Constructive Aspects for the Generalized Orthogonal Group

by

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A dissertation submitted to the Graduate Faculty of
Auburn University
in partial fulfillment of the
requirements for the Degree of
Doctor of Philosophy

Auburn, Alabama
May 14, 2010

Keywords: generalized orthogonal group, generalized orthogonal matrix, generalized Householder matrix, indefinite inner product, elementary reflection

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Abstract

Our main result is a constructive proof of the Cartan-Dieudonné-Scherk Theorem in the real or complex fields. The Cartan-Dieudonné-Scherk Theorem states that for fields of characteristic other than two, every orthogonality can be written as the product of a certain minimal number of reflections across hyperplanes. The earliest proofs were not constructive, and more recent constructive proofs either do not achieve minimal results or are restricted to special cases. For the real or complex fields, this paper presents a constructive proof for decomposing a generalized orthogonal matrix into the product of the minimal number of generalized Householder matrices.

A pseudo code and the MATLAB code of our algorithm are provided. The algorithm factors a given generalized orthogonal matrix into the product of the minimal number of generalized Householder matrices specified in the CDS Theorem.

We also look at some applications of generalized orthogonal matrices. Generalized Householder matrices can be used to study the form of Pythagorean n-tuples and generate them. All matrices can not be factored in a QR-like form when a generalized orthogonal matrix in used in place of a standard orthogonal matrix. We find conditions on a matrix under which an indefinite QR factorization is possible, and see how close we can bring a general matrix to an indefinite QR factorization using generalized Householder eliminations.

Acknowledgments

I would like to thank my advisor, Dr. Uhlig, for all of his guidance throughout my master's and PhD programs. His experience and suggestions have often been crucial to my progress. I appreciate the assistance of the AU math department, my committee members, and other influencial professors at Auburn. I would also like to thank my family and friends for their support, particularly my dad whose encouragement and sacrifices have always made reaching my goals possible and my wife, Torri, for all that she does and all that she means to me.

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Chapter 1

Introduction

Over a field $\mathbb{F}$ with char $\mathbb{F} \neq 2$, the Cartan-Dieudonné-Scherk Theorem states that a generalized orthogonal matrix can be factored into the product of a certain minimal number of generalized Householder matrices. Thus the CDS Theorem states that the elements of the generalized orthogonal group can be decomposed into the group's "basic building blocks." The CDS Theorem has been called the Fundamental Theorem of Algebraic Groups because of this. The identity matrix I_n is the most basic orthogonal as well as generalized orthogonal matrix. It is the unit element of the group. Generalized Householder matrices are rank one modifications of the identity I_n and generalized orthogonal matrices. Thus they are the simplest generalized orthogonal matrices different from the identity. The CDS Theorem itself can be used to show that every generalized orthogonal matrix that is rank one removed from the identity is a generalized Householder matrix. Thus the general orthogonal group's "basic building blocks" are these generalized Householder matrices.

Cartan-Dieudonné-Scherk Theorem (CDS Theorem)**.** *Let* $\mathbb{F}$ *be a field with* char $\mathbb{F} \neq 2$ *and* $S \in M_n(\mathbb{F})$ *be nonsingular symmetric. Then every* S*-orthogonal matrix* $Q \in M_n(\mathbb{F})$ *can be expressed as the product of* $\operatorname{rank}(Q - I_n)$ *generalized* S*-Householder matrices, unless* $S(Q - I_n)$ *is skew-symmetric.*

If $S(Q - I_n)$ *is skew-symmetric, then the same holds with* $\operatorname{rank}(Q - I_n) + 2$ *generalized* S*-Householder matrices.*

Furthermore, the number of factors is minimal in either case.

In this paper, we will present a constructive proof of the CDS Theorem with $\mathbb{F}$ equal to $\mathbb{R}$ or $\mathbb{C}$. We address the complications that arise when the inner product defined by a nonsingular symmetric matrix S is indefinite. For a given S-orthogonal matrix Q, we will explicitly determine a set of S-Householder matrix factors whose product is Q. Our construction, which relies mainly on the diagonalization of a symmetric matrix, factors Q into the product of the minimal number of S-Householder matrix factors as stated in the theorem.

We begin by establishing some notations that we use. Let $\mathbb{F}$ be a field and $S \in M_n(\mathbb{F})$ be a nonsingular symmetric matrix. A vector $x \in \mathbb{F}^n$ is called *S-isotropic* if $x^T Sx = 0$ and *non-S-isotropic* otherwise. A matrix $S = S^T$ defines a symmetric bilinear inner product which may allow nonzero S-isotropic vectors. Two vectors x and y in $\mathbb{F}^n$ are called *S-orthogonal* if $x^T Sy = y^T Sx = 0$, and a matrix $Q \in M_n(\mathbb{F})$ is called *S-orthogonal* provided $Q^T SQ = S$.

In a positive-definite inner product space over $\mathbb{F}$ with $S = I_n$ the orthogonal Householder matrix has the form $H = I_n - 2uu^T/(u^T u)$ for a nonzero vector $u \in \mathbb{F}^n$. The transformation induced by H represents a reflection across the hyperplane orthogonal to u. In Numerical Linear Algebra, Householder matrices over both $\mathbb{R}$ or $\mathbb{C}$ are often used to transform a matrix to Hessenberg form by similarity or to find a QR decomposition of a matrix. More on Householder matrices can be found in [8, 11] for example. For a general nonsingular symmetric matrix $S \in M_n(\mathbb{F})$, Householder matrices generalize to S-Householder matrices which have the form

$$H_{S,u} := I_n - \frac{2uu^T S}{u^T Su}$$

for a non-S-isotropic vector $u \in \mathbb{F}$. Similar to the standard $S = I_n$ case, we have $H_{S,u} = H_{S,u}^{-1}$ and $H_{S,u}$ is S-orthogonal; however, $H_{S,u}^T$ does not necessarily equal $H_{S,u}^{-1}$ for S-Householder matrices with general $S = S^T$. By construction, both the standard Householder matrices and the S-Householder matrices are rank one modifications of the identity matrix. Having to avoid S-isotropic vectors when forming S-Householder matrices is the main complication when trying to apply Householder matrices in indefinite inner product spaces. Householder matrices were generalized in [10] not only to symmetric bilinear inner products but also to skew-symmetric bilinear and Hermitian and skew-Hermitian sesquilinear inner products.

While the CDS Theorem states a precise minimum number of generalized Householder matrix factors that is required to express a generalized orthogonal matrix, this minimal factorization is not unique. The CDS Theorem applied to the identity I_n is an interesting case for which the factorization is not unique. Since the zero matrix is trivially skew-symmetric, two generalized Householder matrix factors are needed to express I_n. Used as its own inverse, any generalized Householder matrix times itself is a factorization of I_n. Hence in the CDS Theorem, the identity is to be considered a repeated reflection rather than a lack of reflections.

The earliest results regarding the CDS Theorem date back to 1938 by E. Cartan. Working over $\mathbb{R}$ or $\mathbb{C}$, Cartan proved that every orthogonal transformation of $\mathbb{R}^n$ (or $\mathbb{C}^n$) is the product of at most n reflections [3]. In 1948 J. Dieudonné extended the result to arbitrary fields with characteristic not two [5]. Finally, P. Scherk obtained the minimal number and dealt with arbitrary fields $\mathbb{F}$ of char $\mathbb{F} \neq 2$ in 1950. Part of Scherk's proof [13] relies on an existence argument and is not entirely constructive. In the literature the CDS Theorem is often stated with the non-minimal upper bound of n factors and Scherk's name is omitted, see [6, 14]. From an algebraic point of view, the fact that every generalized orthogonal group over a field $\mathbb{F}$ with char $\mathbb{F} \neq 2$ is generated by products of reflections, regardless of the minimal number of factors, is the important notion behind the CDS Theorem [14]. However, from a numerical standpoint, an algorithm that factors an S-orthogonal matrix into the product of the minimal number of S-Householder matrices is desirable. The structure of generalized orthogonal groups is studied in [15], and the CDS Theorem is not only presented with the minimal upper bound of factors but also extended to fields with characteristic two; the conclusion being that every generalized orthogonal group except in a space of dimension four over a field of characteristic two is generated by reflections.

Over general fields the CDS Theorem is used in algebraic geometry and group theory. Our interest lies in numerical applications, and hence we work over $\mathbb{R}$ or $\mathbb{C}$. Generalized real and complex orthogonal Householder matrices have applications in computer graphics, crystallography, and signal processing where a least-squares problem is repeatedly modified and solved [1, 12]. Some of these applications show less sensitivity to rounding errors compared to other methods while only slightly increasing and at times even decreasing computation requirements [12].

Our goal is to prove the CDS Theorem with $\mathbb{F}$ equal $\mathbb{R}$ and $\mathbb{C}$ constructively. It should be noted that we use matrix transposes for both the real and complex case. Typically, matrix conjugate-transposes are used for extensions to the complex case. However, the work leading up to the CDS Theorem deals with general fields and only with orthogonal matrices. An extension of the CDS Theorem to the complex field with matrix conjugate-transposes and unitary matrices is an interesting, but different, case. This is open.

Existing proofs of the CDS Theorem are not constructive, and constructive proofs either do not achieve minimal results or are restricted to special cases. Scherk's proof [13] uses construction in parts, but some key steps are proved through existence arguments. Specifically, the existence of a non-isotropic vector that is needed to form a Householder factor [13, Lemma 4] is not proved in a constructive way by Scherk. The outline of our proof closely resembles [13] when restricted to $\mathbb{F}$ equal $\mathbb{R}$ or $\mathbb{C}$, however, we construct all elements for the S-Householder factorization of a generalized orthogonal matrix explicitly rather than rely on their existence.

In 2001, F. Uhlig gave a constructive proof over $\mathbb{R}$ in the case of $S = I_n$ and in the general real or complex case he found a constructive factorization requiring a non-minimal number of $2n - 1$ S-Householder matrices [16]. Moreover, he noted that for the generalized real problem one may deal with a nonsingular diagonal matrix D that is congruent to the nonsingular symmetric matrix S rather than work with the more general matrix S; this is also mentioned in [7]. The proof of Uhlig's first result cannot be extended directly to general S because in the case of $S = I_n$ the complication of nonzero isotropic vectors does not exist. His second result requires up to $2n - 1$ factors by applying $n - 1$ generalized Householder matrices to reduce a matrix U to a matrix $\mathrm{diag}(\pm 1)$. To complete the factorization, up to n additional generalized Householder matrices are needed to reduce the diagonal matrix $\mathrm{diag}(\pm 1)$ to the identity I_n. By sorting the order in which the columns of U are updated, his method can be modified to obtain a smaller, but still non-minimal, upper bound of $n - 1 + \min\{n_+, n_-\}$ factors, where n_+ and n_- are the number of $+1$ and -1 entries in D respectively. Whether the method can be further improved to construct the minimal number of factor matrices is unclear. There is a constructive proof [1] over $\mathbb{R}$, $\mathbb{C}$, or $\mathbb{Q}$ using Clifford algebras, but it requires up to n reflections to represent an orthogonal transformation of an n-dimensional inner product space.

Chapter 2

A constructive proof of the CDS Theorem

2.1 Outline

In Section 2.2 we detail a diagonalization process for real or complex symmetric matrices that will be utilized throughout the paper. Following [16], Section 2.3 establishes that the construction of the S-Householder factors of an S-orthogonal matrix Q can be reduced via a matrix $D = \text{diag}(\pm 1)$ that is congruent to S to constructing the D-Householder matrix factors of a D-orthogonal matrix U that is similar to Q.

Then we constructively prove the CDS Theorem over $\mathbb{R}$ or $\mathbb{C}$ by induction on $\text{rank}(U - I_n)$. The base case is verified by showing that U is a D-Householder matrix whenever $\text{rank}(U - I_n) = 1$. This establishes the generalized Householder matrices as elementary building blocks of the generalized orthogonal group. For $\text{rank}(U - I_n) > 1$, we address the two cases that $D(U - I_n)$ is skew-symmetric or not.

