Efficient generalized Hessenberg form and applications

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This paper proposes an efficient algorithm for reducing matrices to the generalized Hessenberg form by unitary similarity, and recommends using it as a preprocessor in a variety of applications. As an illustration of its power, two cases from control theory are analyzed in detail: a solution procedure for a sequence of shifted linear systems with multiple right hand sides (e.g. evaluating transfer function of a linear time invariant (LTI) dynamical system, with multiple inputs and outputs, at many complex values) and computation of the staircase form. The proposed algorithm for the generalized Hessenberg reduction introduces two levels of aggregation of Householder reflectors, thus allowing efficient BLAS 3 based computation. Another level of aggregation is introduced when solving many shifted systems by processing the shifts in batches. Numerical experiments confirm that the proposed methods have superior efficiency.

Categories and Subject Descriptors: G1 [**Numerical Analysis**]: Numerical Linear Algebra—*Error Analysis*; G4 [**Mathematical Software**]: —*Reliability*; *Robustness*

General Terms: Algorithms, Reliability, Theory

Additional Key Words and Phrases: Hessenberg form, shifted linear systems, staircase algorithm, transfer function

1. INTRODUCTION

Hessenberg form belongs to the tools of trade of numerical linear algebra. We say that $H \in \mathbb{R}^{n\times n}$ is *m-Hessenberg* matrix, $m < n$, if $H_{ij} = 0$ for all $i, j = 1, \ldots, n$ such that $i > j + m$. Any $A \in \mathbb{R}^{n\times n}$ can be written as $A = UHU^T$, where U is orthogonal and H is m-Hessenberg form of A. Such a generalized Hessenberg structure naturally arises e.g. in the block Arnoldi algorithm, and it is very frequent in the computational control. For instance, the *controller Hessenberg form* of $(A, B) \in \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times m}$ is $(H, \left(\begin{smallmatrix} R \\ 0 \end{smallmatrix}\right)) = (Q^T AQ, Q^T B)$, where Q is orthogonal, H is m-Hessenberg and R is upper triangular.

For computing the standard (1-)Hessenberg form, the state of the art software package LAPACK [Anderson et al. 1992] contains an optimized subroutine `xGEHRD`. Recent work by Tomov and Dongarra [Tomov and Dongarra 2009] shows that on a hybrid CPU/GPU parallel computing machinery, a considerable speedup over `xGEHRD` is possible; see also [Tomov et al. 2010]. In a distributed parallel computing environment, ScaLAPACK [ScaLAPACK 2009] provides parallel subroutines `PxGEHRD`. For the controller Hessenberg form, the computational control library SLICOT [SLICOT 2009] contains the subroutine `TB01MD`, which also computes the m-Hessenberg form. Unlike `xGEHRD`, the subroutine `TB01MD` does not use aggregated transformations (block reflectors). As a consequence, its low flop–to–memory–reference ratio cannot provide optimal efficiency. Our goal is high performance CPU and CPU/GPU software for the generalized Hessenberg form and its applications. We are in particular interested in the computational control applications and contributions to the control library SLICOT.

In the first stage of the development, we give detailed block CPU implementa-

tions. Section 2 describes the new algorithm for m-Hessenberg reduction. In §3, we apply the m-Hessenberg form as a preprocessor and improve the efficiency of the staircase reduction, which is one of the structure revealing canonical forms of LTI systems [Dooren 1979]. In §4, we show how to use the m-Hessenberg form and a variant of incomplete RQ factorization to compute $C(\sigma I - A)^{-1}B$ very efficiently for possibly large number of complex values σ. Numerical experiments in §5 show that the new algorithms provide superior performances. The second part of this work, in a separate report [Bosner et al. 2011], contains parallel hybrid CPU/GPU implementations of the algorithms from this paper.

2. A BLOCK ALGORITHM FOR M-HESSENBERG FORM

As with the QR and the 1-Hessenberg LAPACK routines, the main idea for a faster m-Hessenberg algorithm is to partition the $n \times n$ matrix[1] A into blocks of b consecutive columns, $A = (A^{(1)} \;\; A^{(2)} \;\; \ldots \;\; A^{(l)})$, $l = \lceil n/b \rceil$. Each of the leading $l-1$ blocks carries b columns, while the last one contains the remaining $n-(l-1)b$ ones. After determining suitable block size b, the blocks are processed one at a time, from left to right, and the computation is organized to enhance temporal and spatial data locality. In particular, some transformations are postponed until the very last moment in which the updated content is actually needed for the next step. Accumulated transformations are then applied in a block fashion, thus increasing the flop count per memory reference. Many details and tricks are involved, and this section contains the blueprints of the new algorithm.

2.1 Processing a single block

Processing a block consists of constructing b Householder reflectors that annihilate appropriate elements in each of the block's columns. For the i-th block $A^{(i)} = (a_1^{(i)} \; a_2^{(i)} \; \ldots \; a_b^{(i)})$, define a sequence of Householder reflectors: for $j = 1, 2, \ldots, b$, let $H_j = I - \tau_j v_j v_j^\tau$ be the Householder reflector such that the vector $H_j H_{j-1} \cdots H_1 a_j^{(i)}$ has zeros as its $(k+j+1)$-th, $(k+j+2)$-th, …, n-th element (with an offset k that will be a function of i and b). Here τ_j is a scalar and v_j is a vector such that $v_j(1 : k+j-1) = 0$ and $v_j(k+j) = 1$. These vectors are stored in the matrices $V_j = (v_1 \;\; v_2 \;\; \ldots \;\; v_j)$. (The introduction of the V_j matrices is for explanatory purposes only.) As in `xGEHRD`, the non-trivial elements of the vectors v_j are stored in the matrix A in places of entries that have been zeroed by the H_j's. In our description of the algorithm, we overwrite the initial data, thus there will be no "time stepping" index in our notation.

To set the stage for the new algorithm and to introduce necessary notation, we briefly describe block reflectors. For more details we refer the reader to [Schreiber and van Loan 1989].

PROPOSITION 1. *The product $Q_j = H_1 H_2 \ldots H_j$ can be represented as $Q_j = I - V_j T_j V_j^\tau$, where T_j is an upper triangular $j \times j$ matrix.*

PROOF. The construction of T_j is inductive: we first set $V_1 = (v_1)$, $T_1 = \tau_1$, and

[1] For the sake of brevity, we describe only the real case. The algorithm is easily extended, mutatis mutandis, to complex matrices.

then we easily verify that, for $t_+ = -\tau_j T_{j-1} V_{j-1}^\tau v_j$, it holds

$$\begin{aligned} Q_j &= Q_{j-1} H_j = (I - V_{j-1} T_{j-1} V_{j-1}^\tau) \cdot (I - \tau_j v_j v_j^\tau) \\ &= I - (V_{j-1} \;\; v_j) \cdot \begin{pmatrix} T_{j-1} & t_+ \\ 0 & \tau_j \end{pmatrix} \cdot (V_{j-1} \; v_j)^\tau . \end{aligned}$$

Thus, setting $T_j = \begin{pmatrix} T_{j-1} & t_+ \\ 0 & \tau_j \end{pmatrix}$ completes the proof. □

Once the block is processed, we will have to update

$$A \leftarrow Q^\tau A Q = (I - V T^\tau V^\tau) A (I - V T V^\tau) = (I - V T^\tau V^\tau)(A - Y V^\tau) \,, \qquad (1)$$

where $V = V_b$, $T = T_b$, $Q = Q_b$ and $Y = AVT$. The auxiliary matrix Y will be used for fast update of the matrix A "from the right-hand side" ($A \leftarrow A - YV^\tau$).

PROPOSITION 2. *The matrices $Y_j = Y(:, 1:j) = AV_jT_j$ satisfy:*

$$Y_1 = \tau_1 A v_1; \;\; Y_j = \left(Y_{j-1} \;\; \tau_j(-Y_{j-1} \cdot V_{j-1}^\tau v_j + A v_j) \right). \qquad (2)$$

PROOF. Starting with $Y_1 = \tau_1 A v_1$ and using Proposition 1, we have

$$\begin{aligned} Y_j &= A \cdot \left(V_{j-1} \;\; v_j \right) \cdot \begin{pmatrix} T_{j-1} & t_+ \\ 0 & \tau_j \end{pmatrix} = \left(A V_{j-1} T_{j-1} \;\; A V_{j-1} t_+ + \tau_j A v_j \right) \\ &= (\text{since } t_+ = -\tau_j T_{j-1} V_{j-1}^\tau v_j) = \left(Y_{j-1} \;\; \tau_j(-Y_{j-1} \cdot V_{j-1}^\tau v_j + A v_j) \right). \qquad (3) \end{aligned}$$

□

In order to compute the reflector that annihilates the elements in the j-th column of the block, we must have already updated this part of the matrix A with the accumulated product $H_{j-1} \cdots H_1$. To that end, we use Y_{j-1}, following (1). Note that computing the reflectors requires only the elements of A in the rows from $(k+1)$-st on – thus the update will also require only the elements of Y_{j-1} with the same row indices. The processing of a single block is outlined in Algorithm 1 and the details are given in §2.1.1-§2.1.4.

