Fast and backward stable computation of the eigenvalues of matrix polynomials

Leonardo Robol, KU Leuven <leonardo.robol@cs.kuleuven.be>

joint work with Jared L. Aurentz (University of Oxford), Thomas Mach (Nazarbayev University), Raf Vandebril (KU Leuven) and David S. Watkins (WSU)

24 Oct 2016, Luminy

The problem

We are interested in solving Polynomial Eigenvalue Problems, that is finding the *eigenvalues* λ such that:

$$\det P(\lambda)v = 0, \qquad P(\lambda) = \sum_{j=0}^d P_j \lambda^j, \qquad P_j \in \mathbb{C}^{m \times m}.$$

The problem

We are interested in solving Polynomial Eigenvalue Problems, that is finding the *eigenvalues* λ such that:

$$\det P(\lambda)v = 0, \qquad P(\lambda) = \sum_{j=0}^d P_j \lambda^j, \qquad P_j \in \mathbb{C}^{m \times m}.$$

- Only square $(m \times m)$ matrix polynomials.
- We are mainly interested in the *eigenvalues*.
- We want a method with an optimal asymptotic cost.

The classical way

The usual strategy to solve a PEP is to build the Frobenius companion linearization:

$$W - \lambda V = \begin{bmatrix} 0_m & \dots & 0_m & -P_0 \\ I_m & & & -P_1 \\ & \ddots & & \vdots \\ & & I_m & -P_{d-1} \end{bmatrix} - \lambda \begin{bmatrix} I_m & & & \\ & \ddots & & \\ & & & I_m \\ & & & & P_d \end{bmatrix}$$

and solve it via the QZ method. The cost is cubic in the size $\implies \mathcal{O}(m^3d^3)$ flops.

We claim that we can do better than that!

Let's look at some specific cases we are all familiar with:

Let's look at some specific cases we are all familiar with:

d = 1 Eigenvalues of an $m \times m$ matrix pencil: we expect the cost to be $\mathcal{O}(m^3)$.

Let's look at some specific cases we are all familiar with:

- d = 1 Eigenvalues of an $m \times m$ matrix pencil: we expect the cost to be $\mathcal{O}(m^3)$.
- m = 1 Roots of a scalar polynomial: exploiting the structure we are able to do that in $\mathcal{O}(d^2)$ flops (in a proven backward stable way!).

Let's look at some specific cases we are all familiar with:

- d = 1 Eigenvalues of an $m \times m$ matrix pencil: we expect the cost to be $\mathcal{O}(m^3)$.
- m = 1 Roots of a scalar polynomial: exploiting the structure we are able to do that in $\mathcal{O}(d^2)$ flops (in a proven backward stable way!).

By combining the above remarks, we aim for $\mathcal{O}(d^2m^3)$ flops.

Some background

We extend the work of Aurentz et al. for the scalar case, which exploits writing a scalar companion matrix in a special structured form.

Some background

We extend the work of Aurentz et al. for the scalar case, which exploits writing a scalar companion matrix in a special structured form.

Let $p(\lambda)$ be a scalar (monic) polynomial of degree d. Its roots are the eigenvalues of the companion matrix:

$$\begin{bmatrix} & & -p_0 \\ 1 & & -p_1 \\ & \ddots & & \vdots \\ & & 1 & -p_{d-1} \end{bmatrix} = \begin{bmatrix} & & 1 \\ 1 & & \\ & \ddots & & \\ & & 1 & \end{bmatrix} + \begin{bmatrix} -p_0 - 1 \\ -p_1 \\ & \vdots \\ -p_{d-1} \end{bmatrix} e_d^T$$

イロト 不同下 イヨト イヨト

The companion matrix is unitary plus rank 1, and this structure is preserved by the QR (or QZ) iterations. How to parametrize it?

The companion matrix is unitary plus rank 1, and this structure is preserved by the QR (or QZ) iterations. How to parametrize it?