In Section 2.4, we treat the case of a D-orthogonal matrix U for which $D(U - I_n)$ is not skew-symmetric. A non-D-isotropic vector w is found satisfying certain conditions in order to form an appropriate Householder update matrix $H_{D,w}$. Because of our choice of w, this $H_{D,w}$ will guarantee two conditions, namely that $D(H_{D,w}U - I_n)$ is not skew-symmetric and that $\text{rank}(H_{D,w}U - I_n) = \text{rank}(U - I_n) - 1$. This determines one D-Householder factor of U and reduces the problem. Repetition finally establishes

$$\text{rank}\left(\left(H_{D,w_{r-1}} H_{D,w_{r-2}} \cdots H_{D,w_1}\right) U - I_n\right) = 1 \ .$$

In Section 2.5, we deal with a skew-symmetric $D(U - I_n)$. We first update U via $H_{D,w}$ so that $\operatorname{rank}(H_{D,w}U - I_n) = \operatorname{rank}(U - I_n) + 1$. Here the rank increases rather than decreases, but our update forces $D(H_{D,w}U - I)$ to be not skew-symmetric. Thus after one extra update, the method in Section 2.4 for $D(U - I_n)$ not skew-symmetric can be used for all subsequent iterations. This accounts for the additional two factors that are required in the CDS Theorem when $D(U - I_n)$ is skew-symmetric.

Finally we discuss the details of our construction in Section 2.6.

2.2 Diagonal Congruence of a Symmetric Matrix

Given a symmetric matrix A in $M_n(\mathbb{R})$ or $M_n(\mathbb{C})$, in several instances we will need to find a full rank matrix C in $M_n(\mathbb{R})$ or $M_n(\mathbb{C})$, respectively, such that $C^T AC$ is diagonal. Over the reals, it is well-known that a real symmetric matrix is orthogonally diagonalizable. If $A \in M_n(\mathbb{R})$ is symmetric and the columns of $C \in M_n(\mathbb{R})$ are orthonormal eigenvectors of A, then $C^T AC = \Lambda$ where $C^T C = I_n$ and $\operatorname{diag}(\Lambda) = (\lambda_1 \ \lambda_2 \ ... \ \lambda_n)$ for the eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$ of A. While not all complex symmetric matrices can be diagonalized in the usual sense using a unitary matrix and its conjugate-transpose, any complex symmetric matrix can be diagonalized with a unitary matrix and its transpose.

Takagi Factorization ([9, Corollary 4.4.4])**.** *If $A \in M_n(\mathbb{C})$ is symmetric, there is a unitary matrix $C \in M_n(\mathbb{C})$ with $C^*C = I_n$ and a nonnegative diagonal matrix $\Sigma \in M_n(\mathbb{R})$ such that $C^T AC = \Sigma$.*

These factorizations not only exist but they can be constructed, see [9, Section 4.4]. Note that the entries of Σ are real and nonnegative. We only need this C to be invertible, but it happens to be unitary. This is the only place we use a unitary matrix in this paper.

We will refer to the eigenvalue decomposition of a real symmetric matrix or to the Takagi factorization of a complex symmetric matrix as a T-*diagonalization.*

2.3 Problem Reduction

S-orthogonality of a matrix Q is equivalent to D-orthogonality of a matrix U that is similar to Q. Here $D = \text{diag}(\pm 1)$ is the inertia matrix of the nonsingular matrix $S = S^T$ in $M_n(\mathbb{R})$. Following the same reduction in $M_n(\mathbb{C})$, the nonsingular matrix $S = S^T$ is always congruent to $D = I_n$. Thus a generalized S-orthogonal matrix in $M_n(\mathbb{C})$ is equivalent to a standard orthogonal matrix in $M_n(\mathbb{C})$. Our construction is valid for both $\mathbb{R}$ and $\mathbb{C}$ so we will continue to treat them together. For the remainder of this paper we will limit $\mathbb{F}$ to be either $\mathbb{R}$ or $\mathbb{C}$.

Lemma 2.1. *If $S = S^T \in M_n(\mathbb{F})$ is nonsingular symmetric, then*

(i) S is congruent to a diagonal matrix D with diagonal entries ± 1 via an invertible matrix $Y \in M_n(\mathbb{F})$, i.e., $S = Y^T D Y$, and

(ii) a matrix $Q \in M_n(\mathbb{F})$ is S-orthogonal if and only if Q is similar to a D-orthogonal matrix $U = YQY^{-1}$ via the same Y from (i).

Proof. (i) This is Sylvester's law of inertia [8, 9] over $\mathbb{R}$, but a similar proof holds for $\mathbb{C}$.

According to Section 2.2, T-diagonalize the nonsingular symmetric matrix $S \in M_n(\mathbb{F})$ so that

$$V^T S V = \Lambda$$

for a real diagonal matrix $\Lambda \in M_n(\mathbb{R})$ and an invertible matrix $V \in M_n(\mathbb{F})$. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the diagonal entries of Λ. If $L = \text{diag}\left(\dfrac{1}{\sqrt{|\lambda_j|}}\right)$, then

$$L^T V^T S V L = L^T \,\text{diag}(\lambda_j) L = \text{diag}(\text{sign}(\lambda_j)) = \text{diag}(\pm 1) = D \ .$$

Working over $\mathbb{C}$, all λ_j are positive according to the Takagi Factorization so that $D = I_n$. Over $\mathbb{R}$ or $\mathbb{C}$, letting $Y = (VL)^{-1}$ we have

$$S = Y^T D Y \ . \tag{2.1}$$

(ii) Let S be a nonsingular symmetric matrix with (2.1) for Y invertible and $D = \operatorname{diag}(\pm 1)$ according to part (i). Then

$$\begin{aligned}
Q \text{ is } S\text{-orthogonal} \quad &\Longleftrightarrow \quad Q^T S Q = S \\
&\Longleftrightarrow \quad Q^T (Y^T D Y) Q = Y^T D Y \\
&\Longleftrightarrow \quad Y^{-T} (Q^T Y^T D Y Q) Y^{-1} = Y^{-T} (Y^T D Y) Y^{-1} = D \\
&\Longleftrightarrow \quad U^T D U = D \;\text{ for } U = Y Q Y^{-1} \\
&\Longleftrightarrow \quad U \text{ is } D\text{-orthogonal and } Q \text{ is similar to } U
\end{aligned}$$

□

If $H_{D,w}$ is the D-Householder matrix formed from a non-D-isotropic vector w, then

$$H_{D,w} = Y H_{S,Y^{-1}w} Y^{-1} \tag{2.2}$$

for S, D, and Y as in Lemma 2.1 because

$$\begin{aligned}
H_{D,w} &= I_n - \frac{2ww^T D}{w^T D w} \\
&= I_n - \frac{2(YY^{-1})ww^T(Y^{-T}Y^T)D(YY^{-1})}{w^T(Y^{-T}Y^T)D(YY^{-1})w} \\
&= I_n - Y\left(\frac{2Y^{-1}ww^T Y^{-T}(Y^T D Y)}{w^T Y^{-T}(Y^T D Y)Y^{-1}w}\right)Y^{-1} \\
&= Y\left(I_n - \frac{2Y^{-1}w(Y^{-1}w)^T S}{(Y^{-1}w)^T S Y^{-1} w}\right)Y^{-1} \\
&= Y H_{S,Y^{-1}w} Y^{-1} \; .
\end{aligned}$$

This shows the relationship between D-Householder and S-Householder matrices.

Consequently, if a D-orthogonal matrix $U \in M_n(\mathbb{F})$ is written as the product of r D-Householder matrix factors as

$$U = \prod_{j=1}^{r} H_{D,\,w_j} \ ,$$

for a set of r non-D-isotropic vectors $\{w_j \in \mathbb{F}^n\}$, then by Lemma 2.1 and (2.2) we have

$$\begin{aligned} Q &= Y^{-1}UY \\ &= Y^{-1}H_{D,\,w_1}H_{D,\,w_2}\cdots H_{D,\,w_r}Y \\ &= H_{S,\,Y^{-1}w_1}H_{S,\,Y^{-1}w_2}\cdots H_{S,\,Y^{-1}w_r} \ . \end{aligned}$$

Hence, $Q \in M_n(\mathbb{F})$ is the product of the r S-Householder matrices $H_{S,\,Y^{-1}w_i}$. Thus a factorization of an S-orthogonal matrix Q into a product of S-Householder matrices is equivalent to one for the corresponding D-orthogonal matrix U into a product of D-Householder matrices.

For the remainder of this paper we denote H_w with a single subscript to be the D-Householder matrix formed by the non-D-isotropic vector w and a fixed sign matrix $D = \text{diag}(\pm 1)$.

2.4 Case of $D(U - I_n)$ not skew-symmetric

Assume that $D = \text{diag}(\pm 1)$, $U \in M_n(\mathbb{F})$ is D-orthogonal with rank $D(U - I_n) > 1$, and $D(U - I_n)$ is not skew-symmetric. In this case we show how to construct a D-Householder matrix H_w such that $D(H_wU - I_n)$ is not skew-symmetric and rank $D(H_wU - I_n) = \text{rank}\, D(U - I_n) - 1$. The remaining cases are treated separately in the sections that follow.

Later we see that finding a D-Householder H_w that reduces the rank of $D(H_wU - I_n)$ by one is easier than finding one that ensures that $D(H_wU - I_n)$ is not skew-symmetric. For this reason, we will focus on the more difficult second goal first. For either task we need to find a vector $v \in \mathbb{F}^n$ with $v^T N v \neq 0$ where $N = D(U - I_n)$. This v generates a non-D-isotropic vector $w = (U - I_n)v$ used to form H_w.

Lemma 2.2. *For an arbitrary non-skew-symmetric matrix* $N \in M_n(\mathbb{F})$*, a vector* v *with* $v^T N v \neq 0$ *can always be constructed.*

Proof. Since N is not skew-symmetric, we may T-diagonalize the nonzero symmetric matrix $N + N^T$

$$C^T(N + N^T)C = \Lambda$$

where C has full rank and Λ is a diagonal matrix with $\mathrm{rank}(N + N^T) \geq 1$ nonzero diagonal entries. If v is a column of C corresponding to a nonzero diagonal entry λ of Λ, then $v^T(N + N^T)v = \lambda$. Since $v^T N v = (v^T N v)^T$, we have $v^T N v = \lambda/2 \neq 0$. $\square$

The vector v of Lemma 2.2 will be useful in some cases, but there is no assurance that the corresponding $D(H_w U - I_n)$ will not be skew-symmetric. In Lemma 2.5, a test is established to determine whether $D(H_w U - I_n)$ is skew-symmetric or not. The test relies on the inequality

$$N + N^T \neq \frac{1}{v^T N v}\left(N v v^T N + N^T v v^T N^T\right) \ . \tag{2.3}$$

The following lemma is used repeatedly in our main construction step (Lemma 2.4).

Lemma 2.3. *For* $N \in M_n(\mathbb{F})$*, let* $v, b \in \mathbb{F}^n$ *satisfy* $v^T N v \neq 0$*,* $b^T(N + N^T)b = 0$*, and* $b^T N v v^T N b \neq 0$*. Then (2.3) is satisfied.*

Proof. First $b^T N v v^T N b = (b^T N v v^T N b)^T = b^T N^T v v^T N^T b$. Now (2.3) follows by comparing

$$b^T(N + N^T)b = 0$$

and

$$b^T\left[\frac{1}{v^T N v}\left(N v v^T N + N^T v v^T N^T\right)\right]b = \frac{2 b^T N v v^T N b}{v^T N v} \neq 0 \ .$$

$\square$

The next result explains how to choose a vector v satisfying both $v^T N v \neq 0$ and (2.3) in order to form $w = (U - I_n)v$ and the Householder update H_w. This lemma is similar to a previous result [13, Lemma 4, pg. 484] that establishes the existence of such a vector only. The proof in [13] finds a contradiction when assuming that all non-isotropic vectors satisfy the negation of (2.3) by examining the dimension of a certain isotropic subspace. Here we construct a vector with the desired properties by finding a diagonal congruence of the symmetric matrix $N + N^T$ and choosing a suitable linear combination of the columns of the diagonalizing matrix.

