

\mathbb{G} -Reflectors: Analogues of Householder Transformations in Scalar Product Spaces*

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Abstract

We characterize the analogues of Householder transformations in matrix groups associated with scalar products, and precisely delimit their mapping capabilities: given a matrix group \mathbb{G} and vectors x, y , necessary and sufficient conditions are derived for the existence of a Householder-like analogue $G \in \mathbb{G}$ such that $Gx = y$. When G exists, we show how it can be constructed from x and y . Examples of matrix groups to which these results apply include the symplectic and pseudo-unitary groups.

Key words. scalar product, bilinear, sesquilinear, orthosymmetric, isotropic, Householder transformation, hyperbolic transformation, symmetries, transvections, symplectic, pseudo-unitary, structure-preserving.

AMS subject classification. 65F30, 15A04, 15A57, 15A63

1 Introduction

Elementary reflectors in the Euclidean spaces \mathbb{R}^n and \mathbb{C}^n are a widely used tool in linear algebra. Often called Householder transformations, they are useful in unitary reductions and provide efficient and stable means to compute various matrix factorizations. Their first appearance has been credited [12] to Turnbull and Aitken [31, 1932, pp. 102–105], who show that if $p, q \in \mathbb{C}^n$ with $p^*p = q^*q = 1$, then the transformation

$$R = \frac{(p+q)(p+q)^*}{1+q^*p} - I \tag{1.1}$$

is rational and unitary (though not Hermitian), and takes p to q . Should it happen that $q^*p = -1$, replacing q by $-q$ in (1.1) is recommended. This yields a well-defined R taking p to $-q$. Follow this with $-I$ and p is sent to q as desired¹.

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¹Note that for unit vectors p and q , $q^*p = -1$ implies $q = -p$, so the first step in their two-step recommendation is superfluous.

Turnbull and Aitken preface their solution to this unitary mapping problem with a comment on the unsuitability of using the quadratic form $p^T p$ in place of $p^* p$. Indeed, they point out that if $p^T = [1 \ i]$, then $p^T p = 0$, and

“... the vector p is in fact *isotropic*, and cannot be normalized; and this, as we shall see, renders it useless for our purpose.” [31, p. 103].

Our purpose in this paper is to solve the analogue of the unitary mapping problem in matrix groups associated with general scalar product spaces, including those that admit isotropic vectors. Examples of such groups include the symplectic and pseudo-unitary groups.

Given a matrix group \mathbb{G} , we give a complete characterization of all Householder-like analogues in \mathbb{G} ; and given vectors x, y , we give necessary and sufficient conditions for the existence of a Householder-like analogue $G \in \mathbb{G}$ such that $Gx = y$. When G exists, we show how it can be constructed from x and y in a simple manner, akin to the construction of a Householder reflector.

The transformations we develop are mathematically equivalent to those first used in a more abstract framework to study the nature of the classical matrix groups. Depending on the properties of the underlying scalar product — whether it was bilinear, sesquilinear, symmetric, skew-symmetric, etc. — these transformations were variously distinguished as reflections, symmetries, transvections, quasi-symmetries, etc. [3], [6], [7], [15].

To our knowledge, this is the first time these transformations together with their mapping properties have all been presented under a common rubric and developed from a constructive matrix perspective. As a special case of our unified presentation, we obtain a complete specification of all the unitary reflectors together with a full description of their mapping capabilities, a result that can also be found in Laurie [18]. A partial treatment can be found in Uhlig [32] for the case when the scalar product is symmetric bilinear; for skew-symmetric bilinear forms some of our results can be found in Mehrmann [24]. In the case of the pseudo-unitary groups, special instances of \mathbb{G} -reflectors have been studied from the numerical perspective in [5], [27], [30].

2 Preliminaries

2.1 Scalar products

We begin with a brief review of scalar products. More detailed discussions can be found in [15], [17], or [29].

Let \mathbb{K} denote either the field \mathbb{R} or \mathbb{C} . Consider a map $(x, y) \mapsto \langle x, y \rangle$ from $\mathbb{K}^n \times \mathbb{K}^n$ to \mathbb{K} . If such a map is linear in each argument, that is,

$$\begin{aligned} \langle \alpha_1 x_1 + \alpha_2 x_2, y \rangle &= \alpha_1 \langle x_1, y \rangle + \alpha_2 \langle x_2, y \rangle, \\ \langle x, \beta_1 y_1 + \beta_2 y_2 \rangle &= \beta_1 \langle x, y_1 \rangle + \beta_2 \langle x, y_2 \rangle, \end{aligned}$$

then it is called a *bilinear form*. If $\mathbb{K} = \mathbb{C}$, and the map $(x, y) \mapsto \langle x, y \rangle$ is conjugate linear in the first argument and linear in the second,

$$\begin{aligned} \langle \alpha_1 x_1 + \alpha_2 x_2, y \rangle &= \bar{\alpha}_1 \langle x_1, y \rangle + \bar{\alpha}_2 \langle x_2, y \rangle, \\ \langle x, \beta_1 y_1 + \beta_2 y_2 \rangle &= \beta_1 \langle x, y_1 \rangle + \beta_2 \langle x, y_2 \rangle, \end{aligned}$$

then it is called a *sesquilinear form*.

Proposition 2.1. *Given a bilinear or sesquilinear form on \mathbb{K}^n , there exists a unique $M \in \mathbb{K}^{n \times n}$ such that for all $x, y \in \mathbb{K}^n$,*

$$\langle x, y \rangle = \begin{cases} x^T M y & \text{if the form is bilinear,} \\ x^* M y & \text{if the form is sesquilinear.} \end{cases}$$

M is called the matrix associated with the form (with respect to the standard basis); we will denote $\langle x, y \rangle$ by $\langle x, y \rangle_M$ as needed.

A bilinear form is said to be symmetric if $\langle x, y \rangle = \langle y, x \rangle$, and skew-symmetric if $\langle x, y \rangle = -\langle y, x \rangle$. It follows that the matrix associated with a symmetric form is symmetric; similarly, the matrix of a skew-symmetric form is skew-symmetric. A sesquilinear form is Hermitian if $\langle x, y \rangle = \overline{\langle y, x \rangle}$ and skew-Hermitian if $\langle x, y \rangle = -\overline{\langle y, x \rangle}$. The matrices associated with such forms are Hermitian and skew-Hermitian, respectively.

A bilinear or sesquilinear form $\langle \cdot, \cdot \rangle_M$ is *nondegenerate* if

$$\langle x, y \rangle_M = 0, \forall y \Rightarrow x = 0 \quad \text{and} \quad \langle x, y \rangle_M = 0, \forall x \Rightarrow y = 0.$$

It can readily be shown that $\langle \cdot, \cdot \rangle_M$ is non-degenerate if and only if M is non-singular. We will consider only nondegenerate forms.

Definition 2.2. A *scalar product* is a nondegenerate bilinear or sesquilinear form. The space \mathbb{K}^n equipped with a fixed scalar product is said to be a *scalar product space*.

We make no a priori assumption about the positive definiteness of our scalar product. One of the points of this development is to highlight how much the positive definite and indefinite cases have in common².

We will frequently need the associated quadratic functional $q(x) \stackrel{\text{def}}{=} \langle x, x \rangle_M$, which is the natural analogue in a scalar product space of the squared norm $\|x\|_2^2$ in Euclidean space.

2.2 Adjoints

Let $\langle \cdot, \cdot \rangle_M$ be any fixed scalar product on \mathbb{K}^n . For any matrix $A \in \mathbb{K}^{n \times n}$ there is a unique matrix A^\star , the *adjoint* of A with respect to $\langle \cdot, \cdot \rangle_M$, defined by

$$\langle Ax, y \rangle_M = \langle x, A^\star y \rangle_M, \quad \forall x, y \in \mathbb{K}^n.$$

It is straightforward to show that

$$A^\star = \begin{cases} M^{-1} A^T M & \text{if the form is bilinear,} \\ M^{-1} A^* M & \text{if the form is sesquilinear.} \end{cases}$$

Observe that if $M = I$, then A^\star reduces to just A^T or A^* . The following properties of adjoint, all analogous to properties of transpose (or conjugate transpose), follow easily (except the last). We omit the proofs.

1. $(A + B)^\star = A^\star + B^\star$, $(AB)^\star = B^\star A^\star$, $(A^{-1})^\star = (A^\star)^{-1}$.

2. $(\alpha A)^\star = \begin{cases} \alpha A^\star & \text{for bilinear forms,} \\ \bar{\alpha} A^\star & \text{for sesquilinear forms.} \end{cases}$

²A similar view is expressed in Shaw [29, Preface].

$$3. (A^\star)^\star = A \text{ for all } A \in \mathbb{K}^{n \times n} \Leftrightarrow \begin{cases} M^T = \pm M & \text{for bilinear forms,} \\ M^\star = \alpha M, |\alpha| = 1 & \text{for sesquilinear forms.} \end{cases}$$

Further information on scalar products for which the adjoint satisfies the involutory property, $(A^\star)^\star = A$, is given in section 7.

