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GENERALIZING THE HERMITIAN STRUCTURE IN A HOUSEHOLDER REFLECTOR*

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Abstract. Householder's classic 1958 paper popularized a Hermitian unitary matrix now well-known as the Householder reflector. The reflector has a special structure $I - 2P$, where P is a rank-1 orthogonal projector. The reflector plays a key role in several significant algorithms for solving least squares and eigenvalue problems. The influential paper, however, left a subtle oversight that still lingers in recent books and course materials. To correct this oversight, we show that the structure $I - 2P$ needs to be extended. In particular, the Hermitian property must be forsaken when the source of reflection and its target do not obey a certain symmetry condition. We introduce extended structures that fulfill the task of reflection without requiring this condition on symmetry. For reflecting a single vector, we extend the $I-2P$ structure into $I-\eta P$ using a specific $\eta \in \mathbb{C}$. This is in the same spirit of a standard fix of the Householder reflector. For the more general scenario of reflecting multiple vectors simultaneously, we first study the norm-preserving linear targeting problem: we extend the $I - 2P$ structure into $I - (P_1 + P_2)$, where only P_1 is required to be an orthogonal projector; the $I - (P_1 + P_2)$ structure naturally leads to another structure $I - USU^*$, where U has orthonormal columns and S is a square matrix of a suitable size. We further show that the $I - (P_1 + P_2)$ structure also arises in a linear targeting problem with a requirement on positive-definiteness instead of norm-preservation.

Key words. Householder reflector, Symmetry, Projector, Non-Hermitian unitary, Essentially Hermitian, Polar angle, Extended Householder matrix, Linear targeting problem.

AMS subject classifications. 65F25, 65F30, 15A57.

1. Introduction. In [15] Householder introduced a Hermitian matrix of the form $I-2uu^*$, where u is a vector of unit length. The matrix has since played a significant role in numerical linear algebra, particularly in computing QR decompositions, which are essential for stabilizing key algorithms solving least squares and eigenvalue problems. Due to its significance, a matrix of the form $I - 2uu^*$ with $\|u\|_2 = 1$ is named after Householder and is referred to by various terms such as Householder matrix, Householder transformation, and Householder reflector.

Although named after Householder, the Householder matrix was known considerably earlier than 1958. Higham [12, p. 383] and Stewart [19, p. 289] trace the first known Householder matrix to the 1932 book by Turnbull and Aitken [21, pp. 102–105]. Golub and Van Loan in [8, p. 222] point to the same origin, citing the third edition [22] of this book.

Nonetheless, as aptly pointed out by Stewart [19, p. 289], "Householder, who discovered the transformations independently, was the first to realize their computational significance." It was the computational efficiency revealed by Householder that popularized the unitary triangularization method he introduced in [15].

Householder's independent discovery of the reflector may be supported by two observations. First, he developed the essential components that make his reflector work efficiently in digital calculations — a field still in its early stage of development in the late 1950s; second, he left two technical oversights in [15]. In

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scientific discoveries, it is fairly common that an original inventor of a certain theory or method missed some initial subtleties.

The first oversight, as pointed out in [19, p. 290], is that "Householder seems to have missed the fact that there are two transformations that will reduce a vector to a multiple of e_1 and that the natural construction of one of them is unstable." This oversight is related to potential numerical cancellations. In [16], Overton and Yu noted that virtually all later books on numerical linear algebra, when discussing a Householder transformation, focus on the issue about numerical cancellations.

In comparison, the second oversight in [15] has received almost no attention. This oversight is hidden in the only lemma presented in [15]. The lemma claims that for any two vectors x and y of same norm, there is always a unit vector u such that $(I - 2uu^*)x = y$.

Influenced by this lemma, a subtle but somewhat persistent error is to believe that a given vector $x \in \mathbb{C}^n$ can always be reflected to $z\|x\|e_1$ via a Householder reflector $I - 2uu^*$, as long as z is a complex scalar with $|z| = 1$. This error appeared in [20, p. 72], it was not spotted but seconded in [13]. Even until recently, the same error still exists in some influential and overall excellent course materials, for example [1].