Lemma 2.4. *Let* $N \in M_n(\mathbb{F})$ *satisfy* $\operatorname{rank}(N) > 1$ *and* $N + N^T \neq 0$. *Unless* $\operatorname{rank}(N) = \operatorname{rank}(N+N^T) = 2$, *a vector* v *with* $v^T N v \neq 0$ *that satisfies (2.3) can be found by construction.*

The case of $\operatorname{rank}(N) = \operatorname{rank}(N + N^T) = 2$ and, furthermore, any case with $\operatorname{rank}(N)$ even and $N + N^T \neq 0$, is treated after Lemma 2.7.

Proof. We determine a vector v in three separate cases that depend on the rank of the matrix $N + N^T$.

Case 1. Suppose $\operatorname{rank}(N + N^T) = 1$.

T-diagonalize the symmetric matrix $N + N^T$

$$C^T (N + N^T) C = \Lambda$$

where C is full rank and Λ is a diagonal matrix. Without loss of generality let the columns of C be ordered so that $\operatorname{diag}(\Lambda) = (\lambda\ 0 \cdots 0)$ for $\lambda \neq 0$. Hence we have $c_1^T (N + N^T) c_1 = \lambda$ and $c_j^T (N + N^T) c_k = 0$ for j and k not both one. Since $c_j^T (N + N^T) c_k = c_j^T N c_k + c_j^T N^T c_k = c_j^T N c_k + c_k^T N c_j$, we have

$$c_j^T N c_k = \begin{cases} \lambda/2 & \text{if } j = k = 1 \\ 0 & \text{if } j = k \neq 1 \\ -c_k^T N c_j & \text{if } j \neq k\ . \end{cases}$$

Thus the matrix $C^T(N + N^T)C$ is the zero matrix except for its $(1, 1)$ entry λ, and only one diagonal entry of C^TNC is nonzero, namely $(C^TNC)_{11} = \lambda/2$. However, in C^TNC there must be at least one nonzero off-diagonal entry since $\text{rank}(C^TNC) = \text{rank}(N) > 1$ is assumed.

$$\underset{C^T(N+N^T)C}{\begin{pmatrix} \lambda & & 0 \\ & 0 & \\ & & \ddots & \\ 0 & & 0 \end{pmatrix}} \qquad \underset{C^TNC}{\begin{pmatrix} \lambda/2 & & * \\ & 0 & \\ & & \ddots & \\ * & & 0 \end{pmatrix}}$$

Case 1 (a) If there is a nonzero off-diagonal entry in the first column or row of C^TNC, then for some $j \neq 1$, $c_j^TNc_1 = -c_1^TNc_j \neq 0$. In this case we let $v = c_1$ and $b = c_j$. Then $v^TNv = \lambda/2 \neq 0$, $b^T(N + N^T)b = 0$, and $b^TNvv^TNb = c_j^TNc_1c_1^TNc_j = -(c_1^TNc_j)^2 \neq 0$. By Lemma 2.3, v satisfies (2.3).

Case 1 (b) Next suppose $c_1^TNc_j$ and $c_j^TNc_1$ are both zero for all $j \neq 1$. Then C^TNC has a nonzero entry that is neither on the diagonal nor in its first row or column. Thus there exists a $c_j^TNc_k = -c_k^TNc_j \neq 0$ with $k \neq j$ and neither j nor k equal to 1. In this case we let $v = c_1 + c_j$ and $b = c_k$. Then

$$v^TNv = c_1^TNc_1 + c_1^TNc_j + c_j^TNc_1 + c_j^TNc_j = c_1^TNc_1 \neq 0 \ ,$$

$b^T(N + N^T)b = 0$, and

$$b^TNvv^TNb = (c_k^TNc_1 + c_k^TNc_j)(c_1^TNc_k + c_j^TNc_k) = -(c_j^TNc_k)^2 \neq 0 \ .$$

By Lemma 2.3, v satisfies (2.3). Of course, $v = c_1 + c_k$ will also satisfy the three conditions. This allows some freedom of choice in the implementation of the construction.

$$\begin{array}{cc} & \begin{array}{cccc} & & j & \end{array} \\ j & \left(\begin{array}{c|ccc} \lambda/2 & & * & \\ \hline & 0 & & \\ * & & \ddots & \\ & & & 0 \end{array}\right) \end{array} \qquad \begin{array}{cc} & \begin{array}{cccc} & j & & k \end{array} \\ \begin{array}{c} \\ j \\ \\ k \end{array} & \left(\begin{array}{c|ccc} \lambda/2 & 0 & \cdots & 0 \\ \hline 0 & 0 & & * \\ \vdots & & \ddots & \\ 0 & * & & 0 \end{array}\right) \end{array}$$

C^TNC – Case 1 (a) $\qquad$ C^TNC – Case 1 (b)

Case 2. Suppose $\text{rank}(N + N^T) = 2$ and $\text{rank}(N) > 2$.

Again we T-diagonalize the symmetric matrix $N + N^T$ as

$$C^T(N + N^T)C = \Lambda = \text{diag}(\lambda\ \mu\ 0 \cdots 0)$$

where C has full rank with columns ordered so that the two nonzero entries λ and μ are first and second along the diagonal of Λ, i.e.,

$$c_j^T(N + N^T)c_k = \begin{cases} \lambda & \text{if } j = k = 1 \\ \mu & \text{if } j = k = 2 \\ 0 & \text{otherwise.} \end{cases}$$

As before $c_j^T(N + N^T)c_k = c_j^TNc_k + c_j^TN^Tc_k = c_j^TNc_k + c_k^TNc_j$, so

$$c_j^TNc_k = \begin{cases} \lambda/2 & \text{if } j = k = 1 \\ \mu/2 & \text{if } j = k = 2 \\ 0 & \text{if } j = k \notin \{1, 2\} \\ -c_k^TNc_j & \text{if } j \neq k\ . \end{cases}$$

The matrix C^TNC has only two nonzero diagonal entries, namely $(C^TNC)_{11} = \lambda/2$ and $(C^TNC)_{22} = \mu/2$. Since $\text{rank}(C^TNC) = \text{rank}(N) > 2$, there must be a nonzero off-diagonal entry in C^TNC. Furthermore, there must be at least one nonzero entry in C^TNC that is neither along the diagonal nor in the leading 2×2 block.

$$
\underset{C^T(N+N^T)C}{\begin{pmatrix} \lambda & & & 0 \\ & \mu & & \\ & & 0 & \\ 0 & & & \ddots & \\ & & & & 0 \end{pmatrix}}
\qquad\qquad
\underset{C^TNC}{\begin{pmatrix} \lambda/2 & & & * \\ & \mu/2 & & \\ & & 0 & \\ * & & & \ddots & \\ & & & & 0 \end{pmatrix}}
$$

Case 2 (a) Suppose there is a nonzero off-diagonal entry in the first or second row or column of C^TNC that is not in the leading 2×2 block. Then $c_j^TNc_k = -c_k^TNc_j \neq 0$ for $j \in \{1,2\}$ and $k \in \{3,4,...,n\}$. In this case we let $v = c_j$ and $b = c_k$. Then v^TNv equals $\lambda/2$ or $\mu/2$ depending on j, $b^T(N+N^T)b = 0$ since $k \notin \{1,2\}$, and

$$
b^TNvv^TNb = c_k^TNc_jc_j^TNc_k = -(c_j^TNc_k)^2 \neq 0 \ .
$$

By Lemma 2.3, v satisfies (2.3).

Case 2 (b) Next suppose all entries in the first or second row and column of C^TNC outside the leading 2×2 are zero. Then there exist $j,k \in \{3,4,...,n\}$ such that $c_j^TNc_k = -c_k^TNc_j \neq 0$. In this case we let $v = c_1 + c_j$ and $b = c_k$. Then

$$
v^TNv = c_1^TNc_1 + c_1^TNc_j + c_j^TNc_1 + c_j^TNc_j = c_1^TNc_1 = \lambda/2 \neq 0 \ ,
$$

$b^T(N+N^T)b = 0$, and

$$
b^TNvv^TNb = (c_k^TNc_1 + c_k^TNc_j)(c_1^TNc_k + c_j^TNc_k) = -(c_j^TNc_k)^2 \neq 0 \ .
$$

By Lemma 2.3, v satisfies (2.3). Again, $v = c_2 + c_j$ will satisfy the conditions, and thus the constructive process is flexible.

$$
\left(\begin{array}{cc|ccc}
\lambda/2 & * & & & \\
 & & & *_{(j,k)} & \\
* & \mu/2 & & & \\
\hline
 & & 0 & & \\
\multicolumn{2}{c|}{*_{(k,j)}} & & \ddots & \\
 & & & & 0
\end{array}\right)
\qquad
\left(\begin{array}{cc|ccc}
\lambda/2 & * & & & \\
 & & & 0 & \\
* & \mu/2 & & & \\
\hline
 & & 0 & & *_{(j,k)} \\
\multicolumn{2}{c|}{0} & & \ddots & \\
 & & *_{(k,j)} & & 0
\end{array}\right)
$$

C^TNC – Case 2 (a) $\qquad$ C^TNC – Case 2 (b)

Case 3. Suppose $\operatorname{rank}(N + N^T) > 2$.

In this case, any vector v with $v^TNv \neq 0$ will satisfy (2.3) because $Nvv^TN + N^Tvv^TN$ is the sum of two dyads and can have rank at most 2. We can construct v according to Lemma 2.2.

$\square$

Next we show that a vector v constructed to satisfy both $v^TNv \neq 0$ and (2.3) provides a non-D-isotropic vector $w = (U - I_n)v$ that guarantees that $D(H_wU - I_n)$ is not skew-symmetric for the D-Householder matrix H_w formed by w.

Lemma 2.5. *Let $D = \operatorname{diag}(\pm 1)$, $U \in M_n(\mathbb{F})$ be D-orthogonal, $N = D(U - I_n)$, and $v \in \mathbb{F}^n$ satisfy $v^TNv \neq 0$. Then*

(*i*) *$w = (U - I_n)v$ is non-D-isotropic, and*

(*ii*) *if H_w is the D-Householder matrix formed by w, $D(H_wU - I_n)$ is not skew-symmetric if and only if (2.3) holds for v.*

Proof. Notice that for a D-orthogonal matrix U

$$D(U - I_n) + (D(U - I_n))^T = -(U^T - I_n)D(U - I_n) \tag{2.4}$$

because

$$
\begin{aligned}
D(U-I_n)+(D(U-I_n))^T &= DU-D+U^TD-D \\
&= -(U^TDU-DU-U^TD+D) \\
&= -(U^T-I_n)D(U-I_n)\ .
\end{aligned}
$$

Then the first claim (i) can be seen directly:

$$
w^TDw = v^T(U-I_n)^TD(U-I_n)v = -v^T(N+N^T)v = -2v^TNv\ . \tag{2.5}
$$

Thus w is non-D-isotropic if and only if $v^TNv \neq 0$.

