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## A Tight and Explicit Representation of $Q$ in Sparse $QR$ Factorization

Esmond G. Ng  
Barry W. Peyton

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Engineering Physics and Mathematics Division

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IN SPARSE  $QR$  FACTORIZATION**

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# A TIGHT AND EXPLICIT REPRESENTATION OF $Q$ IN SPARSE $QR$ FACTORIZATION

Esmond G. Ng  
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## Abstract

In  $QR$  factorization of a sparse  $m \times n$  matrix  $A$  ( $m \geq n$ ) the orthogonal factor  $Q$  is often stored *implicitly* as a lower trapezoidal matrix  $H$  known as the Householder matrix. This paper presents a simple characterization of the row structure of  $Q$ , which could be used as the basis for a sparse data structure that can store  $Q$  *explicitly*. The new characterization is a simple extension of a well known row-oriented characterization of the structure of  $H$  [9]. Hare, Johnson, Olesky, and van den Driessche [15] have recently provided a complete sparsity analysis of the  $QR$  factorization. Let  $U$  be the matrix consisting of the first  $n$  columns of  $Q$ . Using results from [15], we show that the data structures for  $H$  and  $U$  resulting from our characterizations are *tight* when  $A$  is a strong Hall matrix. We also show that  $H$  and the lower trapezoidal part of  $U$  have the same sparsity characterization when  $A$  is strong Hall. We then show that this characterization can be extended to any weak Hall matrix that has been permuted into *block upper triangular* form. Finally, we show that permuting to block upper triangular form never increases the fill incurred during the factorization.



## 1. Introduction

Let  $\mathbf{A}$  be an  $m \times n$  sparse matrix with  $m \geq n$  and assume that  $\mathbf{A}$  has full column rank. Consider the reduction of  $\mathbf{A}$  to upper triangular form using orthogonal factorization:

$$\mathbf{A} = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix}, \quad (1.1)$$

where  $\mathbf{Q}$  is  $m \times m$  orthogonal and  $\mathbf{R}$  is  $n \times n$  upper triangular. Since  $\mathbf{A}$  has full column rank,  $\mathbf{R}$  is nonsingular. The orthogonal matrix  $\mathbf{Q}$  can be partitioned conformally with the matrix it premultiplies to obtain

$$\mathbf{Q} = \begin{bmatrix} \mathbf{U} & \mathbf{V} \end{bmatrix},$$

where  $\mathbf{U}$  is  $m \times n$  and  $\mathbf{V}$  is  $m \times (m - n)$ . Thus, we have

$$\mathbf{A} = \mathbf{U}\mathbf{R}. \quad (1.2)$$

If the computation is organized so that the entries on the main diagonal of  $\mathbf{R}$  are positive, the factorization in (1.2) is unique regardless of the method used to compute  $\mathbf{U}$  and  $\mathbf{R}$ , assuming that there are no round-off errors. Of course, only the first  $n$  columns of  $\mathbf{Q}$  (i.e.,  $\mathbf{U}$ ) are uniquely determined, since any orthonormal basis for the null space of  $\mathbf{A}^T$  may serve as the last  $m - n$  columns of  $\mathbf{Q}$ .

For any matrix  $\mathbf{B}$ , its  $i$ -th row and  $j$ -th column are denoted respectively by  $\mathbf{B}_{i,*}$  and  $\mathbf{B}_{*,j}$ . The  $(i, j)$ -element of  $\mathbf{B}$  is written as  $B_{i,j}$ . We use  $\mathit{Struct}(\mathbf{B})$  to denote the *structure* of  $\mathbf{B}$ :

$$\mathit{Struct}(\mathbf{B}) := \{(i, j) \mid B_{i,j} \neq 0\}.$$

Similarly, for any vector  $\mathbf{x}$ , we let

$$\mathit{Struct}(\mathbf{x}) := \{i \mid x_i \neq 0\}.$$

Let  $\mathcal{M}(\mathbf{A})$  contain every full-rank  $m \times n$  matrix  $\mathbf{B}$  for which  $\mathit{Struct}(\mathbf{B}) = \mathit{Struct}(\mathbf{A})$ . We define  $\mathcal{Q}(\mathbf{A})$  by

$$\mathcal{Q}(\mathbf{A}) := \bigcup_{\mathbf{B} \in \mathcal{M}(\mathbf{A})} \mathit{Struct}(\mathbf{Q}^{\mathbf{B}}),$$

where

$$\mathbf{B} = \mathbf{Q}^{\mathbf{B}} \begin{bmatrix} \mathbf{R}^{\mathbf{B}} \\ \mathbf{O} \end{bmatrix}$$

is the  $QR$  factorization of  $\mathbf{B}$ . The sets  $\mathcal{U}(\mathbf{A})$  and  $\mathcal{R}(\mathbf{A})$  are defined in similar fashion.

Note that these sets are the *smallest* sets such that  $Struct(\mathbf{Q}^B) \subseteq \mathcal{Q}(\mathbf{A})$ ,  $Struct(\mathbf{U}^B) \subseteq \mathcal{U}(\mathbf{A})$ , and  $Struct(\mathbf{R}^B) \subseteq \mathcal{R}(\mathbf{A})$  for any matrix  $\mathbf{B} \in \mathcal{M}(\mathbf{A})$ . Thus, the three sets  $\mathcal{Q}(\mathbf{A})$ ,  $\mathcal{U}(\mathbf{A})$  and  $\mathcal{R}(\mathbf{A})$  are the ideal target of any efficient storage scheme or data structure for storing the nonzeros of the factor matrices.

Hare, Johnson, Olesky, and van den Driessche [15] have given a complete characterization of  $\mathcal{U}(\mathbf{A})$ . After first proving that a certain set of ordered pairs must be excluded from  $\mathcal{U}(\mathbf{A})$ , they then show that for any ordered pair  $(i, j)$  not in the excluded set, there exists a matrix  $\mathbf{B} \in \mathcal{M}(\mathbf{A})$  for which  $U_{i,j}^B \neq 0$ . Using a different approach, Pothén [19] further proves that there exists a matrix  $\mathbf{B} \in \mathcal{M}(\mathbf{A})$  for which  $U_{i,j}^B \neq 0$  for every ordered pair  $(i, j) \in \mathcal{U}(\mathbf{A})$ . Hare et al. also show that  $\mathcal{R}(\mathbf{A})$  can be obtained by forming symbolically the product of  $\mathbf{U}^T$  and  $\mathbf{A}$  based on  $\mathcal{U}(\mathbf{A})$  and  $Struct(\mathbf{A})$ ; we refer to the product as the *symbolic product* of  $\mathbf{U}^T$  and  $\mathbf{A}$ .

Earlier work in this area was primarily concerned with efficient storage of  $\mathbf{R}$  and  $\mathbf{Q}$  for use in sparse matrix computations [1,7,9,11]. In this setting  $\mathbf{Q}$  is stored as a sequence of Householder transformations or Givens rotations. For definiteness we consider Householder transformations in this paper. The orthogonal matrix  $\mathbf{Q}$  is stored *implicitly* in the *Householder matrix*  $\mathbf{H}$ , which is an  $m \times n$  lower trapezoidal matrix, each column of which contains a *Householder vector* used to construct a Householder transformation. (A more detailed description of the Householder matrix  $\mathbf{H}$  is given in Section 3.1. Note also that we will be using the pattern  $\mathcal{H}(\mathbf{A})$ , which is defined in the manner  $\mathcal{Q}(\mathbf{A})$ ,  $\mathcal{U}(\mathbf{A})$ , and  $\mathcal{R}(\mathbf{A})$  were defined.) In [11], George and Ng gave a fast symbolic factorization algorithm for generating (from  $Struct(\mathbf{A})$ ) zero-nonzero patterns  $\overline{\mathcal{H}}(\mathbf{A})$  and  $\overline{\mathcal{R}}(\mathbf{A})$  such that  $\mathcal{H}(\mathbf{A}) \subseteq \overline{\mathcal{H}}(\mathbf{A})$  and  $\mathcal{R}(\mathbf{A}) \subseteq \overline{\mathcal{R}}(\mathbf{A})$ . George, Liu, and Ng [9] introduced a simple characterization of  $\overline{\mathcal{H}}(\mathbf{A})$ , which is based on  $\overline{\mathcal{R}}(\mathbf{A})$ . Using this characterization, they presented row-oriented data structures that can be used to store the nonzero entries of  $\mathbf{H}$  and  $\mathbf{R}$ . There are circumstances, however, under which this data structure is not *tight*: i.e., circumstances under which  $\mathcal{H}(\mathbf{A}) \subset \overline{\mathcal{H}}(\mathbf{A})$  and/or  $\mathcal{R}(\mathbf{A}) \subset \overline{\mathcal{R}}(\mathbf{A})$ .

In this paper, we use the results in [15] to extend the results and techniques introduced in [9] in two different ways. First, we modify the row-oriented characterization of  $\overline{\mathcal{H}}(\mathbf{A})$  in [9] to obtain a row-oriented characterization of a set  $\overline{\mathcal{Q}}(\mathbf{A})$ , which has the property that  $\mathcal{Q}(\mathbf{A}) \subseteq \overline{\mathcal{Q}}(\mathbf{A})$ . Using  $\overline{\mathcal{Q}}(\mathbf{A})$ , the row-oriented data structure for  $\mathbf{H}$  described in [9] can be extended to provide a data structure for storing  $\mathbf{Q}$  *explicitly*. Note that it is trivial to obtain  $\overline{\mathcal{U}}(\mathbf{A})$  from  $\overline{\mathcal{Q}}(\mathbf{A})$  so that  $\mathcal{U}(\mathbf{A}) \subseteq \overline{\mathcal{U}}(\mathbf{A})$ . Second, we give sufficient conditions under which set equalities are achieved. That is, we give conditions under which  $\mathcal{R}(\mathbf{A}) = \overline{\mathcal{R}}(\mathbf{A})$ ,  $\mathcal{U}(\mathbf{A}) = \overline{\mathcal{U}}(\mathbf{A})$ , and  $\mathcal{H}(\mathbf{A}) = \overline{\mathcal{H}}(\mathbf{A})$ . Whenever these sets are equal, the data structures based on  $\overline{\mathcal{H}}(\mathbf{A})$ ,  $\overline{\mathcal{U}}(\mathbf{A})$ , and  $\overline{\mathcal{Q}}(\mathbf{A})$  are therefore *tight*.