In Section 2, we focus on correcting the second oversight in [15]. Given $x, y \in \mathbb{C}^n$ with $\|x\|_2 = \|y\|_2$, every unitary U satisfies $\|Ux\|_2 = \|y\|_2$, and there exist infinitely many unitary matrices that also satisfy $Ux = y$. The tricky part is to make the unitary matrix observe the Householder structure $I - 2P$, which is an identity matrix minus *twice* of a rank-1 orthogonal projector ($P = uu^*$ with $\|u\|_2 = 1$). This structure makes $I - 2P$ Hermitian unitary, thus involutory. The name "reflector" for the Householder matrix stems from it being involutory.

To address the second technical oversight in [15], forsaking the Hermitian property becomes necessary when a certain symmetry condition is broken. In this case, the extended Householder matrix becomes non-involutory, causing it to lose the geometric interpretation of a reflector intuitive in a real space. But our extension largely keeps the Householder structure and can indeed transform any $x \in \mathbb{C}^n$ into any $y \in \mathbb{C}^n$ as long as $\|x\|_2 = \|y\|_2$.

Householder reflector was initially designed to reflect vectors, i.e., $Ax = y$ where $x, y \in \mathbb{C}^n$. It is a special case of finding an A such that $AX = Y$ for multiple known vectors $X, Y \in \mathbb{C}^{n\times k}$, $k > 1$. Finding such an A is known as the linear targeting problem [4], where Y is called the target and X the source. The linear targeting problem is related to a wide-range of applications, including the Procrustes problems [18, 11], dynamical system identification and control [5], manifold optimization [2], and machine learning [10].

In Section 3, we extend the Householder reflector for a norm-preserving linear targeting problem in [4], generalizing the formula so that it can work for a wider class of matrices than those addressed in [4]. We develop two extensions to the Householder structure: one of them is $I - USU^*$, where U is a low-rank matrix with orthonormal columns; the other is $I - (P_1 + P_2)$, which separates the $2P$ in the standard Householder matrix into two low-rank matrices P_1 and P_2; here, only P_1 is an orthogonal projector, while P_2 is not necessarily a projector.

In Section 4, we extend the Householder reflector to address a class of symmetric positive definite (SPD) linear targeting problem. Interestingly, the structure $I - (P_1 + P_2)$, which works for the norm-preserving targeting problem, also arises naturally in this type of usually not norm-preserving SPD targeting problem.

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As for notation, we use $(\cdot)^*$ for the conjugate transpose, $(\cdot)^+$ for the Moore–Penrose pseudo-inverse, and I for the identity matrix when its size is clear from context (otherwise, we specify it with a subscript, e.g., I_k for the $k \times k$ identity matrix). For simplicity, we use $\|\cdot\|$ solely for the 2-norm from here onward.

2. Householder reflector and its extension for reflecting a vector to a specific target. In the now classic paper [15], Householder stated the following Lemma for all vectors in $\mathbb{C}^n$. (To keep the notations consistent with [15], in this section, we use a and v to represent the reflection source and its target.)

LEMMA 2.1. *[15]: For any vector $a \neq 0$, and any unit vector v, there exists a unit vector u such that*

$$(I - 2uu^*)a = \|a\|v. \tag{2.1}$$

Householder provided a proof in [15]; however, he made a subtle error in his proof. But this error only shows up in a specific and quite rare situation. Outside this specific situation, the statement of Lemma 2.1 is perfectly true.

To see the subtle error, one only needs to multiply (2.1) by a^* from the left to get

$$a^*(I - 2uu^*)a = \|a\|a^*v,$$

leading to

$$\|a\|^2 - 2|a^*u|^2 = \|a\|a^*v.$$

The left-hand side being real forces a^*v to be real. But a^*v is not guaranteed to be real by the conditions given in Lemma 2.1. In fact, for any v for which $a^*v \notin \mathbb{R}$, there exists no such u that can make (2.1) to hold.

