

A Fast QR Eigenvalue Method for a Class of Structured Matrices

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Outline

- 1 Introduction
- 2 Structured Matrices and Their Representation
- 3 The Algorithm
- 4 Numerical Experiments

Computing Eigenvalues

Problem

Given $A \in \mathbb{R}^{n \times n}$ or $\mathbb{C}^{n \times n}$, compute all its eigenvalues.

This task is usually accomplished by applying the **QR method**:

- Computational cost: $\mathcal{O}(n^3)$
- Storage: $\mathcal{O}(n^2)$.

The method is effective but not suitable for large matrices. But the structure of A can be exploited to achieve a computational cost of $\mathcal{O}(n^2)$ with linear memory space.

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The structure we are interested in...

We consider matrices $A \in \mathbb{C}^{n \times n}$ which are **upper Hessenberg** and have the form

$$A = U - pq^T$$

where

- $U \in \mathbb{C}^{n \times n}$ is **unitary**,
- $p, q \in \mathbb{C}^n$ (**perturbation vectors**).

Observe that U belongs to the class \mathcal{U}_n of $n \times n$ unitary matrices which can be written as a rank one correction of an upper Hessenberg matrix.

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Some History

- **Restarted QR:**
 - Calvetti, Kim, Reichel (2002)
- Explicit structured QR for companion, fellow, unitary-quasiseparable matrices:
 - Bini, Daddi, Gemignani (2004)
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Our Result

For theoretical background, see also the 2006 SIAM Annual Meeting (Boston), session on Structured Matrices and Fast Algorithms.

We present here a new algorithm which

- is based on the implicit QR method,
- computes the eigenvalues of Hessenberg matrices which are unitary + rank 1,
- achieves quadratic computational cost and linear memory,
- shows good stability properties.

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Representation of U

$$U = A + pq^T$$

with U unitary, A upper Hessenberg. We will use two different representations for U :

- as product of "small" unitary matrices,
- as a quasiseparable matrix.

About product structure: compare Schur parametrization (Gragg) and generalized Givens representation (Leuven group).

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Product Structure

Choose 2×2 unitary matrices $\{V_i\}_{i=2,\dots,n-1}$ such that

$$V_i^* \cdot \begin{bmatrix} p_i \\ \beta_{i+1} \end{bmatrix} = \begin{bmatrix} \beta_i \\ 0 \end{bmatrix}, \quad i = n-1, \dots, 2$$

for some complex numbers $\{\beta_i\}_{i=2,\dots,n}$, with $\beta_n = p(n)$. For each i set

$$\tilde{V}_i = \begin{bmatrix} I_{i-1} & & \\ & V_i & \\ & & I_{n-i-1} \end{bmatrix}$$

and define $V = \tilde{V}_{n-1} \cdot \tilde{V}_{n-2} \cdot \dots \cdot \tilde{V}_2$.

Product Structure

 $U =$

$$\begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ p(3)q(1) & \times & \times & \times & \times & \times \\ p(4)q(1) & p(4)q(2) & \times & \times & \times & \times \\ p(5)q(1) & p(5)q(2) & p(5)q(3) & \times & \times & \times \\ p(6)q(1) & p(6)q(2) & p(6)q(3) & p(6)q(4) & \times & \times \end{bmatrix}$$

Product Structure

$$\tilde{V}_5^* \cdot U =$$

$$\begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ p(3)q(1) & \times & \times & \times & \times & \times \\ p(4)q(1) & p(4)q(2) & \times & \times & \times & \times \\ \beta(5)q(1) & \beta(5)q(2) & \beta(5)q(3) & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \end{bmatrix}$$

Product Structure

$$\tilde{V}_4^* \cdot \tilde{V}_5^* \cdot U =$$

$$\begin{bmatrix} \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \\ p(3)q(1) & \times & \times & \times & \times & \times & \times \\ \beta(4)q(1) & \beta(4)q(2) & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times & \times \end{bmatrix}$$

