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Unitary k-Hessenberg Matrices

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ABSTRACT

In 1971, Householder and Fox [26] introduced a method for computing an orthonormal basis for the range of a projection. Using a Cholesky decomposition on a symmetric idempotent matrix A produced $A = LL^T$, where the columns of the lower triangular matrix L form said basis. Moler and Stewart [32] performed an error analysis on the Householder-Fox algorithm in 1978. It was shown that in most cases reasonable results can be expected, however a recent paper by Parlett and Barszcz [36] included a numerical experiment by Kahan in which the Householder-Fox method performed poorly. Parlett proposed an alternate method which focused on exploiting the structure of the $n \times n$ projection $I - qq^T$. In the case where the Householder-Fox algorithm produced an error of 1, this new method produced full accuracy. In what follows, additional algorithms will be introduced, exploiting the decomposable, Green's $(H, 1)$-quasiseparable and Green's $(H, 1)$-semiseparable structure of unitary Hessenberg matrices. It will be shown that the more general and newly defined unitary k-Hessenberg matrices also have a great deal of structure, and further, that the structure exploiting algorithms mentioned above are readily generalizable to this new unitary k-Hessenberg case.

Unitary k-Hessenberg Matrices

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Unitary k-Hessenberg Matrices

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Contents

List of Figures

1 Introduction

For the sake of completeness, we begin with the definitions of order k quasiseparable and order k semiseparable matrices, along with some previously known results. Because the primary focus of this paper involves Hessenberg matrices, the more useful definitions of (H, k)-quasiseparable and (H, k)-semiseparable matrices are introduced.

1.1 Quasiseparable and Semiseparable Matrices

1.1.1 Order k Quasiseparable Matrices

There are two equivalent characterizations of quasiseparable matrices. We begin with the "rank" definition.

Definition 1.1 (Rank)**.** *An $n \times n$ matrix A is quasiseparable of order k provided that $\max(rank(A_{21})) = \max(rank(A_{12})) = k$ where the maxima are taken over all symmetric partitions of the form:*

$$A = \left[\begin{array}{c|c} * & A_{12} \\ \hline A_{21} & * \end{array}\right]$$

The definition above is useful in the theoretical sense, however in order to take advantage of the structure of such matrices when designing an algorithm, the equivalent "generator" definition is necessary.

Definition 1.2 (Generator)**.** *An $n \times n$ matrix A is quasiseparable of order*

k if there exist parameters $\mathfrak{G} = \{p_t, a_u, r_v, g_v, b_u, h_t, d_w\}$ for $t = 2, \ldots, n$, $u = 2, \ldots, n-1$, $v = 1, \ldots, n-1$, $w = 1, \ldots, n$, where each is a matrix of size $1 \times k$, $k \times k$, $k \times 1$, 1×1, $1 \times k$, $k \times k$ and $k \times 1$ respectively, such that

$$A_{ij} = \begin{cases} p_i a_{ij}^{\times} r_j, & i > j \\ d_i, & i = j \\ g_i b_{ij}^{\times} h_j & i < j \end{cases}$$

where

$$a_{ij}^{\times} = \begin{cases} a_{i-1} a_{i-2} \cdots a_{j+1}, & i > j+1 \\ I_k & i = j+1 \end{cases}$$

$$b_{ij}^{\times} = \begin{cases} b_{i+1} b_{i+2} \cdots b_{j-1}, & i < j-1 \\ I_k & i = j-1 \end{cases}$$

The elements of $\mathfrak{G}$ are called a set of order k quasiseparable generators for A.

Now, suppose we have two lower triangular order 1 quasiseparable matrices A and B, and we wish to compute the product of the two. It turns out that the structure of A and B carries over to the desired product. Indeed, AB is lower triangular order 2 quasiseparable, and hence can be constructed via its order 2 quasiseparable generators. The next theorem (see [18]) generalizes this result, and will be of use in the sections that follow.

Theorem 1.3. *Let A and B be $n \times n$ lower triangular matrices. If A has order j quasiseparable generators $\mathfrak{G}_1 = \{p_t^{(A)}, a_u^{(A)}, r_v^{(A)}, d_w^{(A)}\}$ and B has order* *k quasiseparable generators* $\mathfrak{G}_2 = \{p_t^{(B)}, a_u^{(B)}, r_v^{(B)}, d_w^{(B)}\}$*, then the product* AB *has order* $(j+k)$ *quasiseparable generators* $\mathfrak{G}_{12} = \{p_t^{(AB)}, a_u^{(AB)}, r_v^{(AB)}, d_w^{(AB)}\}$ *given by:*

$$p_i^{(AB)} = \begin{bmatrix} p_i^{(A)} & d_i^{(A)} p_i^{(B)} \end{bmatrix}, \quad a_i^{(AB)} = \begin{bmatrix} a_i^{(A)} & r_i^{(A)} p_i^{(B)} \\ 0 & a_i^{(B)} \end{bmatrix}$$

$$r_i^{(AB)} = \begin{bmatrix} r_i^{(A)} d_i^{(B)} \\ r_i^{(B)} \end{bmatrix}, \quad d_i^{(AB)} = d_i^{(A)} d_i^{(B)}$$

for $t = 2, \ldots, n$, $u = 2, \ldots, n-1$, $v = 1, \ldots, n-1$, *and* $w = 1, \ldots, n$. *It is noted that since* A, B *and* AB *are lower triangular, one can take the generators above the main diagonal to be* 0.

1.1.2 Order k Semiseparable Matrices

We now briefly turn our attention to a subclass of quasiseparable matrices, namely, matrices with semiseparable structure. As in the previous section, we offer two equivalent characterizations.

Definition 1.4 (QS Generator)**.** *An* $n \times n$ *matrix* A *is semiseparable of order* k *if there exists a choice of order* k *quasiseparable generators* $\mathfrak{G} = \{p_t, a_u, r_v, g_v, b_u, h_t, d_w\}$ *for* A *such that* a_u *and* b_u *are invertible for* $u = 2, \ldots, n-1$.

It is obvious that by definition, order k semiseparable matrices form a subclass of order k quasiseparable matrices. These two classes are not equivalent however. As a simple example when $k = 1$, consider an irreducible tridiagonal matrix. That is, a matrix of the form

$$\begin{bmatrix} \alpha_1 & \gamma_1 & 0 & 0 & 0 \\ \beta_1 & \alpha_2 & \gamma_2 & 0 & 0 \\ 0 & \beta_2 & \alpha_3 & \gamma_3 & 0 \\ 0 & 0 & \beta_3 & \alpha_4 & \gamma_4 \\ 0 & 0 & 0 & \beta_4 & \alpha_5 \end{bmatrix}$$

where β_i and γ_i are nonzero for $i = 1, \ldots, 4$. This matrix certainly satisfies the rank requirements for order 1 quasiseparability. Thus, we have

$$\begin{bmatrix} \alpha_1 & \gamma_1 & 0 & 0 & 0 \\ \beta_1 & \alpha_2 & \gamma_2 & 0 & 0 \\ 0 & \beta_2 & \alpha_3 & \gamma_3 & 0 \\ 0 & 0 & \beta_3 & \alpha_4 & \gamma_4 \\ 0 & 0 & 0 & \beta_4 & \alpha_5 \end{bmatrix} = \begin{bmatrix} d_1 & g_2h_1 & g_3b_2h_1 & g_4b_3b_2h_1 & g_5b_4b_3b_2h_1 \\ p_2r_1 & d_2 & g_3h_2 & g_4b_3h_2 & g_5b_4b_3h_2 \\ p_3a_2r_1 & p_3r_2 & d_3 & g_4h_3 & g_5b_4h_3 \\ p_4a_3a_2r_1 & p_4a_3r_2 & p_4r_3 & d_4 & g_5h_4 \\ p_5a_4a_3a_2r_1 & p_5a_4a_3r_2 & p_5a_4r_3 & p_5r_4 & d_5 \end{bmatrix}$$

Since $\beta_i \neq 0$ and $\gamma_i \neq 0$, it must be the case that r_i, h_i, p_j and g_j are nonzero for $i = 1, \ldots, 4$ and $j = 2, \ldots, 5$, and hence the conditions $a_l \neq 0$ and $b_l \neq 0$ for all l are not satisfied. That is, irreducible tridiagonal matrices are quasiseparable, but not semiseparable.

In the case of order k semiseparability, the invertibility of each a_u and b_u permits the following equivalent definition.

Definition 1.5 (SS Generator)**.** *An $n \times n$ matrix A is semiseparable of order k if*

$$tril(A, -1) = tril(r_l t_l, -1), \quad triu(A, 1) = triu(r_u t_u, 1) \tag{1}$$

for some matrices r_l and r_u of size $n \times k$, and t_l and t_u of size $k \times n$ and where $tril(\cdot, -1)$ denotes the strictly lower triangular parts of A and $r_l t_l$, and $triu(\cdot, 1)$ denotes the strictly upper triangular parts of A and $r_u t_u$.[1] *In other words, the lower and upper triangular parts of A coincide with the lower and upper triangular parts of some rank k matrix.*

In the case of order k quasiseparability, we could alternatively refer to the restriction on the lower triangular part of A as order k lower quasiseparability and the restriction on the upper triangular part of A as order k upper quasiseperability. Then A is said to be order k quasiseparable provided it is both order k lower and upper quasiseparable. Similarly, A is order k semiseparable provided it is both order k lower and upper semiseparable.

1.2 (H, k)-quasiseparable and (H, k)-semiseparable Matrices

In this section, following suit with [11], [12], versions of quasiseparability and semiseparability that are more specific to this paper are discussed. We begin with the following definition.

[1]This is consistent with the Matlab functions $tril(\cdot)$ and $triu(\cdot)$

Definition 1.6. *An $n \times n$ matrix A is called lower 1-Hessenberg if the entries above it's first superdiagonal are all zero. If additionally all of the elements along the first superdiagonal are non-zero, we say that A is strongly lower 1-Hessenberg. For simplicity, throughout this paper lower 1-Hessenberg matrices will be referred to as Hessenberg matrices.*

1.2.1 (H, k)-quasiseparable Matrices

We provide two characterizations of (H, k)-quasiseparable structure.

Definition 1.7 (Rank). *An $n \times n$ matrix A is (H, k)-quasiseparable if* **(i)** *it is strongly Hessenberg and* **(ii)** *if* $\max(rank(A_{21})) = k$*, where the maxima are taken over all symmetric partitions of the form:*

$$A = \left[\begin{array}{c|c} * & * \\ \hline A_{21} & * \end{array}\right]$$

Just as with order k quasiseparability, the following generator definition is often of more use when designing structure exploiting algorithms.

Definition 1.8 (Generator). *An $n \times n$ matrix A is called (H,k)-quasiseparable if* **(i)** *it is strongly Hessenberg and* **(ii)** *it can be represented in the form*

$$\begin{bmatrix} d_1 & g_2h_1 & & \\ & \ddots & \ddots & \\ & p_i a_{ij}^{\times} r_j & \ddots & g_n h_{n-1} \\ & & & d_n \end{bmatrix}$$

where the entries above the first super-diagonal are zero, and

$$a_{ij}^{\times} = \begin{cases} a_{j+1} \cdots a_{i-1} & i > j+1 \\ 1 & i = j+1 \end{cases}$$

The elements of $\mathfrak{G} = \{p_t, a_u, r_v, d_w, g_t, h_v\}$*, for* $t = 2, \dots, n$*,* $u = 2, \dots, n-1$*,* $v = 1, \dots, n-1$ *and* $w = 1, \dots, n$*, are matrices of sizes* $1 \times k$*,* $k \times k$*,* $k \times 1$*,* 1×1*,* $1 \times k$ *and* $k \times 1$ *respectively and are called a set of* (H, k)*-quasiseparable generators for the matrix* A*.*

1.2.2 (H, k)-semiseparable Matrices

Finally, we introduce a subclass of (H, k)-quasiseparable matrices, namely, those with (H, k)-semiseparable structure.

Definition 1.9 (QS Generator)**.** *An* $n \times n$ *matrix* A *is* (H, k)*-semiseparable if* **(i)** *it is strongly Hessenberg and* **(ii)** *if there exists a choice of* (H, k)*-quasiseparable generators* $\mathfrak{G} = \{p_t, a_u, r_v, , d_w, g_v, h_t\}$ *for* A *such that* a_u *is invertible for* $u = 2, \dots, n-1$*.*

The invertibility of each a_u allows for the following equivalent characterization of (H, k)-semiseparability.

Definition 1.10 (SS Generator)**.** *An* $n \times n$ *matrix* A *is* (H, k)*-semiseparable if* **(i)** *it is strongly Hessenberg and* **(ii)** *if*

$$tril(A, -1) = tril(rt, -1) \tag{2}$$

for some matrices r and t of sizes $n \times k$ and $k \times n$ respectively, and where $tril(\cdot, -1)$ denotes the strictly lower triangular parts of A and rt. In other words, the strictly lower triangular part of A coincides with the strictly lower triangular part of some rank k matrix.

2 Unitary Hessenberg Matrices

Definition 2.1. *An $n \times n$ matrix U is called unitary Hessenberg if it satisfies (1.6) and if $U^*U = UU^* = I$.*

2.1 Motivation

Unitary Hessenberg matrices appear in a wide variety of areas, a few of which are discussed next. The main focus of this paper is to extend the results of a recent paper, described in the Recent Results section below.

2.1.1 Orthogonal Polynomials on the Unit Circle

Szegö polynomials $\Phi = \{\phi_k(x)\}_{k=0}^{n}$ are polynomials orthonormal on the unit circle with respect to an inner product of the form

$$\langle p(x), q(x) \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} p(e^{i\theta}) q(e^{i\theta})^* w^2(\theta) d\theta$$

For any such inner product there exist Verblunsky coefficients $\{\rho_k\}$ satisfying

$$\rho_0 = -1, \quad |\rho_k| < 1, \quad k = 1, \ldots, n-1, \quad |p_n| \leq 1$$

and complementary parameters $\{\mu_k\}$ defined by

$$\mu_k = \begin{cases} \sqrt{1 - |\rho_k|^2} & |\rho_k| < 1 \\ 1 & |\rho_k| = 1 \end{cases}$$

such that the corresponding Szegö polynomials satisfy the two term recurrence relations

$$\begin{bmatrix} \phi_0(x) \\ \phi_0^{\#}(x) \end{bmatrix} = \frac{1}{\mu_0} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} \phi_{k+1}(x) \\ \phi_{k+1}^{\#}(x) \end{bmatrix} = \frac{1}{\mu_{k+1}} \begin{bmatrix} 1 & -\overline{\rho}_{k+1} \\ -\rho_{k+1} & 1 \end{bmatrix} \begin{bmatrix} \phi_k(x) \\ x\phi_k^{\#}(x) \end{bmatrix} \tag{3}$$

for $k = 0, \ldots, n-1$. The recurrence relations above are completely characterized by the equation

$$\phi_k^{\#}(x) = \frac{1}{\mu_1 \cdots \mu_k} det(xI - U)_{(k \times k)}$$

where $det(xI-U)_{(k\times k)}$ denotes the kth leading principal minor of the matrix $(xI-U)$ and

$$U = \begin{bmatrix} -\rho_1\overline{\rho}_0 & -\rho_2\mu_1\overline{\rho}_0 & -\rho_3\mu_2\mu_1\overline{\rho}_0 & \cdots & -\rho_n\mu_{n-1}\cdots\mu_3\mu_2\mu_1\overline{\rho}_0 \\ \mu_1 & -\rho_2\overline{\rho}_1 & -\rho_3\mu_2\overline{\rho}_1 & \cdots & -\rho_n\mu_{n-1}\cdots\mu_3\mu_2\overline{\rho}_1 \\ 0 & \mu_2 & -\rho_3\overline{\rho}_2 & \cdots & -\rho_n\mu_{n-1}\cdots\mu_3\overline{\rho}_2 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \mu_{n-1} & -\rho_n\overline{\rho}_{n-1} \end{bmatrix}$$

is "almost" unitary Hessenberg, differing from a unitary matrix only in its last column. The above relationship between U and the Szegö polynomials was established by Gragg [23]. Numerical methods exploiting this relation, for example computing the zeros of $\phi_n(x)$, can be found in the work of Ammar, Calvetti, Gragg and Reichel [1]-[2].

2.1.2 Numerical Analysis

In numerical analysis unitary matrices (Hessenberg or not) are desirable for a variety of reasons. For one, if λ is an eigenvalue of a unitary matrix U, then $|\lambda| = 1$, and hence $\kappa(U) = 1$ where κ is the condition number of U. In other words, unitary matrices have the minimum possible condition number, and thus errors will not be magnified when multiplying by such a matrix. Another benefit in terms of cost is that by definition $U^*U = UU^* = I$ and hence $U^{-1} = U^*$. That is, the inverse of a unitary matrix is it's conjugate transpose, which makes computation trivial. Unitary Hessenberg matrices and their applications have been studied in great detail by Ammar, Calvetti, Gragg, He, and Reichel [1]-[7],[24], as well as Bunse-Gerstner, Elsner, and He [13]-[14] to name a few, and it is likely the case that some of this work may generalize to some of the results in this paper. Further studies exploiting the structure of unitary Hessenberg matrices, and in more generality quasiseparable matrices, can be found in the work of Bella, Eidelman, Gohberg, Haimovici, Kailath, Koltracht, Mastronardi, Olshevsky, Van Barel, Vanderbril and Zhlobich [9], [10], [12], [15]-[19], [22], [28], [30], [31], [34].