A simple counter example to (2.1) is found in the $n = 2$ case: Let $a = [i, 0]^T$ and $v = [1, 0]^T$. There exists no unit vector u that can satisfy $(I - 2uu^*)a = \|a\|v$.

This subtle error is mostly missed in later literature on Householder reflectors, and the same error appears in several books. For example, on [3, p. 75], an exercise is assigned to show that $y = (I - \frac{2}{\|w\|^2}ww^*)x$ whenever $\|x\| = \|y\|$ and $w = \pm(x - y)$. This is essentially identical to Lemma 2.1, but the conclusion can fail without the additional condition $x^*y \in \mathbb{R}$.

Trefethen and Bau [20, p. 72] stated that a vector x can be reflected to $z\|x\|e_1$, where z is any scalar with $|z| = 1$: "In the complex case, there is a circle of possible reflections,..." This means a vector x can be reflected by the Householder reflector in the form of $I - 2uu^*$ to $z\|x\|e_1$ for any chosen z on the unit circle $|z| = 1$. Indeed, their statement would be naturally implied by Lemma 2.1 (via $v = ze_1$) if the lemma is fully true.

However, in order for u to exist such that

$$(I - 2uu^*)x = z\|x\|e_1, \tag{2.2}$$

it is critical for x^*ze_1 to be real. Therefore, contrary to the more generally accepted claim that (2.2) can hold for any chosen complex sign z, the z cannot be arbitrarily located on the unit circle $|z| = 1$. In fact there are only two z's that can make (2.2) to hold, both of them must obey the condition $x^*ze_1 \in \mathbb{R}$. Thus, in both the real case and the complex case, the x can be reflected to only two vectors parallel to e_1.

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In order to reflect x to $z\|x\|e_1$ for any chosen z satisfying $|z|=1$, we need to extend the Householder reflector to a more general matrix. The standard reflector $I-2uu^*$ is Hermitian unitary, but when $x^*ze_1 \notin \mathbb{R}$, our extension has to forsake the Hermitian property.

An extended Householder reflector for such a purpose is developed in [23] as

$$H(\eta) = I - \eta uu^*, \tag{2.3}$$

where $\|u\|=1$, and $\eta \in \mathbb{C}$. That is, the scalar 2 in $I-2uu^*$ should be allowed to take a complex value (represented by the η in (2.3)) when necessary. But $H(\eta)$ must be unitary to fulfill the norm-preserving requirement, thus the η cannot be arbitrary either, it must be located on the unit circle $|1-\eta|=1$.

With the extended Householder reflector (2.3), we can reflect any vector x to $z\|x\|e_1$ for an arbitrary z with $|z|=1$. We construct u in (2.3) as

$$u = \hat{u}/\|\hat{u}\|, \qquad \text{where } \ \hat{u} = x - z\|x\|e_1,$$

and construct the η in (2.3) via any of the following equivalent formula

$$\eta = \frac{u^*\hat{u}}{u^*x} = \frac{\|\hat{u}\|}{u^*x} = \frac{\|\hat{u}\|^2}{\hat{u}^*x} = \frac{x^*\hat{u}}{|x^*u|^2}. \tag{2.4}$$

With the choices of u and η, it is straightforward to verify that $H(\eta)x = z\|x\|e_1$. It can also be proved that any η obtained via (2.4) satisfies $|1-\eta|=1$; thus, the constructed $H(\eta)$ is unitary.

For numerical stability, especially in the case that x is close to $z\|x\|e_1$, we can choose $\hat{u} = x + z\|x\|e_1$ and normalize it to construct the unit u in (2.3), while the formulas for η stay the same as in (2.4). The choice of such u and η can construct an $H(\eta)$ such that $H(\eta)x = -z\|x\|e_1$ for any $|z|=1$. (This is similar to constructing a standard Householder reflector which avoids numerical cancellation in $x - z\|x\|e_1$.)