As we shall see in Section 2,  $\mathbf{A}$  is a *Hall matrix* (defined in Section 2.1) if it is a full-rank matrix; consequently, Hall matrices play a key role throughout this paper, along with a subclass known as *strong Hall matrices*. After presenting background material for Hall and strong Hall matrices, Section 2 reviews the characterizations of  $\mathbf{U}(\mathbf{A})$  and  $\mathcal{R}(\mathbf{A})$  presented in [15], with special emphasis on the role played by sets of so-called Hall columns and Hall rows. In Section 3, after reviewing some material in [9], we modify the characterization of  $\overline{\mathcal{H}}(\mathbf{A})$  in [9] to obtain a characterization of  $\overline{\mathcal{Q}}(\mathbf{A})$ . Coleman et al. [1] have shown that when  $\mathbf{A}$  is a strong Hall matrix,  $\mathcal{R}(\mathbf{A})$  and  $\overline{\mathcal{R}}(\mathbf{A})$  are identical, where  $\overline{\mathcal{R}}(\mathbf{A})$  is generated using one of the symbolic factorization procedures in [7,9,11]. We use the results in [15] to show that the set  $\overline{\mathcal{H}}(\mathbf{A})$  generated by the symbolic factorization procedure in [9,11] is identical to  $\mathcal{H}(\mathbf{A})$  when  $\mathbf{A}$  is strong Hall. We further show that the set  $\overline{\mathcal{U}}(\mathbf{A})$  described in Section 3 is the same as  $\mathcal{U}(\mathbf{A})$  for any strong Hall matrix  $\mathbf{A}$ . Since the characterization of  $\mathcal{U}(\mathbf{A})$  and  $\mathcal{R}(\mathbf{A})$  in [15] applies to an arbitrary full-rank Hall matrix with the columns permuted in any order, it is natural to consider whether or not the new results in Section 3 can be extended to obtain row-oriented characterizations of  $\mathcal{H}(\mathbf{A})$ ,  $\mathcal{U}(\mathbf{A})$ , and  $\mathcal{R}(\mathbf{A})$  for any such matrix. We suspect that there is no way to do so.

Coleman et al. [1] have shown however that when a Hall matrix  $\mathbf{A}$  is permuted to a particular block upper triangular form, the zero-nonzero pattern  $\overline{\mathcal{R}}(\mathbf{A})$  in [7,9,11] for  $\mathcal{R}$  (obtained by applying symbolic Givens rotations or Householder transformations to  $\mathbf{A}$ ) is again identical to  $\mathcal{R}(\mathbf{A})$ . Let  $\widehat{\mathbf{A}}$  be the matrix  $\mathbf{A}$  after it has been permuted into block upper triangular form, and let

$$\widehat{\mathbf{A}} = \widehat{\mathbf{Q}} \begin{bmatrix} \widehat{\mathbf{R}} \\ \mathbf{O} \end{bmatrix}$$

be the  $QR$  factorization of  $\widehat{\mathbf{A}}$ . Moreover let  $\widehat{\mathbf{U}}$  be the matrix consisting of the first  $n$  columns of  $\widehat{\mathbf{Q}}$ . In Section 4, again using the results in [15], we extend the results in Section 3 to obtain row-oriented characterizations of  $\mathcal{U}(\widehat{\mathbf{A}})$ ,  $\mathcal{R}(\widehat{\mathbf{A}})$ , and  $\mathcal{H}(\widehat{\mathbf{A}})$ . We further show that if the column ordering of  $\widehat{\mathbf{A}}$  is *consistent* with that of  $\mathbf{A}$  (consistent in a sense defined in Section 4), then for every nonzero entry in  $\widehat{\mathbf{U}}$  ( $\widehat{\mathbf{R}}$ ,  $\widehat{\mathbf{H}}$ ), the corresponding permuted entry in  $\mathbf{U}$  ( $\mathbf{R}$ ,  $\mathbf{H}$ ) is also nonzero. In consequence, permuting a Hall matrix to block upper triangular form permits the use of clean, simple, tight data structures for  $\widehat{\mathbf{U}}$ ,  $\widehat{\mathbf{H}}$ , and  $\widehat{\mathbf{R}}$ , while maintaining or actually lowering the number of nonzero entries in the factors. Some concluding remarks are provided in Section 5.

## 2. A recent sparsity analysis of $QR$ factorization

Recently, Hare et al. [15] have provided a characterization of the sparsity patterns  $\mathcal{U}(\mathbf{A})$  and  $\mathcal{R}(\mathbf{A})$  for any Hall matrix  $\mathbf{A}$  having full column rank. After providing background material on Hall matrices and so-called *Hall rows* and *Hall columns*, we summarize the main results from their paper, which will be used extensively in later sections of this paper.

### 2.1. Hall matrices

An  $m \times n$  matrix  $\mathbf{A}$ , with  $m \geq n$ , is a *Hall matrix* if every  $m \times k$  submatrix,  $1 \leq k \leq n$ , has at least  $k$  nonzero rows. The matrix  $\mathbf{A}$  is a *strong Hall matrix* if every  $m \times k$  submatrix,  $1 \leq k < m$ , has at least  $k + 1$  nonzero rows. Note that  $k < m$  in the second definition because the number of nonzero rows cannot exceed  $k$  when  $k = m = n$ . The concept of Hall and strong Hall matrices apparently was first introduced by Coleman et al. in [1] when they were investigating the structure of  $\mathbf{R}$  obtained in the reduction of  $\mathbf{A}$  to upper triangular form using Givens rotations. Clearly, if  $\mathbf{A}$  is strong Hall, then it is also Hall. We will refer to any Hall matrix that is not strong Hall as a *weak Hall matrix*.

The following lemma is a direct consequence of a result due to Hall [14] on finding a distinct representative member from each set in a collection of subsets. It says that the rows of a Hall matrix can always be permuted so that the entries on the diagonal of the permuted matrix are all nonzero. The permuted matrix is then said to possess a *zero-free diagonal*. For further details consult [4,18].

**Lemma 2.1 (Hall [14]).** *There exists a permutation matrix  $\mathbf{P}$  such that  $\mathbf{PA}$  has a zero-free diagonal if and only if  $\mathbf{A}$  is a Hall matrix.*

In the previous section we assumed that  $\mathbf{A}$  has *full* column rank. As we shall see in subsequent sections, this paper deals primarily with the zero-nonzero structure of matrices. It is therefore sufficient if the following weakened condition holds true for the matrix  $\mathbf{A}$ : Given  $\text{Struct}(\mathbf{A})$ , there exists an assignment of numerical values to the nonzero positions of the matrix so that the matrix has full *numerical* rank and hence has a unique  $QR$  factorization. Thus, it makes more sense to assume that the *structure* of  $\mathbf{A}$  has *full* column rank. We define the *structural rank* of  $\mathbf{A}$  as the maximum number of linearly independent columns in  $\mathbf{B}$ , over all  $m \times n$  matrices  $\mathbf{B}$  for which  $\text{Struct}(\mathbf{B}) = \text{Struct}(\mathbf{A})$ . Clearly, if the  $m \times n$  matrix  $\mathbf{A}$  has full column rank (i.e., rank  $n$ ), its structural rank is also  $n$ . The next result, relating the structural rank of a matrix to the Hall property, follows easily from similar results for square matrices [4,12] and the fact that the column rank and row rank of  $\mathbf{A}$  are the same.

**Corollary 2.2.** *An  $m \times n$  matrix  $\mathbf{A}$ ,  $m \geq n$ , has structural rank  $n$  if and only if it is a Hall matrix.*

Based on Corollary 2.2, we can relax our assumption that  $\mathbf{A}$  has full numerical rank; we can consider Hall matrices throughout the rest of the paper.

## 2.2. Hall sets

One of the key contributions of Hare et al. [15] is their recognition of the subtle interplay of sparsity and column orthogonality in  $\mathbf{U}$  when  $\mathbf{A}$  is a weak Hall matrix. To deal with this issue they introduced the notion of *Hall sets*. Let  $J$  be any subset of the column indices  $\{1, 2, \dots, n\}$ , and let  $\mathbf{A}[J]$  denote the set of columns  $\mathbf{A}_{*,j}$  where  $j \in J$ . A Hall set of size  $k$  in  $\mathbf{A}[J]$  is a set of  $k$  columns from  $\mathbf{A}[J]$  such that the  $m \times k$  matrix formed by these columns has *exactly*  $k$  nonzero rows. It is easy to show that the union of two distinct Hall sets from  $\mathbf{A}[J]$  is also a Hall set in  $\mathbf{A}[J]$ . It follows that there is a unique Hall set of maximum cardinality for any given subset of columns  $\mathbf{A}[J]$ . However, when  $\mathbf{A}$  is a strong Hall matrix, clearly the Hall set of maximum cardinality is empty for any subset of columns  $\mathbf{A}[J]$ .

For convenience, let  $\mathbf{A}[j]$  be the set containing the first  $j$  columns of  $\mathbf{A}$ ; i.e.,  $\mathbf{A}[j] = \mathbf{A}[J]$ , where  $J = \{1, 2, \dots, j\}$ ,  $1 \leq j \leq n$ . Playing a key role in [15] is the maximum cardinality Hall set of  $\mathbf{A}[j]$ , which shall be denoted by  $\mathbf{S}^{[j]}$ . The set containing the column indices of the Hall set, denoted by  $S_C^{[j]}$ , will be referred to as a set of *Hall columns*. Similarly, the row index set for the nonzero rows associated with  $\mathbf{S}^{[j]}$ , denoted by  $S_R^{[j]}$ , will be referred to as the set of *Hall rows*. If the matrix  $\mathbf{A}$  has a zero-free diagonal, then it is easy to see that

$$S_C^{[j]} = S_R^{[j]}, \quad \text{for } 1 \leq j \leq n.$$

To simplify notation we will also use  $\mathbf{A}[j]$  to denote the *matrix* formed by the columns in the *set*  $\mathbf{A}[j]$ . The  $(s, t)$ -element of the  $m \times j$  matrix  $\mathbf{A}[j]$  will be denoted by  $A_{s,t}^{[j]}$ .

## 2.3. Characterizations of $\mathcal{U}(\mathbf{A})$ and $\mathcal{R}(\mathbf{A})$

To determine the sparsity pattern  $\mathcal{U}(\mathbf{A})$ , Hare et al. found it most useful to consider  $QR$  factorization obtained via the Gram-Schmidt orthogonalization procedure. As a natural consequence they examine the sparsity pattern  $\mathcal{U}(\mathbf{A})$  column by column.

Hare et al. associate a bipartite graph  $B^{[k]} = (R^{[k]}, C^{[k]}, E^{[k]})$  with each submatrix  $\mathbf{A}[k]$ . This bipartite graph  $B^{[k]}$  describes the zero-nonzero pattern of  $\mathbf{A}[k]$  with the Hall rows  $S_R^{[k-1]}$  and Hall columns  $S_C^{[k-1]}$  removed. More specifically, the graph  $B^{[k]}$  is

defined as follows:

$$\begin{aligned} C^{[k]} &:= \{c_j \mid 1 \leq j \leq k \text{ and } j \notin S_C^{[k-1]}\}, \\ R^{[k]} &:= \{r_i \mid 1 \leq i \leq m, i \notin S_R^{[k-1]} \text{ and } \exists c_j \in C^{[k]} \text{ such that } A_{ij}^{[k]} \neq 0\}, \\ E^{[k]} &:= \{\{r_i, c_j\} \mid r_i \in R^{[k]}, c_j \in C^{[k]} \text{ and } A_{ij}^{[k]} \neq 0\}. \end{aligned}$$

Now, define a set of row indices  $F^{[k]}$  by

$$F^{[k]} = \{i \mid r_i \notin R^{[k]} \text{ and } i \notin S_R^{[k-1]}\}.$$

Note that  $F^{[k]}$ ,  $S_R^{[k-1]}$ , and  $\{i \mid r_i \in R^{[k]}\}$  partition the row indices  $\{1, 2, \dots, m\}$  into three sets. The set  $\{i \mid r_i \in R^{[k]}\}$  is further partitioned into two sets as follows. Let  $D^{[k]}$  contain the row indices  $i$  for which  $r_i \in R^{[k]}$  and there exists *no* path in  $B^{[k]}$  from  $c_k$  to  $r_i$ ; let  $P^{[k]}$  contain the row indices  $i$  for which  $r_i \in R^{[k]}$  and there exists a path in  $B^{[k]}$  from  $c_k$  to  $r_i$ . That is,  $D^{[k]}$  contains the row vertices in  $B^{[k]}$  that are *disconnected* from the last column vertex  $c_k$ , while  $P^{[k]}$  contains the row vertices in  $B^{[k]}$  that are connected by a *path* to  $c_k$ . Theorem 2.3 states that three of the four sets in this partition of  $\{1, 2, \dots, m\}$  contain every row index  $1 \leq i \leq m$  for which  $(i, k) \notin \mathcal{U}(\mathbf{A})$ , i.e., every row index  $i$  for which  $U_{i,k}^B$  is necessarily zero for any matrix  $B \in \mathcal{M}(\mathbf{A})$ . A proof can be found in [15].

