Fast QR iterations for unitary plus low rank matrices

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The Problem

- Eigenvalues computation $Av = \lambda v$
- if we need all the eigenvalues
- Shifted QR algorithm

$$A_k - \mu_k I = QR$$
$$A_{k+1} = RQ + \mu_k I$$

repeat!

- Textbook approach
- First reduce the matrix to Hessenberg form

The implicit QR algorithm

On upper Hessenberg matrices

- Inizialization phase:
  - Pick the shift μ,
  - Retrieve the vector $x = (A - \mu I)e_1$.
  - x which has only two nonzeros.
  - Compute G_1 such that $G_1 x = \alpha e_1$.
  - Perform the similarity transformation $\tilde{A} = G_1 A G_1^H$.

$\tilde{A}$ is no more in Hessenberg form: a bulge is formed

- Chasing the bulge to restore the Hessenberg structure

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No QR decomposition needed!! Only 2×2 Givens rotations

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No QR decomposition needed!! Only 2×2 Givens rotations
Implicit Q Theorem $\rightarrow$ the same of an explicit QR step

The implicit QR algorithm

On upper Hessenberg matrices

- Inizialization phase:
  - Pick the shift μ,
  - Retrieve the vector $x = (A - \mu I)e_1$.
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  - Perform the similarity transformation $\tilde{A} = G_1 A G_1^H$.

$\tilde{A}$ is no more in Hessenberg form: a bulge is formed

- Chasing the bulge to restore the Hessenberg structure

No QR decomposition needed!! Only 2×2 Givens rotations
Works fabulously with multiple shifts

The implicit QR algorithm

$$A - \mu I = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

Apply Q_0: combine the first two rows and the first two columns of A

The implicit QR algorithm

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Apply Q_0: combine the first two rows and the first two columns of A

The implicit QR algorithm

$$A = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

Chase the Bulge

$$\tilde{A} = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ \otimes & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

Chase the Bulge

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Chase the Bulge

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ {\color{red}0} & \times & \times & \times & \times \\ 0 & {\color{red}\otimes} & \times & \times & \times \\ 0 & 0 & \times & \times & \times \end{bmatrix}$$

Chase the Bulge

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & {\color{red}0} & \times & \times & \times \\ 0 & 0 & {\color{red}\otimes} & \times & \times \end{bmatrix}$$

Chase the Bulge

$$A_1 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & {\color{red}0} & \times & \times \end{bmatrix}$$

The Hessenberg structure is restored

Chase the Bulge

$$A_1 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

The Hessenberg structure is restored

Each step on unstructured matrix costs $O(n^2)$ flops.
Better results with structured matrices!

The Problem

Efficient computation of the eigenvalues of a Unitary-plus-low-rank

$$p(z) = \sum_{i=0}^{n} a_i \phi_i(z)$$

- If $\Phi = \{1, z, z^2, \dots, z^n\}$ we associate the Companion matrix

$$C = \begin{bmatrix} -\frac{a_{n-1}}{a_n} & -\frac{a_{n-2}}{a_n} & \cdots & -\frac{a_0}{a_n} \\ 1 & 0 & \cdots & 0 \\ & \ddots & \ddots & \vdots \\ & & 1 & 0 \end{bmatrix}$$

  the eigenvalues are the roots of $p(z)$.
- Fast algorithms exploit the fact that companion are unitary plus rank-one

$$C = U + e_1 p^T, \quad UU^T = I, U \text{ upper Hessenberg}$$

The Problem

- Companion and block companion matrices
- Fellow matrices (whose eigenvalues are the zeros of a linear combination of Szegö polynomials)
- Perfectly unitary structure corrupted by a low rank error
- Unitary-diagonal matrix plus low rank (interpolation techniques for solving nonlinear eigenproblems)

We assume $A = U + XY^H$ already in Hessenberg form.

The problem

- QR implicit steps on unitary-plus-rank-k
- Need to take advantage from the structure of the matrix otherwise to compute all the eigenvalues we need $O(n^3)$ flops.

$$A = U + XY^H,$$

$U \in \mathbb{C}^{n\times n}$ unitary, $X, Y \in \mathbb{C}^{n\times k}$.

$$\begin{aligned} A &= QR \\ A^{(1)} &= Q^H A Q = Q^H U Q + Q^H X\, Y^H Q = U_1 + X_1 Y_1^H \end{aligned}$$

is still Unitary plus low rank!