2.1.2.1 Generalized Horner Polynomials and Polynomial-Vandermonde Matrices

This section borrows heavily from the results in [22] and [34]. Let the polynomials $R = \{r_0(x), r_1(x), \ldots, r_{n-1}(x), r_n(x)\}$ be defined by the recurrence relations

$$r_k = \alpha_k x r_{k-1}(x) - a_{k-1,k} r_{k-1}(x) - a_{k-2,k} r_{k-2}(x) - \cdots - a_{0,k} r_0(x) \qquad (4)$$

and for the polynomial

$$b(x) = b_0 r_0(x) + b_1 r_1(x) + \cdots + b_{n-1} r_{n-1}(x) + b_n r_n(x) \qquad (5)$$

define its confederate matrix

$$C_R(b) = \begin{bmatrix} \frac{a_{01}}{\alpha_1} & \frac{a_{02}}{\alpha_2} & \frac{a_{03}}{\alpha_3} & \cdots & \cdots & (\frac{a_{0,n}}{\alpha_n} - \frac{1}{\alpha_n} \cdot \frac{b_0}{b_n}) \\ \frac{1}{\alpha_1} & \frac{a_{12}}{\alpha_2} & \frac{a_{13}}{\alpha_3} & \cdots & \cdots & (\frac{a_{1,n}}{\alpha_n} - \frac{1}{\alpha_n} \cdot \frac{b_1}{b_n}) \\ 0 & \frac{1}{\alpha_2} & \frac{a_{23}}{\alpha_3} & \cdots & \cdots & (\frac{a_{2,n}}{\alpha_n} - \frac{1}{\alpha_n} \cdot \frac{b_2}{b_n}) \\ 0 & 0 & \ddots & \ddots & & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & \frac{1}{\alpha_{n-1}} & (\frac{a_{n-1,n}}{\alpha_n} - \frac{1}{\alpha_n} \cdot \frac{b_{n-1}}{b_n}) \end{bmatrix} \quad (6)$$

By design, the columns of $C_R(b)$ capture the recursion of the r_k's. Define the "generalized" Horner polynomials $\tilde{R} = \{\tilde{r}_0(x), \tilde{r}_1(x), \ldots, \tilde{r}_{n-1}(x), \tilde{r}_n(x)\}$ by the confederate matrix satisfying

$$C_{\tilde{R}}(\tilde{r}_n) = \tilde{I} C_R(r_n)^T \tilde{I} \quad (7)$$

The relationship above translates to the following recursion for the "generalized" Horner polynomials.

$$\tilde{r}_0(x) = \tilde{\alpha}_0, \quad \tilde{r}_k(x) = \tilde{\alpha}_k x \tilde{r}_{k-1}(x) - \tilde{a}_{k-1,k}\tilde{r}_{k-1}(x) - \cdots - \tilde{a}_{1,k}\tilde{r}_1(x) - \tilde{a}_{0,k}\tilde{r}_0(x) \quad (8)$$

where

$$\tilde{\alpha}_k = \alpha_{n-k}, \quad (k = 0, 1, \ldots, n)$$

and

$$\tilde{a}_{k,j} = \frac{\alpha_{n-j}}{\alpha_{n-k}} a_{n-j,n-k}, \qquad (k = 0, 1, \ldots, n-1; j = 1, 2, \ldots, n)$$

With the definitions above, a generalization of the well know Parker-Forney-Traub ([35],[21],[37]) algorithm for inverting a Vandermonde matrix can be constructed.

Theorem 2.2. *Let*

$$V_R(x) = \begin{bmatrix} r_0(x_1) & r_1(x_1) & \cdots & r_{n-1}(x_1) \\ r_0(x_2) & r_1(r_2) & \cdots & r_{n-1}(x_2) \\ \vdots & \vdots & & \vdots \\ r_0(x_n) & r_1(x_n) & \cdots & r_{n-1}(x_n) \end{bmatrix} \tag{9}$$

be a polynomial Vandermonde matrix, where $R = \{r_0(x), r_1(x), r_2(x), \ldots, r_{n-1}(x)\}$ *whose nodes* $\{x_k\}$ *are the zeros of*

$$b(x) = \prod_{k=1}^{n} (x - x_k) = x^n + b_{n-1} r_{n-1}(x) + \cdots + b_2 r_2(x) + b_1 r_1(x) + b_0 r_0(x)$$

Then the inverse of $V_R(x)$ *is given by*

$$V_R(x)^{-1} = \begin{bmatrix} \tilde{r}_{n-1}(x_1) & \tilde{r}_{n-1}(x_2) & \cdots & \tilde{r}_{n-1}(x_n) \\ \vdots & \vdots & & \vdots \\ \tilde{r}_1(x_1) & \tilde{r}_1(x_2) & \cdots & \tilde{r}_1(x_n) \\ \tilde{r}_0(x_1) & \tilde{r}_0(x_2) & \cdots & \tilde{r}_0(x_n) \end{bmatrix} \cdot diag(c_1, \ldots, c_n) \tag{10}$$

where $\tilde{R} = \{\tilde{r}_0(x), \tilde{r}_1(x), \tilde{r}_2(x), \ldots, \tilde{r}_{n-1}(x)\}$ *are the "generalized" Horner polynomials associated with* R *satisfying the recursion in (8) and where*

$$c_i = \frac{1}{b'(x_i)} = \frac{1}{\prod_{\substack{k=1 \\ k \neq i}}^{n} (x_k - x_i)} \tag{11}$$

The recursions for the polynomials in $\tilde{R}$ are contained in the matrix $C_{\tilde{R}}(\tilde{r}_n)$. Thus, by the relationship in (7), one can determine these recursions by computing $C_R(r_n)$. This however first requires computation of the coefficients of $b(x)$. One way to achieve this is as follows:

1. Set

$$\left[\begin{array}{cccc} -a_0^{(0)} & \cdots & -a_{n-1}^{(0)} & -\alpha_n^{(0)} \end{array} \right] = \left[\begin{array}{cccc} \frac{1}{\alpha_0} & 0 & \cdots & 0 \end{array} \right]$$

2. For $k = 1 : n$

$$\begin{bmatrix} -a_0^{(k)} \\ \vdots \\ -a_{n-1}^{(k)} \\ \alpha_n^{(k)} \end{bmatrix} = \left(\left[\begin{array}{c|c} C_{\bar{R}}(xr_{n-1}(x)) & 0 \\ \hline 0 \ \cdots \ 0 \ 1 & 0 \end{array} \right] - x_k I \right) \begin{bmatrix} -a_0^{(k-1)} \\ \vdots \\ -a_{n-1}^{(k-1)} \\ \alpha_n^{(k-1)} \end{bmatrix} \tag{12}$$

where $\bar{R} = \{r_0(x), \ldots, r_{n-1}(x), xr_{n-1}(x)\}$. Now, if an efficient means of multiplying this confederate matrix by a vector and a nice recursion formula for the polynomials in $\tilde{R}$ can be found, one can compute $V_R(x)^{-1}$ in just $O(n^2)$

operations as opposed to standard $O(n^3)$ inversion methods.[2] The Parker-Forney-Traub algorithm is one of these special cases, and another relevant to this paper is discussed below.

2.1.2.2 Fast $O(n^2)$ Inversion of Szegö-Vandermonde Matrices

The two term recurrence for the Szegö polynomials in (3) is widely known, but the following n-term recursion also holds

$$\phi_0(x) = 1, \qquad \phi_1(x) = \frac{1}{\mu_1}(x\phi_0(x) + \rho_1\overline{\rho}_0)$$

where $\rho_0 = -1$, and

$$\phi_k(x) = \frac{1}{\mu_k}(x\phi_{k-1}(x) + \rho_k\overline{\rho}_{k-1}\phi_{k-1}(x) + \rho_k\mu_{k-1}\overline{\mu}_{k-2}\phi_{k-2}(x) + \cdots \\ + \rho_k\mu_{k-1}\cdots\mu_2\overline{\rho}_1\phi_1(x) + \rho_k\mu_{k-1}\cdots\mu_1\overline{\rho}_0\phi_0(x)) \tag{13}$$

Then for a polynomial of the form

$$b(x) = b_n\phi_n(x) + b_{n-1}\phi_{n-1}(x) + \cdots + b_1\phi_1(x) + b_0\phi_0(x) \tag{14}$$

[2] The n-term recurrence relation is the general case, but in special cases the number of terms can be reduced significantly

its corresponding confederate matrix is "almost" unitary Hessenberg

$$C_\Phi(b) = \begin{bmatrix} -\rho_1\overline{\rho}_0 & -\rho_2\mu_1\overline{\rho}_0 & -\rho_3\mu_2\mu_1\overline{\rho}_0 & \cdots & -\rho_n\mu_{n-1}\cdots\mu_3\mu_2\mu_1\overline{\rho}_0 - \frac{b_0}{b_n}\mu_n \\ \mu_1 & -\rho_2\overline{\rho}_1 & -\rho_3\mu_2\overline{\rho}_1 & \cdots & -\rho_n\mu_{n-1}\cdots\mu_3\mu_2\overline{\rho}_1 - \frac{b_1}{b_n}\mu_n \\ 0 & \mu_2 & -\rho_3\overline{\rho}_2 & \cdots & -\rho_n\mu_{n-1}\cdots\mu_3\overline{\rho}_2 - \frac{b_2}{b_n}\mu_n \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & \mu_{n-1} & -\rho_n\overline{\rho}_{n-1} - \frac{b_{n-1}}{b_n}\mu_n \end{bmatrix}$$

This is convenient, because in step (2) of (12), multiplication of a unitary Hessenberg matrix by a vector can be done efficiently thanks to its decomposition into a product of Givens rotations, as shown in (21) in section (2.3). Further, though the matrix $C_{\tilde{\Phi}}(\tilde{\phi}_n)$ suggests an n-term recurrence relation for the Horner-Szegö polynomials $\tilde{\Phi} = \{\tilde{\phi}_0(x), \tilde{\phi}_1(x), \tilde{\phi}_2(x), \ldots, \tilde{\phi}_{n-1}(x)\}$, this can be reduced to the following two term recursion

$$\begin{bmatrix} \tilde{\phi}_0(x) \\ \tilde{\phi}_0^{\#}(x) \end{bmatrix} = \frac{1}{\tilde{\mu}_0}\begin{bmatrix} -\tilde{\rho}_0 b_n \\ b_n \end{bmatrix}, \qquad \begin{bmatrix} \tilde{\phi}_k(x) \\ \tilde{\phi}_k^{\#}(x) \end{bmatrix} = \frac{1}{\tilde{\mu}_k}\begin{bmatrix} 1 & -\overline{\tilde{\rho}}_k \\ -\tilde{\rho}_k & 1 \end{bmatrix}\begin{bmatrix} \tilde{\phi}_{k-1}(x) \\ x\tilde{\phi}_{k-1}^{\#}(x) + b_{n-k} \end{bmatrix}$$

with $\tilde{\rho}_k = \overline{\rho}_{n-k}$ for $k = 0, 1, \ldots, n$ and $\tilde{\mu}_k = \sqrt{1 - |\tilde{\rho}_k|^2}$, $\tilde{\mu}_n = 1$, and where $\tilde{\mu}_0 := 1$ if $|\tilde{\rho}_0| = 1$. This allows one to invert

$$V_\Phi(x) = \begin{bmatrix} \phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_{n-1}(x_1) \\ \phi_0(x_2) & \phi_1(x_2) & \cdots & \phi_{n-1}(x_2) \\ \vdots & \vdots & & \vdots \\ \phi_0(x_n) & \phi_1(x_n) & \cdots & \phi_{n-1}(x_n) \end{bmatrix} \tag{15}$$

via

$$V_\Phi(x)^{-1} = \begin{bmatrix} \tilde{\phi}_{n-1}(x_1) & \tilde{\phi}_{n-1}(x_2) & \cdots & \tilde{\phi}_{n-1}(x_n) \\ \vdots & \vdots & & \vdots \\ \tilde{\phi}_1(x_1) & \tilde{\phi}_1(x_2) & \cdots & \tilde{\phi}_1(x_n) \\ \tilde{\phi}_0(x_1) & \tilde{\phi}_0(x_2) & \cdots & \tilde{\phi}_0(x_n) \end{bmatrix} \cdot diag(c_1, \ldots, c_n) \quad (16)$$

where c_i is defined in (11), in just $O(n^2)$ operations. Additionally, the relationship

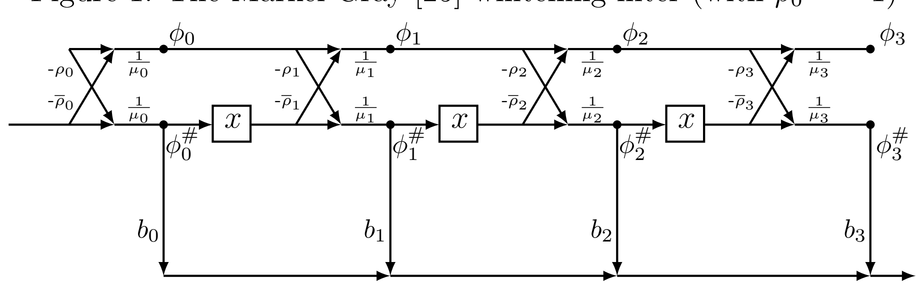
$$C_\Phi(b) V_\Phi^{-1}(x) = V_\Phi^{-1}(x) \cdot diag(x_1, \ldots, x_n) \quad (17)$$

suggests an efficient method for computing the eigenvectors of the "almost" unitary Hessenberg matrix $C_\Phi(b)$

2.1.3 Electrical Engineering

Using the relation in (3), the polynomial in (14) can be conveniently realized via a signal flow graph (see appendix (B)) as shown below

Figure 1: The Markel-Gray [25] whitening filter (with $\rho_0 = -1$)



It is noted that this is not the only possible realization of the Szegö polynomials, this is the one that coincides with the well known two term recursion. See Kimura [29] for more on lattice-ladder realizations of digital filters. In [33], Olshevsky discusses multiple recursions satisfied by the Szegö polynomials and their realizations, analogous to figure (1). The nice thing about the realization of $\Phi = \{\phi_0, \ldots, \phi_n\}$ via a signal flow graph is that it is relatively easy to visualize the recurrence for the Horner-Szegö Polynomials simply by reversing the direction of the flow. The steps below outline this procedure:

1. Given the recursion (3) for the polynomials $\Phi = \{\phi_0, \ldots, \phi_n\}$ and a polynomial $b(x) = b_n\phi_n(x) + b_{n-1}\phi_{n-1}(x) + \cdots + b_1\phi_1 + b_0\phi_0$, draw a signal flow graph for the linear time-invariant system with the overall transfer function $b(x)$, such that the $\phi_k(x)$'s are the partial transfer functions to the input of the kth delay element for $k = 1, 2, \ldots, n-1$ as shown in figure (1).

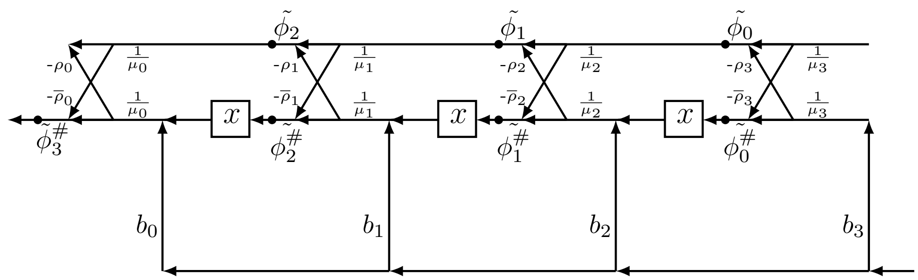
2. Pass to the dual system by reversing the direction of the flow.

3. Identify the Horner-Szegö polynomials $\tilde{\Phi} = \{\tilde{\phi}_k\}$ as the partial transfer functions from the input of the line to the input of the delay elements.

4. Read a recursion from this signal flow graph for $\tilde{\Phi} = \{\tilde{\phi}_0, \ldots, \tilde{\phi}_n\}$

As an example, the dual to figure (1) is shown below

Figure 2: Dual to the Markel-Gray whitening filter shown in figure 1



from which it can be deduced that the Horner-Szegö polynomials satisfy the following recursion

$$\begin{bmatrix} \tilde{\phi}_0(x) \\ \tilde{\phi}_0^{\#}(x) \end{bmatrix} = \frac{1}{\tilde{\mu}_0} \begin{bmatrix} -\tilde{\rho}_0 b_n \\ b_n \end{bmatrix}, \qquad \begin{bmatrix} \tilde{\phi}_k(x) \\ \tilde{\phi}_k^{\#}(x) \end{bmatrix} = \frac{1}{\tilde{\mu}_k} \begin{bmatrix} 1 & -\overline{\tilde{\rho}}_k \\ -\tilde{\rho}_k & 1 \end{bmatrix} \begin{bmatrix} \tilde{\phi}_{k-1}(x) \\ x\tilde{\phi}_{k-1}^{\#}(x) + b_{n-k} \end{bmatrix}$$

where $\tilde{\rho}_k = \overline{\rho}_{n-k}$ for $k = 0, 1, \ldots, n$ and $\tilde{\mu}_k = \sqrt{1 - |\tilde{\rho}_k|^2}$, $\tilde{\mu}_n = 1$, and where $\tilde{\mu}_0 := 1$ if $|\tilde{\rho}_0| = 1$.