**Theorem 2.3 (Hare et al. [15]).** *Let  $\mathbf{A}$  be an  $m \times n$  Hall matrix with  $m \geq n$ . For  $1 \leq k \leq n$ , we have  $(i, k) \notin \mathcal{U}(\mathbf{A})$  if and only if  $i \in F^{[k]} \cup S_R^{[k-1]} \cup D^{[k]}$ .*

Theorem 2.3 places each row index  $i$  for which  $(i, k) \notin \mathcal{U}(\mathbf{A})$  into one of three categories. First, observe that if  $i \in F^{[k]}$ , then  $A_{i,j}^{[k]} = 0$  for  $1 \leq j \leq k$ , and thus every entry  $A_{i,k}$  of  $\mathbf{A}$  for which  $i \in F^{[k]}$  lies to the left of the *envelope* (or *front*) of  $\mathbf{A}$ . It follows from the Gram-Schmidt process that  $U_{*,k}$  is a linear combination of the columns of  $\mathbf{A}[k]$ ; hence we have  $U_{i,k} = 0$  for  $i \in F^{[k]}$ , as the theorem asserts.

Second, consider  $i \in S_R^{[k-1]}$ . The Gram-Schmidt process implies that  $U_{*,k}$  must be orthogonal to every column of  $\mathbf{A}[k-1]$ ; in particular, it is orthogonal to the columns in the Hall set  $S^{[k-1]}$ . Now the columns in  $S^{[k-1]}$  span a subspace of dimension  $|S_R^{[k-1]}|$ , and for every vector  $\mathbf{x}$  in this space we have  $x_i = 0$  for  $i \notin S_R^{[k-1]}$ . In consequence, any vector  $\mathbf{y}$  such that  $y_i \neq 0$  for some  $i \in S_R^{[k-1]}$  cannot be orthogonal to every vector in this space. Thus,  $U_{i,k} = 0$  for  $i \in S_R^{[k-1]}$ , as the theorem states. This is perhaps the key insight in Hare et al. [15].

Finally, we make a few observations for  $i \in D^{[k]}$ . We will not outline the argument that  $(i, k) \notin \mathcal{U}(\mathbf{A})$  as we did for the previous two cases. The argument is longer and more technical, and we will look at a simplified version of this argument in Section 3.4; thus we refer the reader to [15] for these details. Nonetheless, well-known sparsity

results for Cholesky factorization can be used to suggest why  $(i, k) \notin \mathcal{U}(\mathbf{A})$ . Let  $\mathbf{L}$  be the Cholesky factor of some symmetric positive definite matrix  $\mathbf{B}$ , and suppose  $L_{s,t}$  is a “structural” zero entry in the factor, with  $s > t$ . It is well known that this zero entry is “caused” by lack of a path connecting the vertices  $c_s$  and  $c_t$  in the graph of  $\mathbf{B}$  and passing through vertices  $c_r$ , where  $r < t$  [8]. The absence of paths from  $r_i$  to  $c_k$  in  $B^{[k]}$  for orthogonal factorization is analogous to this absence of paths from  $c_s$  to  $c_t$  in the graph of  $\mathbf{B}$  for Cholesky factorization. It is lack of structural and numerical symmetry in orthogonal factorization that complicates the argument.

Theorem 2.3 says that the only possible nonzero entries in column  $k$  of  $\mathbf{U}$  are the entries  $U_{i,k}$ , where  $i \in P^{[k]}$ . Indeed Hare et al. show that for each  $i \in P^{[k]}$ , there exists a matrix  $\mathbf{B} \in \mathcal{M}(\mathbf{A})$  for which  $U_{i,k}^{\mathbf{B}} \neq 0$ , and consequently  $(i, k) \in \mathcal{U}(\mathbf{A})$  if and only if  $i \in P^{[k]}$ . Using a different approach, Pothen [19] proves that there exists a matrix  $\mathbf{B} \in \mathcal{M}(\mathbf{A})$  such that  $U_{i,k}^{\mathbf{B}} \neq 0$  for every  $(i, k) \in \mathcal{U}(\mathbf{A})$ .

In addition to the analysis for  $\mathcal{U}(\mathbf{A})$ , Hare, et al. also provide the following characterization of  $\mathcal{R}(\mathbf{A})$ .

**Theorem 2.4 (Hare et al. [15]).** *Let  $\mathbf{A}$  be an  $m \times n$  Hall matrix with  $m \geq n$ . The sparsity pattern  $\mathcal{R}(\mathbf{A})$  can be obtained by forming the symbolic product of  $\mathbf{U}^T$  and  $\mathbf{A}$  based on  $\mathcal{U}(\mathbf{A})$  and  $\text{Struct}(\mathbf{A})$  respectively.*

### 3. Row-oriented characterization of $\mathcal{Q}(\mathbf{A})$ for strong Hall matrices

For any sparse matrix factorization, it is desirable to know the sparsity structure of each factor in advance so that space can be pre-allocated for storing the nonzeros. The goal of a symbolic factorization is to *predict* from  $\text{Struct}(\mathbf{A})$  the sparsity structures of each factor. For sparse  $QR$  factorization, we use  $\overline{\mathcal{Q}}(\mathbf{A})$ ,  $\overline{\mathcal{U}}(\mathbf{A})$ ,  $\overline{\mathcal{H}}(\mathbf{A})$ , and  $\overline{\mathcal{R}}(\mathbf{A})$  to denote respectively the sparsity patterns of  $\mathbf{Q}$ ,  $\mathbf{U}$ ,  $\mathbf{H}$ , and  $\mathbf{R}$  predicted by any specific symbolic factorization or other symbolic procedure. Throughout we will follow the convention of denoting any matrix with sparsity pattern  $\overline{\mathcal{Q}}(\mathbf{A})$ ,  $\overline{\mathcal{U}}(\mathbf{A})$ ,  $\overline{\mathcal{H}}(\mathbf{A})$ , and  $\overline{\mathcal{R}}(\mathbf{A})$  as  $\overline{\mathbf{Q}}$ ,  $\overline{\mathbf{U}}$ ,  $\overline{\mathbf{H}}$ , and  $\overline{\mathbf{R}}$ , respectively. We introduce this convention because our symbolic procedure in Section 3.3 is most naturally expressed in terms of matrix operation (specifically, matrix products). Consequently, to prove our results we need matrix “representatives” of patterns generated by symbolic procedures.

As suggested by the results reviewed in the last section, straightforward symbolic procedures for analyzing sparsity in  $QR$  factorization, such as those in [9,10,11], *do not* always exclude positions  $(i, k)$ ,  $i \in S_R^{[k-1]}$ , from the patterns  $\overline{\mathcal{H}}(\mathbf{A})$  or  $\overline{\mathcal{U}}(\mathbf{A})$  that they create. Furthermore, we know of no simple fix for this problem. In consequence, the data structures based on  $\overline{\mathcal{H}}(\mathbf{A})$  and  $\overline{\mathcal{U}}(\mathbf{A})$  generally are not tight. One obvious way to avoid this problem is to restrict  $\mathbf{A}$  to those Hall matrices for which  $S_R^{[k]} = S_C^{[k]} = \emptyset$  for

$1 \leq k \leq n - 1$ . This is precisely what we do in this section: we demonstrate that the zero-nonzero pattern  $\bar{\mathbf{U}}(\mathbf{A})$  generated by a particular symbolic factorization procedure is identical to  $\mathbf{U}(\mathbf{A})$  when the matrix  $\mathbf{A}$  to which the symbolic factorization procedure is applied is strong Hall.

Throughout this section we will be working with  $QR$  factorization computed via Householder reductions. The *Householder matrix*  $\mathbf{H}$  generated by this process stores  $\mathbf{Q}$  implicitly, and as a result our symbolic procedure is somewhat complicated, involving the symbolic product of the entire sequence of Householder transformations. Taking this approach however enables us to work with and extend the results introduced in George et al. [9] and also to establish the close relationship between the sparsity patterns  $\mathcal{H}(\mathbf{A})$  and  $\mathbf{U}(\mathbf{A})$ .

This section is organized as follows. Section 3.1 briefly reviews Householder reductions and needed background material from [9]. Section 3.2 introduces a *generalized elimination forest*, which includes vertices  $n + 1, n + 2, \dots, m$  so that all the columns of  $\mathbf{Q}$  can be included in our analysis. Section 3.3 provides row-oriented characterizations of two sets  $\bar{\mathbf{U}}(\mathbf{A})$  and  $\bar{\mathbf{Q}}(\mathbf{A})$ , both of which are simple extensions of the characterization of  $\bar{\mathcal{H}}(\mathbf{A})$  in [9]. Finally, we show in Section 3.4 that  $\bar{\mathbf{U}}(\mathbf{A}) = \mathbf{U}(\mathbf{A})$  and  $\bar{\mathcal{H}}(\mathbf{A}) = \mathcal{H}(\mathbf{A})$ .

### 3.1. Background

The factorization in (1.1) can be obtained using Householder transformations [13]. The matrix  $\mathbf{A}$  is reduced to upper triangular form by a sequence of Householder reductions:

$$\mathbf{H}_n \mathbf{H}_{n-1} \dots \mathbf{H}_1 \mathbf{A} = \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix}.$$

Since each Householder transformation  $\mathbf{H}_k$  is symmetric and orthogonal, the orthogonal matrix  $\mathbf{Q}$  is then expressed as

$$\mathbf{Q} = \mathbf{H}_1 \mathbf{H}_2 \dots \mathbf{H}_n.$$

Let  $\mathbf{I}_s$  denote the  $s \times s$  identity matrix. Each Householder transformation  $\mathbf{H}_k$  has the form  $\mathbf{I}_m - \mathbf{h}_k \mathbf{h}_k^T$  for some  $m$ -vector  $\mathbf{h}_k$  of the form

$$\begin{bmatrix} \mathbf{O} \\ \alpha_k \\ \mathbf{w}_k \end{bmatrix},$$

where  $\alpha_k$  is a scalar,  $\mathbf{w}_k$  is an  $(m - k)$ -vector, and the first  $k - 1$  entries of  $\mathbf{h}_k$  are zero. (For consistency of notation, we include  $\mathbf{H}_n$  in all cases, even though  $\mathbf{h}_n^T =$

[  $\mathbf{O}$   $\alpha_n$  ] when  $m = n$ .) The vector  $\mathbf{h}_k$  is often referred to as a *Householder vector*. The orthogonal factor  $\mathbf{Q}$  can therefore be represented *implicitly* by the  $m \times n$  lower trapezoidal matrix  $\mathbf{H}$ :

$$\mathbf{H} = \begin{bmatrix} \mathbf{h}_1 & \mathbf{h}_2 & \dots & \mathbf{h}_n \end{bmatrix},$$

which is referred to as the *Householder matrix*.