2.3 Lie algebras, Jordan algebras, and matrix groups

Three important classes of structured matrices are associated with each scalar product: the automorphism group \mathbb{G} , defined by

$$\begin{aligned} \mathbb{G} &\stackrel{\text{def}}{=} \{G \in \mathbb{K}^{n \times n} : \langle Gx, Gy \rangle_M = \langle x, y \rangle_M\} \\ &= \{G \in \mathbb{K}^{n \times n} : G^\star = G^{-1}\}, \end{aligned}$$

the Jordan algebra \mathbb{J} defined by

$$\begin{aligned} \mathbb{J} &\stackrel{\text{def}}{=} \{A \in \mathbb{K}^{n \times n} : \langle Ax, y \rangle_M = \langle x, Ay \rangle_M\} \\ &= \{A \in \mathbb{K}^{n \times n} : A^\star = A\}, \end{aligned}$$

and the Lie algebra \mathbb{L} , defined by

$$\begin{aligned} \mathbb{L} &\stackrel{\text{def}}{=} \{B \in \mathbb{K}^{n \times n} : \langle Bx, y \rangle_M = -\langle x, By \rangle_M\} \\ &= \{B \in \mathbb{K}^{n \times n} : B^\star = -B\}. \end{aligned}$$

The matrices in \mathbb{G} are sometimes called *isometries*, since they preserve the value of the scalar product [3], [15], [17], [29]. If \mathbb{G} is associated with a bilinear form, then $\det G = \pm 1$ for any $G \in \mathbb{G}$. In the case of a sesquilinear form, $|\det G| = 1$.

\mathbb{G} always forms a multiplicative group (indeed a Lie group), although it is not a linear subspace. By contrast, the sets \mathbb{J} and \mathbb{L} are linear subspaces, but they are not closed under multiplication. Instead \mathbb{L} is closed with respect to the Lie bracket $[K_1, K_2] = K_1K_2 - K_2K_1$, while \mathbb{J} is closed with respect to the Jordan product $\{S_1, S_2\} = \frac{1}{2}(S_1S_2 + S_2S_1)$.

Since for any $G \in \mathbb{G}$ we have

$$A \in \mathbb{S} \Rightarrow G^{-1}AG \in \mathbb{S}, \quad \text{where } \mathbb{S} = \mathbb{G}, \mathbb{L}, \text{ or } \mathbb{J},$$

the automorphism groups \mathbb{G} provide the natural classes of structure-preserving similarities for matrices in \mathbb{G} , \mathbb{L} , and \mathbb{J} ; they are therefore central to the development of structure-preserving algorithms involving any of these classes of matrices. For more on these three types of structured matrix, see [1], [9], [16].

The rest of this paper will focus only on matrices in \mathbb{G} . Table 2.1 shows a sample of well-known structured matrices associated with a scalar product, and introduces notation for the corresponding automorphism groups \mathbb{G} . Note that the results in this paper are not confined to the examples listed in Table 2.1.

Table 2.1: A sampling of structured matrices associated with scalar products.

$$J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \quad \Sigma_{p,q} = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}, \quad \text{with } p + q = n.$$

Space	Bilinear Form $\langle x, y \rangle$	Adjoint $A \in M_n(\mathbb{K})$	Automorphism Group $\mathbb{G} = \{G : G^* = G^{-1}\}$	Jordan Algebra $\mathbb{J} = \{S : S^* = S\}$	Lie Algebra $\mathbb{L} = \{K : K^* = -K\}$
\mathbb{R}^n	$x^T y$ symmetric form	$A^* = A^T$	Real orthogonals $O(n, \mathbb{R})$	Symmetrics	Skew-symmetrics
\mathbb{C}^n	$x^T y$ symmetric form	$A^* = A^T$	Complex orthogonals $O(n, \mathbb{C})$	Complex symmetrics	Complex skew-symmetrics
\mathbb{R}^n	$x^T \Sigma_{p,q} y$ symmetric form	$A^* = \Sigma_{p,q} A^T \Sigma_{p,q}$	Pseudo-orthogonals $O(p, q, \mathbb{R})$	Pseudo symmetrics	Pseudo skew-symmetrics
\mathbb{R}^{2n}	$x^T J y$ skew-symm. form	$A^* = -J A^T J$	Real symplectics $Sp(2n, \mathbb{R})$	Skew-Hamiltonians	Hamiltonians
\mathbb{C}^{2n}	$x^T J y$ skew-symm. form	$A^* = -J A^T J$	Complex symplectics $Sp(2n, \mathbb{C})$	J -skew-symmetric	J -symmetric

Space	Sesquilinear Form $\langle x, y \rangle$	Adjoint $A \in M_n(\mathbb{C})$	Automorphism Group $\mathbb{G} = \{G : G^* = G^{-1}\}$	Jordan Algebra $\mathbb{J} = \{S : S^* = S\}$	Lie Algebra $\mathbb{L} = \{K : K^* = -K\}$
\mathbb{C}^n	$x^* y$ Hermitian form	$A^* = A^*$	Unitaries $U(n)$	Hermitian	Skew-Hermitian
\mathbb{C}^n	$x^* \Sigma_{p,q} y$ Hermitian form	$A^* = \Sigma_{p,q} A^* \Sigma_{p,q}$	Pseudo-unitaries $U(p, q)$	Pseudo Hermitian	Pseudo skew-Hermitian
\mathbb{C}^{2n}	$x^* J y$ skew-Herm. form	$A^* = -J A^* J$	Conjugate symplectics $Sp^*(2n, \mathbb{C})$	J -skew-Hermitian	J -Hermitian

3 \mathbb{G} -reflectors and their geometry

Following the terminology of Householder [14], we define an *elementary transformation* to be a linear map $T: \mathbb{K}^n \rightarrow \mathbb{K}^n$ of the form $T = I + uv^T$ for some nonzero $u, v \in \mathbb{K}^n$. Equivalently, T may be expressed as $I + uv^*$. It is not hard to see that these maps can also be geometrically characterized. This is done in the following Lemma. We omit the proof.

Lemma 3.1. $T: \mathbb{K}^n \rightarrow \mathbb{K}^n$ is an elementary transformation if and only if $\mathcal{H} \stackrel{\text{def}}{=} \{x \in \mathbb{K}^n : Tx = x\}$ is a hyperplane, that is, $\dim \mathcal{H} = n - 1$.

The focus of this paper are the elementary transformations in automorphism groups \mathbb{G} associated with scalar products. In the case of the real orthogonal group $\mathbb{G} = O(n, \mathbb{R})$, elementary transformations are well-known. Expressible in the form $I - 2uu^T$, with $u^T u = 1$, they are precisely the perpendicular reflections through hyperplanes and are referred to as reflectors [26], or Householder transformations [10].

Definition 3.2. Let \mathbb{G} be the automorphism group of a scalar product on \mathbb{K}^n . Then the elementary transformations in \mathbb{G} will be called *generalized \mathbb{G} -reflectors*, or \mathbb{G} -reflectors for short.

Since \mathbb{G} is a group, any \mathbb{G} -reflector G must be invertible. And since G^{-1} must fix the same hyperplane as G , G^{-1} is also a \mathbb{G} -reflector. Thus the set of \mathbb{G} -reflectors is closed under inverses. It is not closed under products: although the product of \mathbb{G} -reflectors with a common fixed hyperplane is a \mathbb{G} -reflector, the product of \mathbb{G} -reflectors that fix different hyperplanes is not.

When \mathbb{G} is the automorphism group of a general symmetric bilinear form, all \mathbb{G} -reflectors act geometrically as reflections through hyperplanes, although usually these are oblique reflections³. They have been referred to as “symmetries” [3], [7], [15], [28], and are shown by the Cartan-Dieudonné theorem [3], [6], [7], [15], [28], [32] to generate the automorphism group \mathbb{G} of any symmetric bilinear form. That is, any $G \in \mathbb{G}$ can be expressed as a finite product of symmetries. More recently, various authors, for example [5], [27], [30], have referred to \mathbb{G} -reflectors (and some closely related matrices) in the pseudo-orthogonal groups $O(p, q, \mathbb{R})$ as “hyperbolic Householders”.

For the symplectic groups $Sp(2n, \mathbb{K})$, where the scalar product is skew-symmetric bilinear, \mathbb{G} -reflectors have been referred to as “transvections” or “symplectic transvections” [3], [7], [15], [24]. In this case, \mathbb{G} -reflectors do *not* act geometrically as reflections through the fixed hyperplane, but rather by shearing the hyperplanes parallel to \mathcal{H} ; that is, these hyperplanes remain invariant, but undergo a translation. This is a consequence of the fact that the determinant of any real or complex symplectic matrix can only be $+1$ (see [20], for example, for a collection of different proofs of this result).

Indeed, viewed as transformations of \mathbb{K}^n , \mathbb{G} -reflectors in general have a very limited range of possible geometric actions. Because any \mathbb{G} -reflector G has a fixed hyperplane \mathcal{H} , it must have eigenvalue $\lambda = 1$ with geometric multiplicity $n - 1$ and algebraic multiplicity $n - 1$ or n . In particular, $\det G = \lambda_n$, where λ_n is the remaining eigenvalue of G .

For a bilinear form, $\det G = \pm 1$, so $\lambda_n = \pm 1$. If $\lambda_n = -1$, then G is diagonalizable and thus acts geometrically as a (perhaps oblique) reflection. If $\lambda_n = 1$, then G is *not*

³Oblique, that is, with respect to the Euclidean scalar product. With respect to the given scalar product $\langle \cdot, \cdot \rangle_M$, they are *all* perpendicular reflections, in the sense that $\langle u, \mathcal{H} \rangle_M = 0$, where u is the reflected vector (i.e. $Gu = -u$), and \mathcal{H} is the fixed hyperplane.

diagonalizable (otherwise G would have to be I), and the Jordan block structure of G consists of $n - 2$ 1×1 blocks and one 2×2 block. In other words, G acts as a shear (aka transvection) along hyperplanes parallel to \mathcal{H} . Thus for bilinear forms, \mathbb{G} -reflectors can only be reflections or shears/transvections.