2.1.1 *Updating $a_j^{(i)}(k{+}1 : n)$ from the right.* In line 4 of Algorithm 1, the column $a_j^{(i)}(k+1:n)$ is updated by the transformation from the right. The details of this update are given in Algorithm 2 and in Figure 1, which illustrates the situation in the case $n = 15$, $m = 2$ and the block size $b = 5$. The current block $A^{(i)}$ is shaded ($i = 2$); the parameter k is equal to $(i-1) \cdot b + m = 7$. The elements of a particular column $a_j^{(i)}$ are shown as diamonds and filled circles ($j = 4$). All elements below the m-th subdiagonal in the columns to the left of $a_j^{(i)}$ have already been set to zero by the algorithm, and our goal now is to use a Householder reflector and zero out those elements of the column $a_j^{(i)}$ that are shown as filled circles.

Prior to that, we have to apply to this column the previously generated block reflector $I - V_{j-1} T_{j-1} V_{j-1}^\tau$ from both the left and the right. During the block processing, only the row indices $k+1:n$ of $a_j^{(i)}$ will be updated – the remaining indices are not involved in computation of the Householder reflectors for the current block. For the same reason, only the rows $k+1:n$ of Y_{j-1} and V_{j-1} will be

ALGORITHM 1: Processing of a block to reduce it to m-Hessenberg form

Input: block $A^{(i)}$, block size b, index k
Output: partially updated block $A^{(i)}$, transformation matrices Y and T, auxiliary array TAU; details in §2.1.1, 2.1.2, 2.1.3.

1 **for** $j = 1, 2, \ldots, b$ **do**
2 **if** $j > 1$ **then**
3 Update $a_j^{(i)}(k+1:n)$:
4 $a_j^{(i)}(k+1:n) = a_j^{(i)}(k+1:n) - (Y_{j-1}V_{j-1}^{\tau})(k+1:n, k+j-m)$;
5 Multiply $a_j^{(i)}(k+1:n)$ with $I - V_{j-1}T_{j-1}^{\tau}V_{j-1}^{\tau}$ from the left;
6 **end**
7 Generate the elementary reflector H_j to annihilate $a_j^{(i)}(k+j+1:n)$;
8 Set $TAU(j) = \tau_j$, and compute $Y_j(k+1:n, j)$;
9 Compute $T_j(:, j)$;
10 **end**
11 Compute $Y(1:k, 1:b)$;

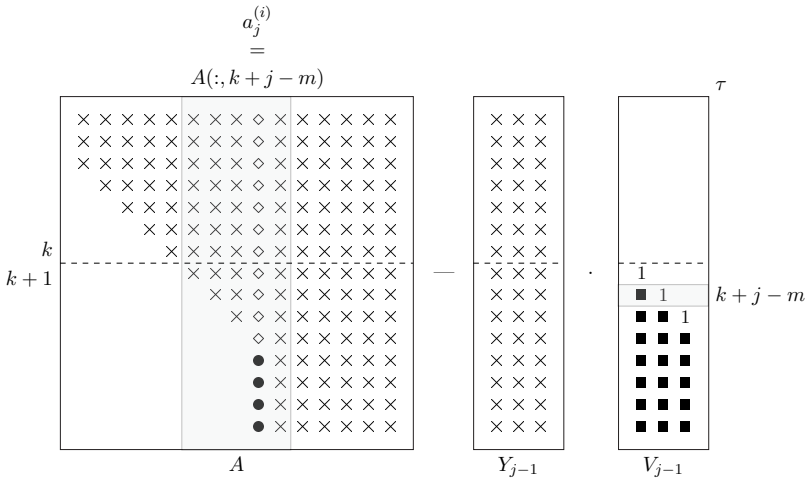


Fig. 1: Updating column $a_j^{(i)}(k+1:n)$ from the right (line 4 in Algorithm 1)

referenced. The horizontal dashed line separates the rows $1:k$ and $k+1:n$ of all matrices in the figure. All action takes place below this line.

The non-trivial elements of the matrix V_{j-1} are shown as ■ – these are actually stored in places of the elements of $A^{(i)}$ that have already been zeroed out. All elements above the ones in the matrix V_{j-1} are zero. Note that the j-th column of the block $A^{(i)}$ is the $((i-1)\cdot b + j = k + j - m)$-th column of the original matrix A. Thus, updating the column $a_j^{(i)}$ involves only the row $k+j-m$ of the matrix V_{j-1} – the shaded one in Figure 1. In fact, what is needed from this row are the leading $j-m-1$ elements stored in $A^{(i)}(k+j-m, 1:j-m-1)$, and a single

ALGORITHM 2: Details of line 4 in Algorithm 1

4.1 **if** $j > m$ **then**
4.2 $\quad temp = a^{(i)}_{j-m}(k+j-m)$;
4.3 $\quad a^{(i)}_{j-m}(k+j-m) = 1$;
4.4 $\quad$ Call `xGEMV` (`BLAS 2`) to compute
$\quad\quad a^{(i)}_{j}(k+1:n) = a^{(i)}_{j}(k+1:n) -$
$\quad\quad\quad Y_{j-1}(k+1:n, 1:j-m) \cdot \left(A^{(i)}(k+j-m, 1:j-m)\right)^{\tau}$;
4.5 $\quad a^{(i)}_{j-m}(k+j-m) = temp$;
end

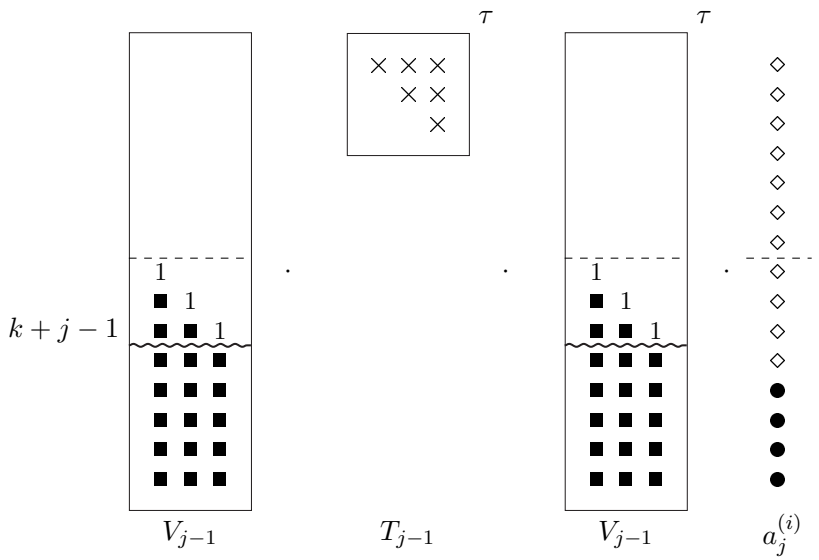


Fig. 2: Updating column $a^{(i)}_j(k+1:n)$ from the left

element 1 (thus the trick with introducing 1 in line 4.3 in Algorithm 2).

2.1.2 *Updating $a^{(i)}_j(k+1:n)$ from the left.* The details of the implementation of line 5 in Algorithm 1 are given in Algorithm 3, and illustrated in Figure 2.

The lines 5.2 and 5.3 compute the product $V^{\tau}_{j-1}a^{(i)}_j$. This multiplication is carried out in two phases: first, we multiply the triangular block $V_{j-1}(k+1:k+j-1, 1:j-1)$ using the `xTRMV` routine. This routine can be deployed to "pretend" as if the lower triangular matrix has ones on its diagonal without explicitly looking up matrix elements, enabling us to avoid the temporary backup of elements of $A^{(i)}$ which occupy that place. (This triangular block of V_{j-1} is between the dashed and the wavy line in Figure 2.) Then the rectangular block $V_{j-1}(k+j:n, 1:j-1)$ multiplies the rest of vector $a^{(i)}_j$.

In line 5.4, the vector $T^{\tau}_{j-1}V^{\tau}_{j-1}a^{(i)}_j$ is formed, and lines 5.5–5.7 complete the

ALGORITHM 3: Details of line 5 in Algorithm 1

5.1 Copy $a_j^{(i)}(k+1:k+j-1)$ to $T(1:j-1,j)$;
5.2 Call `xTRMV` (`BLAS 2`) to compute
$T(1:j-1,j) = \left(A^{(i)}(k+1:k+j-1,1:j-1)\right)^\tau \cdot T(1:j-1,j)$;
5.3 Call `xGEMV` to compute
$T(1:j-1,j) = T(1:j-1,j) + \left(A^{(i)}(k+j:n,1:j-1)\right)^\tau \cdot a_j^{(i)}(k+j:n)$;
5.4 Call `xTRMV` to compute $T(1:j-1,j) = T_{j-1}^\tau \cdot T(1:j-1,j)$;
5.5 Call `xGEMV` to compute
$a_j^{(i)}(k+j:n) = a_j^{(i)}(k+j:n) - A^{(i)}(k+j:n,1:j-1) \cdot T(1:j-1,j)$;
5.6 Call `xTRMV` to compute
$T(1:j-1,j) = A^{(i)}(k+1:k+j-1,1:j-1) \cdot T(1:j-1,j)$;
5.7 $a_j^{(i)}(k+1:k+j-1) = a_j^{(i)}(k+1:k+j-1) - T(1:j-1,j)$;

ALGORITHM 4: Details of line 8 in Algorithm 1

8.1 $temp = a_j^{(i)}(k+j)$; $a_j^{(i)}(k+j) = 1$;
8.2 Call `xGEMV` to compute
$Y_j(k+1:n,j) = A(k+1:n,k+j:n) \cdot a_j^{(i)}(k+j:n)$;
8.3 Call `xGEMV` to compute
$T_j(1:j-1,j) = \left(A^{(i)}(k+j:n,1:j-1)\right)^\tau \cdot a_j^{(i)}(k+j:n)$;
8.4 Call `xGEMV` to compute
$Y_j(k+1:n,j) = Y_j(k+1:n,j) - Y_{j-1}(k+1:n,:) \cdot T_j(1:j-1,j)$;
8.5 Scale $Y_j(k+1:n,j)$ by multiplying it with $\tau_j = TAU(j)$;

transformation by multiplying that vector by V_{j-1} from the left.