Step 0: Enlarge the matrix by adding a row and a column:

$$\begin{bmatrix} & -p_0 & 1 \\ 1 & -p_1 & \vdots \\ & \ddots & \vdots & \vdots \\ & 1 & -p_{d-1} & 0 \\ 0 & \dots & \dots & 0 & 0 \end{bmatrix}$$

The companion matrix is unitary plus rank 1, and this structure is preserved by the QR (or QZ) iterations. How to parametrize it?

Step 1: Compute its QR factorization

$$QR = \begin{bmatrix} 1 & 1 & 0 \\ 1 & & & \\ & \ddots & & \\ & 1 & 0 \\ & & & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -p_1 & 0 \\ & \ddots & \vdots & \vdots \\ & 1 & -p_{d-1} & \vdots \\ & & -p_0 & 1 \\ 0 & \cdots & 0 & 0 \end{bmatrix}$$

The companion matrix is unitary plus rank 1, and this structure is preserved by the QR (or QZ) iterations. How to parametrize it?

Step 2: Decompose the R factor as unitary plus rank 1:

$$R = Y + xy^{T} = \begin{bmatrix} 1 & 0 & 0 \\ & \ddots & 0 & \vdots \\ & 1 & \vdots & \vdots \\ & & 0 & 1 \\ 0 & \cdots & \cdots & 1 & 0 \end{bmatrix} + \begin{bmatrix} -p_{1} \\ \vdots \\ -p_{d-1} \\ -p_{0} \\ -1 \end{bmatrix} e_{d}^{T}$$

6 / 27

The companion matrix is unitary plus rank 1, and this structure is preserved by the QR (or QZ) iterations. How to parametrize it?

Step 3: "Roll up" the column with the coefficients

$$\mathcal{C}\begin{bmatrix} -p_1\\ \vdots\\ -p_{d-1}\\ -p_0\\ -1 \end{bmatrix} = \alpha e_1,$$

and set $\mathcal{B} := \mathcal{C}^* Y$, $y = \alpha e_d^T$, so $W = \mathcal{Q}\mathcal{C}^*(\mathcal{B} + e_1 y^T)$.

Core transformations

The matrices Q, C, and B are sequences of *core transformations*, that are essentially 2×2 matrices. We can write R as:



7 / 27

The same kind of factorization can be done for the leading coefficient, but there is no need for the Q.

The same kind of factorization can be done for the leading coefficient, but there is no need for the Q.

We have

$$V = \mathcal{C}_V^*(\mathcal{B}_V + e_1 y_V^T), \qquad W = \mathcal{Q}\mathcal{C}_W^*(\mathcal{B}_W + e_1 y_V^T).$$

The same kind of factorization can be done for the leading coefficient, but there is no need for the Q.

We have

$$V = \mathcal{C}_V^*(\mathcal{B}_V + e_1 y_V^T), \qquad W = \mathcal{Q}\mathcal{C}_W^*(\mathcal{B}_W + e_1 y_V^T).$$

Basic idea for the QZ: perform unitary similarities with core transformations until W is upper triangular.

The same kind of factorization can be done for the leading coefficient, but there is no need for the Q.

We have

$$V = \mathcal{C}_V^*(\mathcal{B}_V + e_1 y_V^T), \qquad W = \mathcal{Q}\mathcal{C}_W^*(\mathcal{B}_W + e_1 y_V^T).$$

Basic idea for the QZ: perform unitary similarities with core transformations until W is upper triangular.

In our language, that means Q = I.

The matrix polynomial case

We know how to perform the QZ efficiently on unitary plus rank 1 matrices. What about unitary plus rank m?

Treating the unitary plus rank *m* directly is difficult, and easily leads to high complexities in *m*, or instabilities.

The matrix polynomial case

We know how to perform the QZ efficiently on unitary plus rank 1 matrices. What about unitary plus rank m?

- Treating the unitary plus rank *m* directly is difficult, and easily leads to high complexities in *m*, or instabilities.
- Unitary plus rank *m* representations can be cumbersome to work with: it is very difficult to get efficient implementations.

The matrix polynomial case

We know how to perform the QZ efficiently on unitary plus rank 1 matrices. What about unitary plus rank m?