For sesquilinear forms, $\det G$ can be any complex number on the unit circle. If $\det G = \pm 1$, then G is a reflection or shear, as before. Otherwise we have a third possibility, $|\det G| = |\lambda_n| = 1$ with $\lambda_n \in \mathbb{C}, \lambda_n \neq \pm 1$. These \mathbb{G} -reflectors have been referred to as “quasi-symmetries” [7].

In summary, then, we see that there are only three possible geometric types of \mathbb{G} -reflector: reflections, shears/transvections, and quasi-symmetries.

4 General characterization

We give necessary and sufficient conditions for an elementary transformation to belong to the automorphism group \mathbb{G} of any scalar product on \mathbb{K}^n .

Lemma 4.1. *Suppose $w, x, y, z \in \mathbb{K}^n$ with $y, z \neq 0$.*

(a) $wx^T = yz^T \Leftrightarrow y = \beta w$ and $x = \beta z$ for some nonzero $\beta \in \mathbb{K}$.

(b) $wx^* = yz^* \Leftrightarrow y = \beta w$ and $x = \overline{\beta}z$ for some nonzero $\beta \in \mathbb{K}$.

Proof. (a): The proof is almost identical to (b).

(b): $z \neq 0 \Rightarrow \exists v \in \mathbb{K}^n$ such that $z^*v \neq 0$. Then $wx^*v = yz^*v \Rightarrow y = \left(\frac{x^*v}{z^*v}\right)w = \beta w$, with $\beta \neq 0$ and $w \neq 0$, because $y \neq 0$. Finally, $wx^* = yz^* \Rightarrow wx^* = \beta w z^* \Rightarrow w(x - \overline{\beta}z)^* = 0 \Rightarrow x = \overline{\beta}z$. \square

Theorem 4.2 (General Characterization of \mathbb{G} -reflectors).

Let \mathbb{G} be the automorphism group of a scalar product $\langle \cdot, \cdot \rangle_M$ on \mathbb{K}^n defined by the nonsingular matrix M , and let $q(u) = \langle u, u \rangle_M$.

(a) *If G is a \mathbb{G} -reflector then it is expressible in the form*

$$G = \begin{cases} I + \beta uu^T M & \text{if } \langle \cdot, \cdot \rangle_M \text{ is bilinear,} \\ I + \beta uu^* M & \text{if } \langle \cdot, \cdot \rangle_M \text{ is sesquilinear,} \end{cases} \quad (4.1)$$

for some $\beta \in \mathbb{K} \setminus \{0\}$ and $u \in \mathbb{K}^n \setminus \{0\}$.

(b) *Not every G given by (4.1) is in \mathbb{G} ; the parameters β and u must satisfy an additional relation:*

$$\text{bilinear forms: } G \in \mathbb{G} \Leftrightarrow (M + (1 + \beta q(u))M^T)u = 0, \quad (4.2)$$

$$\text{sesquilinear forms: } G \in \mathbb{G} \Leftrightarrow (\beta M + (\overline{\beta} + |\beta|^2 q(u))M^*)u = 0. \quad (4.3)$$

Proof. We prove only the sesquilinear case; the bilinear case is similar.

Suppose G is a \mathbb{G} -reflector. Then we can write $G = I + uv^*$ for some nonzero $u, v \in \mathbb{K}^n$. Now $G^* \stackrel{\text{def}}{=} M^{-1}G^*M = I + M^{-1}vu^*M$, so we get

$$\begin{aligned} G^*G &= (I + M^{-1}vu^*M)(I + uv^*) \\ &= I + M^{-1}vu^*M + uv^* + M^{-1}v(u^*Mu)v^* \\ &= I + M^{-1}(v(M^*u)^* + (Mu + q(u)v)v^*). \end{aligned}$$

Thus $G^*G = I \Leftrightarrow (Mu + q(u)v)v^* = -v(M^*u)^*$. Then by Lemma 4.1 we have

$$-v = \beta(Mu + q(u)v), \quad (4.4)$$

$$v = \bar{\beta}M^*u, \quad (4.5)$$

for some nonzero $\beta \in \mathbb{K}$. Using (4.5) we obtain part (a) of the theorem:

$$G = I + uv^* = I + u(\bar{\beta}M^*u)^* = I + \beta uu^*M.$$

To prove part (b), rearrange (4.4), and substitute in (4.5) to get

$$\begin{aligned} \beta Mu + (1 + \beta q(u))v &= 0, \\ (\beta M + (\bar{\beta} + |\beta|^2 q(u))M^*)u &= 0. \end{aligned} \quad (4.6)$$

Thus $G \in \mathbb{G} \Rightarrow (4.6)$. To prove the converse, let $G = I + \beta uu^*M$, so that $G^* = I + \bar{\beta}M^{-1}M^*uu^*M$. Then

$$\begin{aligned} G^*G &= (I + \bar{\beta}M^{-1}M^*uu^*M)(I + \beta uu^*M) \\ &= I + M^{-1}(\beta M + (\bar{\beta} + |\beta|^2 q(u))M^*)uu^*M, \end{aligned}$$

and hence (4.6) $\Rightarrow G^*G = I \Rightarrow G \in \mathbb{G}$. □

When u is isotropic, that is, when $q(u) = 0$, conditions (4.2) and (4.3) in Theorem 4.2 simplify considerably. The following example illustrates a situation where \mathbb{G} -reflectors can be readily constructed using an isotropic u .

Example 4.1. Consider the bilinear form on \mathbb{R}^2 defined by $M = \begin{bmatrix} 2 & 1 \\ -1 & 0 \end{bmatrix}$. Then $u = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ is isotropic, and condition (4.2) simplifies to checking that $(M + M^T)u = 0$. Since $M + M^T = \begin{bmatrix} 4 & 0 \\ 0 & 0 \end{bmatrix}$, this is clearly satisfied for any $\beta \in \mathbb{R}$. Thus

$$G = I + \beta uu^T M = I + \beta \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ -1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -\beta & 1 \end{bmatrix}$$

is a \mathbb{G} -reflector for any β . This can be independently confirmed by checking that

$$G^* \stackrel{\text{def}}{=} M^{-1}G^T M = \begin{bmatrix} 1 & 0 \\ \beta & 1 \end{bmatrix} = G^{-1}.$$

The next example shows that for some scalar products there may not be any \mathbb{G} -reflectors at all.

Example 4.2. Consider \mathbb{R}^2 equipped with the bilinear form $\langle x, y \rangle_M = x^T M y$ where $M = \begin{bmatrix} 2 & 1 \\ 0 & 2 \end{bmatrix}$. Letting $c = 1 + \beta q(u)$, condition (4.2) becomes $(M + cM^T)u = 0$. But $M + cM^T = \begin{bmatrix} 2c+2 & 1 \\ c & 2c+2 \end{bmatrix}$ is nonsingular for all $c \in \mathbb{R}$, since $\det(M + cM^T) = 4c^2 + 7c + 4 > 0$ for all $c \in \mathbb{R}$. Consequently there is no nonzero vector u that can satisfy (4.2), and thus this scalar product has no \mathbb{G} -reflectors at all.

We shall see in Theorem 7.3 that there is always a generous supply of \mathbb{G} -reflectors for any bilinear form $\langle \cdot, \cdot \rangle_M$ with $M^T = \pm M$, or sesquilinear form with $M^* = \alpha M$, $|\alpha| = 1$; for these scalar products the situation in Example 4.2 cannot arise.

5 Variant forms of \mathbb{G} -reflectors

An alternate version of the basic form (4.1) for \mathbb{G} -reflectors is found by solving (4.5) for u before substituting into $G = I + uv^*$. One obtains:

$$G = \begin{cases} I + \beta M^{-T} v v^T & \text{if } \langle \cdot, \cdot \rangle_M \text{ is bilinear,} \\ I + \beta M^{-*} v v^* & \text{if } \langle \cdot, \cdot \rangle_M \text{ is sesquilinear,} \end{cases} \quad (5.1)$$

for suitable choice of scalar $\beta \in \mathbb{K}$ and vector $v \in \mathbb{K}^n$. This alternate form will in general be less convenient than the form (4.1). However, in many commonly occurring examples we have $M^{-1} = M^T$ (or $M^{-1} = M^*$ for sesquilinear forms), so that the alternate form simplifies to

$$G = \begin{cases} I + \beta M v v^T & \text{if } \langle \cdot, \cdot \rangle_M \text{ is bilinear,} \\ I + \beta M v v^* & \text{if } \langle \cdot, \cdot \rangle_M \text{ is sesquilinear.} \end{cases} \quad (5.2)$$

A further consequence of $M^{-1} = M^T$ ($M^{-1} = M^*$) is that $M^{-1} \in \mathbb{G}$, so that the matrices

$$M^{-1}G = \begin{cases} M^T + \beta v v^T & \text{if } \langle \cdot, \cdot \rangle_M \text{ is bilinear,} \\ M^* + \beta v v^* & \text{if } \langle \cdot, \cdot \rangle_M \text{ is sesquilinear,} \end{cases} \quad (5.3)$$

are also elements of \mathbb{G} , although they no longer have a fixed hyperplane and thus are not \mathbb{G} -reflectors.

The form given in (5.2) is used by Stewart and Stewart [30] for \mathbb{G} -reflectors in $\mathbb{G} = O(p, q, \mathbb{R})$. On the other hand, Rader and Steinhardt [27] used the non- \mathbb{G} -reflector form given in (5.3) under the name ‘‘hyperbolic Householder’’. In both cases, $M = I_p \oplus -I_q$.