2.2 Recent Results in Numerical Analysis

A recent paper by Parlett and Barszcz [36] proposed the following problem: Given an unit vector q, compute the orthogonal Hessenberg matrix A with first column q. In complex form, this translates to completing the unitary Hessenberg matrix U with first column q. Looking at the matrix $I - qq^*$ in the special form

$$I - qq^* = LD^2L^*$$

where L is $n \times (n-1)$ and lower triangular with $1's$ on it's main diagonal and $D^2 = diag(\mu_1^2, \ldots, \mu_{n-1}^2)$ is positive definite, Parlett observed that for $i > j$ the entries of $\tilde{L} = LD$ can be written as

$$\tilde{l}_{ij} = -q_i \overline{q}_j \mu_j / \rho_j \tag{18}$$

where $\overline{q}$ denotes the complex conjugate of q and

$$\rho_i = \sum_{j=i+1}^{n} |q_j|^2, \quad \rho_n = 0, \quad \mu_i = \sqrt{\rho_i/\rho_{i-1}}, \quad i = 1, \ldots, n. \tag{19}$$

Furthermore, one solution to this problem is $U = [q\ \tilde{L}]$. Finally as a quick note, Parlett acknowledged that if $P = diag(\rho_1, \ldots, \rho_{n-1}, 1)$ then the strictly lower triangular part of $\tilde{L} = LD$ coincides with the strictly lower triangular part of the rank one matrix $-qq^* P^{-1}(D \oplus 0)$. Appendix (A) provides details on the derivation of Parlett's formula in (18). Now, given the definition in (1), it becomes apparent that Parlett was in fact exploiting the order 1 semiseparable structure of unitary Hessenberg matrices. The rest of section (2) is devoted to presenting alternative solutions to Parlett's problem, all of which exploit the structure of unitary Hessenberg matrices. The purpose of these algorithms is that each of the alternate solutions can be extended to solve a much more general problem, which is the main result discussed in section (4).

2.3 Schur Parameters and Decomposable Structure

It is well known that an $n \times n$ unitary Hessenberg matrix U has the following form

$$\begin{bmatrix} \rho_1 & \mu_1 & 0 & \cdots & 0 \\ \rho_2\mu_1 & -\rho_2\overline{\rho}_1 & \mu_2 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & 0 \\ \rho_{n-1}\mu_{n-2}\cdots\mu_1 & -\rho_{n-1}\mu_{n-2}\cdots\mu_2\overline{\rho}_1 & -\rho_{n-1}\mu_{n-2}\cdots\mu_3\overline{\rho}_2 & \cdots & \mu_{n-1} \\ \rho_n\mu_{n-1}\cdots\mu_1 & -\rho_n\mu_{n-1}\cdots\mu_2\overline{\rho}_1 & -\rho_n\mu_{n-1}\cdots\mu_3\overline{\rho}_2 & \cdots & -\rho_n\overline{\rho}_{n-1} \end{bmatrix} \tag{20}$$

for some complex $\{\rho_i\}_{i=1}^n$ with $|\rho_i| < 1$ and $\mu_i = \sqrt{1 - |\rho_i|^2}$ for $i = 1, \ldots, n-1$ and $|\rho_n| = 1$. Hence, the matrix in (20) is uniquely determined by its first column. Further, multiplying U on the left by the $n-1$ Givens rotations

$$G_i = \begin{bmatrix} I_{i-1} & & & \\ & \overline{\rho}_i & \mu_i & \\ & \mu_i & -\rho_i & \\ & & & I_{n-i-1} \end{bmatrix} \tag{21}$$

where $i = 1, \ldots, n-1$, and the matrix $G_n = diag(1, \ldots, 1, \overline{\rho}_n)$ transforms U into the identity. In other words, $G_1 \cdots G_n U = I$. This implies that U can be written as the product $U = G_n^* \cdots G_1^*$. The μ_i's (or ρ_i's) are often referred to as Schur parameters, though depending on the source they may be labeled Verblunsky, parcor, or reflection coefficients. The first algorithm presented below exploits the decomposable structure of unitary Hessenberg matrices.

Algorithm 2.3 (Decomp1.1)**.** *Let* $q \in \mathbb{C}^n$ *denote the first column of the unitary Hessenberg matrix* U*. Recalling the structure in (20), we know*

$$\begin{bmatrix} \rho_1 \\ \rho_2\mu_1 \\ \vdots \\ \rho_{n-1}\mu_{n-2}\cdots\mu_1 \\ \rho_n\mu_{n-1}\cdots\mu_1 \end{bmatrix} = \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_{n-1} \\ q_n \end{bmatrix} = q$$

Equating the first components, we have $\rho_1 = q_1$*. Because we know that* $\mu_1 = \sqrt{1-|\rho_1|^2}$*, we can equate the second components to and compute* $\rho_2 = q_2/\mu_1$*. This in turn allows us to compute* μ_2*. Exhausting this process completely determines each* $\{\rho_i, \mu_i\}$ *for* $i = 1, \ldots, n-1$*. Letting* $\rho_n = e^{i\cdot arg(q_n)}$*, compute* $U = G_n^* \cdots G_1^*$*, where* $G_n = diag(1, \ldots, 1, \overline{\rho}_n)$ *and* G_i *is defined in (21) for* $i = 1, \ldots, n-1$*.*

```
function [L] = Decomp1.1(q)

n=length(q);
p(1)=q(1);
```

```
m1=sqrt(1-abs(p(1))^2);
m(1)=m1;

for i=2:1:n-1
  p(i)=q(i)/m1;
  m(i)=sqrt(1-abs(p(i))^2);
  if i<n-1
    m1=m1*m(i);
  else
    m1=m1*m(i);
    p(i+1)=exp(1i*angle(q(end)));
  end
end

U = blkdiag( eye(n-1), p(n));

for i = n-1:-1:1
  U=U*blkdiag(eye(i-1),[p(i) m(i); m(i) -conj(p(i))]
  eye(n-i-1));
end

L = U(:,2:n);

end
```

An issue that may arise in the above algorithm is the fact that $n-1$ subtractions are needed to compute the μ_i's. Theoretically this is not a problem, however the use of floating point arithmetic may result in severe cancellation. As shown in table 1, this algorithm performs fine when randomly generated vectors are used, but it is not difficult to find a case in which the algorithm fails. A simple example is the normalized version of the vector $q = (1, 1/9, 1/9^2, \ldots, 1/9^{15})$, for which $||L^*L - I_{15}|| \approx 0.8623$.

An alternate method is presented, avoiding the use of subtraction. This alternate version of (2.3) given below results in full accuracy using the same vector q, $||L^*L - I_{15}|| \approx 6.7008e-16$.

Algorithm 2.4 (Decomp2.1)**.** *Let* $q \in \mathbb{C}^n$ *and* $\rho_n = e^{i \cdot arg(q_n)}$*. First, compute the vector* $q^{(0)}$

$$\begin{bmatrix} I_{n-1} & \\ & \overline{\rho}_n \end{bmatrix} q = q^{(0)}$$

Define

$$r_n = \sqrt{|q_{n-1}^{(0)}|^2 + |q_n^{(0)}|^2}$$

and set

$$\rho_{n-1} = \frac{q_{n-1}^{(0)}}{r_n}, \qquad \mu_{n-1} = \frac{q_n^{(0)}}{r_n}$$

Then $\mu_{n-1} = \sqrt{1 - |\rho_{n-1}|^2}$ *and we have*

$$\begin{bmatrix} I_{n-2} & & \\ & \overline{\rho}_{n-1} & \mu_{n-1} \\ & \mu_{n-1} & -\rho_{n-1} \end{bmatrix} q^{(0)} = \begin{bmatrix} * \\ \vdots \\ r_n \\ 0 \end{bmatrix} = q^{(1)}$$

Next, define

$$r_{n-1} = \sqrt{|q_{n-2}^{(1)}|^2 + |q_{n-1}^{(1)}|^2}$$

and set

$$\rho_{n-2} = \frac{q_{n-2}^{(1)}}{r_{n-1}}, \qquad \mu_{n-2} = \frac{q_{n-1}^{(1)}}{r_{n-1}}$$

Then

$$\begin{bmatrix} I_{n-3} & & & \\ & \overline{\rho}_{n-2} & \mu_{n-2} & \\ & \mu_{n-2} & -\rho_{n-2} & \\ & & & 1 \end{bmatrix} q^{(1)} = \begin{bmatrix} * \\ \vdots \\ r_{n-1} \\ 0 \\ 0 \end{bmatrix} = q^{(2)}$$

Continue this process until reaching the vector e_1*, the first column of the identity* I_n*. This completely determines* $\{\rho_i, \mu_i\}$ *for* $i = 1, \ldots, n-1$*. Then* $U = G_n^* \cdots G_1^*$*, where* $G_n = diag(1, \ldots, 1, \overline{\rho}_n)$ *and* G_i *is defined in (21) for* $i = 1, \ldots, n-1$*.*

```
function [ L ] = Decomp2.1( q )

n=length(q);
t = q.*conj(q);
r(1) = 1;

for k=2:n
```

```
    r(k) = sqrt(sum(t(k:n)));
end

for i = n-1:-1:1
    p(i) = q(i)/r(i);
    m(i) = r(i+1)/r(i);
end

p(n) = exp(1i*angle(q(n)));
U = blkdiag( eye(n-1), p(n));

for i = n-1:-1:1
    U=U*blkdiag(eye(i-1),[p(i) m(i); m(i) -conj(p(i))]
    eye(n-i-1));
end

L = U(:,2:n);

end
```

2.4 Green's $(H, 1)$-quasiseparable Structure

The first two algorithms presented exploit the well know decomposable structure of unitary Hessenberg matrices, however this is not the only type of structure possessed by such a matrix. Keeping in mind the definitions in (1.2), we introduce the stricter Green's $(H, 1)$-quasiseparable structure.

Definition 2.5 (Rank). *An $n \times n$ matrix A is Green's $(H, 1)$-quasiseparable if* **(i)** *it is strongly Hessenberg and* **(ii)** *if $max(rank(A_i)) = 1$, where*

$$A_i = A(i : n, 1 : i), \quad i = 1, \ldots, n$$

Recall that in definition (1.7), the rank conditions are imposed on submatrices formed below the main diagonal. In the above definition, we extend this notion to submatrices formed below the first superdiagonal. For example, if A is 5×5, then A_2 is the submatrix formed by the $*$'s below:

$$A = \left[\begin{array}{ccc|cc} \times & \times & 0 & 0 & 0 \\ \times & \times & \times & 0 & 0 \\ \hline * & * & * & \times & 0 \\ * & * & * & \times & \times \\ * & * & * & \times & \times \end{array}\right]$$

Now, considering (20), one can easily see that unitary Hessenberg matrices satisfy the rank condition above. For example, if U is 5×5 unitary Hessenberg, a typical submatrix has the form

$$U_{21} = \begin{bmatrix} \rho_3\mu_2\mu_1 & -\rho_3\mu_2\overline{\rho}_1 & -\rho_3\overline{\rho}_2 \\ \rho_4\mu_3\mu_2\mu_1 & -\rho_4\mu_3\mu_2\overline{\rho}_1 & -\rho_4\mu_3\overline{\rho}_2 \\ \rho_5\mu_4\mu_3\mu_2\mu_1 & -\rho_5\mu_4\mu_3\mu_2\overline{\rho}_1 & -\rho_5\mu_4\mu_3\overline{\rho}_2 \end{bmatrix}$$

from which it can be seen $rank(U_{21}) = 1$.

The equivalent generator definition of Green's $(H, 1)$-quasiseparability is given below.

Definition 2.6 (Generator). *An $n \times n$ matrix A is Green's $(H, 1)$-quasiseparable* *if* **(i)** *it is strongly Hessenberg and* **(ii)** *if it can be represented in the form:*

$$\begin{bmatrix} p_2 r_1 & d_2 & & & \\ & \ddots & \ddots & & \\ & & \ddots & \ddots & \\ & p_i a_{ij}^{\times} r_j & & \ddots & d_n \\ & & & & p_{n+1} r_n \end{bmatrix} \tag{22}$$

where the entries above the first super-diagonal are zero, and

$$a_{ij}^{\times} = a_{j+1} \cdots a_i \quad \textit{for} \quad i > j$$

The scalar elements of $\mathfrak{G}_1 = \{p_t, a_u, r_v, d_w\}$, *for* $t = 2, \ldots, n+1$, $u = 2, \ldots, n$, $v = 1, \ldots, n$ *and* $w = 2, \ldots, n$, *are called a set of Green's* $(H,1)$*-quasiseparable generators for the matrix* A.

Again, comparing (22) with the matrix in (20), it should be obvious that unitary Hessenberg matrices are Green's $(H,1)$-quasiseparable. In fact, given the first column q of a unitary Hessenberg matrix U, if we let $f_i = \sqrt{\sum_{j=i}^{n} |q_j|^2}$ for $i = 1, \ldots, n$ and set $r_1 = 1$, then one possible set of Green's $(H,1)$-quasiseparable generators is given in the table below.

Given First Column q	$\frac{q_{t-1}}{f_{t-1}}$	$\frac{f_u}{f_{u-1}}$	$\frac{-\overline{q}_{v-1}}{f_{v-1}}$	$\frac{f_w}{f_{w-1}}$
Quasiseparable Generators	p_t	a_u	r_v	d_w

(23)

where $t = 2, \ldots, n+1$, $u = 2, \ldots, n$, $v = 1, \ldots, n$ and $w = 2, \ldots, n$. The next algorithm presented constructs U directly via its Green's $(H, 1)$-quasiseparable generators.

Algorithm 2.7 (GH1Quasi)**.** *Let $q \in \mathbb{C}^n$ denote the first column of U. First compute*

$$f_i = \sqrt{\sum_{j=i}^{n} |q_j|^2}$$

for $i = 1, \ldots, n$ and set $r_1 = 1$. Next, use the relations

$$p_t = \frac{q_{t-1}}{f_{t-1}}, \quad a_u = \frac{f_u}{f_{u-1}}, \quad r_v = \frac{-\overline{q}_{v-1}}{f_{v-1}}, \quad d_w = \frac{f_w}{f_{w-1}}$$

for $t = 2, \ldots, n+1$, $u = 2, \ldots, n$, $v = 1, \ldots, n$ and $w = 2, \ldots, n$, to compute a set, $\mathfrak{G}_1$, of Green's $(H, 1)$-quasiseparable generators for U, and use the generators to construct the remaining columns of the matrix as in (22).

```
function [ L ] = GH1Quasi( q )

n=length(q);
t = q.*conj(q);
f(1) = 1;
U = zeros(n);

for k=2:n
    f(k) = sqrt(sum(t(k:n)));
end
r(1) = 1;
for i = 2:n+1
    p(i) = (q(i-1))/(f(i-1));
```

```
    if i<n+1
        a(i) = (f(i))/(f(i-1));
        d(i) = (f(i))/(f(i-1));
        r(i) = (-conj(q(i-1)))/(f(i-1));
    end
end

U(:,1)=q;

for i = 1:n-1
    U(i,i+1)=d(i+1);
end

for j = 2:n
    for i = j:n
        if i==j
            U(i,j) = p(i+1)*r(j);
        else
            U(i,j) = p(i+1)*prod(a(j+1:i))*r(j);
        end
    end
end
L = U(:,2:n);
end
```

2.5 Green's $(H,1)$-semiseparable Structure

Green's $(H,1)$-semiseparable matrices form a subclass of matrices with Green's $(H,1)$-quasiseparable structure. As it turns out, unitary Hessenberg matrices also satisfy the two equivalent characterizations of Green's $(H,1)$-semiseparability below.

Definition 2.8 (QS Generators)**.** *An $n \times n$ matrix A is Green's $(H,1)$-*

semiseparable if **(i)** *it is strongly Hessenberg and* **(ii)** *if there exists a choice of Green's* $(H,1)$*-quasiseparable generators* $\{p_t, a_u, r_v, d_w\}$ *for* A *such that* $a_u \neq 0$ *for* $u = 2, \ldots, n-1$*.*

Definition 2.9 (SS Generators)**.** *A matrix* A *is Green's* $(H,1)$*-semiseparable if* **(i)** *it is strongly Hessenberg and* **(ii)** *if*

$$tril(A) = tril(rt)$$

for some matrices r *and* t*, where* r *is* $n \times 1$ *and* t *is* $1 \times n$*, and where* $tril(\cdot)$ *denotes the lower triangular parts of the matrices* A *and* rt*. In other words, the lower triangular part of* A *coincides with the lower triangular part of a rank 1 matrix. The matrices* r *and* t *are referred to as a set of Green's* $(H,1)$*-semiseparable generators for* A*.*

Observe that if p_t, a_u and r_v defined as in (23), the lower triangular part of the matrix in (22) coincides with the lower triangular part of the matrix qt, where

$$q = \begin{bmatrix} p_2 \\ p_3 a_2 \\ \vdots \\ p_n a_{n-1} \ldots a_2 \\ p_{n+1} a_n \ldots a_2 \end{bmatrix}, \qquad t = \begin{bmatrix} r_1 & r_2/a_2 & r_3/(a_3 a_2) & \cdots & r_n/(a_n \cdots a_2) \end{bmatrix}$$

and q is simply the first column of U. The algorithm below takes advantage of the Green's $(H,1)$-semiseparable structure of unitary Hessenberg matrices. That is, given the first column q of the unitary Hessenberg matrix U, U is constructed via a set of Green's $(H,1)$-semiseparable generators.