The extended reflector fixes the subtle error in Lemma 2.1 as follows:

Lemma 2.2. *For any vector $a \neq 0$, and any unit vector v, there exists a unit vector u and a scalar $\eta \in \mathbb{C}$ such that $I-\eta uu^*$ is unitary, and*

$$(I - \eta uu^*)a = \|a\|v. \tag{2.5}$$

Proof. In the trivial case $a = \|a\|v$, the u can be any unit vector orthogonal to a, and η can be any value. So we assume $\hat{u} = a - \|a\|v \neq 0$. Let $u = \hat{u}/\|\hat{u}\|$, then, in order for $(I-\eta uu^*)a = \|a\|v$ to hold, we need $a^*(I-\eta uu^*)a = \|a\|a^*v$, which means $\eta|u^*a|^2 = a^*(a-\|a\|v) = a^*\hat{u}$, therefore $\eta = \frac{a^*\hat{u}}{|u^*a|^2}$. With the constructed u and η, it can be directly verified that

$$(I-\eta uu^*)a = a - \frac{a^*\hat{u}}{|u^*a|^2}uu^*a = a - \hat{u} = \|a\|v.$$

Since $\eta = \frac{a^*\hat{u}}{|u^*a|^2}$, and $\hat{u} = \|\hat{u}\|u = a - \|a\|v$, we have

$$\begin{aligned}
\eta\bar{\eta} &= \frac{a^*\hat{u}\hat{u}^*a}{|u^*a|^4} = \frac{\|\hat{u}\|^2 a^*uu^*a}{|u^*a|^4} = \frac{\|\hat{u}\|^2}{|u^*a|^2},\\
\eta + \bar{\eta} &= \frac{a^*\hat{u} + \hat{u}^*a}{|u^*a|^2} = \frac{2\|a\|^2 - \|a\|(a^*v + v^*a)}{|u^*a|^2}.
\end{aligned}$$

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Since $\|\hat{u}\|^2 = (a - \|a\|v)^*(a - \|a\|v) = 2\|a\|^2 - \|a\|(a^*v + v^*a)$, we obtain $|\eta|^2 = \bar{\eta} + \eta$. Therefore,

$$(I - \eta uu^*)^*(I - \eta uu^*) = I - (\bar{\eta} + \eta)uu^* + |\eta|^2 uu^* = I.$$

So the chosen η makes $I - \eta uu^*$ unitary. $\square$

Since $|\eta|^2 = \bar{\eta} + \eta$ is equivalent to $|1 - \eta| = 1$, it means any η that makes $I - \eta uu^*$ unitary must be located on the unit circle centered at $(1, 0)$ on the complex plane, as shown in Figure 1.

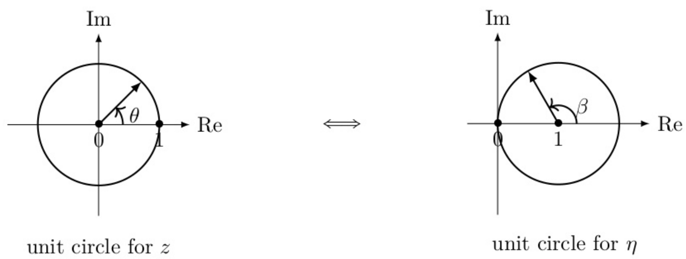

FIG. 1. *Given two unit vectors v and u, in order to achieve $(I - \eta uu^*)a = \|a\|v$ for $a \neq 0$, the η cannot be fixed at 2 but needs to adjust to a value η located on the unit circle $|1 - \eta| = 1$. If $z = \frac{a^*v - \|a\|}{|a^*v - \|a\||}$, then the two depicted polar angles satisfy $\beta = 2\theta$.*

Although [23] introduced the extended Householder reflector (2.3), it did not reveal that the magic number 2 in the standard Householder reflector is in fact retained implicitly in the extended reflector. To finish this step, we need to look deeper into the relationship between two angles: Figure 1 shows that η has to be on the circle $|1 - \eta| = 1$, but the β angle shown in Figure 1 is far from arbitrary, it has to be precisely determined by another angle θ that we describe in Lemma 2.3.