The various forms (4.1), (5.1), and (5.3) may sometimes have other structure in addition to being elements of \mathbb{G} . We will not give a complete analysis here, but just note a few examples. When $\langle \cdot, \cdot \rangle_M$ is a symmetric bilinear form, then the corresponding matrices in (4.1) and (5.1) are also in the Jordan algebra of the scalar product, while the matrices in (5.3) are symmetric. Similarly, for sesquilinear forms $\langle \cdot, \cdot \rangle_M$, the \mathbb{G} -reflectors in (4.1) and (5.1) are in the Jordan algebra when $\beta \in \mathbb{R}$ and M is Hermitian, or when $\beta \in i\mathbb{R}$ and M is skew-Hermitian. The matrices $M^* + \beta v v^* \in \mathbb{G}$ from (5.3) are Hermitian when $\beta \in \mathbb{R}$ and M is Hermitian.

6 Isotropic vectors

Recall that a nonzero vector $x \in \mathbb{K}^n$ is *isotropic* with respect to a given scalar product if $\langle x, x \rangle_M = 0$, and non-isotropic otherwise. For example, when $\langle x, y \rangle \stackrel{\text{def}}{=} x^* y$, no vector in \mathbb{K}^n is isotropic. At the other extreme, with respect to a skew-symmetric bilinear form, every nonzero vector in \mathbb{K}^n is isotropic.

As described in section 3, the geometric action of a \mathbb{G} -reflector is completely determined by its n th eigenvalue, equivalently by $\det G$. The following proposition shows that this geometric information can be more directly inferred from (4.1), simply by determining whether the vector u is isotropic or not.

Proposition 6.1. *For a \mathbb{G} -reflector G given by (4.1), we have*

$$u \text{ is isotropic} \Leftrightarrow G \text{ is a shear/transvection} \quad (6.1a)$$

$$u \text{ is non-isotropic} \Leftrightarrow G \text{ is a reflection or a quasi-symmetry.} \quad (6.1b)$$

Proof. First recall that reflections, quasi-symmetries, and shears/transvections exhaust all the possible types of \mathbb{G} -reflector (see section 3). Thus statements (6.1a) and (6.1b) are just negations of each other, so that it suffices to prove just the forward implication (\Rightarrow) of each statement. Next note that u is always an eigenvector of G , since $Gu = (1 + \beta q(u))u \stackrel{\text{def}}{=} \lambda u$. Clearly

$$\begin{aligned} u \text{ is isotropic} &\Rightarrow q(u) = 0 \Rightarrow \lambda = 1 \Rightarrow u \in \mathcal{H}, \\ u \text{ is non-isotropic} &\Rightarrow q(u) \neq 0 \Rightarrow \lambda \neq 1 \Rightarrow u \notin \mathcal{H}, \end{aligned}$$

where \mathcal{H} is the fixed hyperplane of G . But $u \notin \mathcal{H}$ means that G is diagonalizable, and hence a reflection or a quasi-symmetry. This establishes the forward implication (\Rightarrow) of (6.1b).

On the other hand, if $u \in \mathcal{H}$, then we claim that G must be non-diagonalizable. Consider an arbitrary vector $x \notin \mathcal{H}$. By (4.1), $Gx - x = \beta \langle u, x \rangle_M u \in \mathcal{H}$. But if x was an eigenvector of G with eigenvalue k ($k \neq 1$, since otherwise $G = I$), then $Gx - x = (k - 1)x \notin \mathcal{H}$, a contradiction. Thus G has no eigenvectors outside of \mathcal{H} , and therefore must be non-diagonalizable. This forces $\lambda = 1$ to be the only eigenvalue of G ; and hence G is a shear/transvection, as described in section 3. This establishes the forward implication (\Rightarrow) of (6.1a). \square

The following proposition gives an alternate way to express the results of the preceding argument.

Proposition 6.2. *For a \mathbb{G} -reflector G given by (4.1), we have*

$$\begin{aligned} u \text{ is isotropic} &\Leftrightarrow G \text{ is non-diagonalizable,} \\ u \text{ is non-isotropic} &\Leftrightarrow G \text{ is diagonalizable.} \end{aligned}$$

7 Orthosymmetric scalar products

We turn now from arbitrary scalar products to focus on a special class of scalar products that includes symmetric and skew-symmetric bilinear forms as well as Hermitian and skew-Hermitian sesquilinear forms. The following result, proved in [21], gives four characterizations of this class of scalar products.

Theorem 7.1. *For a scalar product $\langle \cdot, \cdot \rangle_M$ on \mathbb{K}^n , the following properties are equivalent:*

1. *Vector orthogonality is a symmetric relation, i.e., $\langle x, y \rangle_M = 0 \Leftrightarrow \langle y, x \rangle_M = 0$, $\forall x, y \in \mathbb{K}^n$.*
2. *Adjoint with respect to $\langle \cdot, \cdot \rangle_M$ is involutory, i.e., $(A^\star)^\star = A$, $\forall A \in \mathbb{K}^{n \times n}$.*
3. $\mathbb{K}^{n \times n} = \mathbb{L} \oplus \mathbb{J}$.
4. $M^T = \pm M$ for bilinear forms;
 $M^\star = \alpha M$ with $\alpha \in \mathbb{C}$, $|\alpha| = 1$ for sesquilinear forms.

In light of this result, we make the following definition.

Definition 7.2. A scalar product with any one (and hence all) of the properties in Theorem 7.1 will be referred to as an *orthosymmetric* scalar product.

The term "orthosymmetric" is motivated by the first property⁴ in Theorem 7.1, following the usage in Shaw [29]. Two further reasons for the special significance and centrality of orthosymmetric scalar products among all scalar products are the following:

- Suppose $\langle \cdot, \cdot \rangle_M$ is an arbitrary scalar product, and $M = S + K$ is the decomposition of M into its symmetric and skew-symmetric parts if the form is bilinear, respectively into its Hermitian and skew-Hermitian parts if the form is sesquilinear. Then, as observed in [8], a map G is an automorphism of $\langle \cdot, \cdot \rangle_M$ if and only if it is simultaneously an automorphism of $\langle \cdot, \cdot \rangle_S$ and $\langle \cdot, \cdot \rangle_K$.
- Orthosymmetric scalar products and their associated automorphism groups are the ones typically encountered in applications, as illustrated by the sampling of examples in Table 2.1.

The treatment of general orthosymmetric sesquilinear forms is greatly simplified by exploiting their close connection to Hermitian sesquilinear forms. Consider $\langle x, y \rangle_M = x^* M y$, where $M^* = \alpha M$ for $\alpha \in \mathbb{C}$ such that $|\alpha| = 1$. Then the sesquilinear form defined by the Hermitian matrix $H \stackrel{\text{def}}{=} \sqrt{\alpha} M$ is just a scalar multiple of $\langle \cdot, \cdot \rangle_M$:

$$\langle x, y \rangle_H = \sqrt{\alpha} \langle x, y \rangle_M \quad \text{for all } x, y \in \mathbb{C}^n.$$

Consequently, the automorphism group of $\langle \cdot, \cdot \rangle_H$ is identical to the automorphism group of $\langle \cdot, \cdot \rangle_M$:

$$\langle Gx, Gy \rangle_H = \langle x, y \rangle_H \Leftrightarrow \sqrt{\alpha} \langle Gx, Gy \rangle_M = \sqrt{\alpha} \langle x, y \rangle_M \Leftrightarrow \langle Gx, Gy \rangle_M = \langle x, y \rangle_M.$$

Similarly, the Lie and Jordan algebras of $\langle \cdot, \cdot \rangle_H$ and $\langle \cdot, \cdot \rangle_M$ are also identical. Thus a result established for Hermitian sesquilinear forms immediately translates into a corresponding result for orthosymmetric sesquilinear forms. Note also that up to a scalar multiple there are really only three distinct types of orthosymmetric scalar products: symmetric and skew-symmetric bilinear, and Hermitian sesquilinear. We will, however, continue to include separately stated results (sans separate proofs) for skew-Hermitian forms for convenience, as this is a commonly occurring special case. In light of the above remarks, the similarities and differences between the results for Hermitian and skew-Hermitian forms found in the rest of the paper should become transparent.

Theorem 7.3 shows that there is always a generous supply of \mathbb{G} -reflectors in orthosymmetric scalar product spaces, unlike the situation illustrated in Example 4.2, when the automorphism group contained none. In particular, for the unitary group $\mathbb{G} = U(n)$, Theorem 7.3(c) provides a continuum of non-Hermitian unitary reflectors that for the most part have not been treated in the literature (notable exceptions include Lehoucq [19] and Laurie [18]).

Theorem 7.3 (\mathbb{G} -reflectors for orthosymmetric scalar products).

- (a) *Symmetric bilinear forms* ($M^T = M$ and $q(u) \in \mathbb{K}$):

$$\text{For } \beta \neq 0 \text{ and } u \neq 0, \quad G = I + \beta u u^T M \in \mathbb{G} \Leftrightarrow u \text{ is non-isotropic and } \beta = \frac{-2}{q(u)}.$$

⁴For bilinear forms, [3], [15], and [29] all show that symmetry of vector orthogonality holds if and only if $M^T = \pm M$; none of these authors consider the corresponding question for sesquilinear forms.

(b) *Skew-symmetric bilinear forms* ($M^T = -M$ and $q(u) \equiv 0$):

$$G = I + \beta uu^T M \in \mathbb{G} \text{ for any } u \in \mathbb{K}^{2n} \text{ and any } \beta \in \mathbb{K}.$$

(c) *Hermitian sesquilinear forms* ($M^* = M$ and $q(u) \in \mathbb{R}$):

$$G = I + \beta uu^* M \in \mathbb{G} \text{ if and only if one of the following holds :}$$

(i) u is isotropic and $\beta \in i\mathbb{R}$.