2.1.3 *Other details of block processing.* The line 7 is a single call of the LAPACK routine `xLARFG`. The Householder vector is stored in $a_j^{(i)}(k+j+1:n)$, while the scalar τ_j is stored in an auxiliary array TAU as the element $TAU(j)$.

Next, in line 8, we append a column to Y_{j-1} to define Y_j as in (2). Note that $a_j^{(i)}(k+j+1:n)$ now contains the non-trivial part of the j-th elementary Householder vector. Algorithm 4 gives the details.

Line 8.2 is the only line in the loop of the block processing algorithm that references elements of A outside of the current block $A^{(i)}$. This is also the only line which deals with a matrix of dimension $\mathcal{O}(n) \times \mathcal{O}(n)$; all others have at least one dimension of block size b or less. Line 8.3 computes the product $V_{j-1}^\tau v_j$ – observe that $v_j(1:k+j-1) = 0$, so we can disregard the rows 1 to $k+j-1$ of the matrix V_{j-1}. The old value of the element $a_j^{(i)}(k+j)$, whose backup copy is in line 8.1, can be restored after the update of the next column $a_{j+1}^{(i)}$.

All that is now left to do in order to complete the matrix T_j is to re-scale the current content of its last column by $TAU(j)$, and to multiply it by T_{j-1} from the left by using yet another call to `xTRMV`. Finally, we show how to compute the first

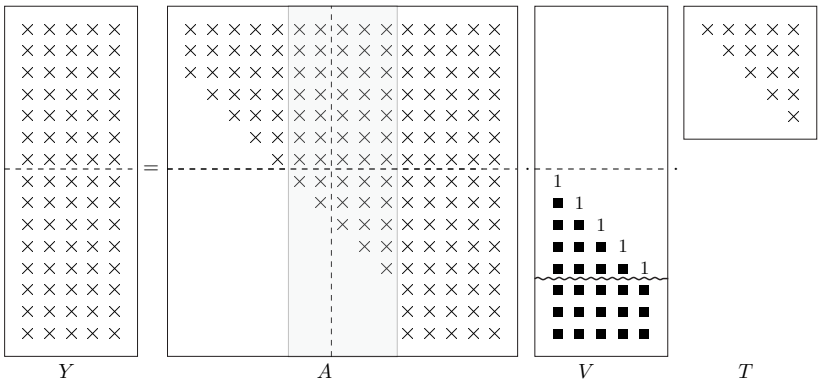


Fig. 3: Updating first k rows of Y

k rows of Y, outside of the main loop in Algorithm 1 (line 11):

ALGORITHM 5: Details of line 11 in Algorithm 1

11.1 Copy $A(1:k, k+1:k+b)$ to $Y(1:k, 1:b)$;

11.2 Call `xTRMM` (`BLAS 3`) to compute

$$Y(1:k,1:b) = Y(1:k,1:b) \cdot A^{(i)}(k+1:k+b,1:b);$$

11.3 Call `xGEMM` (`BLAS 3`) to compute

$$Y(1:k,1:b) = Y(1:k,1:b) + A(1:k,k+b+1:n) \cdot A^{(i)}(k+b+1:n,1:b);$$

11.4 Call `xTRMM` to compute $Y(1:k,1:b) = Y(1:k,1:b) \cdot T$;

In Figure 3, the region below the elements denoted by $\times$ in the current block (shaded) of the matrix A has been zeroed out. It now stores the non-trivial part of the matrix V (elements denoted by $\blacksquare$). Multiplication by the matrix V from the right in lines 11.2 and 11.3 is once again split into triangular and rectangular parts. Line 11.3 references elements not in the current block. Note that only the columns $k+1:n$ of the matrix A (the ones to the right of the vertical dashed line) are referenced while updating Y, because of the zero-pattern in V.

2.1.4 *The concept of mini-blocks.* The first m columns of a block do not need to be updated from the right since the corresponding rows of the matrices V_{j-1} are zero. Moreover, if m is greater than or equal to the block size, then the updates from the right are not needed at all within the current block.[2] When m is less than the block size, this fact permits another variant of Algorithm 1 in which:

(1) The block is split into several disjoint *"mini-blocks"*, each (except maybe the last one) consisting of m consecutive columns.

(2) In each "mini-block", column by column is updated only from the left, and the appropriate elements are annihilated.

[2]We are indebted to Daniel Kressner [Kressner 2010] for pointing this out; a similar concept is also used in [Bischof et al. 2000] for the reduction of a symmetric matrix to the tridiagonal form. The mini-blocks are also successfully used in [Karlsson 2011].

ALGORITHM 6: Processing of a block by using mini-blocks to reduce it to m-Hessenberg form

Input: block $A^{(i)}$, block size b, index k
Output: partially updated block $A^{(i)}$, transformation matrices Y and T, auxiliary array TAU

```
1  for j = 1, 2, ... b do
2      if j > 1 then
3          Update a_j^(i)(k+1 : n) only from the left by applying I − V_{j−1} T_{j−1}^τ V_{j−1}^τ;
4      end
5      Generate the elementary reflector H_j to annihilate a_j^(i)(k + j + 1 : n);
6      Compute T_j(:, j);
7      if j mod m = 0 or j = b then
8          cMini = m or (b mod m); // current miniblock size
9          nMini = min{b − j, m}; // next miniblock size
10         Compute Y_j(k + 1 : n, j − cMini + 1 : j);
11         Call xGEMM to update the entire next miniblock from the right:
           A^(i)(k + 1 : n, j + 1 : j + nMini) =
           A^(i)(k + 1 : n, j + 1 : j + nMini) − (Y_j V_j^τ)(k + 1 : n, j + 1 : j + nMini);
12     end
13 end
14 Compute Y(1 : k, 1 : b);
```

(3) A *"mini-reflector"* $\mathcal{Q}_m = I - \mathcal{V}_m \mathcal{T}_m \mathcal{V}_m^\tau$ is aggregated from m annihilations.

(4) After processing of the "mini-block", the block reflector Q_{j+m} is updated:

$$\left.\begin{aligned} V_{j+m} &= \begin{pmatrix} V_j & \mathcal{V}_m \end{pmatrix}; \\ T_{j+m} &= \begin{pmatrix} T_j & T_{jm} \\ 0 & \mathcal{T}_m \end{pmatrix},\ T_{jm} = -T_j V_j^\tau \mathcal{V}_m \mathcal{T}_m; \\ Y_{j+m} &= \begin{pmatrix} Y_j & (-Y_j V_j^\tau \mathcal{V}_m + A\mathcal{V}_m)\mathcal{T}_m \end{pmatrix}. \end{aligned}\right\} \tag{4}$$

(5) The next m columns of A are updated from the right; these columns are then declared the new current "mini-block".

Note that, in order to update all columns in the next "mini-block" from the right, one only needs the elements of Y that lie in the current and previous "mini-blocks", see line 4.4 in Algorithm 2. Thus, an update from the right of the entire next "mini-block" and the appropriate part of the matrix Y may be computed after all columns in the current "mini-block" have been annihilated.

The details are worked out in Algorithm 6 which, for $m > 1$, makes better use of BLAS 3 operations than the original Algorithm 1 and thus provides better performance. The minimum size of m where this variant is more effective depends on the user's machine setup – on our machine, for $m \geq 3$ the speedup was already notable. (See subsection 5.1 for timing results that illustrate a considerable improvement due to the modification described in Algorithm 6.)

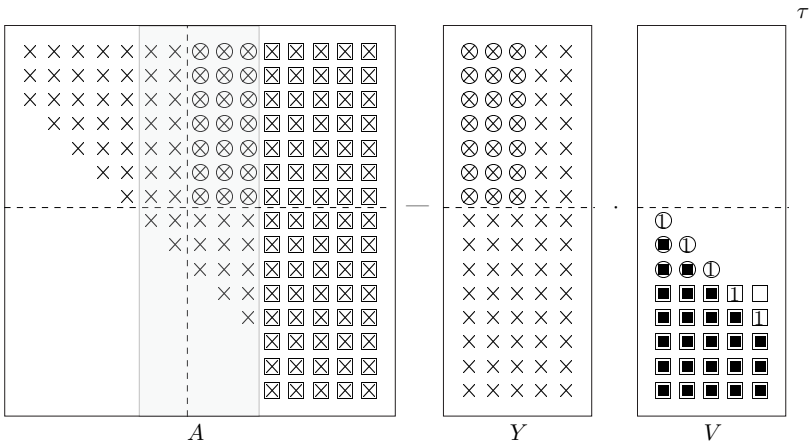


Fig. 4: Updating the matrix A from the right, $A = A - YV^\tau$.

This completes the description of the block processing algorithm. We now turn our attention to the global algorithm on the block level.