Now consider

$$
\begin{aligned}
D(H_wU-I_n) &= D\left(\left(I_n - \frac{2ww^TD}{w^TDw}\right)U - I_n\right) \\
&= D\left(U - I_n - \frac{2ww^TDU}{w^TDw}\right) \\
&= D(U-I_n) - \frac{2Dww^TDU}{w^TDw} \\
&= N - \frac{2D(U-I_n)vv^T(U^T-I_n)DU}{-2v^TNv} \\
&= N + \frac{Nvv^T(D-DU)}{v^TNv} \\
&= N - \frac{Nvv^TN}{v^TNv}\ .
\end{aligned}
$$

Therefore $D(H_wU-I_n)+[D(H_wU-I_n)]^T=0$, or $D(H_wU-I_n)$ is skew-symmetric, if and only if

$$
N - \frac{Nvv^TN}{v^TNv} + N^T - \frac{N^Tvv^TN^T}{v^TNv} = 0\ ,
$$

or if and only if

$$N + N^T = \frac{1}{v^T N v}\left(Nvv^T N + N^T vv^T N^T\right) ,$$

which is the negation of (2.3). $\square$

Lemma 2.6. *For two matrices $A, B \in M_n(\mathbb{F})$*

$$\operatorname{rank}(AB - I_n) \leq \operatorname{rank}(A - I_n) + \operatorname{rank}(B - I_n) \ . \tag{2.6}$$

Lemma 2.6 can easily be seen by considering the dimensions of the kernels of $A - I_n$, $B - I_n$, and $AB - I_n$. It is proved in [13, Lemma 3, pg. 483]. The result is used in the following lemma to show that $\operatorname{rank}(H_w U - I_n)$ is exactly one less than $\operatorname{rank}(U - I_n)$. Lemma 2.6 is also utilized in Section 2.6 to show that the number of D-Householder factors needed to express a D-orthogonal matrix U is minimal.

Lemma 2.7. *Let $D = \operatorname{diag}(\pm 1)$ and $U \in M_n(\mathbb{F})$ be D-orthogonal. If $N = D(U - I_n)$ is not skew-symmetric and $v \in \mathbb{F}^n$ satisfies $v^T N v \neq 0$, then*

$$\operatorname{rank}(H_w U - I_n) = \operatorname{rank}(U - I_n) - 1 \tag{2.7}$$

where

$$H_w = I_n - \frac{2ww^T D}{w^T D w} \tag{2.8}$$

is the generalized Householder transform for $w = (U - I_n)v$.

Proof. Define $w = (U - I_n)v$. By Lemma 2.5, w is not D-isotropic. If $x \in \ker(U - I_n)$, then

$$w^T D x = v^T (U - I_n)^T D x = -v^T \left[(U^T - I_n) D (U - I_n) + D(U - I_n)\right] x = 0 \tag{2.9}$$

by (2.4), and

$$H_w U x = H_w x = x - \frac{2w^T D x}{w^T D w}\, w = x$$

by (2.8) and (2.9). Thus $x \in \ker(H_w U - I_n)$, which shows $\ker(U - I_n) \subseteq \ker(H_w U - I_n)$.

If v satisfies $v^T N v \neq 0$ then

$$v^T D(U - I_n)v = v^T N v \neq 0 \ .$$

Therefore $v \notin \ker(U - I_n)$. We have

$$w^T D w = -2v^T N v = -2v^T D w$$

from (2.5) so that

$$H_w v = v - \frac{2w^T D v}{w^T D w}\, w = v + w = U v \ . \tag{2.10}$$

Thus, $H_w = H_w^{-1}$ and (2.10) imply that

$$v = H_w H_w v = H_w U v \ ,$$

or $v \in \ker(H_w U - I_n)$. Therefore $\ker(U - I_n) \cup \{v\} \subseteq \ker(H_w U - I_n)$ and since $v \notin \ker(U - I_n)$

$$\dim\ker(U - I_n) + 1 \leq \dim\ker(H_w U - I_n) \ .$$

Thus $\operatorname{rank}(H_w U - I_n) \leq \operatorname{rank}(U - I_n) - 1$. Finally by Lemma 2.6,

$$\operatorname{rank}(H_w H_w U - I_n) \leq \operatorname{rank}(H_w - I_n) + \operatorname{rank}(H_w U - I_n) \ ,$$

or

$$\operatorname{rank}(U - I_n) \leq 1 + \operatorname{rank}(H_w U - I_n) \ ,$$

proving (2.7). □

If $N = D(U - I_n)$ is not skew-symmetric and $\operatorname{rank}(N)$ is even, then H_w formed as in Lemma 2.7 by any vector v with $v^T N v \neq 0$ will satisfy (2.7). Therefore $D(H_w U - I_n)$

cannot be skew-symmetric because $\operatorname{rank} D(H_wU - I_n)$ is odd. This addresses the case of $\operatorname{rank} N = \operatorname{rank}(N + N^T) = 2$ that was excluded in Lemma 2.4. Moreover, if $\operatorname{rank}(N)$ is even and greater than two while $N + N^T \neq 0$, any vector v with $v^T N v \neq 0$ will satisfy (2.7) and guarantee that the updated $D(H_wU - I_n)$ is not skew-symmetric. A vector v satisfying $v^T N v \neq 0$ for an arbitrary matrix N with $N + N^T \neq 0$ has been constructed in Lemma 2.2. The vector v constructed in Lemma 2.4 also ensures both properties. The decision of vector used for the case of N not skew-symmetric and $\operatorname{rank}(N)$ even and greater than two leaves a certain freedom of choice with regards to the stability of the implementation.

2.5 Case of $D(U - I_n)$ skew-symmetric

Thus far, a reduction step can be executed as long as $D(U - I_n)$ is not skew-symmetric. If $D(U - I_n)$ is skew-symmetric, we now explain how to perform a generalized orthogonal update so that $D(H_wU - I_n)$ is no longer skew-symmetric. Hence after one such step in the skew-symmetric case, the problem is reduced to the not skew-symmetric case of Section 2.4. In addition to choosing the Householder update matrix H_w, we prove that exactly two additional Householder factors are needed if $D(U - I_n)$ is skew-symmetric.

Lemma 2.8. *Let $D = \operatorname{diag}(\pm 1)$ and $U \in M_n(\mathbb{F})$ be D-orthogonal. Then $D(U - I_n)$ is skew-symmetric if and only if*

$$(U - I_n)^2 = 0 \ . \tag{2.11}$$

Proof. If $D(U - I_n)$ is skew-symmetric, then

$$D(U - I_n) + (D(U - I_n))^T = 0 \ . \tag{2.12}$$

We obtain

$$D(U - I_n)^2 + (U^T - I_n)D(U - I_n) = 0$$

by multiplying (2.12) on the right by $U - I_n$. By (2.4) and (2.12)

$$D(U - I_n)^2 = 0 \ .$$

Multiplying on the left by D gives us (2.11). On the other hand, if (2.11) holds then

$$U(U - I_n) = U - I_n \ . \tag{2.13}$$

In this case

$$\begin{aligned}(U^T - I_n)D(U - I_n) &= (U^T - I_n)DU(U - I_n) \\ &= (U^T DU - DU)(U - I_n) \\ &= -D(U - I_n)^2 \ .\end{aligned}$$

Thus by (2.4) and (2.11), $D(U - I_n)$ is skew symmetric. □

Lemma 2.9. *Let $D = \mathrm{diag}(\pm 1)$, $U \in M_n(\mathbb{F})$ be D-orthogonal, $w \in \mathbb{F}^n$ be any non-D-isotropic vector, and H_w be the D-Householder matrix formed by w. If $D(U - I_n)$ is skew-symmetric, then $\mathrm{rank}(H_w U - I_n) = r + 1$ where $r = \mathrm{rank}(U - I_n)$. Moreover, r is even and $r \leq n/2$.*

Proof. For $D(U - I_n)$ skew-symmetric, we know that $(U - I_n)^2 = 0$ from Lemma 2.8. Therefore

$$\mathrm{im}(U - I_n) \subseteq \ker(U - I_n) \ . \tag{2.14}$$

Hence for $r = \mathrm{rank}(U - I_n)$ we have $r \leq n - r$ or $r \leq n/2$. As D is nonsingular, $r = \mathrm{rank}\, D(U - I_n)$ as well, and since $D(U - I_n)$ is skew-symmetric, r is even.

Next suppose $x \in \ker(U - I_n)$ and $y \in \mathrm{im}(U - I_n)$. Then $y = (U - I_n)z$ for some z, and since $D(U - I_n)$ is skew-symmetric we have

$$y^T Dx = z^T (U^T - I_n) Dx = -z^T D(U - I_n)x = 0 \ .$$

Therefore $\ker(U - I_n) \perp_D \mathrm{im}(U - I_n)$. Along with (2.14) this means all vectors in $\mathrm{im}(U - I_n)$ are D-isotropic.

Let $w \in \mathbb{F}^n$ be any non-D-isotropic vector and define $w^{\perp_D} = \left\{x \in \mathbb{F}^n \mid w^T Dx = 0\right\}$ as the space of vectors that are D-orthogonal to w. Since w is not D-isotropic, $w \notin \mathrm{im}(U - I_n)$. That means that w is not D-orthogonal to $\ker(U - I_n)$ or $w^{\perp_D}$ does not contain $\ker(U - I_n)$. Therefore

$$\dim\left(\ker(U - I_n) \cap w^{\perp_D}\right) = n - r - 1 \ . \tag{2.15}$$

The proof is complete by showing that

$$\ker(U - I_n) \cap w^{\perp_D} = \ker(H_w U - I_n) \ . \tag{2.16}$$

Suppose first that $x \in \ker(U - I_n) \cap w^{\perp_D}$. Since $x \in \ker(U - I_n)$, $Ux = x$ and

$$(H_w U - I_n)x = (H_w - I_n)x = -\frac{2w^T Dx}{w^T Dw} w \ .$$

The latter expression is zero because $x \in w^{\perp_D}$. Next suppose $x \in \ker(H_w U - I_n)$. Then $Ux = H_w H_w Ux = H_w x$ because $H_w = H_w^{-1}$. Hence

$$(U - I_n)x = (H_w - I_n)x = \frac{-2w^T Dx}{w^T Dw} w \ . \tag{2.17}$$

With $D(U - I_n)$ skew-symmetric and $(U^T - I_n)D(U - I_n) = 0$ by (2.4), we have for any x that

$$x^T (U^T - I_n) D(U - I_n)x = 0 \ . \tag{2.18}$$

Substituting (2.17) into (2.18) gives

$$\left(\frac{-2w^T Dx}{w^T Dw} \right)^2 w^T Dw = 0 \ .$$

The left side can only be zero if $w^T Dx = 0$. Hence $x \in w^{\perp_D}$, and $x \in \ker(U - I_n)$ by (2.17).

Therefore (2.16) holds and finally by (2.15)

$$\dim \ker(H_w U - I_n) = n - r - 1$$

or

$$\mathrm{rank}(H_w U - I_n) = \mathrm{rank}(U - I_n) + 1 \ . \qquad \square$$

Lemma 2.9 states that any non-D-isotropic vector w will suffice to form the update matrix H_w for which $\mathrm{rank}(H_w U - I_n) = \mathrm{rank}(U - I_n) + 1$ provided $D(U - I_n)$ is skew-symmetric. For example, any standard unit vector e_j may be used here because $e_j^T De_j = d_j = \pm 1$. In addition, Lemma 2.9 guarantees that $\mathrm{rank}(H_w U - I_n)$ is odd and consequently that $D(H_w U - I_n)$ can not be skew-symmetric.