(ii) u is non-isotropic and $\beta \in \mathbb{C}$ is on the circle $|\beta - r| = |r|$, where $r \stackrel{\text{def}}{=} \frac{-1}{q(u)} \in \mathbb{R}$.

(d) *Skew-Hermitian sesquilinear forms* ($M^* = -M$ and $q(u) \in i\mathbb{R}$):

$$G = I + \beta uu^* M \in \mathbb{G} \text{ if and only if one of the following holds :}$$

(i) u is isotropic and $\beta \in \mathbb{R}$.

(ii) u is non-isotropic and $\beta \in \mathbb{C}$ is on the circle $|\beta - r| = |r|$, where $r \stackrel{\text{def}}{=} \frac{-1}{q(u)} \in i\mathbb{R}$.

Proof. (a): The relation (4.2) simplifies to $(2 + \beta q(u))Mu = 0$. Since M is non-singular this can only occur if $\beta q(u) = -2$. Hence $q(u) \neq 0$, so u is non-isotropic, and $\beta = -2/q(u)$ is the unique choice for the scalar β . This result was also obtained by Scherk [28].

(b): In this case (4.2) simplifies to $-\beta q(u)Mu = 0$. But for a skew-symmetric bilinear form, $q(u) \equiv 0$, so (4.2) is satisfied for all $u \in \mathbb{K}^{2n}$ and all $\beta \in \mathbb{K}$.

(c): The relation (4.3) simplifies to $(\beta + \bar{\beta} + |\beta|^2 q(u))Mu = 0$. Since M is non-singular, we must have

$$\beta + \bar{\beta} + |\beta|^2 q(u) = 0. \quad (7.1)$$

For isotropic u , (7.1) becomes $\beta + \bar{\beta} = 0$, i.e., $\beta \in i\mathbb{R}$. For non-isotropic u we know that $q(u)$ is real, so letting $q(u) = -1/r$ with $0 \neq r \in \mathbb{R}$ and $\beta = a + ib$, (7.1) becomes $-2ar + a^2 + b^2 = 0$. Equivalently, $(a - r)^2 + b^2 = r^2$, or $|\beta - r| = |r|$.

(d): The skew-Hermitian case follows from part (c), as discussed earlier in this section. \square

When combined with Proposition 6.1, Theorem 7.3 gives a complete characterization of the geometric type of all \mathbb{G} -reflectors in certain scalar product spaces. For example, if \mathbb{G} is the automorphism group of a symmetric bilinear form $\langle \cdot, \cdot \rangle_M$, then every \mathbb{G} -reflector must be a reflection. By contrast, when $\langle \cdot, \cdot \rangle_M$ is a skew-symmetric bilinear form, \mathbb{G} -reflectors can only be shears/transvections.

In section 3 it was observed (on geometrical grounds) that the inverse of any \mathbb{G} -reflector G is also a \mathbb{G} -reflector. In all cases $G^{-1} = G^*$, of course, but for the scalar products considered in Theorem 7.3, the formulas for these inverses have a particularly simple form.

- For symmetric bilinear forms with $G = I + \beta uu^T M$, we have $G^{-1} = G^* = G$, and hence $G^2 = I$, so G is involutory. This fits with the geometric characterization of all \mathbb{G} -reflectors for symmetric bilinear forms as reflections.

- For skew-symmetric bilinear forms with $G = I + \beta uu^T M$, we have

$$G^{-1} = G^* = I - \beta uu^T M .$$

- For Hermitian sesquilinear forms with $G = I + \beta uu^* M$, the inverse is given by

$$G^{-1} = G^* = I + \bar{\beta} uu^* M .$$

- For skew-Hermitian sesquilinear forms with $G = I + \beta uu^* M$, we have

$$G^{-1} = G^* = I - \bar{\beta} uu^* M .$$

7.1 β -sets

For each vector $u \in \mathbb{K}^n$ there is a set of scalars $\beta \in \mathbb{K}$ such that $I + \beta uu^T M$ (or $I + \beta uu^* M$) is a \mathbb{G} -reflector. Recall from Example 4.2 that this set may be empty. However, Theorem 7.3 shows this is usually not the case for an orthosymmetric scalar product. The only exception is when the scalar product is symmetric bilinear and the vector u is isotropic.

The possible β -sets for a Hermitian sesquilinear form are shown in Figure 7.1. In this case $q(u) \in \mathbb{R}$, and both the center and radius of the circle of β values are proportional to the reciprocal of $q(u)$. Figure 7.2 depicts the β -sets for a skew-Hermitian sesquilinear form.

Figure 7.1: β -sets (thick lines) for a Hermitian sesquilinear form, $r = \frac{-1}{q(u)}$.

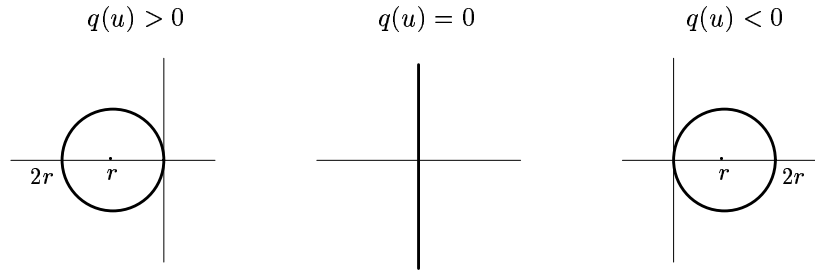
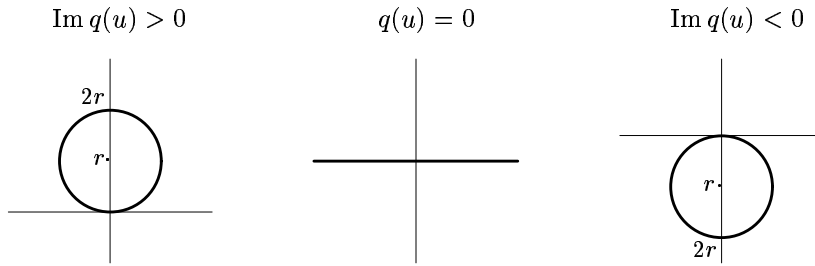


Figure 7.2: β -sets (thick lines) for a skew-Hermitian sesquilinear form, $r = \frac{-1}{q(u)}$.



When viewed on the Riemann sphere, the continuity of these β -sets as a function of the parameter $q(u)$ is apparent. In each case the circular β -sets associated with non-isotropic vectors u approach the linear β -set for isotropic vectors as u gets closer to being isotropic.

7.2 \mathbb{G} -reflectors with extra structure

Among all the β -values for a given u that make $G = I + \beta uu^T M$ (or $I + \beta uu^* M$) into a \mathbb{G} -reflector, there are certain choices of β that impart additional structure to G . For a Hermitian sesquilinear form $\langle \cdot, \cdot \rangle_M$, G is in the Jordan algebra of $\langle \cdot, \cdot \rangle_M$, i.e. $G^* = G$, if and only if $\beta \in \mathbb{R}$. From Figure 7.1 this means $\beta = 2r = -2/q(u)$ is the only such choice, and u must be non-isotropic. A particular instance of this are the unitary reflectors $G = I + \beta uu^*$. For a given u , only $\beta = 2r = -2/q(u)$ gives a unitary reflector that is also in the Jordan algebra, i.e. that is also Hermitian. Every other choice of β on the circular β -set gives a non-Hermitian unitary reflector.

The situation is similar for skew-Hermitian sesquilinear forms. Here a \mathbb{G} -reflector is in the Jordan algebra if and only if $\beta \in i\mathbb{R}$. From Figure 7.2 it is apparent that this can be arranged only by using a non-isotropic u , and from among all the allowed β 's for this u , choosing β to be $2r = -2/q(u) \in i\mathbb{R}$.

Symmetric bilinear forms are a bit of an anomaly in comparison with all other orthosymmetric scalar products. In the latter case, any u can be used to build a \mathbb{G} -reflector, and for any u there is a continuum of choices for β that make (4.1) into a \mathbb{G} -reflector. By contrast, for a symmetric bilinear form only non-isotropic u can be used, and for any such u there is a unique choice of β that yields a \mathbb{G} -reflector. As an unexpected compensation for this lack of freedom in choosing β , though, we find that *every* \mathbb{G} -reflector is also automatically an element of the Jordan algebra (see section 7, formulas for inverses).

8 Mapping problem

Let $\langle \cdot, \cdot \rangle_M$ be a fixed scalar product with associated automorphism group \mathbb{G} . We know from Theorem 4.2 that any \mathbb{G} -reflector can be expressed as

$$G = \begin{cases} I + \beta uu^T M & \text{if } \langle \cdot, \cdot \rangle_M \text{ is bilinear,} \\ I + \beta uu^* M & \text{if } \langle \cdot, \cdot \rangle_M \text{ is sesquilinear.} \end{cases} \quad (8.1)$$

The *mapping problem for \mathbb{G} -reflectors* asks:

1. For which vectors $x, y \in \mathbb{K}^n$ is it possible to find some \mathbb{G} -reflector G such that $Gx = y$?
2. How can such a G be explicitly specified, whenever it exists?

