 2: m = n {Actual problem dimension. m is reduced in the convergence check.}
- 3: while m > 1 do
- 4: $d := (a_{m-1} a_m)/2$; {Compute Wilkinson's shift}
- 5: **if** d = 0 **then**
- 6: $s := a_m |b_m|;$

- The symmetric QR algorithm

Symm. tridiag. QR algo with Wilkinson shifts (cont.)

7: else

8:
$$s := a_m - b_m^2/(d + \operatorname{sign}(d)\sqrt{d^2 + b_m^2});$$

- 9: end if
- 10: x := a(1) s; {Implicit QR step begins here}

11:
$$y := b(2);$$

12: **for**
$$k = 1$$
 to $m - 1$ **do**

13: **if** m > 2 **then**

14:
$$[c,s] := \operatorname{givens}(x,y);$$

- 15: **else**
- 16: Determine [c, s] such that $\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} a_1 & b_2 \\ b_2 & a_2 \end{bmatrix} \begin{bmatrix} c & s \\ -s & c \end{bmatrix}$ is diagonal
- 17: end if

18: w := cx - sy;

- The symmetric QR algorithm

Symm. tridiag. QR algo with Wilkinson shifts (cont.)

19:
$$d := a_k - a_{k+1}; \quad z := (2cb_{k+1} + ds)s;$$

20: $a_k := a_k - z; \quad a_{k+1} := a_{k+1} + z;$
21: $b_{k+1} := dcs + (c^2 - s^2)b_{k+1};$
22: $x := b_{k+1};$
23: if $k > 1$ then
24: $b_k := w;$
25: end if
26: if $k < m - 1$ then
27: $y := -sb_{k+2}; \quad b_{k+2} := cb_{k+2};$
28: end if
29: $Q_{1:n;k:k+1} := Q_{1:n;k:k+1} \begin{bmatrix} c & s \\ -s & c \end{bmatrix};$
30: end for{Implicit QR step ends here}
31: if $|b_m| < \varepsilon(|a_{m-1}| + |a_m|)$ then {Check for convergence}

- The symmetric QR algorithm

Symm. tridiag. QR algo with Wilkinson shifts (cont.)

- 32: m := m 1;
- 33: end if
- 34: end while

The symmetric QR algorithm

Remark on deflation

$$T = \begin{bmatrix} a_1 & b_2 & & & \\ b_2 & a_2 & b_3 & & \\ & b_3 & a_3 & 0 & & \\ & 0 & a_4 & b_5 & \\ & & b_5 & a_5 & b_6 \\ & & & & b_6 & a_6 \end{bmatrix}$$

- Shift for next step is determined from second block.
- First plane rotation is determined from shift and first block!
- The implicit shift algorithm then chases the bulge down the diagonal. Procedure finishes already in row 4 because b₄ = 0.
- This shift does not improve convergence.
- Explicit QR algorithm converges rapidly, but first block is not treated properly

- The symmetric QR algorithm

Complexity of QR algorithm

	nonsymmetric case		symmetric case	
	without	with	without	with
	Schurvectors		eigenvectors	
transformation to Hessenberg/tridiagonal form	$\frac{10}{3} n^3$	$\frac{14}{3} n^3$	$\frac{4}{3} n^3$	$\frac{8}{3} n^3$
real double step Hessenberg/ tridiagonal QR algorithm (2 steps per eigenvalues)	$\frac{20}{3} n^3$	$\frac{50}{3} n^3$	24 <i>n</i> ²	6 n ³
total	10 n ³	25 n ³	$\frac{4}{3} n^3$	9 n ³

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

Theorem (Generalized Schur decomposition)

Let $A, B \in \mathbb{C}^{n \times n}$. Then there are unitary matrices Q and Z such that $Q^*AZ = T$ and $Q^*BZ = S$ are both upper triangular matrices. If for some k, $t_{kk} = s_{kk} = 0$ then $\sigma(A; B) = \mathbb{C}$. Otherwise,

$$\sigma(A;B) = \left\{\frac{t_{ii}}{s_{ii}} \mid s_{ii} \neq 0\right\}.$$

Remark: (1) It is possible that $\infty \in \sigma(A; B)$. This is equivalent with $0 \in \sigma(B; A)$. (2) There is a real version of this theorem. There *T* is quasi-upper triangular and *S* is upper triangular.

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

Proof.

Let B_k a sequence of nonsingular matrices converging to B. Let $Q_k^*(AB_k^{-1})Q_k = R_k$, $k \ge 0$, the Schur decomposition of AB_k^{-1} . Let Z_k be unitary and $Z_k^*(B_k^{-1}Q_k) = S_k^{-1}$ upper triangular. Then

$$Q_k^* A Z_k Z_k^* B_k^{-1} Q_k = R_k \implies Q_k^* A Z_k = R_k S_k$$

is upper triangular.

Bolzano–Weierstrass: the sequence $\{(Q_k, Z_k)\}$ has convergent subsequence, $\lim(Q_{k_i}, Z_{k_i}) = (Q, Z)$. Q, Z are unitary and Q^*AZ , Q^*BZ are upper triangular. Statement on eigenvalues follows from

$$\det(A - \lambda B) = \det(QZ^*) \prod_{i=1}^n (t_{ii} - \lambda s_{ii}).$$

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 1

Step 1: Reduction to Hessenberg-triangular form. Transform *B* into upper triangular form (QR factorization of *B*)

$$A \leftarrow U^* A = \begin{pmatrix} \times \times \times \times \times \\ \times \times \times \times \end{pmatrix}, \quad B \leftarrow U^* B = \begin{pmatrix} \times \times \times \times \times \\ 0 \times \times \times \\ 0 & 0 \times \times \\ 0 & 0 & 0 \times \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 1 (cont.)