2.2 The outer loop

Figure 4 shows the update $A = A - YV^\tau$, where Y and V are computed during the last block processing (the last block $A^{(i)}$ is shaded). This update only affects the columns $k+1:n$ of A – the ones to the right of the vertical dashed line. Only the elements of A that are encircled or boxed have yet to be updated, since the block processing has already updated $A^{(i)}(k+1:n, 1:b)$.

The boxed elements of A will be updated by subtracting the product of Y with the boxed part of V. Since the elements of V above the ones are all zeros and V is stored in $A^{(i)}$, the appropriate part of $A^{(i)}$ has to be replaced with zeros and ones in order to use the `xGEMM` routine for the multiplication. The encircled elements of A will be updated by subtracting the product of encircled elements of Y with the triangular matrix of encircled elements in V.

The Block Algorithm 7 at first just stores all of the block's reflectors, instead of annihilating columns one by one and applying the resulting reflector to the entire matrix A each time. Only after a block is processed, the whole batch of its reflectors is applied to A, first from the left and then from the right.

This brings several important performance benefits into play. The first one is the localization of memory referencing: in the point version, the algorithm has to reference elements of A that are "far away" (in terms of memory addresses) from the current column when applying the reflectors, for each column being annihilated. On the other hand, the block version mostly references only elements local to the block being processed. Elements "far away", i.e. the ones outside of that block are referenced only after all of the block's reflectors have already been computed. If the block size is chosen to fit into the cache memory, there will be much less cache misses during the computation of all the reflectors and less data fetching from the slower main memory. The second advantage is the more effective transformation $A \mapsto Q^\tau AQ$. If Q were a single Householder reflector, one could only use BLAS

ALGORITHM 7: Block algorithm for reduction to the m-Hessenberg form

Input: $n \times n$ matrix A, block size b, bandwidth m
Output: A converted to m-Hessenberg form

for $z = 1,\ 1+b,\ 1+2\cdot b,\ 1+3\cdot b,\ \ldots$ **do**
  $i = (z-1)/b + 1$;
  Process block $A^{(i)} = A(1:n, z:z+b-1)$ with $k = z+m-1$ by Algorithm 6;
  `// Apply block reflector from the right:`
  Backup the upper triangle of $A^{(i)}(k+b-m+1:k+b, b-m+1:b)$ into matrix *temp* and replace it with the upper triangle of identity matrix;
  Call `xGEMM` to compute $A(1:n, z+b:n) = A(1:n, z+b:n) - Y \cdot \left(A^{(i)}(k+b-m+1:n, 1:b)\right)^{\tau}$;
  Restore *temp* to upper triangle of $A^{(i)}(k+b-m+1:k+b, b-m+1:b)$;
  Call `xTRMM` to compute $temp = Y(1:k, 1:b-m) \cdot \left(A^{(i)}(k+1:k+b-m, 1:b-m)\right)^{\tau}$;
  $A(1:k, k+1:z+b-1) = A(1:k, k+1:z+b-1) - temp$;
  `// Apply block reflector from the left:`
  Call `xLARFB` to apply block reflector (V, T) from left onto $A(k+1:n, z+b:n)$;
end

2 operations to apply the transformation, whereas transformation routines such as `xLARFB` use the more efficient BLAS 3 operations (e.g. `xGEMM`, `xTRMM`), taking advantage of the underlying block reflector structure of Q.

3. THE STAIRCASE FORM

The m-Hessenberg form can be used for efficient computation of other useful canonical forms. For instance, the controller Hessenberg form of $(A, B) \in \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times m}$ is easily computed in two steps: first compute the QR factorization $B = Q_1 \left(\begin{smallmatrix} R \\ 0 \end{smallmatrix}\right)$, update A to $A^{(1)} = Q_1^T A Q_1$, and compute the m-Hessenberg form $H = Q_2^T A^{(1)} Q_2$. Then, the transformation $Q = Q_1 Q_2$ produces $Q^T A Q = H$, $Q^T B = \left(\begin{smallmatrix} R \\ 0 \end{smallmatrix}\right)$. We now turn our attention to detecting whether the system is controllable and to determining its controllable part. A numerically reliable method for such task is the computation of a staircase form.

THEOREM 3. *[Dooren 1979] For a pair (A, B), where $A \in \mathbb{R}^{n\times n}$ and $B \in \mathbb{R}^{n\times m}$, there exists an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ such that $\left(\, Q^{\tau}B \,\middle|\, Q^{\tau}AQ \,\right)$ equals*

$$\left(\begin{array}{c|c|c} \bar{B} & \bar{A}_{11} & \bar{A}_{12} \\ \hline 0 & 0 & \bar{A}_{22} \end{array}\right) \equiv \left(\begin{array}{c|cccc|c} X_1 & \hat{A}_{11} & \hat{A}_{12} & \ldots & \hat{A}_{1k} & \hat{A}_{1,k+1} \\ 0 & X_2 & \hat{A}_{22} & \ldots & \hat{A}_{2k} & \hat{A}_{2,k+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & X_k & \hat{A}_{kk} & \hat{A}_{k,k+1} \\ \hline 0 & 0 & \ldots & 0 & 0 & \hat{A}_{k+1,k+1} \end{array}\right),$$

ALGORITHM 8: Computing a staircase form with a full system matrix A

Input: the system (A, B)
Output: the system $(\hat{A}, \hat{B})$ in the staircase form

1 Compute RRD $B = U \begin{pmatrix} \bar{B} \\ 0 \end{pmatrix}$, where $\bar{B}$ has full row rank ρ_1;
2 Update $A = U^\tau A U$;
3 Set $prev = 0$, $curr = \rho_1$, $i = 1$;
4 **while** $curr < n$ **do**
5 Set $Z = A(curr + 1 : n, prev + 1 : prev + \rho_i)$;
6 **if** *Z is a zero matrix* **then**
7 break: the system is uncontrollable;
8 **end**
9 Compute RRD $Z = U \begin{pmatrix} \bar{Z} \\ 0 \end{pmatrix}$, where $\bar{Z}$ has full row rank ρ_{i+1};
10 Update from left:
$A(curr + 1 : n, prev + 1 : n) = UA(curr + 1 : n, prev + 1 : n)$;
11 Update from right: $A(1 : n, curr + 1 : n) = A(1 : n, curr + 1 : n)U^\tau$;
12 $prev = curr$, $curr = curr + \rho_{i+1}$, $i = i + 1$;
13 **end**
14 Set $\hat{A} = A$, $\hat{B} = \begin{pmatrix} \bar{B} \\ 0 \end{pmatrix}$;

where each matrix X_i is of order $\rho_i \times \rho_{i-1}$ and has a full row rank ρ_i (we set $\rho_0 = m$). The initial system (A, B) is controllable if and only if $\bar{A}_{22} = \hat{A}_{k+1,k+1}$ is void, i.e. $\sum_{i=1}^{k} \rho_i = n$. Otherwise, $(\bar{A}_{11}, \bar{B})$ is the controllable part of (A, B).

If the matrix A has no structure, then a common way of computing the staircase form is shown in the Algorithm 8. A series of rank-revealing decompositions of the sub-matrices is computed. By a rank-revealing decomposition (RRD) of the matrix $Z \in \mathbb{R}^{p \times q}$, $p \geq q$, we consider any factorization $Z = U \begin{pmatrix} \bar{Z} \\ 0 \end{pmatrix}$, where U is orthogonal and $\bar{Z}$ has a full row rank. To make the staircase algorithm more efficient, usually a rank-revealing QR-factorization is used instead of the more reliable, but slower singular value decomposition. The SLICOT routine `AB01ND` implements a staircase algorithm which uses the classical QR-factorization with Businger–Golub pivoting and an incremental rank estimator. Note that most of those pivoted QR factorizations run on tall matrices. To compute X_i (line 9), the factorization of a matrix with at least $n-(i-1)m$ rows is required. The corresponding updates (lines 10 and 11) transform the sub-matrix of order at least $(n-(i-1)m) \times (n-(i-1)m)$. Assuming the usual case $m \ll n$, we see that many of these updates are actually on $\mathcal{O}(n) \times \mathcal{O}(n)$ sub-matrices.

3.1 A new scheme

We propose a novel algorithm for computing the staircase form in which the system is first transformed into the controller Hessenberg form using the blocked algorithm described in §2. Then, we use Algorithm 9, specially tailored for the generalized Hessenberg structure. Compared to the Algorithm 8, performance is gained because of these differences, which are due to the m-Hessenberg form of the system matrix:

—RRDs in line 9 are computed on matrices with h rows. The number h is initially

equal to m, and may increase by at most $m-1$ in each pass through the while-loop. Therefore, we expect that RRDs are computed on matrices having only $\mathcal{O}(m)$ rows.

—Update in line 10 transforms a submatrix of order $\mathcal{O}(m) \times \mathcal{O}(n)$.

—Update in line 11 transforms a submatrix of order $\mathcal{O}(n) \times \mathcal{O}(m)$.