Observe that every matrix in \mathbb{G} (not just \mathbb{G} -reflectors) preserves the values of q , since

$$q(Gx) = \langle Gx, Gx \rangle_M = \langle x, x \rangle_M = q(x), \quad \forall x \in \mathbb{K}^n. \quad (8.2)$$

Thus $q(x) = q(y)$ is a necessary condition for there to exist a \mathbb{G} -reflector mapping x to y . The next proposition describes two further necessary conditions, one on the vectors x and y , and the other on the form of the \mathbb{G} -reflector itself. Note that these conditions apply in *any* automorphism group \mathbb{G} . Theorem 8.2 then shows that these conditions are also sufficient when \mathbb{G} arises from an orthosymmetric scalar product. This is done by giving an explicit formula for a \mathbb{G} -reflector G such that $Gx = y$. The G so constructed is also shown to be unique. Some special cases of Theorem 8.2 were obtained by Mehrmann in [24] and Uhlig in [32].

Proposition 8.1. *Suppose $x, y \in \mathbb{K}^n$ are distinct nonzero vectors, and G is a \mathbb{G} -reflector such that $Gx = y$. Then the vectors x and y must satisfy the condition $\langle y - x, x \rangle_M \neq 0$, and in (8.1) G must have $u = \alpha(y - x)$ for some $0 \neq \alpha \in \mathbb{K}$ and $\beta = 1/(\alpha \langle u, x \rangle_M)$.*

Proof. By (8.1), $Gx = x + \beta \langle u, x \rangle_M u$. But then $Gx = y \Rightarrow 0 \neq y - x = \beta \langle u, x \rangle_M u$, so that $\beta \neq 0$ and $\langle u, x \rangle_M \neq 0$. This in turn implies that $u = \alpha(y - x)$ with $\alpha = 1/(\beta \langle u, x \rangle_M) \neq 0$, so that $\beta = 1/(\alpha \langle u, x \rangle_M)$. Finally, $\langle u, x \rangle_M \neq 0 \Rightarrow \langle \alpha(y - x), x \rangle_M \neq 0 \Rightarrow \langle y - x, x \rangle_M \neq 0$. \square

Theorem 8.2 (\mathbb{G} -reflector mapping theorem).

Suppose \mathbb{K}^n is equipped with an orthosymmetric scalar product $\langle \cdot, \cdot \rangle_M$; i.e. a scalar product that is either symmetric bilinear, skew-symmetric bilinear, or sesquilinear with $M^ = \gamma M$ for some $|\gamma| = 1$. Then for distinct nonzero vectors $x, y \in \mathbb{K}^n$, there exists a \mathbb{G} -reflector G such that $Gx = y$ if and only if $q(x) = q(y)$ and $\langle y - x, x \rangle_M \neq 0$. Furthermore, whenever G exists it is unique, and can be specified by taking $u = y - x$ and $\beta = 1/\langle u, x \rangle_M$ in (8.1). Equivalently, G may be specified by taking $u = x - y$ and $\beta = -1/\langle u, x \rangle_M$ in (8.1).*

Proof. The necessity of the conditions $q(x) = q(y)$ and $\langle y - x, x \rangle_M \neq 0$ was established in (8.2) and Proposition 8.1. Their sufficiency is demonstrated by showing that $Gx = y$ and $G \in \mathbb{G}$ for the indicated choices of u and β . Abbreviating $\langle \cdot, \cdot \rangle_M$ to $\langle \cdot, \cdot \rangle$, we have from (8.1) that

$$Gx = x + \beta \langle u, x \rangle u = x + u = y.$$

Thus to establish existence it only remains to show that $G \in \mathbb{G}$ in each case.

- For a symmetric bilinear form, condition (4.2) reduces to showing that $2 + \beta q(u) = 0$. Substituting for β and u we get

$$2 + \beta q(u) = \frac{2\langle u, x \rangle + \langle u, u \rangle}{\langle u, x \rangle} = \frac{\langle u, 2x + u \rangle}{\langle u, x \rangle} = \frac{\langle y - x, y + x \rangle}{\langle u, x \rangle} = 0,$$

since the form is symmetric and $q(x) = q(y)$.

- When the form is skew-symmetric bilinear, then $M^T = -M$ and $q(u) \equiv 0$, and hence $G \in \mathbb{G}$ by (4.2).
- For a sesquilinear form with $M^* = \gamma M$, condition (4.3) reduces to showing that

$$\beta + \gamma \bar{\beta} + \gamma \beta \bar{\beta} q(u) = 0. \quad (8.3)$$

But $M^* = \gamma M$ means that $\overline{\langle u, x \rangle} = \gamma \langle x, u \rangle$, so that with $\beta = 1/\langle u, x \rangle$, we have $\gamma \bar{\beta} = 1/\langle x, u \rangle$. Thus $\beta + \gamma \bar{\beta} + \gamma \beta \bar{\beta} q(u)$ becomes

$$\frac{\langle x, u \rangle + \langle u, x \rangle + \langle u, u \rangle}{\langle x, u \rangle \langle u, x \rangle} = \frac{\langle x, y - x \rangle + \langle y - x, y \rangle}{\langle x, u \rangle \langle u, x \rangle} = 0, \quad (8.4)$$

since $q(x) = q(y)$, establishing (8.3).

To see that G is unique, consider the only other possible choices for u and β . From proposition 8.1 we know that $u = \alpha(y - x)$ and $\beta = 1/(\alpha \langle u, x \rangle_M)$ for some nonzero $\alpha \in \mathbb{K}$. With this u and β in the sesquilinear case of (8.1) we have

$$\begin{aligned} I + \beta u u^* M &= I + \frac{1}{\alpha \langle \alpha(y - x), x \rangle_M} \alpha(y - x) (\alpha(y - x))^* M \\ &= I + \frac{1}{(\alpha \bar{\alpha}) \langle y - x, x \rangle_M} (\alpha \bar{\alpha}) (y - x) (y - x)^* M = G, \end{aligned}$$

for any $\alpha \neq 0$. Thus all choices of u and β produce the same G . A similar argument works in the bilinear case. \square

8.1 Alternative forms for the mapping problem solution

The formula given in Theorem 8.2 for the \mathbb{G} -reflector that maps x to y may often be rewritten in an alternate form that provides some additional insight into the \mathbb{G} -reflector mapping problem, as well as a more direct link to the results of section 7 and to several well-known special cases.

However, this alternate form can be achieved only if the vector $y - x$ is *not* isotropic. This condition on $y - x$ may be a huge restriction, a moderate restriction, or no restriction at all, depending on the scalar product being used. With this caveat firmly in mind, we begin with the following simple lemma.

Lemma 8.3. *Suppose $\langle \cdot, \cdot \rangle$ is any scalar product, and $x, y \in \mathbb{K}^n$ are any two vectors such that $\langle x, x \rangle = \langle y, y \rangle$. If $u = y - x$ then $\langle u, u \rangle = -\langle x, u \rangle - \langle u, x \rangle$.*

Proof.

$$\begin{aligned} \langle u, u \rangle &= \langle u, y \rangle - \langle u, x \rangle = \langle y, y \rangle - \langle x, y \rangle - \langle u, x \rangle \\ &= \langle x, x \rangle - \langle x, y \rangle - \langle u, x \rangle = -\langle x, u \rangle - \langle u, x \rangle. \quad \square \end{aligned}$$

Proposition 8.4. *Suppose $u = y - x$ is non-isotropic, so that $q(u) = \langle u, u \rangle_M \neq 0$. Then $G = I + \frac{uu^*M}{\langle u, x \rangle_M}$ from Theorem 8.2 can be rewritten as*

$$G = I + \left(-1 - \frac{\langle x, u \rangle_M}{\langle u, x \rangle_M} \right) \frac{uu^*M}{q(u)}, \quad (8.5)$$

*Note that (8.5) gives the same G if $u = x - y$. (For bilinear forms, replace uu^*M by $uu^T M$.)*

Proof.

$$\begin{aligned} I + \frac{uu^*M}{\langle u, x \rangle_M} &= I + \left(\frac{\langle u, u \rangle_M}{\langle u, x \rangle_M} \right) \frac{uu^*M}{\langle u, u \rangle_M} \\ &= I + \left(\frac{-\langle u, x \rangle_M - \langle x, u \rangle_M}{\langle u, x \rangle_M} \right) \frac{uu^*M}{q(u)} \\ &= I + \left(-1 - \frac{\langle x, u \rangle_M}{\langle u, x \rangle_M} \right) \frac{uu^*M}{q(u)}. \quad \square \end{aligned}$$

Let us examine how formula (8.5) specializes for particular types of orthosymmetric scalar product.

- If $\langle \cdot, \cdot \rangle_M$ is a symmetric bilinear form, then Lemma 8.3 says that $\langle u, u \rangle = -2\langle u, x \rangle$. Thus $u = y - x$ is non-isotropic if and only if $\langle u, x \rangle \neq 0$. Since $\langle u, x \rangle \neq 0$ is one of the necessary conditions in the \mathbb{G} -reflector mapping theorem, we see that u being non-isotropic is in this case no restriction at all, and (8.5) applies to any \mathbb{G} -reflector from Theorem 8.2. In addition we have $\left(-1 - \frac{\langle x, u \rangle_M}{\langle u, x \rangle_M} \right) = -2$. Substituting in (8.5) gives

$$G = I - \frac{2uu^T M}{q(u)}, \quad (8.6)$$

bringing us back to the form in Theorem 7.3(a), and giving us an expression that resembles the well-known formula for the real orthogonal Householder transformation mapping x to y .