In the case of $D = I_n$, the only D-orthogonal matrix U with $D(U - I_n)$ skew-symmetric is the trivial $U = I_n$ example. However, Section 2.5 is required to address general D. Here are D-orthogonal matrices U with skew-symmetric $D(U - I_n)$ for $n = 4$ and $n = 6$:

$$U = \begin{pmatrix} 1 & -a & a & 0 \\ a & 1 & 0 & -a \\ a & 0 & 1 & -a \\ 0 & -a & a & 1 \end{pmatrix} \text{ for any } a \in \mathbb{F} \text{ and } D = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \ ;$$

$$U = \begin{pmatrix} 1 & a & -b & b & 0 & a \\ -a & 1 & -a & a & -a & 0 \\ b & a & 1 & 0 & b & a \\ b & a & 0 & 1 & b & a \\ 0 & -a & b & -b & 1 & -a \\ a & 0 & a & -a & a & 1 \end{pmatrix} \text{ for any } a, b \in \mathbb{F} \text{ and } D = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

2.6 Construction

Let $S \in M_n(\mathbb{F})$ be a nonsingular symmetric matrix that defines the indefinite inner product space. Let $Q \in M_n(\mathbb{F})$ be S-orthogonal and $r = \operatorname{rank}(Q - I_n)$. Our construction factors Q into the product of a minimal number of S-Householder matrices. Depending on whether $S(Q - I_n)$ is skew-symmetric or not, the minimal number of factors is $r + 2$ or r, respectively. We begin by finding $D = Y^{-T}SY^{-1} = \operatorname{diag}(\pm 1)$ and the D-orthogonal matrix $U = YQY^{-1}$ as detailed in the proof of Lemma 2.1. Note that $\operatorname{rank}(U - I_n) = \operatorname{rank} Y(Q - I_n)Y^{-1} = r$, and $S(Q - I_n)$ is skew-symmetric if and only if $N = D(U - I_n)$ is. As shown in Section 2.3, the factorization of Q into the product S-Householder matrices is equivalent to the factorization of U into the product of D-Householder matrices.

If $r = 1$, then U is a D-Householder matrix. Clearly $U = I_n + xy^T$ for two nonzero vectors $x, y \in \mathbb{F}^n$. Since U is D-orthogonal, or $U^T DU - D = 0$, we have

$$0 = \left[(I_n + yx^T)D(I_n + xy^T) - D\right] = Dxy^T + yx^T D(I_n + xy^T) \ . \tag{2.19}$$

Multiplying on the right by a nonzero vector z we obtain

$$0 = (y^T z)Dx + [x^T D(I_n + xy^T)z]\, y \ .$$

Therefore y and Dx are linearly dependent, or $y = \alpha Dx$ for some nonzero $\alpha \in \mathbb{F}$. Substituting into (2.19) gives

$$0 = \alpha Dxx^T D + \alpha Dxx^T D(I_n + \alpha xx^T D) = \alpha(2 + \alpha x^T Dx)Dxx^T D \ .$$

Since x is nonzero, the dyad $Dxx^T D$ is nonzero. Thus $\alpha = -2/(x^T Dx)$, and we have

$$U = I_n + \alpha xx^T D = I_n - \frac{2xx^T D}{x^T Dx} \ .$$

Hence U is a D-Householder matrix. We next need to construct a non-D-isotropic vector to form U. If $r = 1$, N cannot be skew-symmetric, so there exists a constructible vector v with $v^T Nv \neq 0$ by Lemma 2.2. Then for $w = (U - I_n)v$

$$w = \frac{-2x^T Dv}{x^T Dx} x = \beta x$$

for $\beta \in \mathbb{F}$. We have that w is not D-isotropic from (2.5) and

$$U = I_n - \frac{2xx^T D}{x^T Dx} = I_n - \frac{2\beta x(\beta x)^T D}{\beta x^T D(\beta x)} = I_n - \frac{2ww^T D}{w^T Dw} \ .$$

Next, suppose $r > 1$ and $N = D(U - I_n)$ is not skew-symmetric. If $\operatorname{rank} N = \operatorname{rank}(N + N^T) = 2$, choose any vector v with $v^T Nv \neq 0$ according to the constructive proof of Lemma 2.2. Otherwise, construct a vector v using columns from the T-diagonalization of the symmetric matrix $N + N^T$ as detailed in the proof of Lemma 2.4. Alternatively, we may choose any v with $v^T Nv \neq 0$ as described after Lemma 2.7 whenever r is even, and we may construct v according to Lemma 2.4 whenever r is odd. With either choice of v, let $w = (U - I_n)v$ and H_w be the D-Householder matrix formed by w. If v is chosen according to Lemma 2.4, $D(H_w U - I_n)$ is not skew-symmetric by Lemmas 2.4 and 2.5, and $\operatorname{rank}(H_w U - I_n) = r - 1$ by Lemma 2.7. If r is even and any v satisfying $v^T Nv \neq 0$

is chosen, $D(H_wU - I_n)$ is not skew-symmetric because $\operatorname{rank} D(H_wU - I_n) = r - 1$ is odd by Lemma 2.7. We repeat the process inductively with H_wU in place of U until $\operatorname{rank}(H_{w_{r-1}} H_{w_{r-2}} \cdots H_{w_1} U - I_n) = 1$. Exactly $r - 1$ D-Householder factors have now been constructed. Thus in the case of N not skew-symmetric, U can be expressed as the product of r D-Householder matrices in total. To see that r is the minimal number of factors, suppose U can be expressed as the product of s D-Householder matrices. Using Lemma 2.6 repeatedly, we have $r = \operatorname{rank}(U - I) \leq s$.

Finally suppose $N = D(U - I_n)$ is skew-symmetric. For any non-D-isotropic vector w, we have $\operatorname{rank}(H_wU - I_n) = r + 1$ by Lemma 2.9 and consequently $D(H_wU - I)$ cannot be skew-symmetric. Any standard unit vector e_i may be chosen here for w. The updated matrix H_wU can then be factored inductively as detailed in the previous paragraph. Only one D-Householder matrix is used here, but $\operatorname{rank}(H_wU - I_n) = r+1$ additional D-Householder matrices are now needed to complete the factorization. Thus in the case of N skew-symmetric, U can be expressed as the product of $r + 2$ D-Householder matrices in total. To see that $r + 2$ is the minimal number of factors, suppose U can be expressed as the product of s D-Householder matrices. Then $U = H_wT$ for a D-Householder matrix H_w and a matrix T that is the product of the $s-1$ remaining D-Householder factors. However, we have already seen that expressing $T = H_wH_wT = H_wU$ as a product of D-Householder matrices requires at least $r+1$ factors because $D(H_wU - I_n)$ is not skew-symmetric. Thus $s - 1 \geq r + 1$.

Therefore, setting σ equal to r if $N = D(U - I_n)$ is not skew-symmetric and equal to $r + 2$ if it is skew-symmetric, we have

$$U = \prod_{j=1}^{\sigma} H_{w_j} \ .$$

As shown in Section 2.3, this means that

$$Q = \prod_{j=1}^{\sigma} H_{S,Y^{-1}w_j} \ .$$

Furthermore, the number of factors σ is minimal. The freedom of choice for selecting the vectors w_j in the factorization process above can benefit the numerical stability of our method's implementation.

Chapter 3

Pseudo Code for a CDS Factorization over $\mathbb{R}$ or $\mathbb{C}$

In this section we give a pseudo code for an algorithm to factor a given S-orthogonal matrix Q into the product of S-Householder matrices that uses the minimal number of factors as specified by the CDS Theorem. An outline of the algorithm was given in Section 2.6. Here we omit the earlier explanations of the proof and provide only the steps required. As described in Section 2.6, there are generally several options in selecting a vector v at many of the steps, but for simplicity, we only list one here while making note when a different choice might have been made.

Here $\mathbb{F}$ equals $\mathbb{R}$ or $\mathbb{C}$ and e_j denotes the j^{th} standard unit vector. We use MATLAB notation for matrix columns, i.e., $A(:,j)$ is the j^{th} column of A.

- Input:

  a nonsingular symmetric matrix $S \in M_n(\mathbb{F})$ and an S-orthogonal matrix $Q \in M_n(\mathbb{F})$

- Reduce S to $D = \text{diag}(\pm 1)$ and the S-orthogonal Q to a D-orthogonal U:

  T-diagonalize S so that $V^T S V = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ see Section 2.2

  Set $L = \text{diag}\left(1/\sqrt{|\lambda_j|}\right)$

  Set $D = LV^T SVL$

  Set $U = L^{-1}V^{-1}QVL$

- Factor the D-orthogonal matrix U into a product of D-Householder matrices.

  Set $r = \text{rank}(U - I_n)$

  - If $D(U - I_n)$ is skew-symmetric, update so that $D(HU - I_n)$ is not

    If $D(U - I_n)$ is skew-symmetric

Set $W(:,1) = e_1$ free choice of any e_j

Set $H_1 = I_n - \dfrac{2e_1 e_1^T D}{e_1^T D e_1}$ Householders never explicitly formed, see below

Update $U \leftarrow H_1 U$

Set $isSkew = 1$

Else

Set $isSkew = 0$

End if

– Iterate until $\text{rank}\left[\left(\prod H_j\right) U - I_n\right] = 1$

For ℓ equal $1 + isSkew$ to $r + 2 \cdot isSkew - 1$

Set $N = D(U - I_n)$

Find C such that $C^T(N + N^T)C = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ see Section 2.2

Sort the columns of C so that $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$

Set $B = C^T N C$

If $\text{rank}\, N = \text{rank}(N + N^T) = 2$ or if $\text{rank}(N + N^T)$ is even

set $v = C(:,1)$ or choose $v = C(:,2)$

Else

If $\text{rank}(N + N^T) = 1$ Lemma 2.4, Case 1

If there is a nonzero entry in $B(1, 2:n)$

Set $v = C(:,1)$

Else there is a $B(j,k) \neq 0$ with $j \neq k$ and $j, k > 1$

Set $v = C(:,1) + C(:,j)$ choice of nonzero entry $B(j,k)$ and

End if choice of $C(:,k)$ instead of $C(:,j)$

Elseif $\text{rank}(N + N^T) = 2$ Lemma 2.4, Case 2

If there is a $B(j,k) \neq 0$ with $j \in \{1,2\}$, $k \in \{3,4,\ldots,n\}$

Set $v = C(:,j)$ choice of nonzero entry $B(j,k)$

Else there is a $B(j,k) \neq 0$ with $j \neq k$ and $j, k \geq 3$

Set $v = C(:,1) + C(:,j)$ choice of nonzero entry $B(j,k)$ and

End if choice of $C(:,1)$ or $C(:,2)$ and $C(:,j)$ or $C(:,k)$

Else $\text{rank}(N + N^T) \geq 3$; Lemma 2.4, Case 3

Set $v = C(:,1)$ $\text{rank}(N + N^T)$ choices

End if

End if

Set $w = (U - I_n)v$

Set $W(:,\ell) = w$

Set $H_\ell = I_n - \dfrac{2ww^TD}{w^TDw}$

Update $U \leftarrow H_\ell U$

End for

- Now $\text{rank}(U - I_n) = 1$ so U is a D-Householder matrix

  Note: This can easily be combined with the previous 'for' loop.

  Set $N = D(U - I_n)$

  Find C such that $C^T(N + N^T)C = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$

  Sort the columns of C so that $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n|$

  Set $v = C(:,1)$

  Set $w = (U - I_n)v$

  Set $W(:, r + 2 \cdot isSkew) = w$

  Set $H_{r+2\cdot isSkew} = I_n - \dfrac{2ww^TD}{w^TDw}$

• Convert D-Householders to S-Householders

For j equal 1 to $r + 2 \cdot isSkew$

Set $H_j = VLH_jL^{-1}V^{-1}$

Set $W(:,j) = VLW(:,j)$

End for

- Output:

  the matrix $W = \begin{pmatrix} | & | & & | \\ w_1 & w_2 & \cdots & w_{r+2\cdot isSkew} \\ | & | & & | \end{pmatrix} \in \mathbb{F}^{n\times(r+2\cdot isSkew)}$ with columns that form the S-Householder factors $H_1, H_2, \ldots, H_{r+2\cdot isSkew}$ such that $Q = \prod_{j=1}^{r+2\cdot isSkew} H_j$

We note that in the MATLAB code, the D-Householder factors

$$H_j = I_n - \frac{2w_j w_j^T D}{w_j^T D w_j}$$

of Q are never explicitly formed as matrices. Instead only their generating vectors w_j are stored. Then, the updates $U \leftarrow H_{w_j} U$ are always performed vector and dyad-wise by evaluating

$$\begin{aligned} H_{w_j} U &= \left(I_n - \frac{2w_j w_j^T D}{w_j^T D w_j} \right) U \\ &= U - \frac{2}{(w_j^T * \mathrm{diag}(D))\, w_j}\, w_j \left((w_j^T * \mathrm{diag}(D))\, U \right) \end{aligned}$$

where the computation of $w_j^T D = w_j^T * \mathrm{diag}(D)$ uses entry-wise multiplication of vectors rather than a vector-matrix multiplication. The operations count is reduced by a factor of n by taking advantage of the structure of D-Householder matrices. We follow the standard practice in numerical linear algebra for using Householder matrices efficiently.