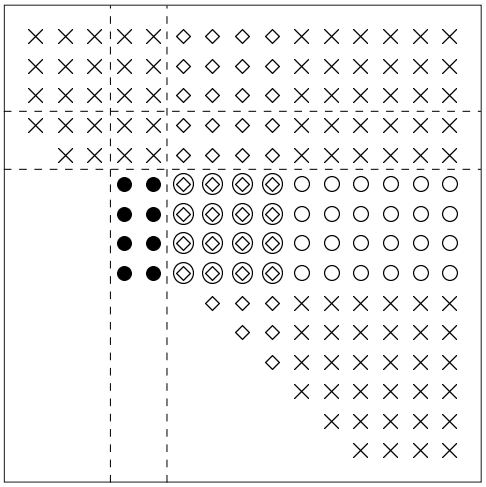


Fig. 5: A typical situation in the loop of Algorithm 9. RRD is computed on the submatrix •; elements ∘ are updated from the left, and elements ⋄ are updated from the right. Here $n = 15$, $m = \rho_0 = \rho_1 = 3$, $\rho_2 = 2$.

4. SHIFTED SYSTEMS AND TRANSFER FUNCTION

Hessenberg reduction is known to be an excellent preprocessing tool in solving shifted linear systems, in particular for evaluating the transfer function $G(\sigma) = C(\sigma I - A)^{-1}B + D$ of a LTI system $(A, B, C, D) \in \mathbb{R}^{n\times n} \times \mathbb{R}^{n\times m} \times \mathbb{R}^{p\times n} \times \mathbb{R}^{p\times m}$ at many values of complex scalar σ. Recently, it has been shown that using the controller Hessenberg form of (A, B) or (A^T, C^T) allows for more efficient and numerically more consistent computation in the case $\min(m, p) = 1$; for details and references see [Beattie et al. 2011]. Here we extend those ideas to the case $\min(m, p) > 1$, where it is tacitly assumed that $\max(m, p)$ is small compared to n.

Henry [Henry 1994] introduced the idea of using the RQ factorization $(A-\sigma I)U = T$, where U is $n \times n$ unitary, and T is $n \times n$ upper triangular. Then, $C(\sigma I - A)^{-1}B = -(CU)(T^{-1}B)$, and the original problem reduces to matrix multiplication and backward substitutions using the upper triangular matrix T. It is immediately clear how the controller Hessenberg structure of (A, B) simplifies this computation. First, performing many RQ factorizations is more efficient if the matrix A is in Hessenberg form simply because part of the matrix is already zero. Next,

$$T^{-1}B = \begin{pmatrix} \hat{T}^{-1}\hat{B} \\ 0 \end{pmatrix}, \quad B = \begin{pmatrix} \hat{B} \\ 0 \end{pmatrix}, \quad T = \begin{array}{c} \\ m \\ n-m \end{array} \begin{array}{c} \begin{array}{cc} m & n-m \end{array} \\ \begin{pmatrix} \hat{T} & * \\ 0 & * \end{pmatrix} \end{array},$$

ALGORITHM 9: Computing a staircase form of a system in controller Hessenberg form

Input: the system $(A, \left(\begin{smallmatrix} B \\ 0 \end{smallmatrix}\right))$ in the controller Hessenberg form
Output: the system $(\hat{A}, \left(\begin{smallmatrix} \hat{B} \\ 0 \end{smallmatrix}\right))$ in the staircase form

```
Compute RRD B = U ( B̄ ; 0 ), where B̄ has full row rank ρ_1;
Update A from left: A(1 : m, 1 : n) = U^τ A(1 : m, 1 : n);
Update A from right: A(1 : 2m, 1 : m) = A(1 : 2m, 1 : m)U;
Set h = m, prev = 0, curr = ρ_1, i = 1;
while curr < n do
    Set Z = A(curr + 1 : curr + h, prev + 1 : prev + ρ_i);
    if Z is a zero matrix then
        break: the system is uncontrollable;
    end
    Compute RRD Z = U ( Z̄ ; 0 ), where Z̄ has full row rank ρ_{i+1};
    Update from left:  A(curr + 1 : curr + h, prev + 1 : n) =
        UA(curr + 1 : curr + h, prev + 1 : n);
    Update from right:  A(1 : curr + h + m, curr + 1 : curr + h) =
        A(1 : curr + h + m, curr + 1 : curr + h)U^τ;
    h = h + m − ρ_{i+1}, prev = curr, curr = curr + ρ_{i+1}, i = i + 1;
end
Set Â = A, B̂ = B̄;
```

and $C(\sigma I - A)^{-1}B = -\hat{C}(\hat{T}^{-1}\hat{B})$, where $\hat{C} = (CU)(1 : p, 1 : m)$. Note that only the leading $m \times m$ matrix $\hat{T}$ of T is needed, which further simplifies the computation of the RQ factorization (both in number of flops and memory management); also, only a part of the transformed C is needed. In short, for each σ the computation is organized to compute only $\hat{T}$ and $\hat{C}$.

The RQ factorization is computed by Householder reflectors, $U = H_1 H_2 \cdots H_{n-1}$, where the i-th reflector H_i annihilates all subdiagonal elements in the $(n - i + 1)$-th row. The reduction starts at the last and finishes at the second row. For $i = n - m + 1, \ldots, n - 1$, during the update of the rows $m, \ldots, 2$, the matrix $\hat{T}$ is built bottom-up and the back-substitution is done on the fly.

4.1 A point algorithm

We first describe an algorithm in which the Householder reflectors are computed and applied one by one. Since the matrix A is in the m-Hessenberg form, in each row we have to annihilate m entries. This means that the corresponding Householder vector has at most $m + 1$ nonzero elements. Further, the application of the corresponding Householder reflector affects only $m + 1$ columns of the matrices $A - \sigma I$ and C. Since we need only a part of the RQ factorization, at no point we need more than $m + 1$ columns of the transformed $A - \sigma I$ and of the transformed C. (The role of C is rather passive – it just gets barraged by a sequence of reflectors, designed to produce triangular structure of $A - \sigma I$, and only $\hat{C}$ is wanted.) For this reason we introduce an auxiliary $(p + n) \times (m + 1)$ array Z which, at any moment, stores

$m+1$ columns of the thus far transformed matrices C and $A-\sigma I$. We can think of Z as a sliding window, moving from the last $m+1$ columns to the left.

ALGORITHM 10: A point algorithm for computing $\mathcal{G}(\sigma)$, where A and B are in the controller Hessenberg form.

Input: $(A,B,C,D) \in \mathbb{R}^{n\times n}\times\mathbb{R}^{n\times m}\times\mathbb{R}^{p\times n}\times\mathbb{R}^{p\times m}$ ((A,B) in the controller Hessenberg form); complex scalar σ

Output: $\mathcal{G}(\sigma) \equiv C(\sigma I - A)^{-1}B + D$

$Z(1:p,1:m) = C(1:p, n-m+1:n)$;
$Z(p+1:p+n,1:m) = (A-\sigma I)(1:n, n-m+1:n)$;
for $k = n:-1:m+1$ **do**
  $Z(1:p+k, 2:m+1) = Z(1:p+k, 1:m)$;
  $Z(1:p,1) = C(1:p, k-m)$;
  $Z(p+1:p+k,1) = (A-\sigma I)(1:k, k-m)$;
  Determine $(m+1)\times(m+1)$ Householder reflector $\bar{H}$ such that $Z(p+k, 1:m+1)\bar{H} = (\,0\ \ 0\ \ \cdots\ \ 0\ \ *\,)$;
  Transform $Z(1:p+k-1, 1:m) = Z(1:p+k-1, 1:m+1)\bar{H}(1:m+1, 1:m)$;
end
$\hat{X} = \hat{B}$;
for $k = m:-1:2$ **do**
  Determine $k\times k$ Householder reflector $\bar{H}$ such that $Z(p+k, 1:k)\bar{H} = (\,0\ \ 0\ \ \cdots\ \ 0\ \ *\,)$;
  Transform $Z(1:p+k-1, 1:k) = Z(1:p+k-1, 1:k)\bar{H}$;
  Compute $\hat{X}(k, k:m) = \hat{X}(k, k:m)/Z(p+k, k)$;
  Compute $\hat{X}(1:k-1, k:m) = \hat{X}(1:k-1, k:m) - Z(p+1:p+k-1, k)\cdot\hat{X}(k, k:m)$;
end
// $\hat{C}(1:p, 1:m)$ `is now stored in` $Z(1:p, 1:m)$
// $\hat{T}$ `is now stored in` $Z(p+1:p+m, 1:m)$.
$\hat{X}(1, 1:m) = \hat{X}(1, 1:m)/Z(p+1, 1)$;
$\mathcal{G}(\sigma) = D - Z(1:p, 1:m)\cdot\hat{X}$;

4.2 A block algorithm

Block algorithm for the RQ factorization by Householder reflectors is based on a special block representation of aggregated product of several reflectors. It is a well-known technology, and we will adjust it to our concrete structure. We will use a "reversed" WY representation of the aggregated Householder reflectors, which is a modification of the WY form from [Bischof and Loan 1987].

PROPOSITION 4. *Let $H_i = I - \tau_i v_i v_i^*$ be a Householder reflector, and let $U_j = H_1 H_2 \cdots H_j$. Then U_j can be represented as $U_j = I - Y_j V_j^*$, where*

$$V_1 = v_1,\ \ Y_1 = \tau_1 v_1;\ V_i = \begin{pmatrix} v_i & V_{i-1}\end{pmatrix},\ \ Y_i = \begin{pmatrix}\tau_i U_{i-1} v_i & Y_{i-1}\end{pmatrix},\ \ i = 2,\ldots,j.$$

The correctness of the above representation is easily checked, and we will see later why this particular form is practical in our framework.