Product Structure

$$\tilde{V}_3^* \cdot \tilde{V}_4^* \cdot \tilde{V}_5^* \cdot U =$$

$$\left[\begin{array}{ccccccc} \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \\ \beta(3)q(1) & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times & \times \end{array} \right]$$

Product Structure

Now choose 3×3 unitary matrices $\{F_i\}_{i=1,\dots,n-2}$ and for each i set

$$\tilde{F}_i = \begin{bmatrix} I_{i-1} & 0 & 0 \\ 0 & F_i & 0 \\ 0 & 0 & I_{n-i-2} \end{bmatrix}.$$

Define $F = \tilde{F}_1 \cdot \tilde{F}_2 \cdot \dots \cdot \tilde{F}_{n-2}$, so that we have...

Product Structure

$$V^* \cdot U =$$

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

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$$\tilde{F}_1^* \cdot V^* \cdot U =$$

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Product Structure

...and the upper triangular factor must be the identity. We obtain a factorization

$$U = V \cdot F$$

where the unitary matrices V and F have the form

$$V = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \times & \times & 0 & 0 & 0 \\ 0 & \times & \times & \times & 0 & 0 \\ 0 & \times & \times & \times & \times & 0 \\ 0 & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \end{bmatrix}, \quad F = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \end{bmatrix}$$

(V is lower Hessenberg and $\text{tril}(F, -3)=0$).

Quasiseparable Structure

First introduced in [Eidelman, Gohberg (1999)].

Definition

$M \in \mathbb{C}^{n \times n}$ is (n_L, n_U) -quasiseparable if

- $n_L = \max_{1 \leq k \leq n-1} \text{rank } M(k+1 : n, 1 : k),$
- $n_U = \max_{1 \leq k \leq n-1} \text{rank } M(1 : k, k+1 : n).$

Quasiseparable matrices can be represented using $\mathcal{O}((n_L + n_U)n)$ parameters.

Quasiseparable Representation of U

Theorem

The upper triangular part of U has the structure

$$U(i, j) = g_i \cdot b_i \cdot b_{i+1} \cdots b_{j-1} \cdot h_j, \quad i \leq j$$

where

- g_1, \dots, g_n are row vectors of length 2,
- h_1, \dots, h_n are column vectors of length 2,
- b_1, \dots, b_{n-1} are 2×2 matrices.

Recall that the $\text{tril}(U, -2)$ is defined by

$$U(i, j) = p(i) \cdot q(j), \quad i > j + 1$$

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Quasiseparable Representation of U

Therefore U can be represented as

$$U = \begin{bmatrix} g_1 \cdot h_1 & g_1 \cdot b_1 \cdot h_2 & g_1 \cdot b_1 \cdot b_2 \cdot h_3 & \dots \\ \sigma_1 & g_2 \cdot h_2 & g_2 \cdot b_2 \cdot h_3 & \dots \\ p(3)q(1) & \sigma_2 & g_3 \cdot h_3 & \dots \\ p(4)q(1) & p(4)q(2) & \sigma_3 & \\ \vdots & & & \end{bmatrix}$$

and it is completely determined by the sets of generators $\{g_i\}$, $\{h_i\}$, $\{b_i\}$, $\{\sigma_i\}$ and the perturbation vectors p and q . [▶ to algorithm](#)

Recovery of Quasiseparable Structure

The quasiseparable representation can easily be recovered from the product representation:

- $h_k = F_k(1 : 2, 1)$ for $k = 1, \dots, n-2$
- $h_{n-1} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, h_n = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
- $b_k = F_k(1 : 2, 2 : 3)$ for $k = 1, \dots, n-2, \quad b_{n-1} = l_2$
- $\gamma_1 = \begin{pmatrix} 0 & 1 \end{pmatrix}, \quad g_1 = \begin{pmatrix} 1 & 0 \end{pmatrix}$
- $\begin{pmatrix} \sigma_k & g_{k+1} \\ q(k) & \gamma_{k+1} \end{pmatrix} = V_{k+1} \begin{pmatrix} \gamma_k & 0 \\ 0 & 1 \end{pmatrix} F_k, \quad k = 1, \dots, n-2$
- $\sigma_{n-1} = \gamma_{n-1} h_{n-1}, \quad g_n = \gamma_{n-1} b_{n-1}$

An Interesting Example: Companion Matrices

Let $P(z) = z^n + \sum_{j=2}^{n+1} c_j z^j$ a real or complex monic polynomial.
Then the associated companion matrix

$$A_P = \begin{bmatrix} -c_2 & -c_3 & \dots & -c_n & -c_{n+1} \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{bmatrix}$$

displays an upper Hessenberg and (unitary + rank one) structure.