- If $\langle \cdot, \cdot \rangle_M$ is a skew-symmetric bilinear form, then *every* vector is isotropic, so formula (8.5) will never be a valid representation for any \mathbb{G} -reflector. In this case the only significant simplification to the formula for G given in Theorem 8.2 is to observe that

$$\langle u, x \rangle_M = \langle y - x, x \rangle_M = \langle y, x \rangle_M - \langle x, x \rangle_M = \langle y, x \rangle_M .$$

Thus we have

$$G = I + \frac{uu^T M}{\langle y, x \rangle_M} , \quad (8.7)$$

with the condition $\langle u, x \rangle_M \neq 0$ replaced by $\langle y, x \rangle_M \neq 0$.

- When $\langle \cdot, \cdot \rangle_M$ is a Hermitian sesquilinear form, then $\langle x, u \rangle_M = \overline{\langle u, x \rangle_M}$, so that (8.5) becomes

$$G = I + \beta uu^* M, \quad \text{where} \quad \beta = \frac{1}{q(u)} \left(-1 - \frac{\overline{\langle u, x \rangle_M}}{\langle u, x \rangle_M} \right) . \quad (8.8)$$

Observe that $\overline{\langle u, x \rangle_M} / \langle u, x \rangle_M$ is a complex number of unit length, and $q(u)$ is a nonzero real number, so the coefficient β can immediately be seen to lie on one of the circles shown in Figure 7.1 of section 7.1.

By contrast with the situation for symmetric bilinear forms, in this case the issue of $u = y - x$ being isotropic or not is independent of whether $\langle u, x \rangle$ is zero or not. That is, for Hermitian sesquilinear forms a \mathbb{G} -reflector mapping x to y may exist even if $u = y - x$ is isotropic, so that the form (8.8) will not be available for every \mathbb{G} -reflector supplied by Theorem 8.2.

In the special case when $M = I$ we have $\langle v, w \rangle \stackrel{\text{def}}{=} v^* w$, and \mathbb{G} is the unitary group. Since in this case there are no isotropic vectors, every \mathbb{G} -reflector given by Theorem 8.2 is expressible in the form (8.8); with unit vector $u = (y - x) / \|y - x\|_2$, this now simplifies to

$$G = I - uu^* - \left(\frac{\overline{u^* x}}{u^* x} \right) uu^* . \quad (8.9)$$

This is the form proposed by Laurie in [18] for unitary reflectors mapping x to y .

- Finally, when $\langle \cdot, \cdot \rangle_M$ is a skew-Hermitian sesquilinear form, then $\langle x, u \rangle_M = -\overline{\langle u, x \rangle_M}$, and (8.5) becomes

$$G = I + \beta uu^* M, \quad \text{where} \quad \beta = \frac{1}{q(u)} \left(-1 + \frac{\overline{\langle u, x \rangle_M}}{\langle u, x \rangle_M} \right) . \quad (8.10)$$

In this case $q(u)$ is a pure imaginary number, and once again we can immediately see that β lies on one of the circles shown in Figure 7.2 of section 7.1.

The alternative forms for solutions to the \mathbb{G} -reflector mapping problem presented in this section can certainly be useful, but their diversity of form and restricted validity gives added emphasis to the simplicity of the common unified formula provided by Theorem 8.2.

8.2 Mapping by unitary reflectors

The more general perspective of the \mathbb{G} -reflector mapping theorem yields a simple development of the properties of complex unitary \mathbb{G} -reflectors as a special case. In this section $\langle u, v \rangle \stackrel{\text{def}}{=} u^*v$.

Lemma 8.5. *Consider $x, y \in \mathbb{C}^n$ such that $\|x\|_2 = \|y\|_2$. Then $\langle y - x, x \rangle = 0 \Leftrightarrow y = x$.*

Proof. The result holds trivially if $x = 0$, so assume that $x \neq 0$.

$$\begin{aligned} \langle y - x, x \rangle = 0 &\Rightarrow \langle y, x \rangle = \langle x, x \rangle \\ &\Rightarrow |\langle y, x \rangle| = \|x\|_2^2 = \|x\|_2 \|y\|_2 \\ &\Rightarrow y = \alpha x, \quad \alpha \in \mathbb{C}, \quad \text{by Cauchy-Schwartz} \\ &\Rightarrow \langle \alpha x, x \rangle = \langle x, x \rangle \\ &\Rightarrow \bar{\alpha} \langle x, x \rangle = \langle x, x \rangle \Rightarrow \alpha = 1 \Rightarrow y = x. \quad \square \end{aligned}$$

Theorem 8.6. *For any distinct $x, y \in \mathbb{C}^n$ such that $\|x\|_2 = \|y\|_2$, there exists a unique unitary reflector G such that $Gx = y$. Furthermore, $G = I + \beta uu^*$, where $u = y - x$ and $\beta = 1/(u^*x)$.*

Proof. By Lemma 8.5, $y \neq x \Rightarrow \langle y - x, x \rangle \neq 0$. The desired conclusion now follows from the \mathbb{G} -reflector mapping theorem. \square

We remark that in contrast to real orthogonal reflectors, the development of complex unitary reflectors is not standard fare in textbooks of numerical linear algebra. The implicit assumption that a unitary reflector should be both unitary and Hermitian leads to a theory that is incomplete, and a tool that is circumscribed in flexibility. Special instances of non-Hermitian unitary reflectors were implemented in the Hammarling-Du Croz NAG subroutine F06HRF [25], and in its slight variant, the LAPACK subroutine CLARFG [2], and discussed in Lehoucq [19]; but to our knowledge, a specification of all the unitary reflectors together with a full description of their mapping capabilities has appeared only in Laurie [18].

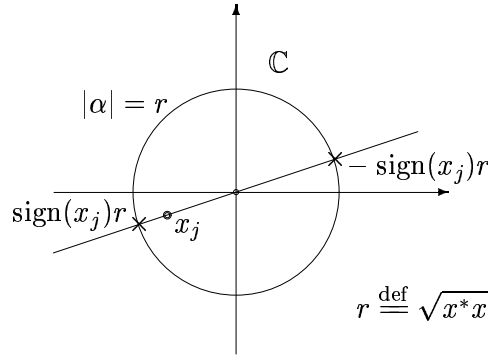
At first glance, requiring that a unitary reflector also be Hermitian seems reasonable since real orthogonal reflectors are symmetric. However, the symmetry of real orthogonal reflectors is automatic, and so in some sense an accidental bonus. Norm preservation together with simplicity of form (i.e., elementary transformation) implies symmetry in the real case⁵, but does not imply Hermitian in the complex case.

From an algorithmic perspective, it is not symmetry that gives a real orthogonal reflector its computational advantage, since its matrix form is not explicitly calculated in practice. The advantage is due to the ease of determining the vector that defines a reflector having a desired mapping property, and also to the efficiency of computing the action of the reflector on other vectors. Theorem 8.6 shows that both Hermitian and non-Hermitian unitary reflectors share these properties.

A comparison of the result of Theorem 8.6 with earlier work is easily made. As shown in section 8.1, the formula for G can be rewritten as in (8.9); this is the form proposed by Laurie in [18]. By contrast, Turnbull and Aitken's non-elementary transformation R that maps p to q (see (1.1)), is the negative of the unique unitary \mathbb{G} -reflector that takes p to $-q$.

⁵Every \mathbb{G} -reflector for a symmetric bilinear form has the additional structure of being in the corresponding Jordan algebra (see section 7.2).

Figure 8.1: Circle of α 's corresponding to unitary reflectors that align x with e_j .



To see this start with $G = I + \beta uu^*$ from Theorem 8.6, with $u = -q - p$ and $\beta = 1/(u^*p)$. Simplifying shows that $G = -R$.

Finally, Theorem 8.6 readily yields a convenient parametrization of the continuum of unitary reflectors that align $0 \neq x \in \mathbb{C}^n$ with e_j . For each $\alpha \in \mathbb{C}$ with $|\alpha| = \sqrt{x^*x}$, the unitary reflector

$$G_\alpha = I + \frac{uu^*}{u^*x} = I + \frac{(x - \alpha e_j)(x - \alpha e_j)^*}{\bar{\alpha}(x_j - \alpha)} \quad (8.11)$$

has the property that $G_\alpha x = \alpha e_j$. Only two choices of α yield a Hermitian reflector; these are identified by \times in Figure 8.1. Note that because this scalar product is positive definite, x_j cannot lie outside the circle of α -values; and if x_j were on the circle, x would already be a multiple of e_j . The inclusion of non-Hermitian reflectors in the toolkit gives one the flexibility to select the polar angle of the scalar multiple of e_j to which x is mapped; for example, one can choose to map x to a real multiple of e_j . This is analogous to the flexibility afforded by unitary Givens rotations, discussed in [4] and [23]. By contrast, limiting oneself to Hermitian reflectors still allows one to map x to αe_j , but α is forced to be $\pm \text{sign}(x_j)\sqrt{x^*x}$, where $\text{sign}(x_j) = x_j/|x_j|$. The importance of this issue is discussed by Lehoucq [19].

8.3 Geometry of the mapping problem

We have seen that the conditions $q(x) = q(y)$ and $\langle y - x, x \rangle_M \neq 0$ are necessary in order for there to exist a \mathbb{G} -reflector mapping x to y , for a general automorphism group \mathbb{G} . It is possible to give a geometric interpretation of these conditions that provides some insight into the scope and limitations of the “mapping power” of \mathbb{G} -reflectors. Let $\mathcal{S}_q(c)$ denote the level surface of the function q with value c , that is,

$$\mathcal{S}_q(c) \stackrel{\text{def}}{=} \{z \in \mathbb{K}^n : q(z) = c\}.$$

Then to have $q(x) = q(y)$ simply means that x and y lie on the same level surface $\mathcal{S}_q(c)$. In \mathbb{R}^3 such a level surface can be an ellipsoid, cone, or hyperboloid.