Let n_b denote the block size, i.e. the number of aggregated reflectors. Since n_b consecutive transformations on n_b rows touch $m + n_b$ consecutive columns of $A - \sigma I$ and C, we extend our auxiliary array Z, and define it as $(p+n) \times (m+n_b)$ to accommodate $m + n_b$ columns of the transformed matrices C and $A - \sigma I$. The sliding window (array Z) will move to the left now with step n_b: its last n_b columns will be discarded, the leading m columns shifted to the right, and new n_b columns from $A-\sigma I$ and C will be brought as the leading columns of Z. During this sliding, the number of rows of Z shrinks by n_b at each step. Only the last n_b rows of the current Z are needed to generate the reflector, and these pivotal parts of the sliding window are trapezoidal matrices sliding upwards along the diagonal of $A - \sigma I$.

The last $m - 1$ Householder reflectors which reduce the rows $m, m-1, \ldots, 2$ of the matrix $A - \sigma I$ compute the dense RQ factorization and for small m are applied as in the point algorithm.

4.2.1 *Auxiliary: Trapezoidal to triangular reduction.* We use an auxiliary RQ routine to reduce an $n_b \times (m + n_b)$ upper trapezoidal matrix to triangular form by right multiplication by a sequence of Householder reflections,

$$\begin{pmatrix} x & x & x & x & x & x & x \\ 0 & x & x & x & x & x & x \\ 0 & 0 & x & x & x & x & x \\ 0 & 0 & 0 & x & x & x & x \end{pmatrix} \longrightarrow \begin{pmatrix} 0 & 0 & 0 & x & x & x & x \\ 0 & 0 & 0 & 0 & x & x & x \\ 0 & 0 & 0 & 0 & 0 & x & x \\ 0 & 0 & 0 & 0 & 0 & 0 & x \end{pmatrix}. \tag{5}$$

In the global scheme, this trapezoidal matrix is an $n_b \times (m + n_b)$ pivotal block of the auxiliary matrix Z. Most of the time we are not interested in the resulting triangle, but in the aggregated product of the reflectors, which will be packed in the reversed WY form and applied to only the part of the copy of the global array (stored in Z) that is needed in subsequent steps.

Updates with Householder reflectors within the auxiliary routine are also done in the blocked manner. The current row which determines current Householder reflector, is not updated by previous reflectors from the block until it is needed. Prior to computing the current Householder vector, aggregated Householder reflectors from previous steps have to be applied to the current row. Moreover, we update only the part of the row that carries information needed to construct the reflector for the next step.

Since the deployed reflectors are determined by Householder vectors with at most $m + 1$ nonzero elements (occupying consecutive positions), the matrix V is banded with bandwidth $m + 1$ and Y is lower trapezoidal:

$$V = \begin{pmatrix} \bullet & 0 & 0 & 0 \\ \bullet & \bullet & 0 & 0 \\ \bullet & \bullet & \bullet & 0 \\ \bullet & \bullet & \bullet & \bullet \\ 0 & \bullet & \bullet & \bullet \\ 0 & 0 & \bullet & \bullet \\ 0 & 0 & 0 & \bullet \end{pmatrix}, \quad Y = \begin{pmatrix} \star & 0 & 0 & 0 \\ \star & \star & 0 & 0 \\ \star & \star & \star & 0 \\ \star & \star & \star & \star \\ \star & \star & \star & \star \\ \star & \star & \star & \star \\ \star & \star & \star & \star \end{pmatrix} \tag{6}$$

Since an application of the block transformation $I - YV^*$ involves V^*, it is convenient to store V^* instead of V. Each time a new $(m+1)$-dimensional Householder vector v is determined, the first m components of v^* are stored in places of m subdiagonal elements that are annihilated by the corresponding reflector. The Householder vector is scaled so that its last component is equal to one, and there is no need for storing it. This procedure is implemented in the LAPACK routine

xLARFG. Hence, combining (5) and (6), the normalized V^* is placed in the last n_b rows of Z as follows:

$$Z(n+p-n_b+1:n+p, 1:m+n_b) \equiv Z_{block} = \begin{pmatrix} \bullet & \bullet & \bullet & x & x & x \\ 0 & \bullet & \bullet & x & x & x \\ 0 & 0 & \bullet & \bullet & x & x \\ 0 & 0 & 0 & \bullet & \bullet & x \end{pmatrix},$$

where Z contains the last $m+n_b$ columns of A and C.

ALGORITHM 11: Reduction of an $n_b \times (m+n_b)$ upper trapezoidal block to the triangular form.

Input: $n_b \times (m+n_b)$ matrix block Z_{block}
Output: V and Y such that $Z_{block}(I - YV^*)$ is triangular as in (5)

1 $V = 0_{(m+n_b)\times n_b}$; $Y = 0_{(m+n_b)\times n_b}$;
2 **for** $k = n_b : -1 : 1$ **do**
3 **if** $k = n_b$ **then**
4 Determine $(m+1)\times(m+1)$ Householder reflector $\bar{H} = I - \tau\bar{v}\bar{v}^*$ such that $Z_{block}(k, k:k+m)\bar{H} = (\ 0\ \ 0\ \cdots\ \ 0\ \ *\ )$;
5 Set $V(k:k+m, k) = \bar{v}$;
6 Set $Y(k:k+m, k) = \tau \cdot \bar{v}$;
7 **else**
8 $m_b = \min\{n_b - k, m\}$;
9 Update of the current row: Call xGEMM twice to compute $Z_{block}(k, k+1:k+m) = Z_{block}(k, k+1:k+m) - (Z_{block}(k, k+1:n_b+m)\cdot Y(k+1:n_b+m, k+1:k+m_b))\cdot V(k+1:k+m, k+1:k+m_b)^*$;
10 Determine $(m+1)\times(m+1)$ Householder reflector $\bar{H} = I - \tau\bar{v}\bar{v}^*$ such that $Z_{block}(k, k:k+m)\bar{H} = (\ 0\ \ 0\ \cdots\ \ 0\ \ *\ )$;
11 Set $V(k:k+m, k) = \bar{v}$;
12 Set $Y(k:k+m, k) = \tau \cdot \bar{v}$;
13 Call xGEMV twice to compute $Y(k+1:n_b+m, k) = Y(k+1:n_b+m, k) - Y(k+1:n_b+m, k+1:k+m_b)\cdot (V(k+1:k+m, k+1:k+m_b)^* \cdot Y(k+1:k+m, k))$;
14 **end**
15 **end**

The banded structure of the matrix V has been used to derive the lines 9 and 13 of Algorithm 11 from their original forms:

line 9 of Algorithm 11. $Z_{block}(k, k+1 : k+m) = Z_{block}(k, k+1 : k+m) - (Z_{block}(k, k+1 : n_b+m)\cdot Y(k+1 : n_b+m, k+1 : n_b))\cdot V(k+1 : k+m, k+1 : n_b)^*$

line 13 of Algorithm 11. $Y(k+1 : n_b+m, k) = Y(k+1 : n_b+m, k) - Y(k+1 : n_b+m, k+1 : n_b)\cdot(V(k+1 : k+m, k+1 : n_b)^* \cdot Y(k+1 : k+m, k))$

In both cases, we have multiplication of some submatrices of V and Y:
$Y(k+1 : n_b+m, k+1 : n_b)\cdot V(k+1 : k+m, k+1 : n_b)^*$
Since, for $n_b - k > m$, $V(k+1 : k+m, k+m+1 : n_b) = 0_{m\times(n_b-k-m)}$, we obtain the forms of these lines as presented in Algorithm 11. A similar modification will be used in Algorithm 12.

4.2.2 *The outer loop.* The global structure of the block algorithm is given in Algorithm 12.

ALGORITHM 12: Block algorithm for computing $\mathcal{G}(\sigma)$, where A and B are in the controller Hessenberg form.

Input: matrices A, B, C, D ((A, B) in the controller Hessenberg form); complex scalar σ, and block dimension n_b

Output: matrix $\mathcal{G}(\sigma)$

1 $l_b = (n-m)/n_b$;
2 $mink = n - (l_b - 1) \cdot n_b$;
3 $Z(1:p, 1:m) = C(1:p, n-m+1:n)$;
4 $Z(p+1:p+n, 1:m) = (A - \sigma I)(1:n, n-m+1:n)$;
5 **for** $k = n : -n_b : mink$ **do**
6 $\quad Z(1:p+k, n_b+1:m+n_b) = Z(1:p+k, 1:m)$;
7 $\quad Z(1:p, 1:n_b) = C(1:p, k-m-n_b+1:k-m)$;
8 $\quad Z(p+1:p+k, 1:n_b) = (A - \sigma I)(1:k, k-m-n_b+1:k-m)$;
9 $\quad$ Compute V and Y by Algorithm 11, such that
$\quad Z(p+k-n_b+1:p+k, 1:m+n_b)(I - YV^*)$ is upper triangular;
10 $\quad$ Call `xTRMM` and `xGEMM` to compute
$\quad Z(1:p+k-n_b, 1:m) = Z(1:p+k-n_b, 1:m) - Z(1:p+k-n_b, 1:m+n_b) \cdot$
$\quad (Y(1:m+n_b, 1:m) \cdot V(1:m, 1:m)^*)$;
11 **end**
12 $l = n - l_b \cdot n_b$;
13 **for** $k = l : -1 : m+1$ **do**
14 $\quad$ Perform lines 4–8 of Algorithm 10;
15 **end**
16 $\hat{X} = \hat{B}$;
17 **for** $k = m : -1 : 2$ **do**
18 $\quad$ Compute $\hat{X}(2:m, 1:m)$ as in lines 12–15 of Algorithm 10;
19 **end**
20 $\hat{X}(1, 1:m) = \hat{X}(1, 1:m)/Z(p+1, 1)$;
21 $\mathcal{G}(\sigma) = D - Z(1:p, 1:m) \cdot \hat{X}$;

In the implementation of the Algorithm 12 we can also exploit the fact that V is banded with bandwidth $m+1$ and Y is lower trapezoidal, hence the form of the implementation of line 10, which in the original reads:

line 10 of Algorithm 12. $Z(1:p+k-n_b, 1:m) \leftarrow Z(1:p+k-n_b, 1:m) - Z(1:p+k-n_b, 1:m+n_b) \cdot (Y \cdot V(1:m, 1:n_b)^*)$

Here we also assumed that $n_b \geq m$. Otherwise, $V(1:m, 1:m)$ does not exist and we have the product $YV(1:m, 1:n_b)^*$ with smaller inner dimension.