We now impose two more assumptions on the Hall matrix  $\mathbf{A}$ . It follows from Lemma 2.1 that there exists a row permutation  $\mathbf{P}$  such that  $\mathbf{PA}$  has a *zero-free diagonal*. Since

$$\mathbf{PA} = \mathbf{PQ} \begin{bmatrix} \mathbf{R} \\ \mathbf{O} \end{bmatrix},$$

the only effect permuting the rows of  $\mathbf{A}$  has on  $\mathbf{Q}$  and  $\mathbf{R}$  is to permute the rows of  $\mathbf{Q}$ . That is, the sparsity patterns of  $\mathbf{Q}$  and  $\mathbf{R}$  remain essentially unchanged when the rows of  $\mathbf{A}$  are permuted. Consequently we can assume without loss of generality that  $\mathbf{A}$  has a zero-free diagonal. We also assume throughout this section that  $\mathbf{A}$  is a strong Hall matrix. We turn our attention to weak Hall matrices in Section 4.

In [11], George and Ng presented an efficient symbolic factorization algorithm for generating, *solely* from  $\text{Struct}(\mathbf{A})$ , two pattern sets  $\overline{\mathcal{H}}(\mathbf{A})$  and  $\overline{\mathcal{R}}(\mathbf{A})$  that have the following properties:  $\text{Struct}(\mathbf{H}) \subseteq \overline{\mathcal{H}}(\mathbf{A})$  and  $\text{Struct}(\mathbf{R}) \subseteq \overline{\mathcal{R}}(\mathbf{A})$ . The symbolic factorization algorithm is based on the following simple observation. Consider applying  $\mathbf{H}_1$  to  $\mathbf{A}$ . It is easy to see that  $\text{Struct}((\mathbf{H}_1\mathbf{A})_{i,*}) = \text{Struct}(\mathbf{A}_{i,*})$ , if  $A_{i,1} = 0$ ; otherwise,  $\text{Struct}((\mathbf{H}_1\mathbf{A})_{i,*}) = \bigcup_{A_{k,1} \neq 0} \text{Struct}(\mathbf{A}_{k,*})$ . The result can be applied to  $\mathbf{H}_1\mathbf{A}$  recursively to obtain  $\overline{\mathcal{H}}(\mathbf{A})$  and  $\overline{\mathcal{R}}(\mathbf{A})$ . The “row-merging” process is the key in an efficient implementation of the symbolic factorization procedure. Since the symbolic procedure does not take numerical values or Hall sets into account, we can conclude that

$$\text{Struct}(\mathbf{H}) \subseteq \mathcal{H}(\mathbf{A}) \subseteq \overline{\mathcal{H}}(\mathbf{A})$$

and

$$\text{Struct}(\mathbf{R}) \subseteq \mathcal{R}(\mathbf{A}) \subseteq \overline{\mathcal{R}}(\mathbf{A}).$$

George et al. [9] then obtained the following simple row-oriented characterization of  $\overline{\mathcal{H}}(\mathbf{A})$ . Consider an upper triangular matrix  $\overline{\mathbf{R}}$ . (Recall that  $\text{Struct}(\overline{\mathbf{R}}) = \overline{\mathcal{R}}(\mathbf{A})$ .) For  $1 \leq k \leq n$ , if  $\text{Struct}(\overline{\mathbf{R}}_{k,*}) \neq \emptyset$ , then we define  $\rho(k)$  by

$$\rho(k) := \min\{j > k \mid j \in \text{Struct}(\overline{\mathbf{R}}_{k,*})\};$$

otherwise, we let  $\rho(k) = k$ . Thus, if  $\rho(k) > k$ , then  $\rho(k)$  is the column index of the *first* off-diagonal nonzero entry in row  $k$  of  $\overline{\mathbf{R}}$ . Since  $\mathbf{A}$  is strong Hall, it follows from

results in Coleman et al. [1] that  $Struct(\mathbf{R}) = Struct(\overline{\mathbf{R}}) = Struct(\mathbf{L}^T)$ , where  $\mathbf{L}$  is the Cholesky factor of  $\mathbf{A}^T \mathbf{A}$ . Thus  $\rho$  is the *parent* function of the *elimination forest* associated with  $\mathbf{L}$ ,  $\mathbf{R}$  and  $\overline{\mathbf{R}}$  [16,17,21]. The elimination forest may consist of one or more trees. When  $\mathbf{A}^T \mathbf{A}$  is irreducible, the elimination forest has exactly one tree. For each tree, there is exactly one node  $r$  for which  $\rho(r) = r$ , and it is called the *root* of the tree.

For  $1 \leq i \leq m$ , if row  $i$  of  $\mathbf{A}$  is nonzero, then we let  $f(i)$  be the column index of the *first* nonzero in that row:

$$f(i) := \min\{j \mid A_{i,j} \neq 0\};$$

otherwise, we let  $f(i) = i$ . Note that  $f(i) \leq i$  for  $1 \leq i \leq n$  because of the zero-free diagonal in  $\mathbf{A}$ . Moreover,  $f(i) \leq n$  for  $n+1 \leq i \leq m$  if and only if row  $i$  is nonzero. It is straightforward to show that if row  $i$  of  $\mathbf{A}$  is zero (i.e.,  $f(i) > n$ ), then row  $i$  in both  $\mathbf{H}$  and  $\overline{\mathbf{H}}$  must be zero; this result follows from the way in which Householder transformations are constructed. For any nonzero row  $i$  of  $\mathbf{A}$ , Theorem 3.1 provides a characterization of  $Struct(\overline{\mathbf{H}}_{i,*})$  in terms of  $f$  and  $\rho$ .

**Theorem 3.1** (George et al. [9]). *Let  $\mathbf{A}$  be a strong Hall matrix with a zero-free diagonal, and assume that  $A_{i,*}$  is nonzero. Then the column indices of the nonzero entries in  $\overline{\mathbf{H}}_{i,*}$  are given by*

$$Struct(\overline{\mathbf{H}}_{i,*}) = \{ f(i), \rho(f(i)), \rho(\rho(f(i))), \dots, t(i) \},$$

where  $t(i)$  is the first node encountered along the path from  $f(i)$  to the root of its elimination tree for which one of the following two conditions holds:

1.  $t(i) = i$  (in which case  $1 \leq i \leq n$ ), or
2.  $\rho(t(i)) = t(i)$ .

Theorem 3.1 presents a row-oriented characterization of  $\overline{\mathcal{H}}(\mathbf{A})$ . (Recall again that  $Struct(\overline{\mathbf{H}}) = \overline{\mathcal{H}}(\mathbf{A})$ .) Proving our main results in Section 3.3 requires additional insight into the column structure of  $\overline{\mathbf{H}}$ , as provided by the following two results. (Lemma 3.2 holds even when  $\mathbf{A}$  is a weak Hall matrix.)

**Lemma 3.2.** *Let  $\mathbf{A}$  be a strong Hall matrix with a zero-free diagonal. Then the following two statements hold true:*

1.  $Struct(\overline{\mathbf{H}}_{*,k}) - \{k\} \subseteq Struct(\overline{\mathbf{H}}_{*,\rho(k)})$ , and
2.  $Struct(\overline{\mathbf{H}}_{*,k}) - \{1, 2, \dots, k-1\} \subseteq Struct(\overline{\mathbf{H}}_{*,k})$ .

**Proof:** Consider the first statement. There is nothing to prove if  $k = \rho(k)$  or  $Struct(\overline{H}_{*,k}) - \{k\} = \emptyset$ . Assume therefore that  $k \neq \rho(k)$  and  $Struct(\overline{H}_{*,k}) - \{k\} \neq \emptyset$ . Choose  $i \in Struct(\overline{H}_{*,k}) - \{k\}$ . It follows that  $k \in Struct(\overline{H}_{i,*})$ ; moreover, by Theorem 3.1,  $Struct(\overline{H}_{i,*})$  is given by

$$\{ f(i), \dots, k, \rho(k), \dots, t(k) \},$$

where  $\rho(k) \leq t(k)$ . Consequently,  $i \in Struct(\overline{H}_{*,\rho(k)})$ , and the first statement is verified.

Turning our attention now to the second statement, we follow the approach in [11] and consider the first Householder reduction step  $H_1 A$ . For convenience we write  $A$  and  $H_1$  as

$$A = \begin{bmatrix} \beta & v^T \\ u & B \end{bmatrix}, \quad H_1 = I_m - hh^T, \quad \text{where } h = \begin{bmatrix} \alpha \\ w \end{bmatrix}.$$

By construction [10,13],  $w$  is some appropriate multiple of  $u$  chosen along with  $\alpha$  so that  $H_1 A$  has the form

$$H_1 A = \begin{bmatrix} \delta & y^T \\ O & C \end{bmatrix}.$$

Because  $\overline{H}_{*,1}$  is chosen so that  $Struct(H_{*,1}) \subseteq Struct(\overline{H}_{*,1})$ , it then follows that

$$Struct(A_{*,1}) \subseteq Struct(H_{*,1}) \subseteq Struct(\overline{H}_{*,1}),$$

as required. By direct computation we have

$$C = B - \alpha w v^T - w w^T B.$$

Assuming no numerical cancellation, it follows that  $Struct(B) \subseteq Struct(C)$ . Applying the argument recursively to  $C$  verifies that the second statement is true.  $\blacksquare$

**Lemma 3.3.** *Let  $A$  be a strong Hall matrix with a zero-free diagonal. Then*

$$Struct(\overline{H}_{*,k}) - \{k\} \neq \emptyset, \quad \text{for } 1 \leq k \leq n-1.$$

**Proof:** Let  $desc(k)$  be the set containing the descendants of node  $k$  in the elimination forest given by  $\rho$ . (Note that  $k \in desc(k)$ .) Now choose  $1 \leq k \leq n-1$ . By recursive

application of Lemma 3.2 to the descendants of  $k$ , it follows that

$$\left( \bigcup_{j \in \text{desc}(k)} \text{Struct}(\mathbf{A}_{*,j}) \right) - \text{desc}(k) \subseteq \text{Struct}(\overline{\mathbf{H}}_{*,k}) - \{k\}. \quad (3.1)$$

Since  $\mathbf{A}$  is strong Hall, the left hand side of (3.1) must be nonempty, thereby proving the result.  $\blacksquare$

### 3.2. Generalized elimination forest

The nodes in the elimination forest are labeled from 1 to  $n$ . To account for all the columns of  $\mathbf{Q}$  in our new results, we will “expand” the elimination forest  $\rho$  to include nodes  $n+1, n+2, \dots, m$ . Consider the root  $r$  of a tree in the elimination forest (i.e.,  $\rho(r) = r$ ). Since  $\mathbf{A}$  is strong Hall, it follows from Lemma 3.3 that  $\text{Struct}(\overline{\mathbf{H}}_{*,r}) - \{r\} \neq \emptyset$ . Suppose that the row indices of  $\text{Struct}(\overline{\mathbf{H}}_{*,r})$  are given by

$$i_1 < i_2 < \dots < i_p,$$

where  $p \geq 2$ . Clearly  $i_1 = r$  and  $i_p \leq m$ . Furthermore,  $i_2 > n$ ; otherwise, the zero-free diagonal in  $\mathbf{A}$  and the row-merging process in [11] would imply that  $\overline{R}_{r,i_2} \neq 0$ , which contradicts the fact that  $r$  is the root of a tree.