Classic Explicit QR

Let $A \in \mathbb{R}^{n \times n}$ or $\mathbb{C}^{n \times n}$. Then the iteration defined by

$$A^{(0)} = A$$

$$A^{(i)} = Q^{(i)} \cdot R^{(i)}$$

$$A^{(i+1)} := R^{(i)} \cdot Q^{(i)}, \quad i = 0, 1, 2, \dots$$

converges to an upper triangular matrix B which has the same eigenvalues as A .

Classic Implicit QR

Let $A \in \mathbb{R}^{n \times n}$ or $\mathbb{C}^{n \times n}$. Then the iteration defined by

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where $A^{(i)} = Q^{(i)} \cdot R^{(i)}$ for $i = 0, 1, 2, \dots$

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Shift Strategies

To accelerate convergence, QR iterations are generally applied to $\mathcal{P}(A^{(i)})$, where $\mathcal{P}(X)$ is a carefully chosen polynomial, rather than to $A^{(i)}$ itself. Usual choices for $\mathcal{P}(X)$ include:

- (single shift) $\mathcal{P}(X) = X - \alpha I$, with $\alpha = X(n, n)$
- (double shift) $\mathcal{P}(X) = (X - \alpha_1 I)(X - \alpha_2 I)$, with α_1 and α_2 eigenvalues of

$$\begin{pmatrix} X(n-1, n-1) & X(n-1, n) \\ X(n, n-1) & X(n, n) \end{pmatrix}$$

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Bulge Chasing

Practical implementation of implicit QR with single shift on an upper Hessenberg matrix A :

- choose Q_1 unitary 2×2 such that

$$Q_1^* \cdot \begin{bmatrix} A(1,1) - \alpha \\ A(2,1) \end{bmatrix} = \begin{bmatrix} \times \\ 0 \end{bmatrix},$$

- perform bulge chasing:

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

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Application to the Quasiseparable Structure

What happens in the structured case?

- The QR iteration preserves the upper Hessenberg and unitary + rank one structure.
- We can carry out each QR iteration working only on the quasiseparable and product representations.

We apply the shifted implicit QR strategy to $A = U - pq^T$. At each iteration:

- the bulge chasing process is applied to A in order to compute the Q_i 's (using the quasiseparable structure), ▷ q.s.rep.
- the product structure of the next iterate $A^{(1)} = Q^* \cdot A \cdot Q$ is computed,
- the quasiseparable structure of $A^{(1)}$ is recovered.

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We apply the shifted implicit QR strategy to $A = U - pq^T$. At each iteration:

- the bulge chasing process is applied to A in order to compute the Q_i 's (using the quasiseparable structure), ▸ q.s.rep.
- the product structure of the next iterate $A^{(1)} = Q^* \cdot A \cdot Q$ is computed,
- the quasiseparable structure of $A^{(1)}$ is recovered.

Numerical Experiments

We implemented this algorithm (**fastQR**) in Fortran 95 for the case of companion matrices. Numerical experiments have been carried out on several families of test polynomials, in order to check:

- growth of running time,
- accuracy of output (comparison with output given by LAPACK),
- (backward) stability,
- comparison of performance with other fast eigenvalue solvers.

Errors

- Absolute forward error: distance between the eigenvalues found by the structured methods and the eigenvalues computed by LAPACK (sort vectors and compute max distance);
- Relative backward error:

$$\text{b.e.} = \frac{\|Q_a^* A_0 Q_a - (V_f F_f - p_f q_f^T)\|_\infty}{\|A_0\|_\infty}$$

where Q_a is the accumulated unitary similarity transformation and V_f, F_f, p_f, q_f are generators for the final iterate A_f .