Algorithm 2.10 (GH1Semi)**.** *Let $q \in \mathbb{C}^n$ denote the first column of U. First compute*

$$f_i = \sqrt{\sum_{j=i}^{n} |q_j|^2}$$

for $i = 1, \ldots, n$ and $r_1 = 1$ and use the relations

$$p_t = \frac{q_{t-1}}{f_{t-1}}, \quad a_u = \frac{f_u}{f_{u-1}}, \quad r_v = \frac{-\overline{q}_{v-1}}{f_{v-1}}, \quad d_w = \frac{f_w}{f_{w-1}}$$

for $t = 2, \ldots, n+1$, $u = 2, \ldots, n$, $v = 1, \ldots, n$ and $w = 2, \ldots, n$ to compute the matrix t

$$t = \begin{bmatrix} r_1 & r_2/a_2 & r_3/(a_3 a_2) & \cdots & r_n/(a_n \cdots a_2) \end{bmatrix}$$

Then q and t make up a set of Green's $(H,1)$-semiseparable generators for U. In other words, the lower triangular part of U coincides with the lower triangular part of qt, and further, the super-diagonal entries of U are given by the d_w's.

```
function [ L ] = GH1Semi( q )

n=length(q);
x = q.*conj(q);
f(1) = 1;
```

```
for k=2:n
    f(k) = sqrt(sum(x(k:n)));
end
r(1) = 1;
for i = 2:n+1
    p(i) = (q(i-1))/(f(i-1));
    if i<n+1
        a(i) = (f(i))/(f(i-1));
        d(i) = (f(i))/(f(i-1));
        r(i) = (-conj(q(i-1)))/(f(i-1));
    end
end
t(1)=r(1);
for j = 2:n
    t(j) = r(j)/prod(a(2:j));
end
U = tril(q*t);
for i = 2:n
    U(i-1,i) = d(i);
end
L = U(:,2:n);

end
```

2.6 Order 1 Numerical Experiments

Numerical experiments were performed with randomly generated normalized vectors q of various sizes. As the table below shows, each of the algorithms produce L in which the orthogonality of its columns is maintained throughout the computation. Additionally, in the numerical experiment by Kahan in which the Householder-Fox method performed poorly, the normalized version of the vector $q = (1, 1/8, 1/8^2, \ldots, 1/8^{15})$ was used. Where Parlett's algorithm produced an error of $2.2291e^{-16}$, the algorithms Decomp1, Decomp2, GH1Quasi and GH1Semi produced errors of $2.3549e-16$, $4.4540e-16$, $4.4507e-16$, and $2.5732e-16$ respectively. In other words, none of the methods suffered from the severe cancellation one encounters using the Cholesky decomposition in the Householder-Fox method.

n	Decomp1.1	Decomp2.1	GH1Quasi	GH1Semi
5	1.441482e-16	2.747310e-16	2.840501e-16	2.900364e-16
6	1.803470e-16	3.216273e-16	3.601083e-16	3.661081e-16
7	2.115891e-16	3.456447e-16	3.306928e-16	3.358801e-16
8	2.201314e-16	4.188025e-16	3.533755e-16	3.564010e-16
9	2.518760e-16	3.647511e-16	3.395976e-16	3.414434e-16
10	2.395479e-16	4.208616e-16	3.788792e-16	4.030267e-16
15	2.891496e-16	4.799696e-16	4.273925e-16	4.385353e-16
20	2.988824e-16	5.486274e-16	4.357952e-16	4.149611e-16
25	3.148853e-16	5.678320e-16	4.447643e-16	4.300907e-16
50	3.882197e-16	6.491263e-16	5.435018e-16	5.359209e-16
75	4.538128e-16	6.685918e-16	5.879911e-16	5.647093e-16
100	4.894567e-16	7.490992e-16	6.510562e-16	6.174313e-16

Table 1: $||L^*L - I||$, given the first column of an $\mathbf{n} \times \mathbf{n}$ unitary Hessenberg matrix

3 Unitary 2-Hessenberg Matrices

In this section, we show how each of the algorithms presented can be extended to solve the following problem: Given two orthonormal vectors q_1 and q_2 of length n, compute the $n \times (n-2)$ matrix L such that $U = [q_1\ q_2\ L]$ is unitary.

We begin by extending the definition of a 1-Hessenberg matrix.

Definition 3.1. *An $n \times n$ matrix A is called* 2*-Hessenberg if the entries above it's second superdiagonal are all zero. If additionally all of the elements along second superdiagonal are non-zero, we say that A is strongly* 2*-Hessenberg.*

Theorem 3.2. *If A is $n \times n$ strongly Hessenberg and B is $n \times n$ and has the form*

$$B = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{B} \end{bmatrix}$$

where $\tilde{B}$ is strongly Hessenberg, then AB is strongly 2*-Hessenberg.*

Proof. This is easily verified by noting that the entries along the second superdiagonal of AB consist of products from the first superdiagonal of A and the first superdiagonal of $\tilde{B}$, which are all nonzero by assumption. □

3.1 Reduction to an Order One Problem

One method of extending the algorithms in the previous section is to use the fact that a unitary 2-Hessenberg matrix can be factored as a product of two unitary Hessenberg matrices.

Theorem 3.3. *An $n \times n$ unitary* 2*-Hessenberg matrix U can be decomposed into a product of* 2 *unitary Hessenberg matrices. In particular, if U is an $n \times n$ unitary* 2*-Hessenberg matrix, then $U = U_1 U_2$, where U_1 is unitary*

Hessenberg and where

$$U_2 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_2 \end{bmatrix} \tag{24}$$

and $\tilde{U}_2$ *is an* $(n-1) \times (n-1)$ *unitary Hessenberg matrix.*

Proof. Suppose U is $n \times n$ unitary 2-Hessenberg with first column $q = (q_1, \ldots, q_n)$, and let $diag(U, i)$ denote the ith superdiagonal of the matrix U. As seen in (2.4), multiplying U by the $n-1$ plane rotations

$$G_i = \begin{bmatrix} I_{i-1} & & & \\ & \overline{\rho}_i & \mu_i & \\ & \mu_i & -\rho_i & \\ & & & I_{n-i-1} \end{bmatrix} \tag{25}$$

where $i = 1, \ldots, n-1$, and the matrix $G_n = diag(1, \ldots, 1, \overline{\rho}_n)$, with $\rho_n = e^{i*arg(q_n)}$ reduces the first column of U to e_1, the first column of the $n \times n$ identity matrix I_n. That is, $G_1 \cdots G_n U = U_2$, where U_2 has the form

$$U_2 = \begin{bmatrix} 1 & u \\ 0 & \tilde{U}_2 \end{bmatrix}$$

However, U_2 is a product of unitary matrices, and thus it must be unitary as well. This implies $u = 0$, so

$$U_2 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_2 \end{bmatrix}$$

Next, note that $diag(U, i) = 0$ for $i = 3, \ldots, n$ and $diag(U_1, j) = 0$ for $j = 2, \ldots, n$ and $diag(U_1, 1) \neq 0$. Thus if

$$U = U_1 \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_2 \end{bmatrix}$$

it must be the case that $diag(\tilde{U}_2, w) = 0$ for $w = 2, \ldots, n$. That is, $\tilde{U}_2$ is unitary Hessenberg.

□

Corollary 3.4. *An $n \times n$ unitary 2-Hessenberg matrix U is strongly 2-Hessenberg.*

Proof. This follows from the fact that the decomposition in (3.3) has exactly the form required in (3.2). □

Using the simple result from (3.3), an order two problem is reduced to solving two order one problems. Since the first column q_1 of U and U_1 coincide, the first column of U can be used to compute U_1. If the first column $\tilde{q}_2$ of $\tilde{U}_2$ is known, it can be used to compute the rest of U_2. Notice however that if e_2 denotes the second column of the $n \times n$ identity matrix

I_n, then

$$q_2 = Ue_2 = U_1 U_2 e_2 = U_1 \begin{bmatrix} 0 \\ \tilde{q}_2 \end{bmatrix}$$

Thus, we can compute $\tilde{q}_2$ using q_2 and U_1 via

$$U_1^* q_2 = \begin{bmatrix} 0 \\ \tilde{q}_2 \end{bmatrix} \tag{26}$$

Once U_1 and U_2 are known, U is simply the product of the two, $U = U_1 U_2$.

It is also observed that this solution is unique, for if q_1 uniquely determines U_1, then $U_1^* q_2$ uniquely determines $\tilde{q}_2$ which in turn uniquely determines $\tilde{U}_2$.

3.2 Decomposable Structure Revisited

Using (3.3) and keeping in mind the observation in (26), we can extend (2.3) and (2.4) to the order two case

Algorithm 3.5 (Decomp1.2)**.** *Let* $q^{(1)}, q^{(2)} \in \mathbb{C}^n$ *denote the first* 2 *columns of* U*. From (3.3), we know* $U = U_1 U_2$ *where both* U_1 *and* U_2 *are unitary*

Hessenberg. So, use $q^{(1)}$ *to compute* U_1

$$\begin{bmatrix} \rho_1^{(1)} \\ \rho_2^{(1)}\mu_1^{(1)} \\ \vdots \\ \rho_{n-1}^{(1)}\mu_{n-2}^{(1)}\cdots\mu_1^{(1)} \\ \rho_n^{(1)}\mu_{n-1}^{(1)}\cdots\mu_1^{(1)} \end{bmatrix} = \begin{bmatrix} q_1^{(1)} \\ q_2^{(1)} \\ \vdots \\ q_{n-1}^{(1)} \\ q_n^{(1)} \end{bmatrix} = q^{(1)}$$

Equating the first components, we have $\rho_1^{(1)} = q_1^{(1)}$*. Because we know that* $\mu_1^{(1)} = \sqrt{1 - |\rho_1^{(1)}|^2}$*, we can equate the second components to and compute* $\rho_2^{(1)} = q_2^{(1)}/\mu_1^{(1)}$*. This in turn allows us to compute* $\mu_2^{(1)}$*. Exhausting this process completely determines* $\{\rho_i^{(1)}, \mu_i^{(1)}\}$ *for* $i = 1, \ldots, n-1$*. Letting* $\rho_n^{(1)} = e^{i \cdot arg(q_n^{(1)})}$*, compute*

$$U_1 = (G_n^{(1)})^*(G_{n-1}^{(1)})^*(G_{n-2}^{(1)})^* \cdots (G_1^{(1)})^*$$

where $G_n^{(1)} = diag(1, \ldots, 1, \overline{\rho}_n^{(1)})$ *and* $G_i^{(1)}$ *is defined as in (21) for* $i = 1, \ldots, n-1$*. Next, compute the second column of* U_2

$$U_1^* q^{(2)} = \tilde{q}^{(2)}$$

and set

$$\begin{bmatrix} 0 \\ \rho_2^{(2)} \\ \rho_3^{(2)}\mu_2^{(2)} \\ \vdots \\ \rho_n^{(2)}\mu_{n-1}^{(2)}\dots\mu_2^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ \tilde{q}_2^{(2)} \\ \tilde{q}_3^{(2)} \\ \vdots \\ \tilde{q}_n^{(2)} \end{bmatrix} = \tilde{q}^{(2)}$$

Equating $\rho_2^{(2)} = \tilde{q}_2^{(2)}$, *repeat the process above to compute*

$$U_2 = (G_n^{(2)})^*(G_{n-1}^{(2)})^*(G_{n-2}^{(2)})^* \cdots (G_2^{(2)})^*$$

Finally, compute $U = U_1U_2$.

```
function [L] = Decomp1.2(q,r)
n=length(q)
U = Decomp1(q); % As defined in (2.2)
X = U'*r;
X = X(2:end);
G = Decomp1(X);
U = U*blkdiag(1,G);
L = U(:,i+1:n);
```

The second decomposable algorithm avoids subtraction in the computation of the μ_i's just as in the order 1 case.

Algorithm 3.6 (Decomp2.2)**.** *Let* $q^{(1)}, q^{(2)} \in \mathbb{C}^n$ *denote the first two columns* *of* U, *and* $\rho_n^{(1)} = e^{i \cdot arg(q_n^{(1)})}$. *First, compute the vector* $q^{(1,1)}$.

$$\begin{bmatrix} I_{n-1} & \\ & \overline{\rho}_n^{(1)} \end{bmatrix} q^{(1)} = q^{(1,1)}$$

Define

$$r_{n-1}^{(1)} = \sqrt{|q_{n-1}^{(1,1)}|^2 + |q_n^{(1,1)}|^2}$$

and set

$$\rho_{n-1}^{(1)} = \frac{q_{n-1}^{(1,1)}}{r_{n-1}^{(1)}}, \qquad \mu_{n-1}^{(1)} = \frac{q_n^{(1,1)}}{r_{n-1}^{(1)}}$$

Then $\mu_{n-1}^{(1)} = \sqrt{1 - |\rho_{n-1}^{(1)}|^2}$, *and*

$$\begin{bmatrix} I_{n-2} & & \\ & \overline{\rho}_{n-1}^{(1)} & \mu_{n-1}^{(1)} \\ & \mu_{n-1}^{(1)} & -\rho_{n-1}^{(1)} \end{bmatrix} q^{(1,1)} = \begin{bmatrix} * \\ \vdots \\ r_{n-1}^{(1)} \\ 0 \end{bmatrix} = q^{(1,2)}$$

Next, define

$$r_{n-2}^{(1)} = \sqrt{|q_{n-2}^{(1,2)}|^2 + |q_{n-1}^{(1,2)}|^2}$$

and set

$$\rho_{n-2}^{(1)} = \frac{q_{n-2}^{(1,2)}}{r_{n-2}^{(1)}}, \qquad \mu_{n-2}^{(1)} = \frac{q_{n-1}^{(1,2)}}{r_{n-2}^{(1)}}$$

Then

$$\begin{bmatrix} I_{n-3} & & & \\ & \overline{\rho}_{n-2}^{(1)} & \mu_{n-2}^{(1)} & \\ & \mu_{n-2}^{(1)} & -\rho_{n-2}^{(1)} & \\ & & & 1 \end{bmatrix} q^{(1,2)} = \begin{bmatrix} * \\ \vdots \\ r_{n-2}^{(1)} \\ 0 \\ 0 \end{bmatrix} = q^{(1,3)}$$

Continue this process until reaching the vector e_1*, the first column of the identity* I_n*. This determines* $\{\rho_i^{(1)}, \mu_i^{(1)}\}$ *for* $i = 1, \ldots, n-1$*. Use these parameters to compute*

$$U_1 = (G_n^{(1)})^*(G_{n-1}^{(1)})^*(G_{n-2}^{(1)})^* \cdots (G_1^{(1)})^*$$

where $G_n^{(1)} = diag(1, \ldots, 1, \overline{\rho}_n^{(1)})$ *and* $G_i^{(1)}$ *is defined as in (21) for* $i = 1, \ldots, n-1$*. Next, compute the second column of* U_2

$$U_1^* q^{(2)} = \tilde{q}^{(2)}$$

and repeat the process above with $\tilde{q}^{(2)}$ *to determine* $\{\rho_i^{(2)}, \mu_i^{(2)}\}$ *for* $i = 2, \ldots, n-$

1 *and construct* U_2

$$U_2 = (G_n^{(2)})^*(G_{n-1}^{(2)})^*(G_{n-2}^{(2)})^* \cdots (G_2^{(2)})^*$$

Finally, compute $U = U_1U_2$.

```
function [L] = Decomp2.2(q,r)
n=length(q)
U = Decomp2(q); % As defined in (2.3)
X = U'*r;
X = X(2:end);
G = Decomp2(X);
U = U*blkdiag(1,G);
L = U(:,i+1:n);
```

3.3 Green's $(H, 2)$-quasiseparable Structure

A more interesting approach to solving the order two problem is to extend the definition of Green's $(H, 1)$-quasiseparability. Doing so allows us to discuss some additional structure of unitary 2-Hessenberg matrices. As per usual, two equivalent definitions are provided.

Definition 3.7 (Rank)**.** *An* $n \times n$ *matrix* A *is Green's* $(H, 2)$*-quasiseparable if* **(i)** *it is strongly* 2*-Hessenberg and* **(ii)** *if* $max(rank(A_i)) = 2$*, where*

$$A_i = \quad A(i : n, 1 : i + 1), \quad i = 1, \ldots, n - 1$$

In light of (3.3), one might conjecture that unitary 2-Hessenberg matrices also possess a great deal of structure, for if $U = U_1U_2$, where U_1 and U_2 are unitary Hessenberg, we know from the previous section that each possess a set of Green's $(H,1)$-quasiseparable generators. Thus, we may be able to construct the unitary 2-Hessenberg matrix U using these generators. The equivalent definition of Green's $(H,2)$-quasiseparability is given below will be of use.

Definition 3.8 (Generator)**.** *An $n\times n$ matrix A is said to be Green's $(H,2)$-quasiseparable if* **(i)** *it is strongly 2-Hessenberg and* **(ii)** *if can be represented in the form:*

$$\begin{bmatrix} p_3a_2r_1 & p_3r_2 & d_3 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & d_n \\ & p_ia_{ij}^{\times}r_j & & & \ddots & p_{n+1}r_n \\ & & & & & p_{n+2}a_{n+1}r_n \end{bmatrix} \tag{27}$$

where the entries above the second super-diagonal are zero, and

$$a_{ij}^{\times} = \begin{cases} a_{j+1}\cdots a_i & i>j \\ 1 & i=j \end{cases}$$

where the elements of $\mathfrak{G}_1 = \{p_t, a_u, r_v, d_w\}$, for $t=3,\dots,n+2$, $u=2,\dots,n+1$, $v=1,\dots,n$, and $w=3,\dots,n$, are called a set of Green's $(H,2)$-quasiseparable generators for A, and are matrices of sizes 1×2, 2×2,

2×1, *and* 1×1 *respectively.*

As it turns out, the product of two Green's $(H, 1)$-quasiseparable matrices produces a Green's $(H, 2)$-quasiseparable matrix. This is not surprising, and additionally, given Green's $(H, 1)$-quasiseparable generators for two matrices A and B, the next theorem shows that one can compute Green's $(H, 2)$-quasiseparable generators for their product AB.

Theorem 3.9. *Let A and B be $n \times n$ unitary Hessenberg matrices. If A has Green's $(H, 1)$-quasiseparable generators $\mathfrak{G}_1 = \{p_i^{(A)}, a_i^{(A)}, r_i^{(A)}, d_i^{(A)}\}$ and B has Green's $(H, 1)$-quasiseparable generators $\mathfrak{G}_2 = \{p_i^{(B)}, a_i^{(B)}, r_i^{(B)}, d_i^{(B)}\}$, then the product AB is unitary 2-Hessenberg, with Green's $(H, 2)$-quasiseparable generators $\mathfrak{G}_{12} = \{p_t^{(AB)}, a_u^{(AB)}, r_v^{(AB)}, d_w^{(AB)}\}$ for $t = 3, \ldots, n+2$, $u = 2, \ldots, n+1$, $v = 1, \ldots, n$, and $w = 3, \ldots, n$, given by:*

$$p_i^{(AB)} = \begin{bmatrix} p_{i-1}^{(A)} & d_{i-1}^{(A)} p_i^{(B)} \end{bmatrix}, \quad a_i^{(AB)} = \begin{bmatrix} a_{i-1}^{(A)} & r_{i-1}^{(A)} p_i^{(B)} \\ 0 & a_i^{(B)} \end{bmatrix} \tag{28}$$

$$r_i^{(AB)} = \begin{bmatrix} r_{i-1}^{(A)} d_i^{(B)} \\ r_i^{(B)} \end{bmatrix}, \quad d_i^{(AB)} = d_{i-1}^{(A)} d_i^{(B)}$$

Proof. That AB is unitary follows from the fact that a product of unitary matrices is again unitary, and it is easily checked that AB is 2-Hessenberg. To compute the generators, begin by embedding A and B into $(n+2) \times (n+2)$ lower triangular matrices as follows:

(a) Take A and add one column of all zeros to the left of its first column.