- Treating the unitary plus rank *m* directly is difficult, and easily leads to high complexities in *m*, or instabilities.
- Unitary plus rank *m* representations can be cumbersome to work with: it is very difficult to get efficient implementations.
- ... so we do what mathematician always do: we go back to the previous case.

A nice factorization trick

Let W be the (block) companion of a matrix polynomial $P(\lambda)$. Assume the constant coefficient P_0 is lower triangular. Then we have:

$$W=W_1\ldots W_m,$$

where W_i are scalar companion matrices of polynomial having as coefficients (some of) the coefficients of $P(\lambda)$, appropriately permuted.

A nice factorization trick

Let W be the (block) companion of a matrix polynomial $P(\lambda)$. Assume the constant coefficient P_0 is lower triangular. Then we have:

$$W = W_1 \ldots W_m,$$

where W_i are scalar companion matrices of polynomial having as coefficients (some of) the coefficients of $P(\lambda)$, appropriately permuted.

In particular, the factorization can be computed at *no cost*!

An example



An example



< □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □

Almost the same trick for the leading coefficient

We can factor the leading coefficient in a similar way, if we assume P_d to be upper triangular

$$V = V_1 \dots V_d$$

Almost the same trick for the leading coefficient

We can factor the leading coefficient in a similar way, if we assume P_d to be upper triangular

$$V = V_1 \dots V_d$$

V is upper triangular, and V_j are all elementary Gauss transformations. Again, no computations needed!

Almost the same trick for the leading coefficient

We can factor the leading coefficient in a similar way, if we assume P_d to be upper triangular

$$V = V_1 \dots V_d$$

V is upper triangular, and V_j are all elementary Gauss transformations. Again, no computations needed!

A quick look at Gaussian decomposition



A quick look at Gaussian decomposition



The required structure

In order to compute these decompositions we need the initial structure of the matrix polynomial to be

$$P_{d} P_{d-1} P_{d-2} \cdots P_{1} P_{0}$$

Not restrictive, can be computed by QZ-like algorithm.

The required structure

In order to compute these decompositions we need the initial structure of the matrix polynomial to be

$$P_d$$
 P_{d-1} P_{d-2} \cdots P_1 P_0

Not restrictive, can be computed by QZ-like algorithm.

Our pencil is now

$$W_1 \ldots W_m - \lambda V_1 \ldots V_m,$$

which we can solve as a product eigenvalue problem!

What's missing

Hessenberg-Triangular reduction The matrices V_j are upper triangular, but each of the W_j is upper Hessenberg, thus the product is *m*-Hessenberg. We need to eliminate m - 1 subdiagonals. Chasing We can implement the chasing passing rotations through the triangular factors.

What's missing

Hessenberg-Triangular reduction The matrices V_j are upper triangular, but each of the W_j is upper Hessenberg, thus the product is *m*-Hessenberg. We need to eliminate m - 1 subdiagonals. Chasing We can implement the chasing passing rotations through the triangular factors.

To understand how this works, we need some basic operations with core transformations.

And then we need to pass rotation through upper triangular matrices:



・ロ ・ < 部 ・ < 言 ・ < 言 ・ 言 ・ う へ で 16 / 27

Exploiting the structure

Since we have structured upper triangular matrices, we can pass rotation through them in a fast way:

(recall that
$$R = \mathcal{C}^*(\mathcal{B} + e_1 y^T))$$



The QZ and the Hessenberg-Triangular reduction are (formally) equivalent to the Hessenberg reduction and QR on WV^{-1} .

The QZ and the Hessenberg-Triangular reduction are (formally) equivalent to the Hessenberg reduction and QR on WV^{-1} .

We can write our factorization in a structured form:

$$WV^{-1} = W_1 \dots W_m V^{-1} = QR_1 \dots QR_m V^{-1}$$

The QZ and the Hessenberg-Triangular reduction are (formally) equivalent to the Hessenberg reduction and QR on WV^{-1} .