Estimate for the forward error:

$$K \cdot \epsilon \cdot \|A\|_2 \cdot \max(\text{condeig}(A)).$$

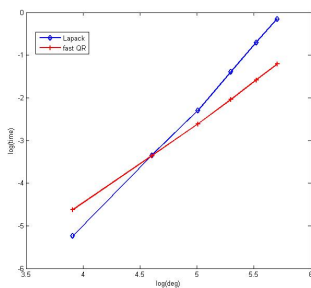
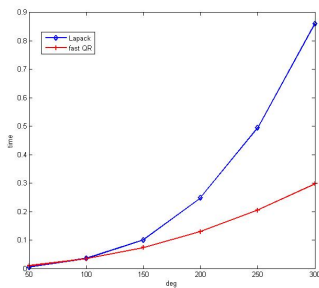
Single Shift, Random Coefficients

Example 1: Monic polynomials with complex pseudorandom coefficients; both the real and imaginary part belong to $[-1, 1]$:

- compare running time to LAPACK (routine ZGEEV),
- check growth of running time,
- check forward and backward errors.

Single Shift, Random Coefficients

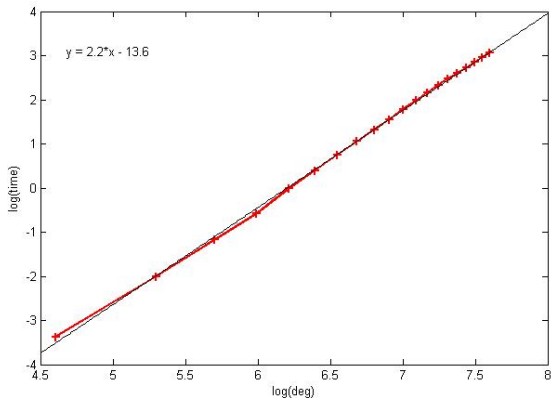
Comparison with LAPACK



Single Shift, Random Coefficients

Time growth, log-log plot

Polynomials of degrees from 50 to 2000



Single Shift, Random Coefficients II

Example 2: $P(z) = z^n + \sum_{j=0}^{n-1} a_j z^j$, with $a_j = u_j \cdot 10^{v_j}$, where $|u_j| \in [-1, 1]$ and $v_j \in [-5, 5]$.

deg	b.e.	f.e.	δ
50	4.91×10^{-15}	6.24×10^{-10}	2.21×10^{-8}
100	6.63×10^{-15}	6.95×10^{-10}	1.61×10^{-8}
150	7.02×10^{-15}	3.19×10^{-10}	1.12×10^{-7}
500	7.43×10^{-15}	8.30×10^{-10}	8.28×10^{-7}
1000	1.44×10^{-14}	1.47×10^{-9}	1.59×10^{-6}

$$\delta = \epsilon \cdot \|A\|_2 \cdot \max(\text{condeig}(A))$$

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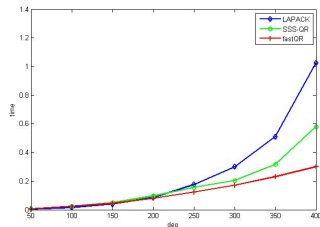
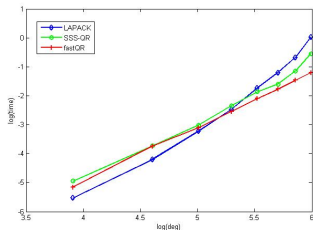
Example 3: Monic polynomials with real pseudorandom coefficients in $[-1, 1]$:

- compare running time to LAPACK (routine DGEEV) and SSS-QR (Chandrasekaran et al.),
- check growth of running time,
- check forward errors.