- Keyword is representation preserved by QR-steps

Related work

Most authors analyze the companion /block companion case... nothing, to the best of our knowledge, on unitary plus low rank

- 2004 Bini, Daddi, Gemignani (explicit QR)
- 2007 Bini, Eidelman, Gemignani, Gohberg (explicit QR on unitary-plus-rank-1)
- 2007 Chandrasekeran, Gu, Xia, Zhu (implicit QR on a QR factorization of the companion)
- 2012 Delvaux, Frederix, Van Barel (block companion, the matrix is stored using the Givens weight representation)
- 2015-2017 Aurentz, Mach, Robol, Vandebril, Watkins different papers where the representation uses only unitary matrices

The algorithm

The algorithm consists of

- a preliminary phase (we embed the original matrix into a $(n+k) \times (n+k)$ matrix still unitary +rank-k

$$\hat{A} = \left[\begin{array}{c|c} A & * \\ \hline 0_{kn} & 0_{kk} \end{array}\right] = \hat{U} + \hat{X}\hat{Y}^H$$

- computation of the representation of $\hat{A}$
- iterative phase - actual implicit shifted QR step

An $\mathcal{O}(nk)$ representation

$A = U + XY^H$, hence

$$\underbrace{\begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} \times & \cdot & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \times & \cdot & \cdot & \cdot \\ \times & \times & \times & \times & \cdot & \cdot \\ \times & \times & \times & \times & \times & \cdot \\ \times & \times & \times & \times & \times & \times \end{bmatrix}}_{U} + \underbrace{\begin{bmatrix} \times & \times \\ \times & \times \\ \times & \times \\ \times & \times \\ \times & \times \\ \times & \times \end{bmatrix}}_{X} \underbrace{\begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \end{bmatrix}}_{Y^H}$$

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that is $\operatorname{rank}(U(h+1:n, 1:h-1)) = k$, $h = 2, \ldots, n-1$

Representation

Consider first the case $k = 1$. $A = U + xy^H$,

- L lower unitary Hessenberg matrix such that $L^H x = \alpha e_1$
- $L^H U$ is a generalized unitary upper Hessenberg with two diagonals

$$L^H U = \begin{bmatrix} \times & \cdot & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \times & \cdot & \cdot & \cdot \\ 0 & \times & \times & \times & \cdot & \cdot \\ 0 & 0 & \times & \times & \times & \cdot \\ 0 & 0 & 0 & \times & \times & \times \end{bmatrix}$$

Representation

$$A = L \left(\underbrace{\begin{bmatrix} \times & \cdot & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \times & \cdot & \cdot & \cdot \\ 0 & \times & \times & \times & \cdot & \cdot \\ 0 & 0 & \times & \times & \times & \cdot \\ 0 & 0 & 0 & \times & \times & \times \end{bmatrix}}_{L^H U} + \underbrace{\begin{matrix} \times & \times & \times & \times & \times & \times \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{matrix}}_{\alpha e_1 y^H} \right)$$

Representation

$$A = L \left(\underbrace{\begin{bmatrix} \times & \cdot & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \times & \cdot & \cdot & \cdot \\ 0 & \times & \times & \times & \cdot & \cdot \\ 0 & 0 & \times & \times & \times & \cdot \\ 0 & 0 & 0 & \times & \times & \times \end{bmatrix}}_{L^H U} + \underbrace{\begin{matrix} \times & \times & \times & \times & \times & \times \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{matrix}}_{\alpha e_1 y^H} \right)$$

- We can "peal off" another diagonal from $L^H U$

Representation

$$A = L \left(\underbrace{\begin{bmatrix} \times & \cdot & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \cdot & \cdot & \cdot & \cdot \\ 0 & \times & \times & \cdot & \cdot & \cdot \\ 0 & 0 & \times & \times & \cdot & \cdot \\ 0 & 0 & 0 & \times & \times & \cdot \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}}_{L^H U R^H} + \underbrace{\begin{matrix} \times & \times & \times & \times & \times & \times \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{matrix}}_{\alpha e_1 z^H} \right) R$$