An estimate of additional workspace is as follows:

- Two-dimensional array of dimension $(m+n_b) \times n_b$ for storing the matrix Y.
- One-dimensional array of dimension m for storing intermediate results in lines 9 and 13 of Algorithm 11
- Two-dimensional array of dimension $(p+n-n_b) \times m$ for storing intermediate

result in line 10 of Algorithm 12
• One-dimensional array of dimension $p+m+n_b-1$ for storing intermediate results occurring in application of Householder reflector to a matrix in lines 14 and 17 of Algorithm 12 (lines 8 and 13 of Algorithm 10)
• Two-dimensional $m \times m$ array for storing the matrix $\bar{X}$. Depending on m/n, $\bar{X}$ may be stored in place of Y, since $\bar{X}$ appears after Y becomes obsolete.

4.2.3 *Batch processing in case of multiple shifts.* The second level of aggregation in the algorithm for solving shifted systems is processing the shifts in batches, see [Beattie et al. 2011]. There are several reasons for introducing this technique. First, we have to access the elements of the same matrices A and C for every shift. In each step of the outer loop, lines 7 and 8 are the same for every shift: the same n_b columns of A and C are copied to the auxiliary array Z (except that different shifts are subtracted from the diagonal elements of A). Second, the most expensive operation in the algorithm, which is the update of Z with the Householder reflectors generated in Z_{block} (line 10), involves large amount of the same data for different shifts. These data are the first n_b columns of Z, containing original elements of A and C, copied in lines 7 and 8.

The main goal of shift aggregation is to avoid all these redundant operations. Let us assume that we evaluate the transfer function $G(\sigma_i)$ for n_s different shifts σ_i, $i = 1, \ldots, n_s$. For all these shifts we will access all the elements of A and C only once, and we will perform one part of the update for all shifts simultaneously, as one call to `xGEMM`. Such approach will require much more memory for storing the auxiliary arrays, but it will reduce communication between different parts of the memory. The original array Z is now split in two parts:

—The first part consists of the first n_b columns of Z and is denoted by Z_1. This part is (almost) the same for all shifts and relates to the original elements of A and C. The "small" differences will be dealt with later.
—The second part consists of the last m columns of Z that are specific to the shift σ_i, and is denoted by $Z_2(i)$. These submatrices are the result of the update from the previous outer loop step, and are different for different shifts.

We do not need to store the pivotal block Z_{block} after its reduction in Algorithm 11, and the Householder vectors which are generated in that block can be exploited immediately after the auxiliary routine implementing Algorithm 11 completes execution. Hence, we use the same $n_b \times (m + n_b)$ array Z_{block} for all shifts. Finally, we will need the matrices $Y(i)$ obtained from Algorithm 11 for different shifts σ_i. The actual placing of these matrices in the workspace will be described later, after some details of the new algorithm are explained.

The update in line 10 of Algorithm 12 is now divided into two parts: one part dealing with shift specific arrays $Z_2(i)$ and the other part dealing with Z_1 which is common to all updates (for all shifts). Actually there is a "small" difference between the array Z_1 and the first n_b columns of the array Z from Algorithm 12, that was mentioned before. For Z_1 to be identical in all updates it cannot include shifts, and that is not the case with Z. A shift is subtracted from the diagonal elements of $Z(p + k - n_b - m + 1 : p + k - n_b, 1 : m)$, which is $m \times m$ bottom-left submatrix of the part of Z involved in update in the k-th outer loop step. Thus,

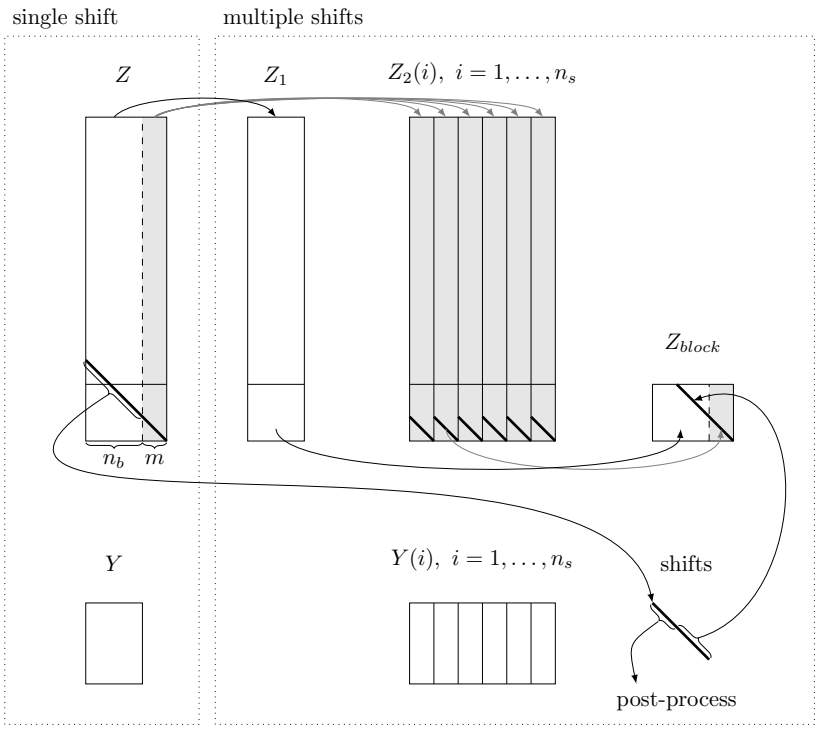


Fig. 6: The layout of the auxiliary arrays within the working space.

Z_1 will contain only elements of the original matrices A and C, and the shifts in the first m columns will be processed separately. The details of the update after reduction of the pivot block in case of multiple shifts are given in Algorithm 13.

Line 10.4 in Algorithm 13 suggests the layout of the auxiliary arrays within the working space. We need only the first m columns of the matrices $Y(i)$, so there is no need for storing all n_b columns (under assumption $n_b \geq m$). Thus, submatrices $Y(i)(1 : m + n_b, 1 : m)$ should occupy $m \cdot n_s$ consecutive columns as well as the matrices $Z_2(i)$. We should also note that the result of the update (lines 10.1–10.4) is already placed on the right position for the next outer loop step, so that copying operation in line 6 of Algorithm 12 can be omitted.

Similar techniques can be applied to the non-blocked part of the algorithm.

4.3 Descriptor systems

Algorithm 12 can be easily adapted for computing the transfer function $\mathcal{G}(\sigma) = C(\sigma E - A)^{-1}B + D$ of a descriptor system. Here $E \in \mathbb{R}^{n\times n}$. For Algorithm 12 to be efficient, the matrices A, B and E have to be in the m-Hessenberg–triangular–triangular form. An efficient block algorithm for the m-Hessenberg–triangular–triangular reduction is described in [Bosner 2011].