Next, add two rows of zeros above the top row of the updated matrix. Finally, add one column of zeros to the right of this second updated matrix. Denote this matrix by L_A.

(b) Take B and add one row of all zeros below its last row. Next, add two columns of zeros to the right of the last column of the updated matrix. Finally, add one row of zeros above the first row of this second updated matrix. Denote this matrix by L_B.

For example, if $n = 4$ and the ⊠'s represent the entries of A and B then

$$L_A = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \boxtimes & \boxtimes & 0 & 0 & 0 \\ 0 & \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\ 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \\ 0 & \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 \end{bmatrix}, \quad L_B = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ \boxtimes & \boxtimes & 0 & 0 & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & 0 & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\ \boxtimes & \boxtimes & \boxtimes & \boxtimes & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{29}$$

By design, the matrices L_A and L_B are both order 1 quasiseparable with generators given by:

$$p_i^{(L_A)} = \begin{cases} p_{i-1}^{(A)} & i = 3, \dots, n+2 \\ 0 & \text{otherwise} \end{cases}, \qquad a_i^{(L_A)} = \begin{cases} a_{i-1}^{(A)} & i = 3, \dots, n+3 \\ 0 & \text{otherwise} \end{cases}$$

$$r_i^{(L_A)} = \begin{cases} r_{i-1}^{(A)} & i = 2, \dots, n+2 \\ 0 & \text{otherwise} \end{cases}, \qquad d_i^{(L_A)} = \begin{cases} d_{i-1}^{(A)} & i = 3, \dots, n+1 \\ 0 & \text{otherwise} \end{cases}$$

$$p_i^{(L_B)} = \begin{cases} p_i^{(B)} & i = 2, \dots, n+1 \\ 0 & \text{otherwise} \end{cases}, \qquad a_i^{(L_B)} = a_i^{(B)}$$

$$r_i^{(L_B)} = \begin{cases} r_i^{(B)} & i = 1, \dots, n \\ 0 & \text{otherwise} \end{cases}, \qquad d_i^{(L_B)} = \begin{cases} d_i^{(B)} & i = 2, \dots, n \\ 0 & \text{otherwise} \end{cases}$$

$$g_i^{(L_A)} = g_i^{(L_B)} = 0, \qquad h_i^{(L_A)} = h_i^{(L_B)} = 0$$

Thus, using (1.3), one can compute a set of order 2 quasiseparable generators for $L_A L_B = L_{AB}$. Then the Green's $(H, 2)$-quasiseparable generators for AB can be read directly from the order 2 quasiseparable generators of L_{AB} using the restriction $AB = L_{AB}(3 : n+2, 1 : n)$, resulting in the generators proposed in the theorem.

$\square$

Algorithm 3.10 (GH2Quasi)**.** *Let* $q_1, q_2 \in \mathbb{C}^n$*. Use (23) to compute a set of Green's* $(H,1)$*-quasiseparable generators,* $\mathfrak{G}_1$*, for* U_1*. Construct the unitary Hessenberg matrix* U_1 *with first column* q_1*. Next, let*

$$\begin{bmatrix} 0 \\ \tilde{q}_2 \end{bmatrix} = U_1^* q_2$$

Use (23) a second time with the new input $\tilde{q}_2$ *to compute a set of Green's* $(H,1)$*-quasiseparable generators,* $\mathfrak{G}_2$*, for* $\tilde{U}_2$*. Compute a set of Green's* $(H,2)$*-quasiseparable generators,* $\mathfrak{G}_{12}$*, for the product* $U = U_1 U_2$ *from* $\mathfrak{G}_1$ *and* $\mathfrak{G}_2$ *using the formulas in (28). Construct* U *via its Green's* $(H,2)$*-quasiseparable generators as in (27).*

3.4 Green's $(H,2)$-semiseparable Structure

Unitary 2-Hessenberg matrices also exhibit Green's $(H,2)$-semiseparable structure.

Definition 3.11 (QS Generator)**.** *An* $n \times n$ *matrix* A *is Green's* $(H,2)$*-semiseparable if* **(i)** *it is strongly* 2*-Hessenberg and* **(ii)** *if there exists a choice of Green's* $(H,2)$*-quasiseparable generators* $\mathfrak{G} = \{p_t, a_u, r_v, d_w\}$ *for* A *such that* a_u *is invertible for* $u = 2, \ldots, n-1$*.*

Just like the order 1 case, it is clear that Green's $(H,2)$-semiseparable matrices form a subclass of matrices with Green's $(H,2)$-quasiseparable structure. An equivalent characterization for this subclass is given below.

Definition 3.12 (SS Generator). *An $n \times n$ matrix A is Green's $(H, 2)$-semiseparable if* **(i)** *it is strongly 2-Hessenberg and* **(ii)** *if*

$$tril(A, 1) = tril(RT, 1)$$

for some matrices R and T of sizes $n \times 2$ and $2 \times n$, respectively. The matrices R and T are called a set of Green's $(H, 2)$-semiseparable generators for A.

Analogous to the Green's $(H, 2)$-quasiseparable case, given a pair of Green's $(H, 1)$-semiseparable generators for two matrices A and B, on can compute a pair of Green's $(H, 2)$-semiseparable generators for their product AB.

Theorem 3.13. *Suppose A is $n \times n$ unitary Hessenberg with Green's $(H, 1)$-semiseparable generators $R^{(A)}$ and $T^{(A)}$ and B is $n \times n$ unitary Hessenberg with Green's $(H, 1)$-semiseparable generators $R^{(B)}$ and $T^{(B)}$. Then the product AB is unitary 2-Hessenberg and has Green's $(H, 2)$-semiseparable generators R and T of sizes $n \times 2$ and $2 \times n$ respectively, given by:*

$$R = \begin{bmatrix} p_3^{(L_{AB})} a_2^{(L_{AB})} \\ p_4^{(L_{AB})} a_3^{(L_{AB})} a_2^{(L_{AB})} \\ \vdots \\ p_{n+2}^{(L_{AB})} a_{n+1}^{(L_{AB})} \cdots a_2^{(L_{AB})} \end{bmatrix}$$

$$T = \begin{bmatrix} r_1^{(L_{AB})} & (a_2^{(L_{AB})})^{-1} r_2^{(L_{AB})} & \cdots & ((a_2^{(L_{AB})})^{-1} \cdots (a_n^{(L_{AB})})^{-1}) r_n^{(L_{AB})} \end{bmatrix}$$

where

$$p_i^{(L_{AB})} = \begin{bmatrix} x_i^{(L_A)} & d_i^{(L_A)} x_i^{(L_B)} \end{bmatrix}, \quad a_i^{(L_{AB})} = \begin{bmatrix} 1 & y_i^{(L_A)} x_i^{(L_B)} \\ 0 & 1 \end{bmatrix} \tag{30}$$

$$r_i^{(L_{AB})} = \begin{bmatrix} y_i^{(L_A)} d_i^{(L_B)} \\ y_i^{(L_B)} \end{bmatrix}, \quad d_i^{(L_{AB})} = d_i^{(L_A)} d_i^{(L_B)}$$

where $L_{AB} = L_A L_B$, *with* L_A *and* L_B *defined as in (3.9), and where the* x_i*'s and* y_i*'s denote the* i*th rows and* i*th columns of the matrices* $X^{(L_A)}, X^{(L_B)}$ *and* $Y^{(L_A)}, Y^{(L_B)}$ *respectively. These matrices are given by*

$$X^{(L_A)} = \begin{bmatrix} 0 \\ 0 \\ R^{(A)} \end{bmatrix}, \quad Y^{(L_A)} = \begin{bmatrix} 0 & T^{(A)} & 0 \end{bmatrix} \tag{31}$$

$$X^{(L_B)} = \begin{bmatrix} 0 \\ R^{(B)} \\ 0 \end{bmatrix}, \quad Y^{(L_B)} = \begin{bmatrix} T^{(B)} & 0 & 0 \end{bmatrix}$$

Proof. First, note that $tril(L_A, -1) = tril(X^{(L_A)} Y^{(L_A)}, -1)$ and $tril(L_B, -1) = tril(X^{(L_B)} Y^{(L_B)}, -1)$ so that L_A and L_B are both order 1 lower semiseperable by (1). Thus, each has a set of order 1 quasiseparable generators in which $a_i \neq 0$ according to (1.4). It is easily checked that the following generators satisfy this condition:

$$\mathfrak{G}_1 = \left\{p_t^{(L_A)}, a_u^{(L_A)}, r_v^{(L_A)}\right\} = \left\{x_t^{(L_A)}, 1, y_v^{(L_A)}\right\}$$

and

$$\mathfrak{G}_2 = \left\{p_t^{(L_B)}, a_u^{(L_B)}, r_v^{(L_B)}\right\} = \left\{x_t^{(L_B)}, 1, y_v^{(L_B)}\right\}$$

for $t = 2, \ldots, n+2$, $u = 2, \ldots, n+1$ and $v = 1, \ldots, n+1$. Using (1.3), compute a set order 2 quasiseparable generators, $\mathfrak{G}_{12}$, for $L_A L_B = L_{AB}$. This results in (30) above. Note however that each $a_i^{(L_{AB})}$ is invertible. This implies that L_{AB} is order 2 semiseparable, and it is easily checked that if

$$R^{(L_{AB})} = \begin{bmatrix} 0 \\ p_2^{(L_{AB})} \\ p_3^{(L_{AB})} a_2^{(L_{AB})} \\ p_4^{(L_{AB})} a_3^{(L_{AB})} a_2^{(L_{AB})} \\ \vdots \\ p_{n+2}^{(L_{AB})} a_{n+1}^{(L_{AB})} \cdots a_2^{(L_{AB})} \end{bmatrix}$$

and

$$T^{(L_{AB})} = \begin{bmatrix} r_1^{(L_{AB})} & (a_2^{(L_{AB})})^{-1} r_2^{(L_{AB})} & \cdots & ((a_2^{(L_{AB})})^{-1} \cdots (a_n^{(L_{AB})})^{-1}) r_n^{(L_{AB})} & 0 \end{bmatrix}$$

then $tril(L_{AB}, -1) = tril(R^{(L_{AB})} T^{(L_{AB})}, -1)$. From here, we can read Green's $(H, 2)$-semiseparable generators for AB using the restrictions $R = R^{(L_{AB})}(3 :$

$n+2,:)$ and $T = T^{(L_{AB})}(:,1:n)$, resulting in the generators proposed in the theorem.

$\square$

Algorithm 3.14 (GH2Semi)**.** *Let $q_1, q_2 \in \mathbb{C}^n$. Use (2.10) to compute a set of Green's $(H,1)$-semiseparable generators, $\mathfrak{S}_1$, for U_1. Construct the unitary Hessenberg matrix U_1 with first column q_1. Next, let*

$$\begin{bmatrix} 0 \\ \tilde{q}_2 \end{bmatrix} = U_1^* q_2$$

Use (2.10) a second time with the new input $\tilde{q}_2$ to compute a set of Green's $(H,1)$-semiseparable generators, $\mathfrak{S}_2$, for $\tilde{U}_2$. Compute a set of Green's $(H,2)$-semiseparable generators, $\mathfrak{S}_{12}$, for the product $U = U_1U_2$ from $\mathfrak{S}_1$ and $\mathfrak{S}_2$ using the formulas in (3.13). Construct U via its Green's $(H,2)$-semiseparable generators.

3.5 Order 2 Numerical Experiments

As in the order one case, numerical experiments were performed using two random orthonormal vectors, and as the table below shows, the order two algorithms continue to give satisfactory results. The first two columns show results using (3.5) and (3.6) respectively, while the last two columns take advantage of the Green's $(H,2)$-quasiseparable and Green's $(H,2)$-semiseparable structure of unitary 2-Hessenberg matrices.

n	Decomp1.2	Decomp2.2	GH2Quasi	GH2Semi
5	2.022212e-16	3.107808e-16	6.417212e-16	7.240132e-16
6	2.441090e-16	4.030848e-16	5.897694e-16	6.314752e-16
7	2.560498e-16	4.497004e-16	6.201739e-16	6.801807e-16
8	2.858382e-16	5.412214e-16	5.816183e-16	6.459664e-16
9	2.865056e-16	4.912225e-16	6.375426e-16	6.449588e-16
10	2.955906e-16	5.493200e-16	5.985178e-16	6.675054e-16
15	3.620075e-16	6.320014e-16	7.202800e-16	7.956039e-16
20	3.637235e-16	6.794206e-16	7.621410e-16	7.910531e-16
25	4.138340e-16	7.336842e-16	7.502287e-16	7.369190e-16
50	4.918858e-16	8.555373e-16	7.594854e-16	8.233958e-16
75	5.326452e-16	8.803149e-16	8.343950e-16	8.022459e-16
100	6.048012e-16	9.238259e-16	9.035018e-16	8.931376e-16

Table 2: $||L^*L - I||$, given the first two columns of an $\mathbf{n} \times \mathbf{n}$ unitary 2-Hessenberg matrix

4 Unitary k-Hessenberg Matrices

The final section provides the main result of this paper, offering a complete generalization of each algorithm presented previously. Once again, we begin with a definition.

Definition 4.1. *An $n \times n$ matrix A is called k-Hessenberg if the entries above it's kth superdiagonal are all zero. If additionally all of the elements along the kth superdiagonal are non-zero, we say that A is strongly k-Hessenberg.*

Theorem 4.2. *If A is $n \times n$ strongly k-Hessenberg and B is $n \times n$ and has the form*

$$B = \begin{bmatrix} I_k & 0 \\ 0 & \tilde{B} \end{bmatrix}$$

where I_k denotes the $k \times k$ identity matrix and $\tilde{B}$ is strongly Hessenberg, then AB is strongly $(k+1)$-Hessenberg.

Proof. This is easily verified by noting that the entries along the $(k+1)$st superdiagonal of AB consist of products from the kth superdiagonal of A and the first superdiagonal of $\tilde{B}$, which are all nonzero by assumption.

□

4.1 Decomposition of Unitary k-Hessenberg Matrices

We have seen that unitary Hessenberg matrices can be decomposed into a product of Givens rotations, and that unitary 2-Hessenberg can be decomposed as a product of two unitary Hessenberg matrices. In this section, we generalize this notion to unitary k-Hessenberg matrices, beginning with the following theorem.

Theorem 4.3. *An $n \times n$ unitary k-Hessenberg matrix U admits a unique decomposition $U = U_1 U_2$, where U_1 is unitary Hessenberg and*

$$U_2 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_2 \end{bmatrix} \tag{32}$$

where $\tilde{U}_2$ is unitary $(k-1)$-Hessenberg.

Proof. Suppose U is $n \times n$ unitary k-Hessenberg with first column $q = (q_1, \ldots, q_n)$, and let $diag(U, i)$ denote the ith superdiagonal of the matrix

U. As seen in (2.4), multiplying U by the $n-1$ plane rotations

$$G_i = \begin{bmatrix} I_{i-1} & & & \\ & \overline{\rho}_i & \mu_i & \\ & \mu_i & -\rho_i & \\ & & & I_{n-i-1} \end{bmatrix} \tag{33}$$

where $i = 1, \ldots, n-1$, and the matrix $G_n = diag(1, \ldots, 1, \overline{\rho}_n)$, with $\rho_n = e^{i \cdot arg(q_n)}$ reduces the first column of U to e_1, the first column of the $n \times n$ identity matrix I_n. That is, $G_1 \cdots G_n U = U_2$, where U_2 has the form

$$U_2 = \begin{bmatrix} 1 & u \\ 0 & \tilde{U}_2 \end{bmatrix}$$

However, U_2 is a product of unitary matrices, and thus it must be unitary as well. This implies $u = 0$, so

$$U_2 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_2 \end{bmatrix}$$

Next, note that $diag(U, i) = 0$ for $i = k+1, \ldots, n$ and $diag(U_1, j) = 0$ for $j = 2, \ldots, n$ and $diag(U_1, 1) \neq 0$. Thus if

$$U = U_1 \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_2 \end{bmatrix}$$

it must be the case that $diag(\tilde{U}_2, w) = 0$ for $w = k, \ldots, n$. That is, $\tilde{U}_2$ is unitary $(k-1)$-Hessenberg. Uniqueness follows from the fact that U_1 is uniquely determined by q, which implies U_2 is uniquely determined by U_1

□

Corollary 4.4. *An $n \times n$ unitary k-Hessenberg matrix U can be expressed uniquely as the product of k unitary Hessenberg matrices. In particular, if U is an $n \times n$ unitary k-Hessenberg matrix, then $U = U_1 U_2 \cdots U_k$, with*

$$U_j = \begin{bmatrix} I_{j-1} & 0 \\ 0 & \tilde{U}_j \end{bmatrix} \tag{34}$$

and $\tilde{U}_j$ is an $(n-j+1) \times (n-j+1)$ unitary Hessenberg matrix for $j = 1, \ldots, k$.