- $A = L(L^H U R^H + \alpha e_1 z^H) R$
-

Representation

$$A = L \left(\underbrace{\begin{bmatrix} \times & \cdot & \cdot & \cdot & \cdot & \cdot \\ \times & \times & \cdot & \cdot & \cdot & \cdot \\ 0 & \times & \times & \cdot & \cdot & \cdot \\ 0 & 0 & \times & \times & \cdot & \cdot \\ 0 & 0 & 0 & \times & \times & \cdot \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}}_{L^H U R^H} + \underbrace{\begin{matrix} \times & \times & \times & \times & \times & \times \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{matrix}}_{\alpha e_1 z^H} \right) R$$

- $A = L{\color{red}F}R$
- O(nk) Givens rotations and O(k) vectors

Representation

Skipping all the technicalities about the embedding

Theorem

Let $\hat{A} = \hat{U} + \hat{X}\hat{Y}^H$, then there exist L unitary k-lower Hessenberg, R unitary k-upper Hessenberg, $F = Q + I_{n+k,k}Z^H$ such that

$$\hat{A} = L \cdot F \cdot R. \tag{1}$$

If A is proper ($a_{i+1,i} \neq 0$) and nonsingular also L and R are proper.

An implicit QR step

Single shift case

- Inizialization phase:
  - Compute the shift μ,
  - Retrieve the vector $x = (A - \mu I)e_1$.
  - x which has only two nonzeros.
  - Compute G_1 such that $G_1 x = \alpha e_1$.
  - Perform the similarity transformation $G_1 A G_1^H$.
- Chasing the bulge to restore the Hessenberg structure

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Matrices L, R and F can be represented in terms of Givens rotations acting on two consecutive rows

An implicit QR step

- $A = L\,(Q + e_1 z^H)\,R$

An implicit QR step

- $A = L\,(Q + e_1 z^H)\,R$
- $G_1 A = G_1 L\,(Q + e_1 z^H)\,R = \tilde{L} G_2\,(Q + e_1 z^H)\,R = \tilde{L}(G_2 Q + G_2 e_1 z^H) R = \tilde{L}(\tilde{Q} + e_1 z^H) R$

An implicit QR step

- $A = L\,(Q + e_1 z^H)\,R$
- $G_1 A = G_1 L\,(Q + e_1 z^H)\,R = \tilde{L} G_2\,(Q + e_1 z^H)\,R = \tilde{L}(G_2 Q + G_2 e_1 z^H)R = \tilde{L}(\tilde{Q} + e_1 z^H)R$
- $$\begin{aligned} \tilde{A} = G_1 A G_1^H &= \tilde{L}(\tilde{Q} + e_1 z^H) R G_1^H \\ &= \tilde{L}(\tilde{Q} + e_1 z^H)\tilde{G}_2^H \tilde{R} \\ &= G_2 \hat{L}(\hat{Q} + e_1 \tilde{z}^H)\tilde{R} \end{aligned}$$

An implicit QR step

- $A = L\,(Q + e_1 z^H)\,R$
- $G_1 A = G_1 L\,(Q + e_1 z^H)\,R = \tilde{L} G_2\,(Q + e_1 z^H)\,R =$
  $\tilde{L}(G_2 Q + G_2 e_1 z^H)R = \tilde{L}(\tilde{Q} + e_1 z^H)R$
- $$\begin{aligned}\tilde{A} = G_1 A G_1^H &= \tilde{L}(\tilde{Q} + e_1 z^H) R G_1^H \\ &= \tilde{L}(\tilde{Q} + e_1 z^H)\tilde{G}_2^H \tilde{R} \\ &= G_2 \hat{L}(\hat{Q} + e_1 \tilde{z}^H)\tilde{R}\end{aligned}$$
- To remove the bulge multiply $G_2^H \tilde{A} G_2$. After $n-1$ steps of bulge chasing we recover the Hessenberg structure

Deflation

- The outermost diagonal entries of L and R are always nonzero,
- Deflations can be detected directly on the representation
- $F = Q + I_{nk} Z^H$, Q unitary Hessenberg tends to the triangular form when Q becomes diagonal

$a_{i+1,i} = 0, i = 1, \dots n-1$ iff $q_{i+k,i} = 0$.

Deflation criteria

If $|q_{i+k+1,i+k}| < \varepsilon \prod_{j=1}^{n} |l_{j,j+k}|$ then $|a_{i+1,i}| < \varepsilon$.