We can write our factorization in a structured form:

$$WV^{-1} = W_1 \dots W_m V^{-1} = \mathcal{Q}R_1 \dots \mathcal{Q}R_m V^{-1}$$









< □ > < @ > < 볼 > < 볼 > 볼 - 의익증 19/27



□ › < @ › < 볼 › < 볼 › 볼 · 의 < ↔ 20/27



(□) < @) < ≧) < ≧) < ≧) < ≧) < 20 / 27



 $\mathcal{O}(md)$ turnovers per core transformation and $\mathcal{O}(m^2d)$ transformations to annihilate $\implies \mathcal{O}(m^3d^2)$ flops.

20 / 27

The same ideas can be used to chase core transformations until $Q \approx I$. We put a $\tilde{}$ on the matrices and transformations obtained after HT-reduction.

The same ideas can be used to chase core transformations until $Q \approx I$. We put a $\tilde{}$ on the matrices and transformations obtained after HT-reduction.



The same ideas can be used to chase core transformations until $Q \approx I$. We put a $\tilde{}$ on the matrices and transformations obtained after HT-reduction.



The same ideas can be used to chase core transformations until $Q \approx I$. We put a $\tilde{}$ on the matrices and transformations obtained after HT-reduction.

and then we chase it by executing a turnover and similarity:



イロト イポト イヨト イヨト

The same ideas can be used to chase core transformations until $Q \approx I$. We put a $\tilde{}$ on the matrices and transformations obtained after HT-reduction.

until we fuse it at the bottom:



イロン イヨン イヨン イヨン 三日

A quick flop count

A QZ sweep can be completed moving a core transformation down of $\mathcal{O}(md)$ rows.

A quick flop count

A QZ sweep can be completed moving a core transformation down of $\mathcal{O}(md)$ rows.

Each "movement" costs $\mathcal{O}(m)$ passthroughs and 1 turnover, thus a QZ sweep amounts to $O(m^2d)$ flops.

A quick flop count

A QZ sweep can be completed moving a core transformation down of $\mathcal{O}(md)$ rows.

Each "movement" costs $\mathcal{O}(m)$ passthroughs and 1 turnover, thus a QZ sweep amounts to $O(m^2d)$ flops.

Assuming $\mathcal{O}(md)$ steps are required to reach convergence, the cost is $\mathcal{O}(m^3d^2)$.

Complexity in d (4 x 4 matrix polynomial)



23 / 27

Complexity in m (d = 10)



24 / 27

Each passthrough and turnover introduces a small backward error of the order of the unit roundoff u on each of the unitary factors.

- Each passthrough and turnover introduces a small backward error of the order of the unit roundoff u on each of the unitary factors.
- We can prove that the rank 1 part (of each factor) can be recovered from the unitary one.

- Each passthrough and turnover introduces a small backward error of the order of the unit roundoff u on each of the unitary factors.
- We can prove that the rank 1 part (of each factor) can be recovered from the unitary one.
- $\mathcal{O}(u)$ backward error on the unitary part introduces a $\mathcal{O}(||y_j||^2 u)$ backward error on the rank 1 part.

- Each passthrough and turnover introduces a small backward error of the order of the unit roundoff u on each of the unitary factors.
- We can prove that the rank 1 part (of each factor) can be recovered from the unitary one.
- $\mathcal{O}(u)$ backward error on the unitary part introduces a $\mathcal{O}(||y_j||^2 u)$ backward error on the rank 1 part.
- Total backward error of the Schur form (on the original matrix pencil): O(||V||²u) and O(||W||)²u).





• The algorithm has the "optimal" complexity $\mathcal{O}(m^3d^2)$.

Conclusions

- The algorithm has the "optimal" complexity $\mathcal{O}(m^3d^2)$.
- It is fast in practice even for small degrees.

Conclusions

- The algorithm has the "optimal" complexity $\mathcal{O}(m^3d^2)$.
- It is fast in practice even for small degrees.
- It is proven backward stable.

Conclusions

- The algorithm has the "optimal" complexity $\mathcal{O}(m^3d^2)$.
- It is fast in practice even for small degrees.
- It is proven backward stable.

Thank you for your attention!

イロン イロン イヨン イヨン 三日

27 / 27