Chapter 4

Some Applications of generalized orthogonal matrices

In this chapter we look at applications that use generalized orthogonal matrices. In Section 4.1 using $D = \mathrm{diag}(1, 1, \ldots, 1, -1)$, we see how D-orthogonal matrices and in particular D-Householder matrices can be used to study Pythagorean n-tuples. The results we consider are known, but we work with matrices and vectors rather than number theory and develop a few nice results. In the standard $D = I_n$ case, the QR matrix factorization plays an important role in many numerical applications. In Section 4.2, we consider conditions which make an indefinite QR factorization possible for a given matrix A. When this is not possible, we study how close we can bring a matrix to triangular form R by applying D-Householder matrices to zero out entries below the diagonal of A.

4.1 Pythagorean n-tuples

A Pythagorean n-tuple is an integer vector $x \in \mathbb{Z}^n$ with $x_1^2 + x_2^2 + x_3^2 + \cdots + x_{n-1}^2 = x_n^2$. Equivalently, a nonzero $x \in \mathbb{Z}^n$ is a Pythagorean n-tuple if x is D-isotropic for $D = \mathrm{diag}(1,\ 1,\ \cdots,\ 1,\ -1)$, i.e., $x^T D x = 0$. Since generalized orthogonal matrices preserve the inner product, one can easily work with Pythagorean n-tuples using generalized orthogonal matrices. In this section we describe a few known number theoretic results with linear algebra techniques in light of indefinite inner product spaces.

For any D-orthogonal integer matrix $U \in M_n(\mathbb{Z})$, note that x is a Pythagorean n-tuple if and only if Ux is a Pythagorean n-tuple since $(Ux)^T D(Ux) = x^T U^T D U x = x^T D x$. Clearly $x = (1, 0, 0, \ldots, 0, 1)^T$ is a Pythagorean n-tuple. We can show that one can map the generic Pythagorean n-tuple $x = e_1 + e_n$ to any other Pythagorean n-tuple using a single D-Householder matrix.

Lemma 4.1. *Let* $D = \mathrm{diag}(1,\ 1,\ \cdots,\ 1,\ -1)$ *be* $n \times n$*,* $x = (1, 0, 0, \ldots, 0, 1)^T$*, and* $y \in \mathbb{Z}^n$ *be any Pythagorean* n*-tuple with* $y \neq \alpha x$*. Then* $w = x - y$ *is not* D*-isotropic and the* D*-Householder matrix* H_w *satisfies* $H_w x = y$*.*

Proof. For $w = x - y$, $w^T Dx = x^T Dx - y^T Dx = y^T Dx$ and

$$\begin{aligned} w^T Dw &= x^T Dx - y^T Dx - x^T Dy + y^T Dy \\ &= 0 - y^T Dx - y^T Dx + 0 \\ &= -2y^T Dx \ . \end{aligned}$$

Since $y \neq \alpha x$ and y satisfies $y^T Dy = 0$, at least one of $y_2, y_3, \ldots, y_{n-1}$ is nonzero. Then $w^T Dw = -2y^T Dx = -2(y_1 - y_n)$ must be nonzero. And

$$\begin{aligned} H_w x &= \left(I - \frac{2ww^T D}{w^T Dw} \right) x \\ &= x - \frac{2w^T Dx}{w^T Dw} w \\ &= x - w \ . \end{aligned}$$

□

Thus any Pythagorean n-tuple is at most one step away from $x = (1, 0, 0, \ldots, 0, 1)^T$ in terms of D-Householder transformations. In general the D-Householder matrix H_w of Lemma 4.1 is not in $M_n(\mathbb{Z})$. H_w maps x to the Pythagorean n-tuple y, as well as y to x. Also, it satisfies $(H_w w)^T DH_w w = w^T Dw = 0$ for any Pythagorean n-tuple w. However, $H_w w$ may not be a Pythagorean n-tuple since it is not necessarily an integer vector for all w. A D-Householder matrix with only integer entries would map any Pythagorean n-tuple to a different Pythagorean n-tuple. If $w \in \mathbb{Z}^n$ and $w^T Dw \in \{1, 2\}$ for example, then the

D-Householder matrix H_w maps Pythagorean n-tuples to Pythagorean n-tuples since no fractions would be involved.

Clearly, for any Pythagorean n-tuple $x \in \mathbb{Z}^n$ and any nonzero constant $k \in \mathbb{Z}$, kx is also a Pythagorean n-tuple. A Pythagorean n-tuple $x = (x_1, x_2, \ldots, x_n)^T$ is called *primitive* if its greatest common divisor $\gcd(x_1, x_2, \ldots, x_n) = 1$. Primitive Pythagorean n-tuples can be generated by applying D-Householder matrices to other primitive Pythagorean n-tuples. For $w = (1, 1, 1, 0, \ldots, 0, 1)$ for example, we have $w^T D w = 2$, and the D-Householder matrix H_w formed by w has the form

$$H_w = I_n - \frac{2ww^TD}{w^TDw} = I_n - ww^TD = \left(\begin{array}{ccc|c|c} 0 & -1 & -1 & & 1 \\ -1 & 0 & -1 & 0 & 1 \\ -1 & -1 & 0 & & 1 \\ \hline & 0 & & I_{n-4} & 0 \\ \hline -1 & -1 & -1 & 0 & 2 \end{array}\right).$$

In [4], Cass and Arpaia show that this H_w generates all primitive Pythagorean n-tuples for $4 \leq n \leq 9$. They prove that for any Pythagorean n-tuple y a sequence of Pythagorean n-tuples w_j can be found starting with $w_0 = (1, 0, \ldots, 0, 1)^T$ so that $w_0, w_1, w_2, \ldots, w_m = y$. The single matrix H_w above for $w = (1, 1, 1, 0, \ldots, 0, 1)$ is used to move through this sequence as described below. However, repeatedly applying any one generalized Householder matrix H is not very useful since $H^{-1} = H$. To avoid this, [4] denotes the set of n-tuples found by permuting the first $n-1$ entries of w_j and/or changing the signs of these entries by $S(w_j)$. It is shown there that H_w maps at least one Pythagorean n-tuple of $S(w_j)$ to an element of $S(w_{j+1})$ for each j.

For other dimensions, the same H_w does generate Pythagorean n-tuples but will not generate all of them if only the single starting Pythagorean n-tuple $x = (1, 0, \ldots, 0, 1)^T$ is used. In the case of $n = 10$ for example, [4] states that there are two orbits of Pythagorean n-tuples formed by $x_1 = (1, 0, \ldots, 0, 1)^T$ and $x_2 = (1, 1, \ldots, 1, 3)^T$.

Aragón et al. [2] use a factorization of an orthogonal transformation into Householder transformations in terms of Clifford algebras to show the structure of Pythagorean n-tuples for n equal to three or four. They prove that (x_1, x_2, x_3) is a primitive Pythagorean triple if and only if

$$x_1 = -\alpha^2 + \beta^2, \quad x_2 = 2\alpha\beta, \quad x_3 = \alpha^2 + \beta^2$$

for $\alpha, \beta \in \mathbb{N}$ relatively prime. They prove an analogous result for $n = 4$ and mention that the process extends to the general formula that

$$x_1 = -\alpha_1^2 + \sum_{j=2}^{n-1} \alpha_j^2, \quad x_k = 2\alpha_1\alpha_k \quad \text{for } 2 \leq k \leq n-1, \quad x_n = \sum_{j=1}^{n-1} \alpha_j^2$$

will be a Pythagorean n-tuple for $\alpha_j \in \mathbb{Z}$.

4.2 Indefinite QR factorization

Our goal in this section is to establish a QR-like factorization of a matrix A using Householder eliminations in the indefinite inner product case. In the standard case with $D = I_n$, a matrix A is factored into $A = QR$ for an orthogonal matrix Q and an upper triangular matrix R. We wish to generalize so that Q is D-orthogonal for a fixed $D = \text{diag}(\pm 1)$. First we note that such a generalized QR factorization is not possible for some pairs A and D.

Lemma 4.2. *Let*

$$A = \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \qquad \text{and} \qquad D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

Then the matrix A cannot be factored into a D-orthogonal matrix Q and an upper triangular matrix R satisfying $A = QR$.

Proof. Suppose there is a D-orthogonal matrix Q and an upper triangular matrix R with $A = QR$. Since R is upper triangular, the columns $a_1, a_2, \ldots, a_n$ of A are linear combinations of the columns $q_1, q_2, \ldots, q_n$ of Q. For $1 \le k \le n$, this gives

$$a_k = \sum_{j=1}^{k} r_{j\,k}\; q_j\ .$$

In particular, $a_1 = r_{11}\, q_1$. Since Q is D-orthogonal, $Q^T D Q = D$. It follows that

$$a_1^T D a_1 = r_{11}^2\ q_1^T D q_1 = r_{11}^2\ d_1\ .$$

For this example, $d_1 = 1$ and $a_1^T D a_1 = 0$ so that r_{11} must be zero. However, the first column of R cannot be zero since A has full rank. $\square$

One way to address this example could be to generalize the indefinite QR factorization to find $A = QB$ for a D-orthogonal matrix Q and a matrix B with rows and/or columns that can be permuted into an upper triangular or nearly upper triangular form. However, the example in Lemma 4.2 cannot be factored in this way either. If $A = QB$, there would have to be a nonzero entry b_{jk} of B with the rest of the entries in the k^{th} row of B all zero. But since $A^T D A = B^T D B$ it follows that $a_k^T D a_k = b_{jk}^2\, d_j$ with $d_j = \pm 1$. Similar to the above result, we find the contradiction that $b_{jk} = 0$ since the A in Lemma 4.2 has $a_k^T D a_k = 0$ for each k.

Choosing the $D = \mathrm{diag}(\pm 1)$ in dependent of the given matrix A is another possibility here. For A of Lemma 4.2, an indefinite QR factorization is possible with $D = \mathrm{diag}(-1, 1, 1, -1)$ or $D = \mathrm{diag}(1, -1, -1, 1)$. It seems that for any given A there might be a $D = \mathrm{diag}(\pm 1)$ for which an indefinite QR factorization is possible, but this question is open. In this section, we study the indefinite QR factorization given both an A and a $D = \operatorname{diag}(\pm 1)$.

A key step in producing an indefinite QR-like factorization is mapping a vector x via a D-Householder matrix to a vector y that has as many zero entries as possible. Such a mapping theorem for $\mathbb{G}$-reflectors is proved in [10]. In a symmetric bilinear form, $\mathbb{G}$-reflectors are generalized Householder transformations, but they further generalize reflections across hyperplanes to skew-symmetric bilinear and sesquilinear Hermitian and skew-Hermitian forms. In our setting, the mapping theorem of [10] states that for distinct, nonzero vectors x, y there is a D-Householder matrix H such that $Hx = y$ if and only if $x^T Dx = y^T Dy$ and $x^T Dy \neq x^T Dx$. In the following lemmas we map a vector x to a vector y that has only one or two nonzero entries using D-Householder matrices.

Lemma 4.3. *Let* $D = \operatorname{diag}(d_1, d_2, \ldots, d_n) = \operatorname{diag}(\pm 1)$, $x \in \mathbb{R}^n$, *and* $e_1, e_2, \ldots, e_n$ *be the standard unit vectors. If* $x^T Dx \neq 0$, *a D-Householder matrix H can be constructed so that* $Hx = \alpha\, e_j$ *for any j with* $d_j \cdot x^T Dx > 0$ *and* $\alpha = \pm\sqrt{d_j \cdot x^T Dx}$.