Computational cost

- Each step costs $\mathcal{O}(nk)$ flops.
- Total cost of the procedure $\mathcal{O}(n^2k)$.

Applying it to the matrix polynomial eigenvalue problem, with $P(\lambda) = A_0 + A_1\lambda + \cdots + I_m\lambda^d$ and $A_i \in \mathbb{C}^{m\times m}$, we have $n = md$, $k = m$, and we get a cost of $O(m^3d^2)$ which is claimed to be the best achievable by implicit QR.

Backward Stability

The algorithm consists of

- a preliminary phase (we embed the original matrix into a $(n+k)\times(n+k)$ matrix still unitary +rank-k

$$\hat{A} = \left[\begin{array}{c|c} A & * \\ \hline 0_{kn} & 0_{kk} \end{array}\right] = \hat{U} + \hat{X}\hat{Y}^H$$

- computation of the representation
- iterative phase

The preliminary phase is backward stable: error$\approx \varepsilon \|A\|_2$.

Backward Stability: representation

Theorem

- Given $\hat{A} = \hat{U} + \hat{X}\hat{Y}^H$ whose the exact representation is $\hat{A} = LFR$
- Denote by $\tilde{A} = \tilde{L}\tilde{F}\tilde{R}$ the computed one.
- $\tilde{A} = \hat{A} + E$ and $\|E\|_2 \leq c\,\varepsilon\,\|A\|_2$

Backward Stability: implicit QR step

Theorem

Let $\hat{A}^{(1)}$ be the result computed in floating point arithmetic of a QR step on matrix A. Then there exists a perturbation ΔA such that $\hat{A}^{(1)} = P^H(A + \Delta A)P$, and $\|\Delta A\|_2 \approx K_{N,\varepsilon}\mathcal{O}(\varepsilon)\|A\|_2$.

The algorithm is backward stable!

Numerical results

We performed experiments on several classes of matrices

- Scalar polynomials whose roots are known
- Scalar polynomials whose roots are unknown
- Random Fellow matrices with a prescribed norm
- Matrix polynomials from the NLEVP collection
- Fiedler penta-diagonal companion matrices associated to scalar polynomials
- Random unitary plus rank k matrices.
- Random unit diagonal plus random rank k matrices.

Error measures

- Let λ be the "correct" eigenvalue and $\hat{\lambda}$ the closest computed
- Let P_m be the accumulated unitary similarity transformation at the end of the iterative process consisting of m-steps
- A_m is the reconstructed matrix from the representation by the factors L_m, F_m, R_m.

- Forward average error $forw_{err} = \frac{1}{n} \sum_{i=1}^{n} \frac{|\lambda_i - \hat{\lambda}_i|}{|\lambda_i|}$
- Backward error $back_{err} = \frac{\|P_m^H A P_m - A_m\|_\infty}{\|A\|_\infty}$

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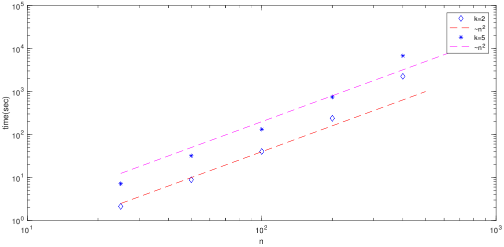
Rule of thumb:

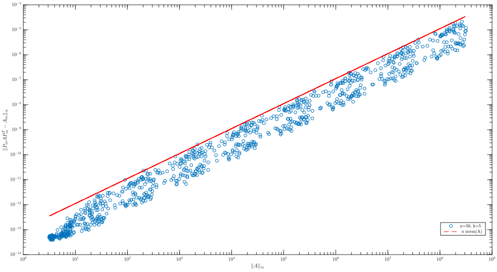
$$\text{forward error} \lesssim \text{condition number} \cdot \text{backward error}$$

Time Complexity



- Confirms that the cost is quadratic in n.
- There is a loss of performance for higher values of n

Backward Error



Dependence of the backward error from the norm of the matrix.