For  $1 \leq s < p$ , we define  $\psi_r(i_s) = i_{s+1}$ . For  $s = p$ , We define  $\psi_r(i_p) = i_p$ . Thus, we view the ordered set  $\text{Struct}(\overline{\mathbf{H}}_{*,r})$  as a *chain* of which  $\psi_r$  is the parent function. There is such a chain for each tree in the elimination forest. We now prove that these chains are disjoint.

**Lemma 3.4.** *Let  $r$  and  $r'$  be two distinct roots in the elimination forest. Then  $\text{Struct}(\overline{\mathbf{H}}_{*,r}) \cap \text{Struct}(\overline{\mathbf{H}}_{*,r'}) = \emptyset$ .*

**Proof:** Without loss of generality, we may assume that  $r < r'$ . By way of contradiction, assume  $\text{Struct}(\overline{\mathbf{H}}_{*,r}) \cap \text{Struct}(\overline{\mathbf{H}}_{*,r'}) \neq \emptyset$ , and choose  $i \in \text{Struct}(\overline{\mathbf{H}}_{*,r}) \cap \text{Struct}(\overline{\mathbf{H}}_{*,r'})$ . It follows that  $r, r' \in \text{Struct}(\overline{\mathbf{H}}_{i,*})$ , whence by Theorem 3.1,  $\text{Struct}(\overline{\mathbf{H}}_{i,*})$  is given by

$$\{ f(i), \rho(f(i)), \dots, r, \rho(r), \dots, r', \dots, t(i) \},$$

with  $f(i) \leq r < \rho(r) \leq r' \leq t(i)$ . But this contradicts our assumption that  $r$  and  $r'$  are both roots, thereby proving the result.  $\blacksquare$

Since the chains constructed above are disjoint, we can omit the subscript  $r$  from the function  $\psi$ . Furthermore, node  $k$  will *not* appear in one of these chains if and only if row  $k$  of  $\mathbf{A}$  is zero. Our assumption of a zero-free diagonal ensures that this condition

can be met only when  $n < k \leq m$ . For each node  $k$  satisfying this condition, we define  $\psi(k) = k$ .

Combining  $\rho$  and  $\psi$ , we now define a new tree structure  $\varphi$ , which we will call the *generalized elimination forest*:

$$\varphi(k) = \begin{cases} \rho(k) & , \text{ for } 1 \leq k \leq n \text{ and } \rho(k) \neq k, \\ \psi(k) & , \text{ for } 1 \leq k \leq n \text{ and } \rho(k) = k, \\ \psi(k) & , \text{ for } n+1 \leq k \leq m. \end{cases}$$

### 3.3. Characterization of $\mathcal{Q}(A)$

Following the approach in [9], we now wish to determine a sparsity pattern  $\overline{\mathcal{Q}}(A)$  such that  $\overline{\mathcal{Q}}(A)$  contains  $\mathcal{Q}(A)$ . This can be achieved by forming the symbolic product of  $\overline{H}_1, \overline{H}_2, \dots, \overline{H}_n$  based on the sparsity patterns  $Struct(\overline{H}_i)$ ,  $1 \leq i \leq n$ , provided by Theorem 3.1 and Lemma 3.2. Toward that end we write each matrix  $\overline{H}_i$  as

$$\overline{H}_i = I_m - \overline{h}_i \overline{h}_i^T, \quad \text{with } \overline{h}_i = \begin{bmatrix} \mathbf{0} \\ \bar{\alpha}_i \\ \overline{w}_i \end{bmatrix},$$

where  $\bar{\alpha} \neq 0$  (by construction) and  $\overline{w}_i$  is an  $(m-i)$ -vector. We also introduce the following sequence of  $m \times m$  matrices:

$$\overline{Q}^{(k)} = \overline{H}_k \overline{H}_{k+1} \dots \overline{H}_n, \quad k = n, n-1, \dots, 1.$$

Moreover we define  $\overline{Q}$  and  $\overline{\mathcal{Q}}(A)$  by  $\overline{Q} := \overline{Q}^{(1)}$  and  $\overline{\mathcal{Q}}(A) := Struct(\overline{Q})$ . Note that we have

$$Struct(\mathcal{Q}) \subseteq \mathcal{Q}(A) \subseteq Struct(\overline{Q}^{(1)}) = Struct(\overline{Q}).$$

We leave it for the reader to verify that for  $1 \leq j \leq k-1$ ,  $\overline{Q}_{*,j}^{(k)} = \mathbf{e}_j$  and  $\overline{Q}_{j,*}^{(k)} = \mathbf{e}_j^T$ , where  $\mathbf{e}_j$  is the  $j$ -th column of the  $m \times m$  identity matrix: this follows easily from the form of  $\overline{H}_i$ 's that are multiplied together to obtain  $\overline{Q}^{(k)}$ . This observation ensures that the following definition, which is crucial to the induction argument in the following proof, is a meaningful construction. For  $k \leq i \leq m$ , we define  $f_k(i)$  by

$$f_k(i) := \min\{s \mid k \leq s \leq n \text{ and } s \in Struct(\overline{H}_{i,*})\}.$$

In other words,  $f_k(i)$  is the index of the "first Householder vector"  $\overline{h}_s$  used in forming the product  $\overline{Q}^{(k)} = \overline{H}_k \overline{H}_{k+1} \dots \overline{H}_n$  that has a nonzero entry in the  $i$ -th position. Note that it follows from Theorem 3.1 that  $f_1(i) = f(i)$  for  $1 \leq i \leq m$ .

The next result provides a row-oriented characterization of the sparsity structure

of each matrix  $\overline{Q}^{(k)}$ ,  $1 \leq k \leq n$ .

**Theorem 3.5.** *Let  $A$  be a strong Hall matrix with a zero-free diagonal. Then for  $1 \leq k \leq n$  and  $k \leq i \leq m$ ,*

$$Struct(\overline{Q}_{i,*}^{(k)}) = \{ f_k(i), \varphi(f_k(i)), \varphi(\varphi(f_k(i))), \dots, \tilde{t}(i) \},$$

where  $\tilde{t}(i)$  is the root of the tree in the generalized elimination forest that contains  $f_k(i)$ .

**Proof:** We prove the result by induction on  $k$ , where  $k = n, n-1, \dots, 1$ .

For the base step  $k = n$  we have

$$\begin{aligned} \overline{Q}^{(n)} &= \overline{H}_n = I_m - \overline{h}_n \overline{h}_n^T = I_m - \begin{bmatrix} \mathbf{O} \\ \overline{\alpha}_n \\ \overline{w}_n \end{bmatrix} \begin{bmatrix} \mathbf{O} & \overline{\alpha}_n & \overline{w}_n^T \end{bmatrix} \\ &= \begin{bmatrix} I_{n-1} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & 1 - \overline{\alpha}_n^2 & -\overline{\alpha}_n \overline{w}_n^T \\ \mathbf{O} & -\overline{\alpha}_n \overline{w}_n & I_{m-n} - \overline{w}_n \overline{w}_n^T \end{bmatrix}. \end{aligned}$$

(Following our convention in Section 3.1,  $\overline{h}_n^T = \begin{bmatrix} \mathbf{O} & \overline{\alpha}_n \end{bmatrix}$  whenever  $m = n$ , in which case  $\overline{w}_n$  is a null vector.) It is trivial to verify from this expression for  $\overline{Q}^{(n)}$  that the result holds for  $k = n$ .

Assume that the result holds for every  $\overline{Q}^{(j)}$ ,  $k < j \leq n$ , and consider  $\overline{Q}^{(k)}$ . By definition,

$$\overline{Q}^{(k)} = \overline{H}_k \overline{H}_{k+1} \dots \overline{H}_n = \overline{H}_k \overline{Q}^{(k+1)}.$$

As we observed in the paragraph preceding this theorem,  $\overline{Q}^{(k+1)}$  has the following form

$$\overline{Q}^{(k+1)} = \begin{bmatrix} I_{k-1} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & 1 & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & B \end{bmatrix}.$$

By direct computation we have

$$\overline{Q}^{(k)} = \overline{H}_k \overline{Q}^{(k+1)} = \begin{bmatrix} I_{k-1} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & 1 - \overline{\alpha}_k^2 & -\overline{\alpha}_k \overline{w}_k^T B \\ \mathbf{O} & -\overline{\alpha}_k \overline{w}_k & (I_{m-k} - \overline{w}_k \overline{w}_k^T) B \end{bmatrix}. \quad (3.2)$$

By Lemma 3.3,  $\overline{w}_k \neq \mathbf{O}$ , and by the symbolic factorization procedure [11],  $\overline{\alpha}_k \neq 0$  also.

First, consider a row  $\overline{Q}_{i,*}^{(k)}$  where  $k \leq i \leq m$  and  $i \notin Struct(\overline{H}_{*,k})$ . It follows from

(3.2) that  $\overline{Q}_{i,*}^{(k)} = \overline{Q}_{i,*}^{(k+1)}$ , and hence

$$\text{Struct}(\overline{Q}_{i,*}^{(k)}) = \text{Struct}(\overline{Q}_{i,*}^{(k+1)}).$$

Moreover, since  $f_k(i) = f_{k+1}(i)$ , it follows directly from the induction hypothesis that the result holds for the row  $\overline{Q}_{i,*}^{(k)}$ .