Double Shift, Random Coefficients

Comparison with LAPACK and SSS-QR

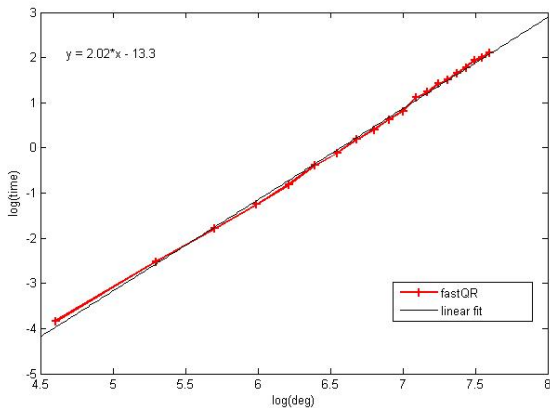
absolute forward errors $\sim 10^{-14}$



Double Shift, Random Coefficients

Time growth, log-log plot

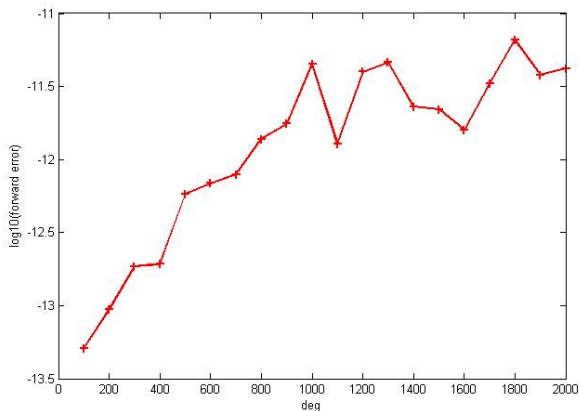
Polynomials of degrees from 50 to 2000



Double Shift, Random Coefficients

Forward errors, log plot

Polynomials of degrees from 50 to 2000



Double Shift, Roots of 1

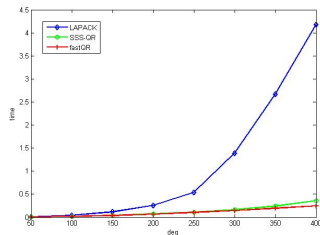
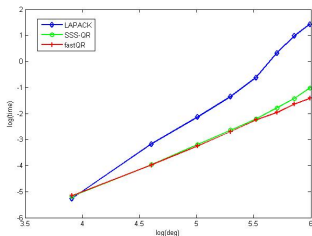
Example 4: $P(x) = x^n - 1$

- compare running time to LAPACK (routine DGEEV) and SSS-QR (Chandrasekaran et al.),
- check forward errors.

Double Shift, Roots of 1

Comparison with LAPACK and SSS-QR

absolute forward errors $\sim 10^{-15}$



Summary and Future Work

- We have developed and implemented a fast version of the implicit QR method for Hessenberg matrices which are rank-one perturbations of unitary matrices.
- Numerical tests show that the algorithm has good stability properties and confirm theoretical estimates on computational cost ($\mathcal{O}(n^2)$) and required memory space ($\mathcal{O}(n)$).
- Open issue: give a theoretical proof of stability (the use of a representation via unitary matrices may prove helpful).

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Computation of New Product Structure (Single Shift)

$$A^{(1)} = \tilde{Q}_{n-1}^* \cdots \tilde{Q}_1^* \cdot \tilde{V}_{n-1} \cdots \tilde{V}_2 \cdot \tilde{F}_1 \cdots \tilde{F}_{n-2} \cdot \tilde{Q}_1 \cdots \tilde{Q}_{n-1}$$

Observe that

- \tilde{Q}_k^* commutes with $\tilde{V}_{n-1}, \dots, \tilde{V}_{k+2}$ for $1 \leq k \leq n-3$
- \tilde{Q}_k commutes with $\tilde{F}_{n-2}, \dots, \tilde{F}_{k+3}$ for $1 \leq k \leq n-4$

so we have

$$A^{(1)} = \tilde{Q}_{n-1}^* \cdots \tilde{V}_4 \cdot \tilde{Q}_2^* \cdot \tilde{V}_3 \cdot \tilde{Q}_1^* \cdot \tilde{V}_2 \cdot \tilde{F}_1 \cdot \tilde{F}_2 \cdot \tilde{Q}_1 \cdot \tilde{F}_3 \cdot \tilde{Q}_2 \cdot \tilde{F}_4 \cdots \tilde{Q}_{n-1}$$