Numerical results

Scalar polynomials

#	degree	$\|\text{condeig}(A)\|_\infty$	forw_{err}	back_{err}	av_{iter}
wil	20	2.47e+27	6.65e-04	2.01e-15	3.29
sswil	20	2.63e+05	7.44e-13	1.93e-15	2.52
proot	20	2.15e+25	4.28e-04	4.61e-15	3.14
2^i	20	6.85e+17	7.34e-05	2.27e-15	4.95
cheb	30	6.31e+10	2.45e-07	2.53e-15	2.61
$\sum x^i$	30	5.57e+00	4.98e-15	2.37e-15	2.64
$(x-1)^n$	10	4.17e+12	4.88e-02	2.36e-15	3.00
clustered	32	4.73e+27	1.58e-01	4.22e-15	3.94
bern	20	9.14e+06	1.86e-13	3.86e-14	3.85
p_1	40	2.08e+01	2.14e-14	2.36e-15	3.00
p_2	29	2.69e+01	5.43e-16	4.23e-15	3.06
p_6	15	2.65e+02	4.00e-16	1.41e-15	3.17
p_7	30	1.87e+05	4.64e-13	9.67e-15	3.32

Table: scalar companion

Numerical results

From the NLEVP collection

#	n	k	$\|\mathrm{condeig}(\mathrm{A})\|_\infty$	$\|A\|_\infty$	$forw_{err}$	$back_{err}$
bicycle	6	2	5.70e+02	9.62e+03	2.60e-15	8.29e-16
clloop	6	2	9.00e+00	3.00e+00	8.99e-16	1.42e-15
qep2	9	3	1.80e+16	4.00e+00	3.31e-09	3.65e-16
spring	15	5	2.33e+00	8.23e+01	3.00e-16	1.93e-15
powplant	24	8	1.72e+05	3.73e+07	7.13e-08	2.68e-15
mtlstrip	27	9	1.71e+02	3.48e+02	7.78e-16	2.42e-15
ocam1	27	9	5.04e+15	1.73e+05	4.03e-07	2.60e-15
acwave1d	30	10	5.96e+01	1.37e+01	1.42e-15	1.02e-14
wiresaw1	30	10	1.57e+01	1.42e+03	6.00e-14	4.20e-15
ocam2	45	15	4.66e+17	6.22e+07	1.16e-02	4.90e-15
orrsom	50	10	1.88e+06	9.67e+00	1.83e-14	6.35e-15
hospital	72	24	4.49e+01	1.11e+04	7.84e-13	2.57e-14
dirac	240	80	2.11e+03	1.38e+03	5.24e-14	1.39e-13
sign1	243	81	3.29e+09	1.53e+01	4.10e-09	5.84e-14
butterfly	320	64	2.97e+01	5.18e+01	5.15e-14	1.29e-13

Numerical results

n	k	$norm(A)$	$\|\text{condeig}(A)\|_\infty$	$back_{err}$
50	1	7.14e+00	4.19e+00	9.45e-15
50	1	9.70e+04	3.52e+01	3.10e-15
50	2	7.19e+00	3.78e+00	9.92e-15
50	2	9.83e+04	3.27e+01	2.91e-15
50	25	8.27e+00	1.00e+15	1.10e-14
50	25	9.98e+04	7.85e+14	3.15e-15
100	1	1.00e+01	1.37e+01	1.79e-14
100	1	9.85e+04	2.04e+02	4.86e-15
100	2	1.01e+01	1.97e+01	1.89e-14
100	2	9.91e+04	1.80e+02	4.78e-15
100	25	1.10e+01	2.18e+07	2.07e-14
100	25	9.99e+04	1.79e+06	5.21e-15

Table: Unitary plus low rank : average on 50 random tests

Numerical results

n	k	$\|\mathrm{condeig(A)}\|_\infty$	$forw_{err}$	$back_{err}$
50	1	2.25e+00	2.66e-16	2.78e-15
50	1	2.25e+00	3.11e-17	2.32e-15
50	2	1.40e+01	1.57e-16	2.78e-15
50	2	2.18e+01	8.83e-14	2.63e-15
50	25	5.59e+01	7.22e-17	2.58e-15
50	25	9.34e+01	8.63e-13	2.21e-15

Table: Unitary diagonal plus low rank: average on 50 random tests

Conclusions and ...

What we have done

- Implicit QR iterations working on the structure
- Algorithm is fast and backward stable
- Everything has been mathematically proved and confirmed by experimental results

What shall be done

- Balancing
- Multishift
- Similar techniques for the QZ