Now consider a row  $\overline{Q}_{i,*}^{(k)}$ , where  $i \in \text{Struct}(\overline{H}_{*,k})$ . We make the following two observations. First, from (3.2) we see that each row  $\overline{Q}_{i,*}^{(k)}$  is computed by accumulating into the original row vector  $\overline{Q}_{i,*}^{(k+1)}$  a nonzero multiple of each row vector  $\overline{Q}_{j,*}^{(k+1)}$ , where  $j \in \text{Struct}(\overline{H}_{*,k}) - \{k\}$ . Second, also from (3.2) we see that  $\overline{Q}_{i,k}^{(k)} \neq 0$ . Thus we can write

$$\text{Struct}(\overline{Q}_{i,*}^{(k)}) = \{k\} \cup \left( \bigcup_{j \in \text{Struct}(\overline{H}_{*,k}) - \{k\}} \text{Struct}(\overline{Q}_{j,*}^{(k+1)}) \right). \quad (3.3)$$

To complete the argument, we next consider the row structure set  $\text{Struct}(\overline{Q}_{i,*}^{(k+1)})$ . We first show that  $f_{k+1}(i) = \varphi(k)$  as follows. Lemma 3.2 states that  $\text{Struct}(\overline{H}_{*,k}) - \{k\} \subseteq \text{Struct}(\overline{H}_{*,\varphi(k)})$ , from which it follows that  $f_{k+1}(i) \leq \varphi(k)$ . Since  $\overline{H}_{i,k} \neq 0$  and  $\overline{H}_{i,\varphi(k)} \neq 0$ , by Theorem 3.1,  $\overline{H}_{i,j} = 0$  for  $k < j < \varphi(k)$ . From the definition of  $f_{k+1}(i)$ , we see that indeed  $f_{k+1}(i) = \varphi(k)$ , and therefore by the induction hypothesis we have

$$\text{Struct}(\overline{Q}_{i,*}^{(k+1)}) = \{ \varphi(k), \varphi(\varphi(k)), \dots, \tilde{i}(i) \}. \quad (3.4)$$

From (3.4), we see that  $\text{Struct}(\overline{Q}_{i,*}^{(k+1)})$  is precisely the same for every  $i \in \text{Struct}(\overline{H}_{*,k})$ . This fact, along with (3.3), implies that

$$\text{Struct}(\overline{Q}_{i,*}^{(k)}) = \{ k, \varphi(k), \varphi(\varphi(k)), \dots, \tilde{i}(i) \}. \quad (3.5)$$

The result follows from (3.5) and the fact that  $f_k(i) = k$ . ■

The next theorem is a direct consequence of Theorem 3.1, Theorem 3.5, and the fact that  $f(i) = f_1(i)$ ,  $1 \leq i \leq m$ .

**Theorem 3.6.** *Let  $A$  be a strong Hall matrix with a zero-free diagonal and denote the matrix consisting of the first  $n$  columns of  $\overline{Q}$  by  $\overline{U}$ .*

(a)  $\text{Struct}(Q) \subseteq \mathcal{Q}(A) \subseteq \text{Struct}(\overline{Q})$ , and for  $1 \leq i \leq m$ ,

$$\text{Struct}(\overline{Q}_{i,*}) = \{ f(i), \varphi(f(i)), \varphi(\varphi(f(i))), \dots, \tilde{i}(i) \},$$

where  $\varphi(\tilde{i}(i)) = \tilde{i}(i)$ .

(b)  $Struct(\mathbf{U}) \subseteq \mathbf{U}(\mathbf{A}) \subseteq Struct(\overline{\mathbf{U}})$ , and for  $1 \leq i \leq m$ ,

$$Struct(\overline{\mathbf{U}}_{i,*}) = \{ f(i), \rho(f(i)), \rho(\rho(f(i))), \dots, t(i) \},$$

where  $\rho(t(i)) = t(i)$ .

(c) The lower trapezoidal part of  $\overline{\mathbf{U}}$  and the lower trapezoidal part of  $\overline{\mathbf{H}}$  have the same structure. That is,

$$\overline{\mathcal{H}}(\mathbf{A}) = \overline{\mathbf{U}}(\mathbf{A}) - \{(i, j) \mid 1 \leq j \leq n, 1 \leq i < j\}.$$

### 3.4. Equivalence of $\mathbf{U}(\mathbf{A})$ and $\overline{\mathbf{U}}(\mathbf{A})$

When  $\mathbf{A}$  is a strong Hall matrix, the results in Coleman et al. [1] showed that the pattern  $\overline{\mathcal{R}}(\mathbf{A})$  generated in George and Ng [11] is identical to  $\mathcal{R}(\mathbf{A})$ . In this section, we provide arguments to show that  $\overline{\mathcal{H}}(\mathbf{A}) = \mathcal{H}(\mathbf{A})$  and  $\overline{\mathbf{U}}(\mathbf{A}) = \mathbf{U}(\mathbf{A})$ . We again assume that  $\mathbf{A}$  is a strong Hall matrix with a zero-free diagonal.

Since we already know that these sparsity patterns are adequate (i.e.,  $\mathcal{H}(\mathbf{A}) \subseteq \overline{\mathcal{H}}(\mathbf{A})$  and  $\mathbf{U}(\mathbf{A}) \subseteq \overline{\mathbf{U}}(\mathbf{A})$ ), it suffices to show that  $\overline{\mathcal{H}}(\mathbf{A}) \subseteq \mathcal{H}(\mathbf{A})$  and  $\overline{\mathbf{U}}(\mathbf{A}) \subseteq \mathbf{U}(\mathbf{A})$ . Toward that end, choose  $(i, k) \notin \mathbf{U}(\mathbf{A})$ . Since  $\mathbf{A}$  is a strong Hall matrix, we have  $S_C^{[k-1]} = S_R^{[k-1]} = \emptyset$ . Consequently, the following two results suffice to show that  $(i, k) \notin \overline{\mathbf{U}}(\mathbf{A})$ .

**Lemma 3.7.** *If  $i \in F^{[k]}$ , then  $(i, k) \notin \overline{\mathbf{U}}(\mathbf{A})$ .*

**Proof:** Suppose that  $i \in F^{[k]}$ . It then follows that  $A_{i,j} = 0$  for  $1 \leq j \leq k$ . Consequently,  $k < f(i)$ , which by Theorem 3.6 ensures that  $(i, k) \notin \overline{\mathbf{U}}(\mathbf{A})$ . ■

**Lemma 3.8.** *If  $i \in D^{[k]}$ , then  $(i, k) \notin \overline{\mathbf{U}}(\mathbf{A})$ .*

**Proof:** Suppose that  $i \in D^{[k]}$ . It follows that  $r_i \in R^{[k]}$ , and thus we have  $f(i) < k$ . To show that  $(i, k) \notin \overline{\mathbf{U}}(\mathbf{A})$ , it is sufficient according to Theorem 3.6 to show that  $k$  is not an ancestor of  $f(i)$  in the elimination forest defined by  $\rho$ .

Consider the symmetric positive definite matrix  $\mathbf{B} = \mathbf{A}^T \mathbf{A}$  and its Cholesky factor  $\mathbf{L}$ . Since  $\mathbf{A}$  is strong Hall, we have (assuming no numerical cancellation)  $Struct(\mathbf{L}^T) = Struct(\overline{\mathbf{R}}) = Struct(\mathbf{R})$  [1], whence  $\overline{\mathbf{R}}$ 's elimination forest and  $\mathbf{L}$ 's elimination forest are identical. Let  $G(\mathbf{B}) = (C^{[n]}, E')$  be the adjacency graph of  $\mathbf{B}$ , i.e., the graph for which there is an edge joining  $c_s$  and  $c_t$  if and only if  $B_{s,t} \neq 0$ . Here,  $C^{[n]} = \{c_1, c_2, \dots, c_n\}$  is the same vertex set used to construct the bipartite graph  $B^{[n]}$  in Section 2.3. Liu [16] has shown that for  $s < t$ , the vertex  $c_t$  is an ancestor of  $c_s$  in  $\mathbf{L}$ 's

elimination forest if and only if they are connected by a path in the subgraph of  $G(\mathbf{B})$  induced by  $C^{[i]} = \{c_1, c_2, \dots, c_i\}$  (Lemma 2.3 in [16]).

Now, membership of  $i$  in  $D^{[k]}$  implies that there exists no path from  $c_k$  to  $r_i$  in the bipartite graph  $B^{[k]}$ . Since  $\{r_i, c_{f(i)}\} \in E^{[k]}$ , there is also no path from  $c_{f(i)}$  to  $c_k$  in  $B^{[k]}$ . Thus, to prove the result it suffices to show that the absence of a path from  $c_{f(i)}$  to  $c_k$  in  $B^{[k]}$  implies the absence of a path from  $c_{f(i)}$  to  $c_k$  in the subgraph of  $G(\mathbf{B})$  induced by  $C^{[k]}$ .

Toward that end, suppose that there is a path

$$(c_{f(i)}, c_{s_1}, c_{s_2}, \dots, c_{s_\tau}, c_k)$$

in  $G(\mathbf{B})$  such that  $s_p < k$  for  $1 \leq p \leq \tau$ . (Recall that  $f(i) < k$ , as well.) It is trivial to verify that  $G(\mathbf{B})$  is the graph on  $C^{[n]}$  with edge set  $E'$  consisting of precisely the edges necessary to make each vertex set  $\{c_j \mid j \in \text{Struct}(\mathbf{A}_{i,*})\}$ ,  $1 \leq i \leq m$ , a clique in the graph (i.e., pairwise adjacent in the graph). Consequently, if  $\{c_s, c_t\} \in E'$  with  $s < t$ , then there must exist some row  $i$  for which  $s, t \in \text{Struct}(\mathbf{A}_{i,*})$ , and therefore  $(c_s, r_i, c_t)$  is a path in  $B^{[i]}$ . It follows that there exists a path

$$(c_{f(i)}, r_{t_1}, c_{s_1}, r_{t_2}, c_{s_2}, \dots, r_{t_\tau}, c_{s_\tau}, r_{t_{\tau+1}}, c_k)$$

in  $B^{[k]}$  such that  $s_p < k$  for  $1 \leq p \leq \tau$  and  $1 \leq t_p \leq m$  for  $1 \leq p \leq \tau + 1$ . This concludes the proof. ■

With these two results and the discussion preceding them we have proven the following result.

**Theorem 3.9.** For  $\overline{\mathbf{U}}(\mathbf{A})$  defined in Theorem 3.6, we have  $\overline{\mathbf{U}}(\mathbf{A}) = \mathbf{U}(\mathbf{A})$ .

The following result shows how the characterization maintains in a natural way the classification of zero entries for a strong Hall matrices from Hare et al. [15].

**Corollary 3.10.**

1.  $i \in F^{[k]}$  if and only if  $k < f(i)$ .
2.  $i \in D^{[k]}$  if and only if  $f(i) < k$  and  $k$  is not an ancestor of  $f(i)$  in the elimination forest  $\rho$ .

**Proof:** The proof follows immediately from Theorem 3.9 and the proofs of Lemma 3.7 and Lemma 3.8. ■

Finally, we have the following result for  $\overline{\mathbf{H}}(\mathbf{A})$ .

**Corollary 3.11.** For  $\overline{\mathcal{H}}(\mathbf{A})$  defined as in Theorem 3.1, we have  $\overline{\mathcal{H}}(\mathbf{A}) = \mathcal{H}(\mathbf{A})$ .

**Proof:** The result follows immediately from Theorem 3.9 and part (c) of Theorem 3.6. ■

#### 4. Weak Hall matrices and block upper triangular forms

We know of no way to generalize the results of the previous section so that they apply to arbitrary Hall matrices. The proofs of those results depend on several properties of strong Hall matrices that do not hold for Hall matrices in general. This problem can be overcome however if one is willing to rearrange the rows and columns of the weak Hall matrix. One can always permute a given weak Hall matrix into *block upper triangular form* so that each diagonal block has the strong Hall property [2,6,20]. (Permuting a weak Hall matrix into such a block upper triangular form is also known as the Dulmage-Mendelsohn decomposition.) The block upper triangular form essentially recaptures the properties of strong Hall matrices needed for our purposes.