Proof. If $x^T Dx < 0$, choose j to correspond to one of the diagonal entries of D with $d_j = -1$. If $x^T Dx > 0$, choose j with $d_j = +1$. Note that if $d_j = +1$ for all j, then $D = I_n$ and $x^T Dx = x^T x > 0$. Also, $x^T Dx$ is clearly negative if $D = -I_n$. Then for $D = \pm I_n$, any j can be chosen. Hence a suitable j is available in all cases.

Let $\alpha = \pm\sqrt{d_j \cdot x^T Dx}$ and $w = x - \alpha e_j$. Then

$$w^T Dx = x^T Dx - \alpha \cdot e_j^T Dx = x^T Dx - \alpha\, d_j\, x_j \ .$$

If $x_j = 0$, then this reduces to $w^T Dx = x^T Dx \neq 0$. If $x_j \neq 0$, choose the sign of α so that $w^T Dx \neq 0$. Then we see from

$$\begin{aligned} w^T Dw &= x^T Dx - \alpha \cdot e_j^T Dx - \alpha \cdot x^T De_j + \alpha^2 \cdot e_j^T De_j \\ &= x^T Dx - 2\alpha \cdot e_j^T Dx + (d_j \cdot x^T Dx) d_j \\ &= 2(x^T Dx - \alpha \cdot e_j^T Dx) \\ &= 2w^T Dx \end{aligned}$$

that w is not D-isotropic. Thus the D-Householder matrix H_w associated with w satisfies $H_w x = \alpha\, e_j$ since

$$\begin{aligned} H_w x &= \left(I - \frac{2ww^T D}{w^T Dw} \right) x \\ &= x - \frac{2w^T Dx}{w^T Dw} w \\ &= x - w \\ &= \alpha\, e_j \end{aligned}$$

□

We would like to find a similar reduction for x with $x^T Dx = 0$. However, there is no D-orthogonal matrix that can reduce a D-isotropic x to a multiple of any standard unit vector e_j as the following lemma shows.

Lemma 4.4. *Let* $D = \operatorname{diag}(d_1, d_2, \ldots, d_n) = \operatorname{diag}(\pm 1)$, $x \in \mathbb{R}^n$, *and* $e_1, e_2, \ldots, e_n$ *be the standard unit vectors. If* $x^T Dx = 0$, *then there is no* D*-orthogonal matrix* $U \in M_n(\mathbb{R})$ *such that* Ux *is a nonzero multiple of* e_j *for any* j.

Proof. Suppose there is a D-orthogonal matrix U with $Ux = \alpha\, e_j$ for a nonzero constant α and some $j \in \{1, 2, 3, \ldots, n\}$. Since U is D-orthogonal, $U^T DU = D$. Then

$$0 = x^T Dx = x^T (U^T DU) x = (Ux)^T D (Ux) = \alpha^2 \cdot e_j^T De_j = \alpha^2 d_j \ .$$

Since $d_j = \pm 1$, it follows that $\alpha = 0$. This contradicts our assumption. □

In the cases of $D = \pm I_n$, Lemma 4.3 shows that there is a D-Householder matrix H to reduce $x \in \mathbb{R}^n$ to a multiple of any of the standard unit vectors $e_1, e_2, \ldots, e_n$. We can use this to work on the case of D-isotropic vectors x. While we can not reduce x to a single standard unit vector with a D-orthogonal matrix, we can use two D-Householder matrices to map x to a linear combination of two standard unit vectors.

Lemma 4.5. *Let $x \in \mathbb{R}^n$ be nonzero, $e_1, e_2, \ldots, e_n$ be the standard unit vectors, and*

$$D = \mathrm{diag}(d_1, d_2, \ldots, d_n) = \begin{pmatrix} I_{n_+} & 0 \\ 0 & -I_{n_-} \end{pmatrix}$$

for $n_+ + n_- = n$ and $n_+, n_- > 0$. If $x^T D x = 0$, then x can be mapped via the product of two D-Householder matrices H_1 and H_2 so that $H_1 H_2 x = \alpha\, e_j + \beta\, e_k$ where α and β are nonzero constants and $d_j = -d_k$. Moreover, $\alpha^2 = \beta^2$.

Proof. Let $D_1 = I_{n_+}$ and $D_2 = I_{n_-}$. For nonzero x with $x^T D x = 0$ we write $x = (x_1,\ x_2)^T$ so that

$$x^T D x = x_1^T D_1 x_1 + x_2^T D_2 x_2 = x_1^T (I_{n_+}) x_1 + x_2^T (-I_{n_-}) x_2 = x_1^T x_1 - x_2^T x_2\ .$$

Since x is nonzero, $x_1^T D_1 x_1 = -x_2^T D_2 x_2 \neq 0$. By Lemma 4.3 there is a D_1-Householder matrix $H_{\hat{w}_1}$ formed by $\hat{w}_1 = x_1 - \alpha \hat{e}_j$ and a D_2-Householder matrix $H_{\hat{w}_2}$ formed by $\hat{w}_2 = x_2 - \beta \hat{e}_{k-n_+}$ such that $H_{\hat{w}_1} x_1 = \alpha \hat{e}_j$ and $H_{\hat{w}_2} x_2 = \beta \hat{e}_{k-n_+}$ for some j and $k - n_+$ with $1 \leq j \leq n_+$ and $1 \leq k - n_+ \leq n_-$. Here $\hat{e}_j$ and $\hat{e}_{k-n_+}$ are the j^{th} and $(k-n_+)^{th}$ column of I_{n_+} and I_{n_-}, respectively.

Finally, we pad $\hat{w}_1$ and $\hat{w}_2$ with n_- and n_+ zeros, respectively, to get $w_1 = (\hat{w}_1,\ 0)^T$ and $w_2 = (0,\ \hat{w}_2)^T$ and form

$$H_{w_1} = \begin{pmatrix} H_{\hat{w}_1} & 0 \\ 0 & I_{n_-} \end{pmatrix} \qquad \text{and} \qquad H_{w_2} = \begin{pmatrix} I_{n_+} & 0 \\ 0 & H_{\hat{w}_2} \end{pmatrix}.$$

In this notation

$$H_{w_1}H_{w_2}x = H_{w_1}\begin{pmatrix} x_1 \\ H_{\hat{w}_2}x_2 \end{pmatrix} = \begin{pmatrix} H_{\hat{w}_1}x_1 \\ H_{\hat{w}_2}x_2 \end{pmatrix} = \begin{pmatrix} \alpha\hat{e}_j \\ \beta\hat{e}_{k-n_+} \end{pmatrix} = \alpha e_j + \beta e_k \ .$$

Since $1 \le j \le n_+$ and $n_+ < k \le n$, clearly $d_j = 1 = -d_k$. Then by

$$\begin{aligned} x^TDx &= x^TH_{w_2}^TH_{w_1}^TDH_{w_1}H_{w_2}x \\ &= (H_{w_1}H_{w_2})^TDH_{w_1}H_{w_2}x \\ &= (\alpha e_j + \beta e_k)^TD(\alpha e_j + \beta e_k) \\ &= \alpha^2 \cdot e_j^TDe_j + 2\alpha\beta \cdot e_j^TDe_k + \beta^2 \cdot e_k^TDe_k \\ &= \alpha^2 d_j + \beta^2 d_k \ , \end{aligned}$$

we see that $\alpha^2 = \beta^2$ since $x^TDx = 0$. □

In Lemma 4.5 we took advantage of the fact that our work is easier in the standard $D = I_n$ case or in the case $D = -I_n$. Thus we were able to reduce x in two stages by splitting the problem according to the signs of $d_1, d_2, \ldots, d_n$ and applying the earlier Lemma 4.3 twice. We would prefer to find a map using only one D-Householder matrix that zeros all but two of the entries of a D-isotropic vector x. The following improves the result from Lemma 4.5.

Lemma 4.6. *Let $x \in \mathbb{R}^n$ be nonzero, $e_1, e_2, \ldots, e_n$ be the standard unit vectors, and $D = \operatorname{diag}(d_1, d_2, \ldots, d_n) = \operatorname{diag}(\pm 1)$. If $x^TDx = 0$, then a D-Householder matrix H can be constructed such that $Hx = e_j + \alpha e_k$ for $\alpha = \pm 1$ and j, k with $d_j = -d_k$.*

Proof. Since x is nonzero and $x^TDx = 0$, there must be two nonzero entries x_j and x_k of x with $d_j = -d_k$. Let $w = x - (e_j + \alpha e_k)$ for $\alpha = \pm 1$. Then

$$w^TDx = x^TDx - e_j^TDx - \alpha e_k^TDx = -d_jx_j - \alpha d_kx_k = -d_j(x_j - \alpha x_k) \ .$$

Choose the sign of α so that $w^T Dx \neq 0$. Then w is not D-isotropic because

$$\begin{aligned}
w^T Dw &= (x - e_j - \alpha e_k)^T D(x - e_j - \alpha e_k) \\
&= x^T Dx - 2x^T De_j - 2\alpha x^T De_k - e_j^T De_j - 2\alpha e_j^T De_k - \alpha^2 e_k^T De_k \\
&= -2x_j d_j - 2\alpha x_k d_k - d_j - d_k \\
&= -2d_j(x_j - \alpha x_k) \\
&= 2w^T Dx \neq 0 \ .
\end{aligned}$$

Finally the D-Householder matrix H_w maps x as desired:

$$\begin{aligned}
H_w x &= \left(I_n - \frac{2ww^T D}{w^T Dw} \right) x \\
&= x - \frac{2w^T Dx}{w^T Dw} \, w \\
&= x - w \\
&= e_j + \alpha e_k \ .
\end{aligned}$$

□

These results are the tools we will use for an indefinite QR factorization of a matrix. As seen in Lemma 4.2, an indefinite QR factorization of a matrix A is not always possible. We will explore different conditions on the matrix A that lead to a indefinite QR factorization of A. Note that any D-orthogonal matrix U can trivially be factored into a D-orthogonal matrix and an upper triangular matrix as UI_n. Other factorizations are also possible by using D-Householder eliminations discussed thus far in this section.

Lemma 4.7. *Let $D = \operatorname{diag}(d_1, d_2, \ldots, d_n) = \operatorname{diag}(\pm 1)$ and $U \in M_n(\mathbb{R})$ be D-orthogonal. Then a diagonal matrix $R = \operatorname{diag}(\pm 1)$ and a D-orthogonal matrix Q with $U = QR$ can be constructed. Here Q is the product of $n-1$ D-Householder matrices $H_1, H_2, \ldots, H_{n-1}$.*

Proof. Let $u_1, u_2, \ldots, u_n$ be the columns of U. Since U is D-orthogonal, $U^T DU = D$ or $u_j^T Du_j = d_j \neq 0$ for each j. By Lemma 4.3 there is a D-Householder matrix H_1 with

$H_1 u_1 = \alpha_1 e_1$. Clearly the first column of $H_1 U$ has all zeros below its first entry. We can also show that the first entries of the remaining columns of $H_1 U$ are also zero. Since the columns of U are pairwise D-orthogonal, for $j \in \{2, 3, \ldots, n\}$

$$\begin{aligned} 0 &= u_1^T D u_j \\ &= u_1^T H_1^T D H_1 u_j \\ &= (H_1 u_1)^T D (H_1 u_j) \\ &= \alpha_1 e_1^T D (H_1 u_j) \\ &= \alpha_1 d_1 e_1^T (H_1 u_j) \ . \end{aligned}$$

Therefore the first entry of $H_1 u_j$ is zero for each $2 \leq j \leq n$. After this first multiplication of U by H_1 we have

$$H_1 U = (H_1 u_1 \ H_1 u_2 \ \cdots \ H_1 u_n) = \begin{pmatrix} \alpha_1 & 0 \\ 0 & U_2 \end{pmatrix} \qquad \text{and} \qquad D = \begin{pmatrix} d_1 & 0 \\ 0 & D_2 \end{pmatrix}$$

where $U_2 \in M_{n-1}(\mathbb{R})$ is D_2-orthogonal. Continuing iteratively through the second to $(n-1)^{th}$ column gives us

$$(H_{n-1} H_{n-2} \cdots H_1) \, U = \text{diag}(\alpha_1, \alpha_2, \ldots, \alpha_n) = R \ .$$

Each of the α_j can be found from Lemma 4.3 and each will be ± 1 since U is D-orthogonal. Thus for

$$Q = \left(\prod_{j=1}^{n-1} H_j \right)$$

we have $U = QR$. $\square$

This lemma can be extended to a constructive factorization of a D-orthogonal matrix U into the product of D-Householder matrices. First $n-1$ D-Householder matrices are needed to reduce U to diag(± 1). Then up to n additional D-Householder matrices are needed to reduce diag(± 1) to I_n. Such a construction was first developed in [16]. This process does not constitute a constructive proof of the minimal number aspect of the CDS Theorem because here up to $2n-1$ D-Householder matrix factors are required while the CDS Theorem states that only $\text{rank}(U - I_n)$ or $\text{rank}(U - I_n) + 2$ are needed. By sorting the order in which the columns are eliminated, the method can be improved to use $n - 1 + \min\{n_+, n_-\}$ factors, where n_+ and n_- are the number of $+1$ and -1 entries in D respectively. While this process is simplier than our construction in Chapter 2, that construction requires only the minimal number of D-Householder matrix factors as specified in the CDS Theorem.