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$$\left[\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & & \\ 0 & V_{k+2} & \end{array} \right] \cdot \left[\begin{array}{c|c} V_{k+1}^{(\tau)} & 0 \\ \hline 0 & 0 \\ \hline 0 & 0 & 1 \end{array} \right]$$

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$$\left[\begin{array}{cc|c} Q_{k+1}^* & 0 & \\ & 0 & \\ \hline 0 & 0 & 1 \end{array} \right] \cdot \quad \left[\begin{array}{ccc} \times & \times & 0 \\ \times & \times & \times \\ \times & \times & \times \end{array} \right]$$

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$$\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \cdot \left[\begin{array}{c|c} H^* & 0 \\ \hline 0 & 0 \\ \hline 0 & 1 \end{array} \right]$$

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$$\left[\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & & \\ 0 & V_{k+2}^{(\tau)} & \end{array} \right] \cdot \left[\begin{array}{c|c} V_{k+1}^{(1)} & 0 \\ \hline 0 & 0 \\ 0 & 0 & 1 \end{array} \right]$$

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$$\left[\begin{array}{c|ccc} & 0 & & & \\ & 0 & & & \\ F_k^{(\tau)} & 0 & & & \\ \hline 0 & 0 & 0 & 1 & \end{array} \right] \cdot \left[\begin{array}{c|ccc} 1 & 0 & 0 & 0 \\ \hline 0 & & & \\ 0 & & F_{k+1} & \\ 0 & & & \end{array} \right] \cdot$$

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$$\begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ 0 & \times & \times & \times \end{bmatrix} \cdot \left[\begin{array}{c|cc} Q_k & 0 & 0 \\ & 0 & 0 \\ \hline 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right]$$

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$$\cdot \left[\begin{array}{cc|cc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 0 & 0 & H & \\ 0 & 0 & & \end{array} \right] \cdot \left[\begin{array}{cccc} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{array} \right]$$

Computation of New Product Structure (Single Shift)

$$A^{(1)} = \tilde{Q}_{n-1}^* \cdot \dots \cdot \tilde{V}_{k+2}^{(\tau)} \cdot \tilde{V}_{k+1}^{(1)} \cdot \tilde{H}^* \cdot \tilde{V}_k^{(1)} \cdot \dots \cdot \tilde{V}_2^{(1)} \cdot \\ \cdot \tilde{F}_1^{(1)} \cdot \dots \cdot \tilde{F}_{k-1}^{(1)} \cdot \tilde{H} \cdot \tilde{F}_k^{(\tau)} \cdot \tilde{F}_{k+1} \cdot \tilde{Q}_k \cdot \dots \cdot \tilde{Q}_{n-1}$$

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

Computation of New Product Structure (Single Shift)

$$A^{(1)} = \tilde{Q}_{n-1}^* \cdot \dots \cdot \tilde{V}_{k+2}^{(\tau)} \cdot \tilde{V}_{k+1}^{(1)} \cdot \tilde{H}^* \cdot \tilde{V}_k^{(1)} \cdot \dots \cdot \tilde{V}_2^{(1)} \cdot \\ \cdot \tilde{F}_1^{(1)} \cdot \dots \cdot \tilde{F}_{k-1}^{(1)} \cdot \tilde{H} \cdot \tilde{F}_k^{(1)} \cdot \tilde{F}_{k+1}^{(\tau)} \cdot \dots \cdot \tilde{Q}_{n-1}$$

$$\left[\begin{array}{c|ccc} & 0 & & & \\ & 0 & & & \\ & 0 & & & \\ \hline 0 & 0 & 0 & 1 \end{array} \right] \cdot \left[\begin{array}{c|ccc} 1 & 0 & 0 & 0 \\ \hline 0 & & & \\ 0 & & & \\ 0 & & & \end{array} \begin{array}{c} \\ F_{k+1}^{(\tau)} \\ \\ \end{array} \right] \cdot$$