In Section 4.1 we briefly review the block upper triangular form. Section 4.2 adapts the characterization of Section 3.3 to obtain a characterization of  $\mathcal{H}(\mathbf{A})$  and  $\mathcal{U}(\mathbf{A})$  when  $\mathbf{A}$  is any weak Hall matrix that is already in block upper triangular form. Finally, let  $\mathbf{A}$  be a weak Hall matrix and let  $\widehat{\mathbf{A}}$  be the same matrix *after it has been permuted* into block upper triangular form. Section 4.3 shows that the factors  $\widehat{\mathbf{U}}$  and  $\widehat{\mathbf{R}}$  of  $\widehat{\mathbf{A}}$  incur no more fill than the factors  $\mathbf{U}$  and  $\mathbf{R}$  of  $\mathbf{A}$ .

##### 4.1. Definitions and notation

Let  $\mathbf{A}$  be a weak Hall matrix and without loss of generality assume that  $\mathbf{A}$  has a zero-free diagonal. Then there exists an  $n \times n$  permutation matrix  $\mathbf{P}$  such that the matrix

$$\widehat{\mathbf{A}} = \begin{bmatrix} \mathbf{P} & \mathbf{O} \\ \mathbf{O} & \mathbf{I}_{m-n} \end{bmatrix} \mathbf{A} \mathbf{P}^T$$

has the form

$$\widehat{\mathbf{A}} = \left[ \begin{array}{cccc|c} \widehat{\mathbf{A}}_{1,1} & \widehat{\mathbf{A}}_{1,2} & \cdots & \widehat{\mathbf{A}}_{1,p} & \widehat{\mathbf{A}}_{1,p+1} \\ \mathbf{O} & \widehat{\mathbf{A}}_{2,2} & \cdots & \widehat{\mathbf{A}}_{2,p} & \widehat{\mathbf{A}}_{2,p+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{O} & \mathbf{O} & \cdots & \widehat{\mathbf{A}}_{p,p} & \widehat{\mathbf{A}}_{p,p+1} \\ \hline \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} & \widehat{\mathbf{A}}_{p+1,p+1} \end{array} \right], \quad (4.1)$$

where  $p \geq 1$ , and for  $1 \leq s \leq p$  the submatrix  $\widehat{\mathbf{A}}_{s,s}$  is a square  $\eta_s \times \eta_s$  matrix that has the strong Hall property. The submatrix  $\widehat{\mathbf{A}}_{p+1,p+1}$  is an  $(\eta_{p+1} + m - n) \times \eta_{p+1}$  matrix that also has the strong Hall property. (In some instances  $\widehat{\mathbf{A}}_{p+1,p+1}$  may be

a null matrix.) Note that  $\hat{\mathbf{A}}$  has the same nonzero diagonal entries as  $\mathbf{A}$ , although they generally will appear in different positions. Note moreover that the block upper triangular form satisfying these properties is essentially unique and is independent of the choice of the zero-free diagonal [2,20].

Let  $\alpha : \{1, 2, \dots, n\} \rightarrow \{1, 2, \dots, n\}$  be the permutation that maps each row (column) index in  $\mathbf{A}$  to its new position in  $\hat{\mathbf{A}}$ . For any respective row and column index pair  $i$  and  $j$ , we let  $\hat{i} := \alpha(i)$  and  $\hat{j} := \alpha(j)$ , so that  $\hat{A}_{\hat{i}, \hat{j}} = A_{i, j}$ . To obtain the results in Section 4.3 we require moreover that the permutation  $\alpha$  be *consistent* with the original ordering in the following sense. The individual columns within a block column of  $\hat{\mathbf{A}}$  must occur in the *same order* in which they are found in  $\mathbf{A}$ . For example, for the first block column we must have

$$\alpha^{-1}(1) < \alpha^{-1}(2) < \alpha^{-1}(3) < \dots < \alpha^{-1}(\eta_1).$$

While the ordering of individual columns within block columns is fixed by the original ordering, there is only one restriction on the ordering of the block columns themselves. When  $m > n$ , block column  $p + 1$  must be composed of all the columns of  $\mathbf{A}$  that belong to no Hall set under *any* column ordering of  $\mathbf{A}$ , if indeed such columns exist. If  $m = n$  or there are no such columns, then there is no restriction on the order of the block columns.

#### 4.2. Characterization of $\mathcal{Q}(\hat{\mathbf{A}})$ for the block upper triangular form

Suppose that  $\hat{\mathbf{A}}$  has the form shown in (4.1), and denote the  $QR$  factorization of  $\hat{\mathbf{A}}$  by

$$\hat{\mathbf{A}} = \hat{\mathbf{Q}} \begin{bmatrix} \hat{\mathbf{R}} \\ \mathbf{O} \end{bmatrix}.$$

Let  $\hat{\mathbf{U}}$  moreover be the matrix consisting of the first  $n$  columns of  $\hat{\mathbf{Q}}$ , and let  $\hat{\mathbf{H}}$  be the Householder matrix for  $\hat{\mathbf{A}}$ . It is well known that for *general* Hall matrices, the zero-nonzero patterns  $\overline{\mathcal{H}}(\hat{\mathbf{A}})$  and  $\overline{\mathcal{R}}(\hat{\mathbf{A}})$  generated by symbolic  $QR$  factorization using Givens rotations or Householder transformations may not be the same as  $\mathcal{H}(\hat{\mathbf{A}})$  and  $\mathcal{R}(\hat{\mathbf{A}})$  respectively. However, Coleman et al. [1] have shown that, when applied to weak Hall matrices that are in block upper triangular form, the pattern  $\overline{\mathcal{R}}(\hat{\mathbf{A}})$  created by symbolic  $QR$  factorization using Givens rotations is indeed identical to  $\mathcal{R}(\hat{\mathbf{A}})$ . This result also holds when Householder transformations are used instead of Givens rotations. In this section we modify the characterization introduced in Section 3 to obtain characterizations of  $\overline{\mathcal{Q}}(\hat{\mathbf{A}})$ ,  $\overline{\mathcal{U}}(\hat{\mathbf{A}})$ , and  $\overline{\mathcal{H}}(\hat{\mathbf{A}})$ , the last two of which are identical to  $\mathcal{U}(\hat{\mathbf{A}})$  and  $\mathcal{H}(\hat{\mathbf{A}})$  respectively.

For convenience, define  $n_s$  to be

$$n_s = \sum_{t=1}^s \eta_t, \quad \text{for } 1 \leq s \leq p+1.$$

Note that  $n = n_{p+1}$ . It should be obvious that the Hall columns  $\widehat{S}_C^{[\hat{k}]}$  and the Hall rows  $\widehat{S}_R^{[\hat{k}]}$  for  $\widehat{A}$  are given by

$$\widehat{S}_C^{[\hat{k}]} = \widehat{S}_R^{[\hat{k}]} = \begin{cases} \emptyset & , \text{ if } 1 \leq \hat{k} \leq n_1 - 1, \\ \{1, 2, \dots, n_1\} & , \text{ if } n_1 \leq \hat{k} \leq n_2 - 1, \\ \{1, 2, \dots, n_2\} & , \text{ if } n_2 \leq \hat{k} \leq n_3 - 1, \\ \vdots & \vdots \\ \{1, 2, \dots, n_{p-1}\} & , \text{ if } n_{p-1} \leq \hat{k} \leq n_p - 1, \\ \{1, 2, \dots, n_p\} & , \text{ if } n_p \leq \hat{k} \leq n_{p+1} - 1. \end{cases} \quad (4.2)$$

We now use Theorem 2.3 to show that  $\widehat{U}$  has the following form:

$$\widehat{U} = \left[ \begin{array}{cccc|c} \widehat{U}_{1,1} & \mathbf{O} & \cdots & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \widehat{U}_{2,2} & \cdots & \mathbf{O} & \mathbf{O} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathbf{O} & \mathbf{O} & \cdots & \widehat{U}_{p,p} & \mathbf{O} \\ \hline \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} & \widehat{U}_{p+1,p+1} \end{array} \right], \quad (4.3)$$

where  $\widehat{U}$  has been partitioned in the same manner as  $\widehat{A}$ .

**Lemma 4.1.** *An  $m \times n$  weak Hall matrix  $\widehat{A}$  in block upper triangular form (4.1) has an  $m \times n$  orthogonal factor  $\widehat{U}$  in block diagonal form (4.3).*

**Proof:** Consider any column  $j$  in  $\widehat{U}$  and let  $\widehat{A}_{i,j}$  be an entry in one of the off-diagonal blocks  $\widehat{A}_{s,t}$  of  $\widehat{A}$ , so that  $n_{s-1} < i \leq n_s$  and  $n_{t-1} < j \leq n_t$ . If  $s > t$ , then it follows from (4.1) that  $\widehat{A}_{i,\hat{p}} = 0$ , for  $1 \leq \hat{p} \leq j$ . Consequently,  $i \in \widehat{F}^{[j]}$  and thus by Theorem 2.3,  $\widehat{U}_{i,j} = 0$ . This observation applies to every entry in  $\widehat{A}_{s,t}$ , and hence  $\widehat{U}_{s,t} = \mathbf{O}$  for  $s > t$ . If on the other hand  $s < t$ , it follows from (4.2) that  $\widehat{S}_C^{[j-1]} = \widehat{S}_R^{[j-1]} = \{1, 2, \dots, n_{t-1}\} \neq \emptyset$ . Since  $s < t$ , we have  $i \leq n_s \leq n_{t-1}$  and thus  $i \in \widehat{S}_R^{[j-1]}$ . It follows then from Theorem 2.3 that  $\widehat{U}_{i,j} = 0$ . Again, this observation applies to every entry in  $\widehat{A}_{s,t}$ , and hence  $\widehat{U}_{s,t} = \mathbf{O}$  for  $s < t$ .  $\blacksquare$

It follows from Lemma 4.1 that the problem of determining  $\mathbf{U}(\widehat{A})$  decomposes into finding  $\mathbf{U}(\widehat{A}_{s,s})$  based solely on  $\text{Struct}(\widehat{A}_{s,s})$  for  $1 \leq s \leq p+1$ . Since each submatrix

$\widehat{\mathbf{A}}_{s,s}$  is strong Hall, the techniques in Section 3.3 can be applied to obtain a row-oriented characterization of  $\mathbf{U}(\widehat{\mathbf{A}}_{s,s})$ .

It is also trivial to use the techniques of Section 3.3 to include the last  $m-n$  columns of  $\widehat{\mathbf{Q}}$  in this characterization. It follows from (4.3) that the matrix  $\widehat{\mathbf{Q}}$  must have the following form:

$$\widehat{\mathbf{Q}} = \left[ \begin{array}{cccc|ccc} \widehat{\mathbf{U}}_{1,1} & \mathbf{O} & \cdots & \mathbf{O} & \mathbf{O} & & \widehat{\mathbf{V}}_{1,p+2} \\ \mathbf{O} & \widehat{\mathbf{U}}_{2,2} & \cdots & \mathbf{O} & \mathbf{O} & & \widehat{\mathbf{V}}_{2,p+2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & & \vdots \\ \mathbf{O} & \mathbf{O} & \cdots & \widehat{\mathbf{U}}_{p,p} & \mathbf{O} & & \widehat{\mathbf{V}}_{p,p+2} \\ \hline \mathbf{O} & \mathbf{O} & \cdots & \mathbf{O} & \widehat{\mathbf{U}}_{p+1,p+1} & & \widehat{\mathbf{V}}_{p+1,p+2} \end{array} \right], \quad (4.4)$$

where  $\widehat{\mathbf{V}}_{s,p+2}$  is  $\eta_s \times (m-n)$  for  $1 \leq s \leq p$ , and  $\widehat{\mathbf{V}}_{p+1,p+2}$  is  $(\eta_{p+1} + m-n) \times (m-n)$ . To ensure orthogonality in the last  $m-n$  columns of  $\widehat{\mathbf{Q}}$ , we must have  $\widehat{\mathbf{V}}_{s,p+2} = \mathbf{O}$ ,  $1 \leq s \leq p$ , by an argument similar to that in the second paragraph following Theorem 2.3. The row structure of  $\widehat{\mathbf{V}}_{p+1,p+2}$  can be obtained using the generalized elimination tree in Section 3.2.