Next we want to relax the conditions on A but still find an indefinite QR factorization, or try to get as close as possible to an indefinite QR factorization of A. A simple next step would address a matrix A with pairwise D-orthogonal columns, i.e., $A^T DA$ would be diagonal but not necessarily equal to D.

Lemma 4.8. *Let $D = \text{diag}(d_1, d_2, \ldots, d_n) = \text{diag}(\pm 1)$ and $A \in M_n(\mathbb{R})$ have pairwise D-orthogonal columns. Then a diagonal matrix R and a D-orthogonal matrix Q with $U = QR$ can be constructed. Here Q is the product of $n-1$ D-Householder matrices $H_1, H_2, \ldots, H_{n-1}$* .

The proof is omitted since the only difference in the proof of this lemma and that of the previous one is that $A^T DA = \text{diag}(\beta_1, \beta_2, \ldots, \beta_n)$ with each $\beta_j \neq 0$ but possibly $\beta_j \neq d_j$. In conclusion, $R = \text{diag}(\pm 1)$ becomes $R = \text{diag}(\alpha_1, \alpha_2, \ldots, \alpha_n)$ with each $\alpha_j \neq 0$ but not necessarily equal to ± 1.

Next we consider an indefinite QR factorization of a general matrix A. A problem generally arises when we move to the next iteration after an update. As we have seen in the proof of Lemma 4.7, the D-Householder update matrix zeros entries not only below the diagonal but also along the row to the right of the diagonal. The same occurs in Lemma 4.8. For a general matrix A, we may not be able to eliminate all entries below the diagonal in a certain column, and there is no reason why the row containing the diagonal entry would have to be simultaneously eliminated simply because it is possible to zero out column entries below the diagonal. If we are able to update A to

$$HA = \begin{pmatrix} \alpha & * \\ 0 & A_2 \end{pmatrix}$$

instead, then the diagonal entries of $A_2^T DA_2$ do not necessarily equal the second through n^{th} diagonal entries of $A^T DA$ as was the case in Lemmas 4.7 and 4.8.

Lemma 4.9. *Let $D = \mathrm{diag}(d_1, d_2, \ldots, d_n) = \mathrm{diag}(\pm 1)$, n_+ equal the number of $+1$'s in D, $n_- = n - n_+$ equal the number of -1's in D, and $A \in M_n(\mathbb{R})$. Then for some k with $0 \le k \le \min\{n_+, n_-\}$*

$$A = Q \left(\begin{array}{c|c} R_{(n-2k)\times(n-2k)} & * \\ \hline 0 & B_{2k\times 2k} \end{array} \right) P$$

where Q is D-orthogonal, P is a permutation matrix, R is upper triangular, and B has the form

$$B = \left(\begin{array}{cccccc|c} * & * & * & \cdots & & * & \\ * & * & * & & & * & \\ & * & * & & & * & \\ & * & * & & & * & \\ & & * & & & * & *_{(2k)\times k} \\ & & * & & & * & \\ & & & \ddots & & \vdots & \\ & & & & & * & \\ 0 & & & & & * & \end{array} \right).$$

When we move from iterate A_j to the next A_{j+1}, we essentially remove a row and column of $H_j A_j$ to obtain A_{j+1}. Since the removed row has nonzero entries, the diagonal entries of $A_{j+1}^T DA_{j+1}$ are not necessarily a subset the diagonal entries of $A_j^T DA_j$. Hence we cannot determine the sizes of R and B in Lemma 4.9 for a given A beyond $0 \le k \le \min\{n_+, n_-\}$ until it is reduced. Also, the order in which the columns are reduced could change the outcome and lead to better factorizations.

In MATLAB, the random examples that we have tested could always be reduced to upper triangular form R, i.e., to $k = 0$ in Lemma 4.9. Of course, random example matrices are not likely to have D-isotropic columns. There exist, however, "bad" examples with $2k = n$ as was the case for A and D in Lemma 4.2 such as

$$A = \begin{pmatrix} I_{n/2} & -S_{n/2} \\ S_{n/2} & I_{n/2} \end{pmatrix} \quad \text{and} \quad D = \begin{pmatrix} I_{n/2} & 0 \\ 0 & -I_{n/2} \end{pmatrix}$$

for any even n. Here

$$S_{n/2} = \begin{pmatrix} 0 & & & 1 \\ & & \iddots & \\ & 1 & & \\ 1 & & & 0 \end{pmatrix}$$

with dimension $n/2$. For such examples, the matrix D itself plays an important role. Changing to a different $D = \operatorname{diag}(\pm 1)$ allows for a factorization with $k = 0$ for each of these example pairs A, D. If the context of the problem does not require a specific D, then D could actually be chosen to minimize k.

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Appendix

MATLAB code for the CDS Theorem factorization

```
function W = CDS_factorization(Q,S,tol)
% -----------------------------------------------------------------------
% Factor an S-orthogonal matrix Q (with Q^TSQ=S) into the product of k
% S-Householder matrices where k is rank(Q-I) or rank(Q-I)+2.
%
% INPUT:
%    S = nonsingular symmetric n by n matrix
%    Q = S-orthogonal n by n matrix
%    tol = tolerance (optional)
% OUTPUT:
%    W = n by k matrix whose columns form the S-Householder matrix factors
% -----------------------------------------------------------------------

if nargin == 2, tol = 10^(-10); end;
n = length(diag(S));
W = [];
I = eye(n);

if norm(abs(S)-I) ~= 0                       % Reduce S to D
    [V,L1] = sym_diag(S,tol);                % Call function sym_diag
    L = diag(1/sqrt(abs(diag(L1))));
    D = L*V.'*S*V*L;
    U = L^-1*V^-1*Q*V*L;                     % Computing inverses can be avoided
    s2d = 1;
else
    D = S;
    U = Q;
    s2d = 0;
end;

d = diag(D);
r = rank(U-I,tol);
if norm(D*(U-I)+(D*(U-I)).') < tol          % D(U-I) is skew symmetric
    w = I(:,1);
    W(:,1) = w;                              % Save w that forms D-Householder H
    wTD=w.'.*d;
    U = U-2/(wTD*w)*w*(wTD*U);               % Update U <-- HU
    isSkew = 1;
```

```
else
    isSkew = 0;
end;

for iter = 1+isSkew:r+2*isSkew              % Iterate until rank(U-I)=0
    N = D*(U-I);
    [C,L] = sym_diag(N+N.',tol);
    B = C.'*N*C;
    r_NNT = rank(N+N.',tol);
    if rank(N,tol) <= 2 & r_NNT == 2        % Include rank(U-I)=1 case here
        v = C(:,1);
    else                                    % Choose v according to Lemma 2.4
        if r_NNT == 1                       % Lemma 2.4 Case 1
            if max(abs(B(1,2:n))) > tol     % Lemma 2.4 Case 1 (a)
                v = C(:,1);
            else                            % Lemma 2.4 Case 1 (b)
                B(:,1) = 0; B(1,:) = 0; B = B-diag(diag(B)); B = abs(B);
                [J,K] = find(B == max(B(:)));
                v = C(:,1) + C(:,J(1));
            end;
        elseif r_NNT == 2                   % Lemma 2.4 Case 2
            if max(abs(B(1:2,3:n))) > tol   % Lemma 2.4 Case 2 (a)
                B(3:n,:) = 0; B(1:2,1:2) = 0; B = abs(B);
                [J,K] = find(B == max(B(:)));
                v = C(:,J(1));
            else                            % Lemma 2.4 Case 2 (b)
                B(1:2,:) = 0; B(:,1:2) = 0; B = B-diag(diag(B)); B = abs(B);
                [J,K] = find(B == max(B(:)));
                v = C(:,1) + C(:,J(1));
            end;
        else   % r_NNT > 2                  % Lemma 2.4 Case 3
            v = C(:,1);
        end;
    end;
    w = U*v-v;
    W(:,iter) = w;                          % Save w that forms D-Householder H
    wTD=w.'.*d';
    U = U-2/(wTD*w)*w*(wTD*U);              % Update U <-- HU
end;

if s2d == 1, W = V*L*W; end;                % Convert back to S-Householders
```

```
function [C,L] = sym_diag(A,tol);
% ----------------------------------------------------------------------
% Find the T-diagonalization of a real or complex symmetric matrix A,
% i.e., find a nonsingular C and diagonal L with C^TAC=L.  If A has only
% real entries, use an eigenvalue decomposition.  If A has complex entries,
% use the Takagi factorization.
% The columns of C are sorted so that the diagonal entries of L appear
% in decreasing magnitude.
%
% INPUT:
%    A = symmetric n by n matrix
%    tol = tolerance (optional)
% OUTPUT:
%    C = nonsingular matrix
%    L = diagonal matrix
% ----------------------------------------------------------------------

[n n] = size(A);
if nargin == 1, tol = 10^(-10); end;

I = eye(n);

if unique(isreal(A)) == 1
    [C,L] = eig(A);
else
    [C,L] = takagi(A,tol);
end;

diag_L = diag(L);
[tmp,srt] = sort(abs(diag_L),'descend');
C = C(:,srt);
L = diag(diag_L(srt));
```

```
function [C,L] = takagi(A,tol)
% -----------------------------------------------------------------------
% Diagonalize a complex symmetric matrix A, i.e., find a nonsingular C
% and diagonal L with C^TAC=L.
% This follows Theorem 4.4.3 and Corollary 4.4.4 in Horn and Johnson's
% Matrix Analysis
%
% INPUT:
%    A = complex n by n symmetric matrix
%    tol = tolerance (optional)
% OUTPUT:
%    C = nonsingular (unitary) matrix
%    L = diagonal matrix
% -----------------------------------------------------------------------

[n n] = size(A);
if nargin == 1, tol = 10^(-10); end;
I = eye(n);

A0 = A; U = I;
for j = 1:n-1
    W=[];
    AA_ = A*conj(A);
    [V,E] = eig(AA_);
    k = find(abs(diag(E)),1);
    x = V(:,k);
    if rank([A*conj(x) x],tol) == 1
        W = x;
    else                               % rank([A*conj(x) x],tol) == 2
        mu = sqrt(E(k,k));
        W = A*conj(x) + mu*x;
        W = W / sqrt(W'*W);
    end;
    W(:,2:n-j+1) = null(W');
    U = U*blkdiag(eye(j-1),W);
    if j < n-1
        tmp = W'*A*conj(W);
        A = tmp(2:n-j+1,2:n-j+1);
    end;
end;

C = conj(U);
L = U'*A0*conj(U);
```