The only changes required for descriptor systems in the m-Hessenberg–triangular–triangular form are in the lines 4, 8 and 14 (line 6 of Algorithm 10) of Algorithm 12 where specific columns of $A - \sigma I$ are copied to the auxiliary array Z. What we

ALGORITHM 13: Details of the update in case of aggregated shifts.

for $k = n : -n_b : mink$ **do**
  Initialize data;
  for $1 = 1 : n_s$ **do**
    Perform necessary copying;
9 Compute $V(i)$ and $Y(i)$ by Algorithm 11, such that
    $Z_{block}(I - Y(i)V(i)^*)$ is upper triangular;
10.1 Call `xTRMM` to compute
    $Y(i)(1 : m + n_b, 1 : m) = Y(i)(1 : m + n_b, 1 : m) \cdot V(i)(1 : m, 1 : m)^*$;
10.2 Call `xGEMM` to compute
    $Z_2(i)(1 : p + k - n_b, 1 : m) = Z_1(1 : p + k - n_b, 1 : m)$
    $-Z_2(i)(1 : p + k - n_b, 1 : m) \cdot Y(i)(n_b + 1 : n_b + m, 1 : m)$;
10.3 $Z_2(i)(p + k - n_b - m + 1 : p + k - n_b, 1 : m) = Z_2(i)(p + k - n_b - m + 1 :$
    $p + k - n_b, 1 : m) + \sigma(i)Y(i)(1 : m, 1 : m) - \sigma(i)I_m$;
  end
10.4 Call `xGEMM` to compute
  $(Z_2(1)\ Z_2(2)\ \cdots\ Z_2(n_s))(1 : p + k - n_b, 1 : m \cdot ns) =$
  $(Z_2(1)\ Z_2(2)\ \cdots\ Z_2(n_s))(1 : p+k-n_b, 1 : m \cdot ns) - Z_1(1 : p+k-n_b, 1 : n_b)$
  $\cdot(Y(1)(1 : n_b, 1 : m)\ Y(2)(1 : n_b, 1 : m)\ \cdots\ Y(n_s)(1 : n_b, 1 : m))$;
end

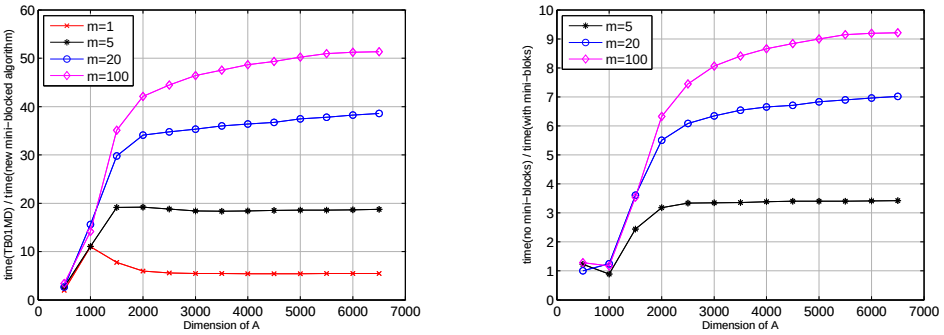
actually do here is copying the specific columns of the matrix A to Z first, and then subtracting σ from the diagonal elements of A. We have to change only the second step and subtract the corresponding columns of E multiplied with σ in order to obtain columns of $A - \sigma E$. Since E is upper triangular, this means that we have to update all elements in the current column of A except subdiagonal ones.

5. NUMERICAL EXPERIMENTS

We have run a series of tests in order to assess the performances of the new software. Our machine was a *Intel® Xeon™ X5470 (quad-core)*, running at 3.33GHz with 8 GB RAM and 6+6MB of Level 2 cache memory, under *Ubuntu Linux 8.10*. The compiler was *Intel® Fortran Compiler 11.0*. We used *-O3* optimization and the BLAS and LAPACK from the *Intel® Math Kernel Library 10.1*. All tests were run using the IEEE double precision and double complex arithmetic. The code was tested for correctness by computing the appropriate residuals and using SLICOT routines for reference values.

5.1 The m-Hessenberg reduction

We have compared the default point implementation found in the routine `TB01MD` from SLICOT with our new algorithms: blocked versions with and without the "mini-blocks". Only the reduction of the matrix A to the m-Hessenberg form is tested, and the code for the QR-factorization of the matrix B is removed from the SLICOT routine, along with the corresponding similarity transformation of the matrix A. We note that the blocked implementation of these transformations would increase the gap between the algorithms even more.



(a) Speedup factors of the new (mini)blocked CPU routine relative to `TB01MD`.

(b) The blocked algorithm: computation with mini-blocks is faster

Fig. 7: Comparisons of the new m-Hessenberg algorithms and `TB01MD` from SLICOT .

Figure 7a shows the speedup factors obtained by the the "mini-block" version of the CPU algorithm versus the SLICOT routine. The tests were run for a batch of matrices A with orders up to 6500 and various bandwidths m. The block size that performed well on our testing hardware was $b = 64$. As Figure 7a shows, the new algorithm can be more than 50 times faster than `TB01MD`. The significance of using the "mini-blocks" is shown in Figure 7b, where we compare two versions of our algorithms: the one using "mini-reflectors" and "mini-blocks" and the one updating each column of the block from the right prior to its annihilation.

The blocking has more effect when m is larger. In fact, to compute 100-Hessenberg form of a 6000×6000 matrix our algorithm needs only about $1/9$ of the time needed for computing the 1-Hessenberg form! One could use this fact to design an algorithm for successive band removal: in order to reduce a matrix to 1-Hessenberg, it is first very quickly reduced to e.g. 100-Hessenberg, and then using a similar process this intermediate matrix is further reduced to a 1-Hessenberg form. However, our attempts to design such an algorithm have failed so far: reduction from a 100-Hessenberg form to a 1-Hessenberg form simply takes too long! In the symmetric case, this scheme is successful; see [Bischof et al. 2000]. (See also [Karlsson 2011].)

5.2 Reduction to the staircase form

We ran a number of numerical tests to demonstrate the efficiency of the Algorithm 9 compared to the Algorithm 8. Both algorithms used the same SLICOT routine `MB03OY` for RRDs; this routine implements a blocked rank-revealing QR algorithm using the Businger–Golub pivoting. We randomly generated systems $(A \quad B)$ of various orders and ran the staircase reduction algorithms. Figure 8 shows that the new algorithm performs up to 19 times faster than the original one. (The timings for the new algorithm include both the reduction to the controller–Hessenberg form and the subsequent transformation into the staircase form.)

5.3 Evaluation of the transfer function

Extensive numerical testing was performed for random systems with various values of n and m; in our tests we set $p = m$. We have compared the SLICOT routine

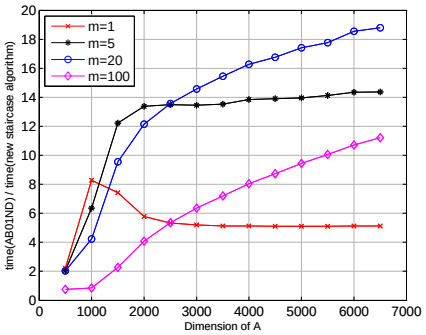
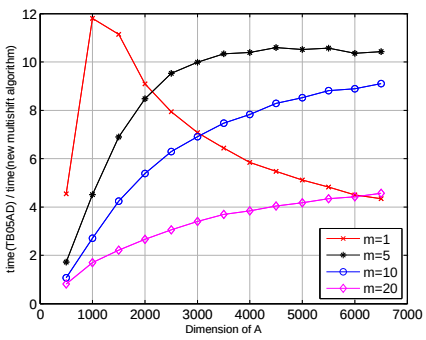


Fig. 8: The staircase reduction: comparison of Algorithm 9 and `AB01ND` from SLICOT .

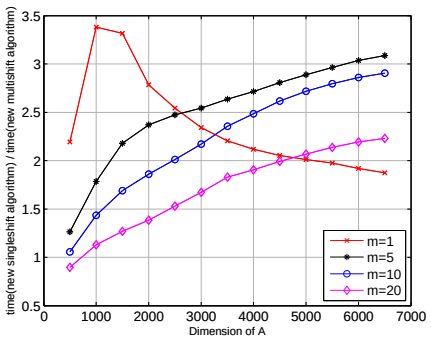
`TB05AD` to our new blocked CPU algorithm for transfer function computation, using $r = 1000$ random complex shifts. The routines were executed as follows:

our routines. CPU implementation of the reduction to the controller Hessenberg form was executed once followed by 1000 executions of our blocked CPU algorithm for computing $\mathcal{G}(\sigma)$;

SLICOT routine TB05AD. at first the routine `TB05AD` was executed with the parameter `INITIA='G'`, indicating that the matrix A is a general matrix, and without balancing and eigenvalues calculations (parameter `BALEIG='N'`). This was followed by 999 executions of `TB05AD` with `INITIA='H'` indicating that the matrix A is in the upper Hessenberg form, which is computed using `DGEHRD` from LAPACK.



(a) Speedup factors of the new blocked CPU routine relative to `TB05AD`.



(b) Aggregation of shifts improves the block algorithm.

Fig. 9: Comparisons of the new transfer function algorithm and `TB05AD` from SLICOT .

The block size in our CPU algorithm was set to $n_b = 64$, which was in most cases the optimal block size for our routine. The results presented in Figure 9a confirm that our block algorithm for evaluating the transfer function is generally faster than the corresponding SLICOT routine `TB05AD`. Figure 9b demonstrates

that aggregation of shifts significantly contributes to the efficiency (we aggregated $n_s = 256$ shifts). Although its efficiency decreases as m increases, we can conclude that, as the dimension n grows, the efficiency of our routines is increasing. We finally note that obvious modifications apply for the cases of purely real shifts, or complex conjugate pairs of shifts.

5.4 Results on a different machine

We run the same test on the different machine with *2 × Intel® Xeon^{TM} E5620 (4 cores)*, running at 2.40GHz with 23.5 GB RAM and 12+12MB of Level 3 cache memory, under *Scientific Linux release 6.0*. The compiler was *Intel® Fortran Composer 2011.4.191* with multithreaded *Intel® Math Kernel Library 10.3*. We obtained slightly weaker speedups than previously shown. The new m-Hessenberg algorithm was up to 32 times faster than `TB01MD` from SLICOT, for $m = 100$. When comparing the new staircase reduction algorithm to `AB01ND` from SLICOT, the best speedup factors were 8.7 for $m = 1$ and 16 for $m = 20$. The best achieved speedup factors of the new blocked transfer function routine relative to `TB05AD` from SLICOT were 3.7 for $m = 20$ and 10 for $m = 1$.

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