We now express these results in a form similar to their analogues in Section 3.3. As in Section 3, we let  $\hat{f}(i)$  be the column index of the *first* nonzero in row  $i$  of  $\widehat{\mathbf{A}}$ . The generalized elimination forest  $\hat{\varphi}$  is defined in exactly the same way as in Section 3.2, using  $\mathcal{R}(\widehat{\mathbf{A}})$  and the structure of the Householder vectors for the “root” columns (in  $\mathcal{H}(\widehat{\mathbf{A}})$ ). However, we need to introduce the *Hall function*  $\hat{v}$ , which is defined as follows. For column  $j$  of  $\widehat{\mathbf{A}}$  belonging to block column  $\widehat{\mathbf{A}}_{*,t}$  (i.e.,  $n_{t-1} < j \leq n_t$ ), we define  $\hat{v}(j) := n_t$ . Thus, for  $1 \leq j \leq n_p$ ,  $\hat{v}(j)$  is the column in whose Hall set column  $j$  first appears. For  $n_p < j \leq m$ , we define  $\hat{v}(j) := 0$ .

**Corollary 4.2.**

(a) For  $1 \leq i, j \leq m$ , if  $(i, j) \in \overline{\mathcal{Q}}(\widehat{\mathbf{A}})$ , then

$$j \in \{ \hat{f}(i), \hat{\varphi}(\hat{f}(i)), \hat{\varphi}(\hat{\varphi}(\hat{f}(i))), \dots, \tilde{t}(i) \},$$

where  $\tilde{t}(i) = \hat{v}(i)$  or  $\hat{\varphi}(\tilde{t}(i)) = \tilde{t}(i)$ .

(b) For  $1 \leq i \leq m$  and  $1 \leq j \leq n$ ,  $(i, j) \in \mathbf{U}(\widehat{\mathbf{A}})$  if and only if

$$j \in \{ \hat{f}(i), \hat{\rho}(\hat{f}(i)), \hat{\rho}(\hat{\rho}(\hat{f}(i))), \dots, t(i) \},$$

where  $t(i) = \hat{v}(i)$  or  $\hat{\rho}(t(i)) = t(i)$ .

(c)  $\mathcal{H}(\widehat{\mathbf{A}}) = \mathbf{U}(\widehat{\mathbf{A}}) - \{(i, j) \mid 1 \leq j \leq n, 1 \leq i < j\}$ .

### 4.3. Minimality of fill in $\widehat{U}$ and $\widehat{R}$

The purpose of this section is to explain the effects of permuting to block upper triangular form on the sparsity of the triangular and orthogonal factors. As noted earlier, reordering the *rows* of  $\mathbf{A}$  has no influence on the sparsity of the triangular factor and merely permutes the rows of the orthogonal factor. Permuting the *columns* of  $\mathbf{A}$  however can dramatically change the amount of fill in either (or both) of the factors. In this subsection, again using the results in [15], we show that when  $\mathbf{A}$  is permuted into block upper triangular form in a fashion that is *consistent* with the original ordering of  $\mathbf{A}$  (see Section 4.1 for the definition of a consistent ordering), then the sparsity of the factors will stay the same or improve.

By direct application of the results in [15], we first prove that the zeros in  $\mathbf{U}$  are preserved in  $\widehat{U}$ .

**Theorem 4.3.** *If  $U_{i,j} = 0$ , then  $\widehat{U}_{i,j} = 0$ .*

**Proof:** We showed in Section 4.2 that  $\widehat{U}$  has a block diagonal form (4.3), and thus we can proceed as follows. Choose diagonal block  $\widehat{\mathbf{A}}_{s,s}$ ,  $1 \leq s \leq p+1$ , and let  $U_{i,j} = 0$  be chosen so that

$$n_{s-1} < \alpha(i), \alpha(j) \leq n_s. \quad (4.5)$$

It now suffices to show that  $\widehat{U}_{i,j} = 0$ . To do so, we consider each of the three cases highlighted in the statement of Theorem 2.3.

First, assume that  $i \in F^{[j]}$ . It follows that  $A_{i,k} = 0$  for  $1 \leq k \leq j$ . From (4.1), the only possible nonzero entries  $\widehat{A}_{i,\hat{k}} \neq 0$  for  $1 \leq \hat{k} \leq \hat{j}$  occur within the diagonal block  $\widehat{\mathbf{A}}_{s,s}$ . However, since  $\alpha$  is a consistent ordering and  $A_{i,k} = 0$  for  $1 \leq k \leq j$ , it follows that  $\widehat{A}_{i,\hat{k}} = 0$  for  $1 \leq \hat{k} \leq \hat{j}$ . Consequently,  $i \in \widehat{F}^{[j]}$  and by Theorem 2.3,  $\widehat{U}_{i,j} = 0$  as desired.

Second, assume that  $i \in D^{[j]}$ . It then follows that  $r_i \in R^{[j]}$  and  $r_i$  is *not* reachable from  $c_j$  by any path in  $B^{[j]}$ . To show that  $\widehat{U}_{i,j} = 0$ , it suffices to show that  $\widehat{B}^{[j]}$  is isomorphic under the bijection  $\alpha$  to a *subgraph* of  $B^{[j]}$ , for then  $\hat{r}_i$  will *not* be reachable from  $\hat{c}_j$  by any path in  $\widehat{B}^{[j]}$ . From (4.2), the only rows (columns)  $1 \leq \hat{k} \leq \hat{j}-1$  that are *not* in  $\widehat{S}_R^{[j-1]}$  ( $= \widehat{S}_C^{[j-1]}$ ) are precisely those rows (columns)  $\hat{k}$  for which  $n_{s-1} < \hat{k} < \hat{j}$ . However, since the ordering  $\alpha$  is consistent with the original ordering and the submatrix  $\widehat{\mathbf{A}}_{s,s}$  is strong Hall, it follows that for each such row (column)  $\hat{k}$  of  $\widehat{\mathbf{A}}$ , the corresponding row (column)  $k$  of  $\mathbf{A}$  is *not* in  $S_R^{[j-1]}$  ( $= S_C^{[j-1]}$ ). Consequently,  $\widehat{B}^{[j]}$  is isomorphic (under  $\alpha$ ) to a subgraph of  $B^{[j]}$ , as required.

Lastly, we consider the possibility that  $i \in S_R^{[j-1]}$ . It follows directly from the argument in the preceding paragraph that if  $k \in S_R^{[j-1]}$ , then  $\hat{k} \in \widehat{S}_R^{[j-1]}$ . Now (4.2) and (4.5) imply that  $i \notin \widehat{S}_R^{[j-1]}$ , and hence  $i \notin S_R^{[j-1]}$ . Thus we do not have to consider this

possibility, and this concludes the proof. ■

We have shown that there can never be more nonzero entries in  $\widehat{U}$  than in  $U$ . Theorem 4.3 can be used to establish a similar result for the upper triangular factor  $\widehat{R}$ .

**Corollary 4.4.** *If  $R_{i,j} = 0$ , then  $\widehat{R}_{i,j} = 0$ .*

**Proof:** Assume that  $\widehat{R}_{i,j} \neq 0$ . Since we can express  $\widehat{R}_{i,j}$  as

$$\widehat{R}_{i,j} = \sum_{\hat{i}=1}^m \widehat{U}_{i,\hat{i}} \widehat{A}_{\hat{i},j},$$

it follows that  $\widehat{U}_{\hat{k},i} \neq 0$  and  $\widehat{A}_{\hat{k},j} \neq 0$  for some  $\hat{k}$ ,  $1 \leq \hat{k} \leq m$ . Clearly then  $A_{k,j} \neq 0$ . By Theorem 4.3,  $\widehat{U}_{\hat{k},i} \neq 0$  implies that  $U_{k,i} \neq 0$ . Proceeding under the usual assumption of no numerical cancellation, we have

$$R_{i,j} = \sum_{t=1}^m U_{t,i} A_{t,j} = \cdots + U_{k,i} A_{k,j} + \cdots \neq 0,$$

which proves the result. ■

## 5. Concluding remarks

In this paper, we have used a recent and complete sparsity analysis of  $QR$  factorization [15,19] to provide a similarly complete extension and analysis of a well-known symbolic factorization procedure for sparse  $QR$  factorization [9,11]. For the purposes of this work, the key insight provided by Hare et al. [15] is the impact that Hall rows and columns in  $A$  have on the sparsity of  $U$ . Essentially, the role of the Hall sets (or the Hall function  $\hat{\nu}$ ) in defining the right profile of  $U$  is perfectly analogous to the role of the function  $f(i)$  in defining the left profile of  $U$ . It should be noted that the efficient symbolic factorization algorithm in [11] can be modified easily to compute  $\overline{Q}(A)$  and  $\overline{U}(A)$ .

We have seen how the Hall sets and the interplay between orthogonality and sparsity disappear for strong Hall matrices. We demonstrated that the characterization of  $\overline{\mathcal{H}}(A)$  given in [9] is identical to  $\mathcal{H}(A)$ . We were able to extend the characterization to obtain a simple characterization of  $\overline{U}(A)$  and prove that  $\overline{U}(A) = U(A)$ . In the strong Hall case, we established that  $\mathcal{H}(A) = U(A) - \{(i,j) \mid 1 \leq j \leq n, 1 \leq i < j\}$ . We were also able to link certain details of the analysis in [15] with certain features found in our structure characterization.

Though we were unable to extend our techniques and analysis to weak Hall matrices in general, we are able to do so for weak Hall matrices that have been permuted into block upper triangular form. We contend however that this is not a serious restriction. Efficient algorithms for finding a zero-free diagonal [3] and for permuting a matrix to block upper triangular form [5,20] have long been used by the sparse matrix research community. Moreover, we have shown here that permuting to block upper triangular form never increases the fill in orthogonal factorization, and may actually reduce it. So given an arbitrary Hall matrix, permuting it to block upper triangular form is both advisable and easily done.

We know of few cases where explicit computation of the orthogonal factor  $U$  is required. There are however many options that fall between explicit computation of  $U$  and implicit computation of the orthogonal factor by computing  $H$ . On advanced architectures, where blocked algorithms are so important for good performance, “partial” computation of  $U$  by multiplying together some but not all of the Householder transformations could be a valuable option. In this paper, we have provided a framework for exploring such possibilities.

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