Proof. From the previous theorem $U = U_1 U_2$, where U_1 is unitary Hessenberg and U_2 has the form

$$U_2 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_2 \end{bmatrix}$$

and $\tilde{U}_2$ is unitary $(k-1)$-Hessenberg. Applying the theorem a second time allows us to write $\tilde{U}_2 = \tilde{U}_2' \tilde{U}_3$, where $\tilde{U}_2'$ is unitary Hessenberg and $\tilde{U}_3$ has the form

$$\tilde{U}_3 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_3' \end{bmatrix}$$

where $\tilde{U}_3'$ is unitary $(k-2)$-Hessenberg. Thus, we can write

$$U = U_1 \begin{bmatrix} 1 & 0 \\ 0 & \tilde{U}_2' \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \tilde{U}_3' \end{bmatrix}$$

Exhausting this process produces $U = U_1 \cdots U_k$ where each U_j is given by (34). Uniqueness follows from the uniqueness in each application of (4.3).

□

Theorem 4.5. *An $n \times n$ unitary k-Hessenberg matrix is strongly k-Hessenberg.*

Proof. This follows directly from the fact that we can write $U = U_1 \cdots U_k$ as in (4.4). If we multiply these matrices out starting with the leftmost factors $U_1 U_2$, then this product, and each of the subsequent products has the form described in (4.2).

□

Finally, in light of the uniqueness of the decomposition in (4.4), we observe that just as a unitary Hessenberg matrix is uniquely determined by its first column, a unitary k-Hessenberg matrix is uniquely determined by its first k columns.

Theorem 4.6. *A unitary k-Hessenberg matrix U is uniquely determined by its first k columns.*

Proof. First, we know that a unitary Hessenberg matrix is uniquely determined by its first column. From of the decomposition in (4.4), where

$U = U_1 U_2 \cdots U_k$, it is clear that U and U_1 must have the same first column, since $U_2 \cdots U_k$ does not affect the first column of U_1 in the product. So, the first column of U uniquely determines U_1. The second column of U uniquely determines U_2, for if q_2 denotes the second column of U then

$$U_1^* q_2 = \begin{bmatrix} 0 \\ \tilde{q}_2 \end{bmatrix}$$

uniquely determines $\tilde{q}_2$, and $\tilde{q}_2$ uniquely determines $\tilde{U}_2$ and hence U_2. Similarly, the third column of U uniquely determines $\tilde{q}_3$

$$U_2^* U_1^* q_3 = \begin{bmatrix} 0 \\ 0 \\ \tilde{q}_3 \end{bmatrix}$$

and hence, uniquely determines U_3. Continuing through the first k columns of U, it is evident that q_i uniquely determines U_i for $i = 1, \ldots, k$ and hence, the first k columns $q_1, \ldots, q_k$ of U uniquely determine $U = U_1 \cdots U_k$.

□

We are now ready to begin the complete generalization of the algorithms in the previous sections. That is, each algorithm completes the unitary k-Hessenberg matrix U, given its first k columns $q_1, \ldots, q_k$.

4.2 Order k Decomposable Structure

In this section, the two algorithms presented generalize the method of exploiting the decomposable structure of unitary k-Hessenberg matrices. That is, (2.3), (3.5), (2.4) and (3.6) are each special cases of (4.7) and (4.8) presented below. Just as in the previous sections, the second decomposable algorithm avoids the use of subtraction while the first does not.

Algorithm 4.7 (Decomp1.k)**.** *Let $q^{(1)}, \ldots, q^{(k)} \in \mathbb{C}^n$ denote the first k columns of U and let $\rho_n^{(1)} = e^{i \cdot \arg(q_n^{(1)})}$. From (4.4), $U = U_1, \ldots, U_k$ where each U_i is unitary Hessenberg, and where the first column of U coincides with the first column of U_1. Recalling the structure of unitary Hessenberg matrices in (20), we know*

$$\begin{bmatrix} \rho_1^{(1)} \\ \rho_2^{(1)}\mu_1^{(1)} \\ \vdots \\ \rho_{n-1}^{(1)}\mu_{n-2}^{(1)}\cdots\mu_1^{(1)} \\ \rho_n^{(1)}\mu_{n-1}^{(1)}\cdots\mu_1^{(1)} \end{bmatrix} = \begin{bmatrix} q_1^{(1)} \\ q_2^{(1)} \\ \vdots \\ q_{n-1}^{(1)} \\ q_n^{(1)} \end{bmatrix} = q^{(1)}$$

Equating the first components, we have $\rho_1^{(1)} = q_1^{(1)}$. Because we know that $\mu_1^{(1)} = \sqrt{1 - |\rho_1^{(1)}|^2}$, we can equate the second components to and compute $\rho_2^{(1)} = q_2^{(1)}/\mu_1^{(1)}$. This in turn allows us to compute $\mu_2^{(1)}$. Exhausting this process completely determines $\{\rho_i^{(1)}, \mu_i^{(1)}\}$ for $i = 1, \ldots, n-1$. Use these *parameters to compute*

$$U_1 = (G_n^{(1)})^*(G_{n-1}^{(1)})^*(G_{n-2}^{(1)})^* \cdots (G_1^{(1)})^*$$

where $G_n = diag(1, \ldots, 1, \overline{\rho}_n^{(1)})$ *and* G_i *is defined as in (21) for* $i = 1, \ldots, n-1$. *Next, compute the second column of* U_2

$$U_1^* q^{(2)} = \tilde{q}^{(2)}$$

and set

$$\begin{bmatrix} 0 \\ \rho_2^{(2)} \\ \rho_3^{(2)}\mu_2^{(2)} \\ \vdots \\ \rho_n^{(2)}\mu_{n-1}^{(2)} \ldots \mu_2^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ \tilde{q}_2^{(2)} \\ \tilde{q}_3^{(2)} \\ \vdots \\ \tilde{q}_n^{(2)} \end{bmatrix} = \tilde{q}^{(2)}$$

Equating $\rho_2^{(2)} = \tilde{q}_2^{(2)}$, *repeat the previous process to determine* $\left\{\rho_i^{(2)}, \mu_i^{(2)}\right\}$ *for* $i = 2, \ldots, n-1$. *Let* $\rho_n^{(2)} = e^{i \cdot \arg(\tilde{q}_n^{(2)})}$ *and compute*

$$U_2 = (G_n^{(2)})^*(G_{n-1}^{(2)})^*(G_{n-2}^{(2)})^* \cdots (G_2^{(2)})^*$$

In general, compute the j*th column of* U_j

$$U_{j-1}^* \cdots U_1^* q^{(j)} = \tilde{q}^{(j)}$$

and set

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ \rho_j^{(j)} \\ \rho_{j+1}^{(j)}\mu_j^{(j)} \\ \vdots \\ \rho_n^{(j)}\mu_{n-1}^{(j)}\cdots\mu_j^{(j)} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tilde{q}_j^{(j)} \\ \tilde{q}_{j+1}^{(j)} \\ \vdots \\ \tilde{q}_n^{(j)} \end{bmatrix} = \tilde{q}^{(j)}$$

Compute $\{\rho_i^{(j)}, \mu_i^{(j)}\}$ *for* $i = j, \dots, n-1$. *Let* $\rho_n^{(j)} = e^{i\cdot\arg(\tilde{q}_n^{(j)})}$ *and compute*

$$U_j = (G_n^{(j)})^*(G_{n-1}^{(j)})^*(G_{n-2}^{(j)})^*\cdots(G_j^{(j)})^*$$

Repeating this process with for $j = 2, \dots, k$ *determines* $U_2, \dots, U_k$, *and finally,* $U = U_1 \cdots U_k$.

```
function [L] = Decomp1.k( varargin )
i = length(varargin);
n = length(varargin{1});
U = Decomp1.1(varargin{1}); % As defined in (2.2)
for j = 2:i
X = U'*varargin{j};
X = X(j:end);
G = Decomp1.1(X);
U = U*blkdiag(eye(j-1),G);
end
L = U(:,i+1:n);
```

4.2.1 Algorithm 1 Numerical Experiments

Order k Decomposable Algorithm 1

n	**k =**	**3**	**4**	**5**	**10**	**15**	**20**	**25**
5		2.0607e-16	1.2212e-16	x	x	x	x	x
6		2.8194e-16	2.1466e-16	1.6653e-16	x	x	x	x
7		2.9803e-16	2.688e-16	2.4685e-16	x	x	x	x
8		3.2406e-16	3.3081e-16	3.2039e-16	x	x	x	x
9		3.3958e-16	3.3772e-16	3.3223e-16	x	x	x	x
10		3.3934e-16	3.9146e-16	4.0605e-16	x	x	x	x
15		4.1993e-16	4.9201e-16	4.9039e-16	5.3781e-16	x	x	x
20		4.4825e-16	5.032e-16	5.733e-16	6.6937e-16	6.0806e-16	x	x
25		4.9812e-16	5.5257e-16	6.0335e-16	7.762e-16	7.9426e-16	6.4866e-16	x
50		5.6809e-16	6.3784e-16	7.0108e-16	9.8065e-16	1.1946e-15	1.2835e-15	1.3849e-15
75		6.1316e-16	7.0837e-16	7.5622e-16	1.0861e-15	1.3038e-15	1.5214e-15	1.6798e-15
100		6.7791e-16	7.7005e-16	8.4405e-16	1.1994e-15	1.4413e-15	1.6828e-15	1.8817e-15

Table 3: $||L^*L-I||$, given the first **k** columns of an **n**×**n** unitary k-Hessenberg matrix $U = [q_1 \cdots q_k \;\; L]$. For comparison, the same given (random) columns were used across Tables 3-9.

Algorithm 4.8 (Decomp2.k)**.** *Let $q^{(1)}, \ldots, q^{(k)} \in \mathbb{C}^n$ denote the first k columns of U, and $\rho_n^{(1)} = e^{i \cdot arg(q_n^{(1)})}$. First, compute the vector $q^{(1,1)}$.*

$$\begin{bmatrix} I_{n-1} & \\ & \overline{\rho}_n^{(1)} \end{bmatrix} q^{(1)} = q^{(1,1)}$$

Define

$$r_{n-1}^{(1)} = \sqrt{|q_{n-1}^{(1,1)}|^2 + |q_n^{(1,1)}|^2}$$

and set

$$\rho^{(1)}_{n-1} = \frac{q^{(1,1)}_{n-1}}{r^{(1)}_{n-1}}, \qquad \mu^{(1)}_{n-1} = \frac{q^{(1,1)}_{n}}{r^{(1)}_{n-1}}$$

Then $\mu^{(1)}_{n-1} = \sqrt{1 - |\rho^{(1)}_{n-1}|^2}$, *and*

$$\begin{bmatrix} I_{n-2} & & \\ & \overline{\rho}^{(1)}_{n-1} & \mu^{(1)}_{n-1} \\ & \mu^{(1)}_{n-1} & -\rho^{(1)}_{n-1} \end{bmatrix} q^{(1,1)} = \begin{bmatrix} * \\ \vdots \\ r^{(1)}_{n-1} \\ 0 \end{bmatrix} = q^{(1,2)}$$

Next, define

$$r^{(1)}_{n-2} = \sqrt{|q^{(1,2)}_{n-2}|^2 + |q^{(1,2)}_{n-1}|^2}$$

and set

$$\rho^{(1)}_{n-2} = \frac{q^{(1,2)}_{n-2}}{r^{(1)}_{n-2}}, \qquad \mu^{(1)}_{n-2} = \frac{q^{(1,2)}_{n-1}}{r^{(1)}_{n-2}}$$

Then

$$\begin{bmatrix} I_{n-3} & & & \\ & \overline{\rho}_{n-2}^{(1)} & \mu_{n-2}^{(1)} & \\ & \mu_{n-2}^{(1)} & -\rho_{n-2}^{(1)} & \\ & & & 1 \end{bmatrix} q^{(1,2)} = \begin{bmatrix} * \\ \vdots \\ r_{n-2}^{(1)} \\ 0 \\ 0 \end{bmatrix} = q^{(1,3)}$$

Continue this process until reaching the vector e_1*, the first column of the identity* I_n*. This determines* $\{\rho_i^{(1)}, \mu_i^{(1)}\}$ *for* $i = 1, \ldots, n-1$*. Use these parameters to compute*

$$U_1 = (G_n^{(1)})^*(G_{n-1}^{(1)})^*(G_{n-2}^{(1)})^* \cdots (G_1^{(1)})^*$$

where $G_n^{(1)} = diag(1, \ldots, 1, \overline{\rho}_n^{(1)})$ *and* $G_i^{(1)}$ *is defined as in (21) for* $i = 1, \ldots, n-1$*. Next, compute the second column of* U_2

$$U_1^* q^{(2)} = \tilde{q}^{(2)}$$

and repeat the process above with $\tilde{q}^{(2)}$ *to determine* $\{\rho_i^{(2)}, \mu_i^{(2)}\}$ *for* $i = 2, \ldots, n-1$ *and construct* U_2

$$U_2 = (G_n^{(2)})^*(G_{n-1}^{(2)})^*(G_{n-2}^{(2)})^* \cdots (G_2^{(2)})^*$$

In general, compute the jth column of U_j

$$U_{j-1}^* \cdots U_1^* q^{(j)} = \tilde{q}^{(j)}$$

Compute $\{\rho_i^{(j)}, \mu_i^{(j)}\}$ for $i = j, \ldots, n-1$ and use these parameters to construct

$$U_j = (G_n^{(j)})^* (G_{n-1}^{(j)})^* (G_{n-2}^{(j)})^* \cdots (G_j^{(j)})^*$$

Finally, $U = U_1 \cdots U_k$.

```
function [L] = Decomp2.k( varargin )
i = length(varargin);
n = length(varargin{1});
U = Decomp2.1(varargin{1}); % As defined in (2.3)
for j = 2:i
X = U'*varargin{j};
X = X(j:end);
G = Decomp2.1(X);
U = U*blkdiag(eye(j-1),G);
end
L = U(:,i+1:n);
```

4.2.2 Algorithm 2 Numerical Experiments

Order k Decomposable Algorithm 2

n	**k =**	**3**	**4**	**5**	**10**	**15**	**20**	**25**
5		3.1686e-16	2.065e-16	x	x	x	x	x
6		4.5428e-16	3.8374e-16	2.6867e-16	x	x	x	x
7		5.0079e-16	4.9495e-16	3.7056e-16	x	x	x	x
8		5.8804e-16	5.3434e-16	4.9411e-16	x	x	x	x
9		6.2551e-16	6.4016e-16	6.4062e-16	x	x	x	x
10		6.2254e-16	6.6357e-16	7.2324e-16	x	x	x	x
15		7.7049e-16	8.6168e-16	9.1097e-16	9.5924e-16	x	x	x
20		8.4399e-16	9.9961e-16	1.0384e-15	1.2428e-15	1.1133e-15	x	x
25		9.063e-16	1.0679e-15	1.1011e-15	1.5023e-15	1.4685e-15	1.3155e-15	x
50		1.0005e-15	1.1526e-15	1.3082e-15	1.8367e-15	2.2364e-15	2.2787e-15	2.3705e-15
75		1.0635e-15	1.238e-15	1.4311e-15	2.0183e-15	2.4821e-15	2.7759e-15	2.9297e-15
100		1.117e-15	1.2324e-15	1.4699e-15	2.1514e-15	2.7141e-15	2.9466e-15	3.0405e-15

Table 4: $||L^*L - I||$, given the first **k** columns of an **n**×**n** unitary k-Hessenberg matrix $U = [q_1 \cdots q_k \;\; L]$. For comparison, the same given (random) columns were used across Tables 3-9.

4.3 Green's (H, k)-quasiseparable Structure

This section completely generalizes the results in (3.3). That is, the $n \times n$ unitary k-Hessenberg matrix U is constructed via a set of (H, k)-quasiseparable generators.

Definition 4.9 (Rank)**.** *An $n \times n$ matrix A is Green's (H, k)-quasiseparable if* **(i)** *it is strongly k-Hessenberg and* **(ii)** *if* $\max(rank(A_i)) = k$*, where*

$$A_i = A(i : n, 1 : i + k - 1), \quad i = 1, \ldots, n - k + 1$$

Definition 4.10 (Generator)**.** *An $n \times n$ matrix A is Green's (H, k)-quasiseparable* *if* **(i)** *it is strongly k-Hessenberg and* **(ii)** *if there exist parameters a set of* $\mathfrak{G} = \{p_t, a_u, r_v, d_w\}$ *for* $t = k+1, \ldots, n+k$, $u = 2, \ldots, n+k-1$, $v = 1, \ldots, n$, $w = k+1, \ldots, n$, *where each is a matrix of sizes* $1 \times k$, $k \times k$, $k \times 1$, *and* 1×1 *respectively, such that*

$$A_{ij} = \begin{cases} p_{i+k} a_{i+k-1} a_{i+k-2} \cdots a_{j+1} r_j, & j < i+k \\ d_i, & j = i+k \\ 0 & j > i+k \end{cases}$$

The elements of the set $\mathfrak{G}$ *are referred to as a set Green's* (H, k)*-quasiseparable generators for* A.

Now that it is known unitary k-Hessenberg matrices can be decomposed into a product of k unitary Hessenberg matrices, a generalization of (3.9) is provided. This result will allow one to compute a set of (H, k)-quasiseparable generators for U via the generators of its factors.