Transform A into Hessenberg form by a sequence of Givens rotations w/o destroying the zero pattern of B

$$A \leftarrow Q_{45}^* A = \begin{pmatrix} \times \times \times \times \times \\ 0 \times \times \times \end{pmatrix}, \quad B \leftarrow Q_{45}^* B = \begin{pmatrix} \times \times \times \times \times \\ 0 \times \times \times \\ 0 & 0 \times \times \\ 0 & 0 & 0 \times \\ 0 & 0 & 0 + \\ \end{pmatrix}$$

$$A \leftarrow AZ_{45} = \begin{pmatrix} \times \times \times \times \times \\ 0 \times \times \times \end{pmatrix}, \quad B \leftarrow BZ_{45} = \begin{pmatrix} \times \times \times \times \times \\ 0 \times \times \times \\ 0 & 0 \times \times \\ 0 & 0 & 0 \times \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 1 (cont.)

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 1 (cont.)

$$A \leftarrow Q_{23}^* A = \begin{pmatrix} \times \times \times \times \times \\ \times \times \times \times \\ 0 \times \times \times \end{pmatrix}, \quad B \leftarrow Q_{23}^* B = \begin{pmatrix} \times \times \times \times \\ 0 \times \times \times \\ 0 + \times \\ 0 +$$

Now the first column of A has the desired structure.

Proceed similarly with columns 2 to n - 2.

— The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 2

Step 2: Deflation. Let us assume

- 1. that A is an irreducible Hessenberg matrix and
- 2. that B is a nonsingular upper triangular matrix.

If 1. is not satisfied, e.g.
$$a_{k+1,k} = 0$$
, then

$$A - \lambda B = \begin{pmatrix} A_{11} - \lambda B_{11} & A_{12} - \lambda B_{12} \\ 0 & A_{22} - \lambda B_{22} \end{pmatrix}$$

and we can treat the smaller problems $A_{11} - \lambda B_{11}$ and $A_{22} - \lambda B_{22}$ individually.

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 2 (cont.)

If 2. is not satisfied, then $b_{k,k} = 0$ for some k.

We chase the zero down the diagonal of B:

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 2 (cont.)

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 2 (cont.)

$$A \leftarrow AZ_{34}^* = \begin{pmatrix} \times \times \times \times \times \\ \times \times \times \times \\ 0 \times \times \times \\ 0 & 0 \times \times \\ 0 & 0 & 0 \times \\ \end{pmatrix}, \quad B \leftarrow BZ_{34}^* = \begin{pmatrix} \times \times \times \times \\ 0 \times \times \times \\ 0 & 0 & 0 \times \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \end{pmatrix}$$
$$A \leftarrow AZ_{45} = \begin{bmatrix} \times \times \times \times \\ \times \times \times \times \\ 0 \times \times \times \\ 0 & 0 \times \times \\ 0 & 0 & 0 & 0 \\ \hline \\ 0$$

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The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 2

Step 3: QZ step.

We now consider the pair (A, B) satisfing assumptions 1 and 2. We execute an iteration that corresponds to a QR algorithm applied to AB^{-1} .

We look at a single step of the QR algorithm. We want to modify A and B,

$$ar{A} - \lambda ar{B} = ar{Q}^* (A - \lambda B) ar{Z}, \qquad ar{Q}, ar{Z} ext{ unitary.}$$

with \overline{A} Hessenberg and \overline{B} upper triangular. $\overline{A}\overline{B}^{-1}$ is the matrix that is obtained by one step of the QR algorithm applied to AB^{-1} .

The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 2 (cont.) Set $M := AB^{-1}$. *M* is Hessenberg. Let

$$\mathbf{v} = (M - aI)(M - bI)\mathbf{e}_1$$

where *a* and *b* are the eigenvalues of the trailing 2×2 block of *M*. (**v** can be computed in $\mathcal{O}(1)$ flops.) Let P_0 be the Householder reflector with

$$P_0\mathbf{v}=\pm\|\mathbf{v}\|\mathbf{e}_1.$$

Then,

$$A = P_0 A = \begin{pmatrix} \times \times \times \times \times \\ \times \times \times \times \\ + \times \times \times \\ 0 & 0 & \times \\ 0 & 0 & 0 & \times \end{pmatrix}, \quad B = P_0 B \begin{pmatrix} \times \times \times \times \times \\ + & \times \times \times \\ + & + & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & \times \\ 0 & 0 & 0 & \times \\ \end{pmatrix}$$

— The QZ algorithm for $A\mathbf{x} = \lambda B\mathbf{x}$

The QZ algorithm: step 2 (cont.)

Now we restore the Hessenberg-triangular form:

and so on, until the bulge drops out at the end of the matrix.

References

 G. H. Golub and C. F. van Loan. *Matrix Computations*. The Johns Hopkins University Press, Baltimore, MD, 4th ed., 2012.