For a general scalar product $\langle \cdot, \cdot \rangle_M$ and fixed nonzero vector $x \in \mathbb{K}^n$, the set $\mathcal{P}_x \stackrel{\text{def}}{=} \{y \in \mathbb{K}^n : \langle y - x, x \rangle_M = 0\}$ is always a hyperplane in \mathbb{K}^n through the point x . The condition $\langle y - x, x \rangle_M \neq 0$ then says that \mathcal{P}_x is a “forbidden plane”; no \mathbb{G} -reflector with respect to

$\langle \cdot, \cdot \rangle_M$ can map x to any point in \mathcal{P}_x . And conversely, because \mathbb{G} -reflectors are closed under inverses, no \mathbb{G} -reflector can map any point in \mathcal{P}_x to x .

When $\langle \cdot, \cdot \rangle_M$ is any orthosymmetric scalar product, then the \mathbb{G} -reflector mapping theorem can now be interpreted as saying that a nonzero $x \in \mathbb{K}^n$ can be mapped by a \mathbb{G} -reflector to any point on the level surface $\mathcal{S}_q(q(x))$, except for those that are also in the “forbidden” plane \mathcal{P}_x .

The next proposition shows that in the case of a symmetric bilinear form, the forbidden plane \mathcal{P}_x has a simple geometric relationship to the level surface $\mathcal{S}_q(q(x))$ at x .

Proposition 8.7. *Let $\langle \cdot, \cdot \rangle_M$ be a symmetric bilinear form on \mathbb{K}^n , $q(u) = \langle u, u \rangle_M$ the associated quadratic form, and $0 \neq x \in \mathbb{K}^n$. Then the set $\mathcal{T}_x\mathcal{S}$ of all tangent vectors to the surface $\mathcal{S}_q(q(x))$ at the point x is the same as the set $(x)_M^\perp \stackrel{\text{def}}{=} \{w \in \mathbb{K}^n : \langle w, x \rangle_M = 0\}$.*

Thus the condition $\langle y - x, x \rangle_M = 0$ says that $y - x$ is a tangent vector at the point x , and hence Proposition 8.7 says that \mathcal{P}_x is the tangent space to $\mathcal{S}_q(q(x))$ at x . Note that this result generalizes the well-known fact that for a sphere \mathcal{S} centered at the origin and $x \in \mathcal{S}$, the tangent space at x is just $\{y \in \mathbb{R}^n : y - x \in x^\perp\}$, where x^\perp is the Euclidean orthogonal complement.

Proof. Since $\mathcal{T}_x\mathcal{S}$ and $(x)_M^\perp$ are both $(n - 1)$ -dimensional subspaces, it suffices to show that $\mathcal{T}_x\mathcal{S}$ is contained in $(x)_M^\perp$. For brevity, let $c = q(x)$. Every tangent vector to $\mathcal{S}_q(c)$ is realized as the tangent vector of some smooth path in $\mathcal{S}_q(c)$, so let $z(t)$ be an arbitrary differentiable path such that $q(z(t)) = c$ for all t , and $z(0) = x$. Then $z'(0)$ is an arbitrary tangent vector to $\mathcal{S}_q(c)$ at x . Differentiating $q(z(t)) = c$ gives

$$\begin{aligned} 0 &= \frac{d}{dt} [q(z(t))] = \frac{d}{dt} [\langle z(t), z(t) \rangle_M] \\ &= \langle z'(t), z(t) \rangle_M + \langle z(t), z'(t) \rangle_M \\ &= 2\langle z'(t), z(t) \rangle_M, \end{aligned}$$

since the scalar product is symmetric. Evaluating at $t = 0$ gives $\langle z'(0), x \rangle_M = 0$, that is $z'(0) \in (x)_M^\perp$. \square

Together with Theorem 8.2, this result shows that among all the y 's with $q(y) = q(x)$, the only ones that *cannot* be mapped to x by any \mathbb{G} -reflector are the y 's that lie on the intersection of the q -level surface $\mathcal{S}_q(q(x))$ with its tangent space at x . When $\langle \cdot, \cdot \rangle_M$ is positive definite, the level surfaces \mathcal{S}_q are all ellipsoids, so this intersection is just the point x . Thus in the positive definite case, *every* y such that $q(y) = q(x)$ can be mapped to x by a \mathbb{G} -reflector; this fits nicely with the well understood behavior of Householder reflectors in \mathbb{R}^n .

On the other hand, when $\langle \cdot, \cdot \rangle_M$ is indefinite, the intersection of q -level surfaces with their tangent spaces may be trivial for some q -values and nontrivial for others. Consider the example of $\mathbb{G} = O(2, 1, \mathbb{R})$ where $M = \Sigma_{2,1} \stackrel{\text{def}}{=} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$, so that $q(x) = x_1^2 + x_2^2 - x_3^2$. Here the q -level surfaces are hyperboloids of two sheets for $q < 0$, a cone for $q = 0$, and hyperboloids of one sheet for $q > 0$, all with axis of symmetry along the z -axis (see Figure 8.2). These three types of surface have different types of intersection with their tangent spaces. When $q < 0$ the intersection is a single point, when $q = 0$ the intersection is a single line, and when $q > 0$ the intersection is a *pair* of lines through the tangency point x . This is

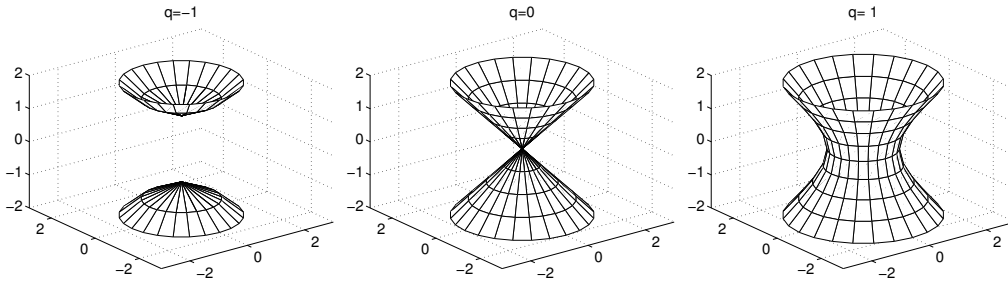


Figure 8.2: q -level surfaces of $x_1^2 + x_2^2 - x_3^2 = q$ for $q = -1$ (hyperboloid of two sheets), $q = 0$ (cone) and $q = 1$ (hyperboloid of one sheet).

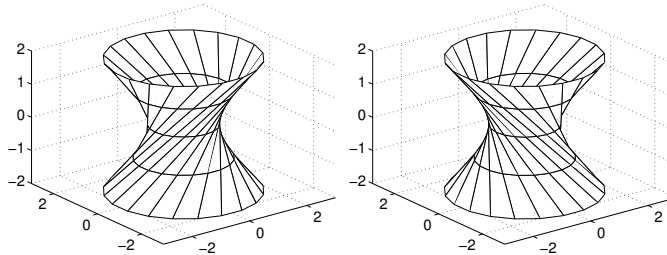


Figure 8.3: Rulings of a hyperboloid of one sheet.

because hyperboloids of one sheet are doubly ruled surfaces (see Figure 8.3) containing two lines through each point x on the surface⁶. These two lines are precisely the intersection of the surface with the tangent plane at x .

Thus in this example we see that whenever $q(x) = q(y) < 0$, then x and y can always be mapped to each other by a \mathbb{G} -reflector. But the situation is different when $q(x) = q(y) > 0$, that is, when x and y lie on a hyperboloid of one sheet. In this case they can be mapped to each other by a \mathbb{G} -reflector only if they do not lie on the same ruling of the hyperboloid.

9 Conclusion

The transformations studied in this paper may be found in a more abstract form in [3], [6], [7], [15], where they are distinguished as symmetries, quasi-symmetries, transvections and reflections, and used to investigate the structure of the classical groups.

By contrast, this work looks at all these transformations from a concrete matrix perspective and under a common rubric: the generalized \mathbb{G} -reflectors, or \mathbb{G} -reflectors for short. Our contribution includes a complete characterization of these transformations for a large class of automorphism groups — those arising in the context of an orthosymmetric scalar product; this includes all symmetric and skew-symmetric bilinear forms as well as all Her-

⁶The Corporation Street pedestrian bridge in Manchester City Centre is a beautiful architectural example of a hyperboloid of one sheet together with its double rulings (see <http://www.ma.man.ac.uk/~higham/photos/manchester/030105-1225-28.htm>). Classic renditions of hyperboloids and their rulings can be found in [13]; for a more technical treatment with a modern flavour see [11].

mitian and skew-Hermitian sesquilinear forms. This in turn is used to determine under what conditions a given vector can be mapped to another by a generalized \mathbb{G} -reflector, and to give a concrete description of the unique \mathbb{G} -reflector that does the task.

The unified matrix treatment of \mathbb{G} -reflectors presented in this paper has been specialized in [23] to derive new structured tools for a number of specific matrix groups. In [22], \mathbb{G} -reflectors have been used to prove the structured mapping theorem: for any orthosymmetric scalar product on \mathbb{K}^n and any $x, y \in \mathbb{K}^n$ such that $q(x) = q(y)$, there is an element A of the automorphism group \mathbb{G} such that $Ax = y$.

The authors hope this work will stimulate further investigations both theoretical and algorithmic, where the preservation of structure is desired.

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