Theorem 4.11. *If* A *is* $n \times n$ *unitary* j*-Hessenberg with Green's* (H, j)*-quasiseparable generators* $\mathfrak{G}_1 = \{p_i^{(A)}, a_i^{(A)}, r_i^{(A)}, d_i^{(A)}\}$, *and if* B *is* $n \times n$ *unitary* k*-Hessenberg with Green's* (H, k)*-quasiseparable generators* $\mathfrak{G}_2 = \{p_i^{(B)}, a_i^{(B)}, r_i^{(B)}, d_i^{(B)}\}$, *then* AB *is unitary* $(j+k)$*-Hessenberg with Green's* $(H, j+k)$*-quasiseparable with generators* $\mathfrak{G}_{12} = \{p_t^{(AB)}, a_u^{(AB)}, r_v^{(AB)}, d_w^{(AB)}\}$ *for* $t = j+k+1, \ldots, n+j+k$, $u = 2, n+j+k-1$, $v = 1, \ldots, n$ *and*

$w = j+k+1, \ldots, n$ given by:

$$p_i^{(AB)} = \begin{bmatrix} p_{i-k}^{(A)} & d_{i-k}^{(A)} p_i^{(B)} \end{bmatrix}, \quad a_i^{(AB)} = \begin{bmatrix} a_{i-k}^{(A)} & r_{i-k}^{(A)} p_i^{(B)} \\ 0 & a_i^{(B)} \end{bmatrix} \tag{35}$$

$$r_i^{(AB)} = \begin{bmatrix} r_{i-k}^{(A)} d_i^{(B)} \\ r_i^{(B)} \end{bmatrix}, \quad d_i^{(AB)} = d_{i-k}^{(A)} d_i^{(B)}$$

Proof. Embed A and B into $(n+j+k) \times (n+j+k)$ lower triangular matrices L_A and L_B as follows:

(a) Take A and add k columns of all zeros to the left of its first column. Then add $j+k$ rows of zeros above the top row of the updated matrix. Finally, add j columns of zeros to the right of the last column of the second updated matrix. Denote this matrix by L_A

(b) Take B and add j rows of all zeros below its last row. Then add $j+k$ columns of zeros to the right of the last column of the updated matrix. Finally, add k rows of zeros above the top row of the second updated matrix. Denote this matrix by L_B.

By design, L_A and L_B are order j lower quasiseparable and order k lower quasiseparable respectively, with generators given by

$$p_i^{(L_A)} = \begin{cases} p_{i-k}^{(A)} & i = j+k+1, \dots, n+j+k \\ 0 & \text{otherwise} \end{cases}, \qquad a_i^{(L_A)} = \begin{cases} a_{i-k}^{(A)} & i = k+2, \dots, n+k+2 \\ 0 & \text{otherwise} \end{cases}$$

$$r_i^{(L_A)} = \begin{cases} r_{i-k}^{(A)} & i = k+1, \dots, n+k+1 \\ 0 & \text{otherwise} \end{cases}, \qquad d_i^{(L_A)} = \begin{cases} d_{i-k}^{(A)} & i = j+k+1, \dots, n+k \\ 0 & \text{otherwise} \end{cases}$$

$$p_i^{(L_B)} = \begin{cases} p_i^{(B)} & i = k+1, \dots, n+k \\ 0 & \text{otherwise} \end{cases}, \qquad a_i^{(L_B)} = a_i^{(B)}$$

$$r_i^{(L_B)} = \begin{cases} r_i^{(B)} & i = 1, \dots, n \\ 0 & \text{otherwise} \end{cases}, \qquad d_i^{(L_B)} = \begin{cases} d_i^{(B)} & i = k+1, \dots, n \\ 0 & \text{otherwise} \end{cases}$$

$$g_i^{(L_A)} = g_i^{(L_B)} = 0, \qquad h_i^{(L_A)} = h_i^{(L_B)} = 0$$

Thus, using (1.3), one can compute a set of order $(j+k)$ quasiseparable generators for $L_A L_B = L_{AB}$. Then the Green's $(H, j+k)$-quasiseparable generators for AB can be read directly from the order $(j+k)$ quasiseparable generators of L_{AB} using the restriction $AB = L_{AB}(j+k+1 : n+j+k, 1 : n)$, resulting in the generators proposed in the theorem.

□

Algorithm 4.12 (GHKQuasi)**.** *Let $q_1, \ldots, q_k \in \mathbb{C}^n$. Use (23) to compute a set of Green's $(H,1)$-quasiseparable generators, $\mathfrak{G}_1$, for U_1. Construct the unitary Hessenberg matrix U_1 with first column q_1. Next, let*

$$\begin{bmatrix} 0 \\ \tilde{q}_2 \end{bmatrix} = U_1^* q_2$$

Use (23) a second time with the new input $\tilde{q}_2$ to compute a set of Green's $(H,1)$-quasiseparable generators, $\mathfrak{G}_2$, for $\tilde{U}_2$. Compute a set of Green's $(H,2)$-quasiseparable generators, $\mathfrak{G}_{12}$ for the product $U = U_1U_2$ from $\mathfrak{G}_1$ and $\mathfrak{G}_2$ using (35) in the previous theorem. Next, let

$$\begin{bmatrix} 0 \\ 0 \\ \tilde{q}_3 \end{bmatrix} = U_2^* U_1^* q_3$$

Use (23) with the new input $\tilde{q}_3$ to compute a set of Green's $(H,1)$-quasiseparable generators, $\mathfrak{G}_3$, for $\tilde{U}_3$. Compute a set of Green's $(H,3)$-quasiseparable generators, $\mathfrak{G}_{123}$ for the product $U = U_1U_2U_3$ from $\mathfrak{G}_{12}$ and $\mathfrak{G}_3$ using (35) in the previous theorem. In general, let

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tilde{q}_i \end{bmatrix} = U_{i-1}^* \cdots U_1^* q_i$$

and compute a set of Green's $(H,1)$-quasiseparable generators, $\mathfrak{G}_i$, for U_i. Compute a set of Green's (H,i)-quasiseparable generators, $\mathfrak{G}_{1\ldots i}$ for the product $U = U_1 \cdots U_i$ from $\mathfrak{G}_{1\ldots i-1}$ and $\mathfrak{G}_i$ using (35) in the previous theorem. Continue this process until a set of Green's (H,k)-quasiseparable generators, $\mathfrak{G}_{1\ldots k}$, for $U = U_1 \cdots U_k$ is reached .

4.3.1 Numerical Experiments

Green's (H,k)-quasiseparable Generators

n	**k =**	**3**	**4**	**5**	**10**	**15**	**20**	**25**
5		9.0144e-16	1.0769e-15	x	x	x	x	x
6		9.0859e-16	1.356e-15	1.37e-15	x	x	x	x
7		9.41e-16	1.4353e-15	1.4761e-15	x	x	x	x
8		9.5432e-16	1.1722e-15	1.5749e-15	x	x	x	x
9		1.0376e-15	1.2489e-15	1.5571e-15	x	x	x	x
10		9.958e-16	1.3651e-15	1.7773e-15	x	x	x	x
15		1.222e-15	1.4326e-15	1.6865e-15	2.6625e-15	x	x	x
20		9.4881e-16	1.3953e-15	1.4001e-15	3.0359e-15	4.1844e-15	x	x
25		1.0853e-15	1.3114e-15	1.6319e-15	2.8843e-15	4.4422e-15	5.4117e-15	x
50		1.2152e-15	1.3262e-15	1.7215e-15	3.2027e-15	5.1509e-15	4.8752e-15	7.2295e-15
75		1.2223e-15	1.6351e-15	2.0011e-15	3.7128e-15	4.7636e-15	5.5513e-15	5.1283e-15
100		1.3408e-15	1.6605e-15	1.7996e-15	3.0208e-15	4.1216e-15	4.7205e-15	6.9105e-15

Table 5: $||L^*L-I||$, given the first **k** columns of an $\mathbf{n}\times\mathbf{n}$ unitary k-Hessenberg matrix $U = [q_1 \cdots q_k \;\; L]$. For comparison, the same given (random) columns were used across Tables 3-9.

4.4 Green's (H,k)-semiseparable Structure

The final generalization exploits the (H,k)-semiseparable structure of unitary k-Hessenberg matrices.

Definition 4.13 (QS Generator)**.** *An $n \times n$ matrix A is Green's (H,k)-*

semiseparable if **(i)** *it is strongly k-Hessenberg and* **(ii)** *if there exists a choice of order Green's (H, k)-quasiseparable generators $\mathfrak{G} = \{d_i, p_i, a_i, r_i\}$ for A such that a_i is invertible for $i = 2, \ldots, n-1$.*

By definition, (H, k)-semiseparable matrices form a subclass of matrices with (H, k)-quasiseparable structure, and just as in the earlier special cases, an equivalent characterization of (H, k)-semiseparability is given below.

Definition 4.14 (SS Generator)**.** *An $n \times n$ matrix A is Green's (H, k)-semiseparable if* **(i)** *it is strongly k-Hessenberg and* **(ii)** *if*

$$tril(A, k-1) = tril(RT, k-1)$$

for some matrices R and T of sizes $n \times k$ and $k \times n$, respectively. The matrices R and T are called a set of Green's (H, k)-semiseparable generators for A.

The final theorem provides a complete generalization of theorem (3.13).

Theorem 4.15. *Suppose A is $n \times n$ unitary j-Hessenberg with Green's (H, j)-semiseparable generators $R^{(A)}$ and $T^{(A)}$ and B is $n \times n$ unitary k-Hessenberg with Green's (H, k)-semiseparable generators $R^{(B)}$ and $T^{(B)}$. Then AB is unitary $(j + k)$-Hessenberg with Green's $(H, j + k)$-semiseparable generators*

R and T given by:

$$R = \begin{bmatrix} p_{j+k+1}^{(L_{AB})} a_{j+k}^{(L_{AB})} \cdots a_2^{(L_{AB})} \\ p_{j+k+2}^{(L_{AB})} a_{j+k+1}^{(L_{AB})} \cdots a_2^{(L_{AB})} \\ \vdots \\ p_{n+j+k}^{(L_{AB})} a_{n+j+k-1}^{(L_{AB})} \cdots a_2^{(L_{AB})} \end{bmatrix}$$

and

$$T = \begin{bmatrix} r_1^{(L_{AB})} & (a_2^{(L_{AB})})^{-1} r_2^{(L_{AB})} & \cdots & ((a_2^{(L_{AB})})^{-1} \cdots (a_n^{(L_{AB})})^{-1}) r_n^{(L_{AB})} \end{bmatrix}$$

where

$$p_i^{(L_{AB})} = \begin{bmatrix} x_i^{(L_A)} & d_i^{(L_A)} x_i^{(L_B)} \end{bmatrix}, \quad a_i^{(L_{AB})} = \begin{bmatrix} I_j & y_i^{(L_A)} x_i^{(L_B)} \\ 0 & I_k \end{bmatrix} \tag{36}$$

$$r_i^{(L_{AB})} = \begin{bmatrix} y_i^{(L_A)} d_i^{(L_B)} \\ y_i^{(L_B)} \end{bmatrix}, \quad d_i^{(L_{AB})} = d_i^{(L_A)} d_i^{(L_B)}$$

and $L_{AB} = L_A L_B$*, with* L_A *and* L_B *defined as in (4.11), and where the* x_i*'s and* y_i*'s are the ith rows and ith columns of the matrices* $X^{(L_A)}, X^{(L_B)}$ *and*

$Y^{(L_A)}, Y^{(L_B)}$ respectively. These matrices are given by

$$X^{(L_A)} = \begin{bmatrix} \mathbf{0}_{j+k,j} \\ R^{(A)} \end{bmatrix}, \quad Y^{(L_A)} = \begin{bmatrix} \mathbf{0}_{j,k} & T^{(A)} & \mathbf{0}_{j,j} \end{bmatrix}$$

$$X^{(L_B)} = \begin{bmatrix} \mathbf{0}_{k,k} \\ R^{(B)} \\ \mathbf{0}_{j,k} \end{bmatrix}, \quad Y^{(L_B)} = \begin{bmatrix} T^{(B)} & \mathbf{0}_{k,j+k} \end{bmatrix}$$

where $\mathbf{0}_{j,k}$ denotes the $j \times k$ zero matrix.

Proof. First, note that $tril(L_A, -1) = tril(X^{(L_A)}Y^{(L_A)}, -1)$ and $tril(L_B, -1) = tril(X^{(L_B)}Y^{(L_B)}, -1)$ so that L_A is order j lower semiseparable and L_B is order k lower semiseperable by (1). Thus, L_A has a set of order k quasiseparable generators with invertible a_{u_1}, and L_B has a set of order j quasiseparable generators with invertible a_{u_2} according to (1.4). It is easily checked that the following generators satisfy this condition:

$$\mathfrak{G}_1 = \left\{p_{t_1}^{(L_A)}, a_{u_1}^{(L_A)}, r_{v_1}^{(L_A)}\right\} = \left\{x_{t_1}^{(L_A)}, I_j, y_{v_1}^{(L_A)}\right\}$$

for $t_1 = j+1, \ldots, n+j$, $u_1 = 2, \ldots, n+j-1$ and $v_1 = 1, \ldots, n+j+k$ and

$$\mathfrak{G}_2 = \left\{p_{t_2}^{(L_B)}, a_{u_2}^{(L_B)}, r_{v_2}^{(L_B)}\right\} = \left\{x_{t_2}^{(L_B)}, I_k, y_{v_2}^{(L_B)}\right\}$$

for $t_2 = k+1, \ldots, n+k$, and $u_2 = 2, \ldots, n+k-1$ and $v_2 = 1, \ldots, n+j+k$. Using (1.3), compute a set order $(j+k)$ quasiseparable generators, $\mathfrak{G}$, for

$L_A L_B = L_{AB}$. This results in (36) above. Note however that each $a_i^{(L_{AB})}$ is invertible. This implies that L_{AB} is order $(j+k)$ semiseparable, and notice that if

$$R^{(L_{AB})} = \begin{bmatrix} 0 \\ p_2^{(L_{AB})} \\ p_3^{(L_{AB})} a_2^{(L_{AB})} \\ p_4^{(L_{AB})} a_3^{(L_{AB})} a_2^{(L_{AB})} \\ \vdots \\ p_{n+j+k}^{(L_{AB})} a_{n+j+k-1}^{(L_{AB})} \cdots a_2^{(L_{AB})} \end{bmatrix}$$

$$T^{(L_{AB})} = \begin{bmatrix} r_1^{(L_{AB})} & (a_2^{(L_{AB})})^{-1} r_2^{(L_{AB})} & \cdots & ((a_2^{(L_{AB})})^{-1} \cdots (a_{n+j+k-1}^{(L_{AB})})^{-1}) r_{n+j+k-1}^{(L_{AB})} & 0 \end{bmatrix}$$

then $tril(L_{AB}, -1) = tril(R^{(L_{AB})} T^{(L_{AB})}, -1)$. From here, we can read Green's $(H, j+k)$-semiseparable generators for AB from the order $(j+k)$ semiseparable generators of L_{AB} using the restrictions $R = R^{(L_{AB})}(j+k+1 : n+j+k, :)$ and $T = T^{(L_{AB})}(:, 1 : n)$, resulting in the generators proposed in the theorem.

□

Algorithm 4.16 (GHKSemi)**.** *Let $q_1, \ldots, q_k \in \mathbb{C}^n$. Use (2.10) to compute a set of Green's $(H,1)$-semiseparable generators, $\mathfrak{G}_1$, for U_1. Construct the unitary Hessenberg matrix U_1 with first column q_1. Next, let*

$$\begin{bmatrix} 0 \\ \tilde{q}_2 \end{bmatrix} = U_1^* q_2$$

Use (2.10) a second time with the new input $\tilde{q}_2$ to compute a set of Green's

$(H,1)$*-semiseparable generators,* $\mathfrak{G}_2$*, for* $\tilde{U}_2$*. Compute a set of Green's* $(H,2)$*-semiseparable generators,* $\mathfrak{G}_{12}$ *for the product* $U = U_1U_2$ *from* $\mathfrak{G}_1$ *and* $\mathfrak{G}_2$ *using (4.15). Next, let*

$$\begin{bmatrix} 0 \\ 0 \\ \tilde{q}_3 \end{bmatrix} = U_2^* U_1^* q_3$$

Use (2.10) with the new input $\tilde{q}_3$ *to compute a set of Green's* $(H,1)$*-quasiseparable generators,* $\mathfrak{G}_3$*, for* $\tilde{U}_3$*. Compute a set of Green's* $(H,3)$*-semiseparable generators,* $\mathfrak{G}_{123}$ *for the product* $U = U_1U_2U_3$ *from* $\mathfrak{G}_{12}$ *and* $\mathfrak{G}_3$ *using (4.15). In general, let*

$$\begin{bmatrix} 0 \\ \vdots \\ 0 \\ \tilde{q}_i \end{bmatrix} = U_{i-1}^* \cdots U_1^* q_i$$

and compute a set of Green's $(H,1)$*-semiseparable generators,* $\mathfrak{G}_i$*, for* U_i *using (2.10). Compute a set of Green's* (H,i)*-semiseparable generators,* $\mathfrak{G}_{1\ldots i}$ *for the product* $U = U_1 \cdots U_i$ *from* $\mathfrak{G}_{1\ldots i-1}$ *and* $\mathfrak{G}_i$ *using (4.15). Continue this process until a set of Green's* (H,k)*-semiseparable generators,* $\mathfrak{G}_{1\ldots k}$*, is reached for* $U = U_1 \cdots U_k$*.*

4.4.1 Numerical Experiments

Green's (H, k)-semiseparable Generators

n	k =	3	4	5	10	15	20	25
5		1.0999e-15	9.7256e-15	x	x	x	x	x
6		1.0895e-15	1.7247e-15	1.7319e-15	x	x	x	x
7		1.3744e-15	2.6376e-15	2.4212e-15	x	x	x	x
8		2.0905e-15	1.3595e-15	3.1603e-15	x	x	x	x
9		3.207e-15	9.6663e-15	4.2031e-15	x	x	x	x
10		3.2048e-15	3.4461e-15	4.4141e-15	x	x	x	x
15		1.583e-15	4.0152e-15	2.1266e-14	1.1355e-14	x	x	x
20		1.7326e-15	2.8304e-15	3.2656e-15	1.6296e-14	2.8941e-14	x	x
25		1.6928e-15	7.0368e-15	5.4041e-15	2.4104e-14	8.6784e-14	8.5927e-14	x
50		1.8701e-15	4.3663e-15	3.8388e-15	2.9725e-14	4.7575e-14	6.5215e-14	1.6737e-13
75		1.7999e-15	8.7258e-15	3.873e-15	2.889e-14	1.8361e-13	1.5344e-13	3.3092e-13
100		2.0246e-15	4.1336e-15	8.4195e-15	2.5193e-14	7.0309e-14	1.1723e-13	2.9288e-13

Table 6: $||L^*L - I||$, given the first **k** columns of an **n**×**n** unitary k-Hessenberg matrix $U = [q_1 \cdots q_k \;\; L]$. For comparison, the same given (random) columns were used across Tables 3-9.

5 Additional Numerical Experiments

In sections (3.3) and (3.4), we solved the order k problem by computing a set of generators for the unitary k-Hessenberg matrix U. Alternatively, once generators for $U_1, \ldots, U_k$ are known, we could simply take the product $U = U_1 \cdots U_k$ as we did with the decomposable algorithms. In other words, only Green's $(H, 1)$-quasiseparable and Green's $(H, 1)$-semiseparable generators are computed using repeated application of the order 1 algorithms. This is described below, followed by numerical results obtained using this method.

Algorithm 5.1 (Alternate). *Let $q_1, \ldots, q_k \in \mathbb{C}^n$. Use (2.7) or (2.10) to* *compute U_1, the unitary Hessenberg matrix with first column q_1. Next, let*

$$\begin{bmatrix} 0 \\ \tilde{q}_2 \end{bmatrix} = U_1^* q_2$$

Use (2.7) or (2.10) a second time with the new input $\tilde{q}_2$ to compute the unitary Hessenberg matrix $\tilde{U}_2$ with first column $\tilde{q}_2$. Next, let

$$\begin{bmatrix} 0 \\ 0 \\ \tilde{q}_2 \end{bmatrix} = U_2^* U_1^* q_3$$

Use (2.7) or (2.10) a third time with the new input $\tilde{q}_3$ to compute the unitary Hessenberg matrix $\tilde{U}_3$ with first column $\tilde{q}_3$. Exhausting this process computes $U_1, \ldots, U_k$, and hence, $U = U_1 \cdots U_k$ is one solution to the order two problem.

5.1 Repeated Green's $(H, 1)$-quasiseparable Generators

```
function [L] = AltGHKQuasi( varargin )
i = length(varargin);
n = length(varargin{1});
U = GH1Quasi(varargin{1}); % As defined in (2.6)
for j = 2:i
X = U'*varargin{j};
X = X(j:end);
G = GH1Quasi(X);
U = U*blkdiag(eye(j-1),G);
end
L = U(:,i+1:n);
```

Repeated Green's $(H,1)$-quasiseparable Generators

n	k =	3	4	5	10	15	20	25
5		9.0805e-16	1.1235e-15	x	x	x	x	x
6		8.8352e-16	1.3474e-15	1.3767e-15	x	x	x	x
7		9.6696e-16	1.4224e-15	1.4647e-15	x	x	x	x
8		9.4519e-16	1.1587e-15	1.5346e-15	x	x	x	x
9		1.0632e-15	1.2732e-15	1.5496e-15	x	x	x	x
10		1.0091e-15	1.3459e-15	1.7781e-15	x	x	x	x
15		1.1904e-15	1.4093e-15	1.6766e-15	2.6105e-15	x	x	x
20		9.3886e-16	1.426e-15	1.463e-15	3.2007e-15	4.3938e-15	x	x
25		1.0781e-15	1.3049e-15	1.6344e-15	2.897e-15	4.1262e-15	5.2959e-15	x
50		1.2082e-15	1.3285e-15	1.7014e-15	3.329e-15	5.1866e-15	5.0003e-15	7.1709e-15
75		1.2307e-15	1.6309e-15	1.9924e-15	3.689e-15	4.9182e-15	5.7156e-15	5.1048e-15
100		1.3296e-15	1.6795e-15	1.8457e-15	3.1246e-15	4.3361e-15	4.7488e-15	7.4499e-15

Table 7: $||L^*L-I||$, given the first $\mathbf{k}$ columns of an $\mathbf{n}\times\mathbf{n}$ unitary k-Hessenberg matrix $U = [q_1 \cdots q_k \;\; L]$. For comparison, the same given (random) columns were used across Tables 3-9.

5.2 Repeated Green's $(H,1)$-semiseparable Generators

```
function [L] = AltGHKSemi( varargin )
i = length(varargin);
n = length(varargin{1});
U = GH1Semi(varargin{1}); % As defined in (2.9)
for j = 2:i
X = U'*varargin{j};
X = X(j:end);
G = GH1Semi(X);
U = U*blkdiag(eye(j-1),G);
end
L = U(:,i+1:n);
```

Repeated Green's $(H, 1)$-semiseparable Generators

n	k =	3	4	5	10	15	20	25
5		9.2088e-16	1.1902e-15	x	x	x	x	x
6		9.1466e-16	1.3058e-15	1.4877e-15	x	x	x	x
7		1.0192e-15	1.4352e-15	1.4829e-15	x	x	x	x
8		9.0206e-16	1.0891e-15	1.4685e-15	x	x	x	x
9		1.0675e-15	1.2965e-15	1.5011e-15	x	x	x	x
10		9.9946e-16	1.388e-15	1.7802e-15	x	x	x	x
15		1.2186e-15	1.4547e-15	1.6457e-15	2.66e-15	x	x	x
20		9.0208e-16	1.4294e-15	1.4759e-15	3.0039e-15	4.3883e-15	x	x
25		1.0799e-15	1.3304e-15	1.5885e-15	2.7952e-15	4.0696e-15	5.2657e-15	x
50		1.2001e-15	1.2689e-15	1.8305e-15	3.2784e-15	5.0455e-15	4.7467e-15	7.1454e-15
75		1.182e-15	1.5618e-15	2.1141e-15	3.5062e-15	4.6846e-15	5.3888e-15	5.2493e-15
100		1.3197e-15	1.7028e-15	1.823e-15	2.9313e-15	3.9402e-15	4.5767e-15	7.1248e-15

Table 8: $||L^*L-I||$, given the first **k** columns of an $\mathbf{n}\times\mathbf{n}$ unitary k-Hessenberg matrix $U = [q_1 \cdots q_k \;\; L]$. For comparison, the same given (random) columns were used across Tables 3-9.

5.3 Repeated Application of Parlett's Algorithm

In this final section, numerical experiments were performed using the method in (5.1) with repeated application of Parlett's exact formulas. For a more detailed discussion on this, see appendix (A). It is noted that the omission of Parlett's algorithm from the main portion of this paper is not to insinuate it should not be used. Indeed, all of the additional numerical experiments in this section give satisfactory results. The order one algorithm is shown below, and table (9) shows repeated application of this algorithm, just as in tables (7) and (8).

```
function [ L ] = Parlett( q )

p(n)=0;

for i = n-1:-1:1
```

```
  p(i) = p(i+1) + q(i+1)*conj(q(i+1));
end

for k = 1:1:n-1
  if k == 1
    d(k) = sqrt(p(1));
  else
    d(k) = sqrt(p(k))/sqrt(p(k-1));
  end
end

D=diag(d);

for i = 2:1:length(q)
  for j = 1:1:i-1
    L(j,j)=1;
    L(i,j)=-q(i)*conj(q(j))/p(j);
  end
end

L=L*D;

end
```

Repeated Application of Parlett's Algorithm

n	k =	3	4	5	10	15	20	25
5		9.597e-16	1.1391e-15	x	x	x	x	x
6		8.9717e-16	1.2516e-15	1.4033e-15	x	x	x	x
7		1.0061e-15	1.3538e-15	1.4842e-15	x	x	x	x
8		8.6623e-16	1.1824e-15	1.616e-15	x	x	x	x
9		1.0791e-15	1.2734e-15	1.5436e-15	x	x	x	x
10		1.0175e-15	1.3752e-15	1.7064e-15	x	x	x	x
15		1.2263e-15	1.4542e-15	1.7127e-15	2.6752e-15	x	x	x
20		8.725e-16	1.4545e-15	1.4759e-15	3.0829e-15	4.2584e-15	x	x
25		1.0797e-15	1.2854e-15	1.6456e-15	2.8587e-15	3.9415e-15	5.4213e-15	x
50		1.1612e-15	1.3244e-15	1.7923e-15	3.3401e-15	5.1369e-15	4.6719e-15	6.7115e-15
75		1.1616e-15	1.6022e-15	2.0506e-15	3.5006e-15	4.7152e-15	5.3983e-15	4.8999e-15
100		1.2682e-15	1.6079e-15	1.7272e-15	2.9938e-15	4.12e-15	4.7137e-15	7.2638e-15

Table 9: $||L^*L-I||$, given the first **k** columns of an $\mathbf{n}\times\mathbf{n}$ unitary k-Hessenberg matrix $U=[q_1\cdots q_k\ \ L]$. For comparison, the same given (random) columns were used across Tables 3-9.

6 Concluding Remarks

The study of quasiseparable and semiseparable matrices is a field of mathematics that is still growing, so extending the definitions of such matrices will surely be of interest. Additionally, even though the desired results of this paper are intended to expand upon results in numerical analysis, it is only logical to think that other fields might benefit as well. The connection of unitary Hessenberg matrices to the study of orthogonal polynomials and electrical engineering might lead one to conjecture that there is a great deal the two could gain from such generalizations.

Appendices

A Parlett's Algorithm

This section is intended to provide a little more detailed information about Parlett's algorithm [36], discussed briefly in section (2.2). As was mentioned, [36] presented a particular numerical experiment by Kahan in which the Householder-Fox method performed poorly. Using the Cholesky factorization technique on $I - qq^T$ with the normalized version of $q = (1, 1/8, 1/8^2, \ldots, 1/8^{15})$ produced L such that $||L^T L - I|| \approx 1$. The source of this poor result is simply cancellation due to subtraction. Parlett suggests a method in which subtraction can be avoided. To begin, recall that if A_k is the $k \times k$ leading principal submatrix of $A = LU$, then $det(A_k) = u_{11} \cdots u_{kk}$ and the kth pivot is given by

$$u_{kk} = \begin{cases} det(A_1) = a_{11} & \text{for } k = 1 \\ det(A_k)/det(A_{k-1}) & \text{for } k = 2, \ldots, n \end{cases} \tag{37}$$

Let $p_0 = 1$ and $p_1, \ldots, p_{n-1}$ denote the leading principal minors of $I - qq^T$, where $p_n = det(I - qq^T) = 0$. Sylvester's determinant theorem states that if A is $n \times m$ and B is $m \times n$, then $det(I_n - AB) = det(I_m - BA)$, where I_n and I_m denote the $n \times n$ and $m \times m$ identity matrices respectively. Thus, for the leading principal minors, we have the formula

$$p_j = det\left(1 - \begin{bmatrix} q_1 & \cdots & q_j \end{bmatrix} \begin{bmatrix} q_1 \\ \vdots \\ q_j \end{bmatrix}\right)$$

$$= 1 - \sum_{i=1}^{j} q_i^2 \tag{38}$$

Parlett however used the simple observation that since

$$\sum_{i=1}^{n} q_i^2 = 1$$

it follows that

$$p_j = 1 - \sum_{i=1}^{j} q_i^2 = \sum_{k=j+1}^{n} q_k^2$$

or defined recursively

$$p_n = 0, \quad p_j = p_{j+1} + q_{j+1}^2 \tag{39}$$

for $j = n-1, \ldots, 1$. Matlab uses the expression in (38) because it must deal with the general case, while Parlett's expression in (39) avoids the use of subtraction entirely. The table below compares the computation of the leading principal minors using (38) and (39) respectively.

p_j	**Matlab using (38)**	**Parlett using (39)**
p_1	0.015625000000000	0.141736677378456
p_2	0.000244140625000	0.017717084672303
p_3	0.000003814697266	0.002214635584034
p_4	0.000000059604645	0.000276829448001
p_5	0.000000000931323	0.000034603680997
p_6	0.000000000014552	0.000004325460121
p_7	0.000000000000227	0.000000540682512
p_8	0.000000000000004	0.000000067585310
p_9	0.000000000000000	0.000000008448160
p_{10}	0.000000000000000	0.000000001056017
p_{11}	0.000000000000000	0.000000000131999
p_{12}	0.000000000000000	0.000000000016496
p_{13}	0.000000000000000	0.000000000002059
p_{14}	0.000000000000000	0.000000000000254
p_{15}	0.000000000000000	0.000000000000028
p_{16}	0.000000000000000	0

Table 10: Cancellation in Matlab's computation of the leading principal minors, using Kahan's vector $q = (1, 1/8, 1/8^2, \dots, 1/8^{15})$

Looking at the special factorization $I - qq^T = \tilde{L}\tilde{L}^T$, where $\tilde{L} = LD$, and recalling (37), we can write

$$d_1^2 = \frac{p_1}{p_0}, \quad d_2^2 = \frac{p_2}{p_1}, \quad \dots, \quad d_{n-1}^2 = \frac{p_{n-1}}{p_{n-2}}, \quad d_n^2 = 0 \tag{40}$$

where L has 1's on its main diagonal and $D^2 = diag(d_1^2, \dots, d_n^2)$. For motivation with the rest of the computation of $\tilde{L} = LD$, consider the following example when $n = 4$. Start by factoring $I - qq^T = LD^2L^T$

$$\begin{bmatrix} 1-q_1^2 & -q_1q_2 & -q_1q_3 & -q_1q_4 \\ -q_2q_1 & 1-q_2^2 & -q_2q_3 & -q_2q_4 \\ -q_3q_1 & -q_3q_2 & 1-q_3^2 & -q_3q_4 \\ -q_4q_1 & -q_4q_2 & -q_4q_3 & 1-q_4^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \\ l_{41} & l_{42} & l_{43} \end{bmatrix} \begin{bmatrix} d_1^2 & 0 & 0 \\ 0 & d_2^2 & 0 \\ 0 & 0 & d_3^2 \end{bmatrix} \begin{bmatrix} 1 & l_{21} & l_{31} & l_{41} \\ 0 & 1 & l_{32} & l_{42} \\ 0 & 0 & 1 & l_{43} \end{bmatrix} \tag{41}$$

Now, multiply (41) through on the left by the permutation matrix that interchanges the third and fourth row, and consider the 3×3 leading principal minor of the updated equality. On the right hand side we have

$$det\left(\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{41} & l_{42} & l_{43} \end{bmatrix} \begin{bmatrix} d_1^2 & 0 & 0 \\ 0 & d_2^2 & 0 \\ 0 & 0 & d_3^2 \end{bmatrix} \begin{bmatrix} 1 & l_{21} & l_{31} \\ 0 & 1 & l_{32} \\ 0 & 0 & 1 \end{bmatrix}\right) = l_{43}p_3$$

keeping in mind (40). Now, the left hand side is much less obvious at first, but also gives an amazingly simple result[3]

$$det\left(\begin{bmatrix} 1-q_1^2 & -q_1q_2 & -q_1q_3 \\ -q_2q_1 & 1-q_2^2 & -q_2q_3 \\ -q_4q_1 & -q_4q_2 & -q_4q_3 \end{bmatrix}\right) = -q_4q_3 \tag{42}$$

Notice that this is simply the $(4,3)$ entry in the matrix $I - qq^T$. Equating

[3]Look at the matrix on the left hand side of (42) in block form $Q = [A \;\; B; \;\; C \;\; D]$ and use the identity $det(Q) = det(D) \cdot det(A - BD^{-1}C)$

the left hand and right hand side, we can conclude that

$$l_{43} = -\frac{q_4 q_3}{p_3}$$

In fact, this result holds in general. For $j > k$, the entries of L in $\tilde{L} = LD$ can be formed explicitly using

$$l_{jk} = -\frac{q_j q_k}{p_k} \tag{43}$$

Finally, using (39), (40) and (43), Parlett's solution to the original posed problem is $U = [q \;\; LD]$.

B Signal Flow Graphs

This is a very brief section pertaining to the reading of the signal flow graphs in figures (1) and (2). The three things one needs to know to interpret the graphs are listed below:

1. The delay operation $\boxed{\text{x}}$ denotes multiplication by x.

2. Diagonal and horizontal arrows denote scaling by the ρ_i's and $1/\mu_i$'s respectively.

3. When two arrowheads meet, this indicates the results from each path are combined via addition.

As an example, consider figure (3), a simplified version of figure (1) in section (2.1.3). We will consider the paths starting from the nodes at $\phi_1(x)$ and $\phi_1^{\#}(x)$ and ending at the node $\phi_2(x)$.

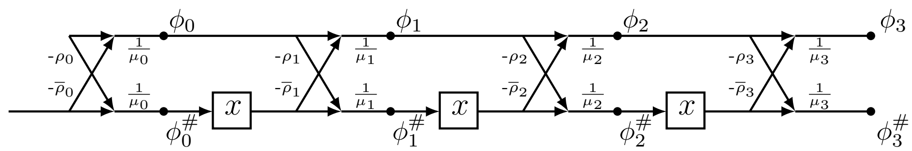


Figure 3: Markel-Gray Filter Structure

The portion of the signal flow graph shown in figure (4) says we take $\phi_1^{\#}(x)$, multiply it by x and scale it by $-\overline{\rho}_2$, then add this result to $\phi_1(x)$. Finally, scale the entire quantity by $\frac{1}{\mu_2}$.

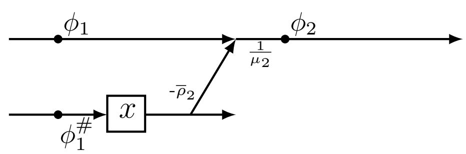


Figure 4: The two possible paths to $\phi_2(x)$

In other words, figure (4) shows that

$$\phi_2(x) = \frac{1}{\mu_2}(-\overline{\rho}_2 x \phi_1^{\#}(x) + \phi_1(x))$$

It is easily checked that this agrees with $\phi_2(x)$ from the recursion in (3).

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