LEMMA 2.3. *Let θ be the polar angle of $a^*v - \|a\|$. Then, the η in (2.5) is $\eta = 1 + \cos(\beta) + i\sin(\beta)$, where $\beta = 2\theta$.*

Proof. For notational simplicity, we normalize the a in (2.5) as $\tilde{a} = a/\|a\|$. Then, (2.5) becomes $(I - \eta uu^*)\tilde{a} = v$, multiplying both sides from the left by u^* leads to $\eta = \frac{u^*\tilde{a} - u^*v}{u^*\tilde{a}} = 1 - \frac{u^*v}{u^*\tilde{a}}$. Since the u is constructed from $u = \frac{\tilde{a} - v}{\|\tilde{a} - v\|}$, we get

$$\eta = 1 + \frac{(\tilde{a} - v)^*v}{(v - \tilde{a})^*\tilde{a}} = 1 + \frac{\tilde{a}^*v - 1}{v^*\tilde{a} - 1}. \tag{2.6}$$

Since the polar angle of $\tilde{a}^*v - 1$ is the same θ as that of $a^*v - \|a\|$ [1], we get $\tilde{a}^*v - 1 = |\tilde{a}^*v - 1|e^{i\theta}$. Since $\tilde{a}^*v - 1 = \overline{v^*\tilde{a} - 1}$, from (2.6), we get $\eta = 1 + e^{2i\theta}$.

Denoting the polar angle of η as β, then the β in $\eta = 1 + e^{i\beta}$ is exactly $\beta = 2\theta$, where θ is the polar angle of $a^*v - \|a\|$. $\square$

When $a^*v \in \mathbb{R}$, we always have $\eta = 2$, which corresponds to the standard Householder reflector. Interestingly, the magic number 2 is still in the reflector even when $a^*v \notin \mathbb{R}$, it is just hidden in the relation of the polar angles ($\beta = 2\theta$) of the two key scalars η and $a^*v - \|a\|$ that decide the extended reflector (2.3).

[1] Here, the θ is not the angle between $\tilde{a} - v$ and v: Although $\tilde{a}^*v - 1 = (\tilde{a} - v)^*v$, it is incorrect to write $(\tilde{a} - v)^*v = \|\tilde{a} - v\|\cos(\theta)$. The angle between two complex vectors is far less intuitive to describe. (See e.g. [17].)

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In numerical computations, the simple choice of $\eta = 2$ is typically preferred. However, when $a^*v \notin \mathbb{R}$, the $(I - 2uu^*)a$ cannot be in the same direction as v, since $(I - 2uu^*)a \neq \|a\|v$ for all unit u. But such a blemish can be easily remedied, we only need to "rotate" the target vector v by a complex sign (represent by some $z \in \mathbb{C}$ with $|z| = 1$) so that its inner produce with a becomes real. This in quantum mechanics is called phase-rotation. Such a remedy has existed for decades. E.g., [9, p. 243] describes it for the case where v is parallel to e_1, which is the typical case in QR decompositions. It was already used in early development of LAPACK (LINPACK, EISPACK). The remedy makes the standard Householder reflector of form $I - 2uu^*$ sufficient for QR decompositions, attested by the great success of LAPACK, which is the workhorse behind Matlab, Numpy, and even PyTorch. For completeness, we present this known remedy for a general v in the following lemma.

Lemma 2.4. *For any vector $a \neq 0$, and any unit vector v, there exists a unit vector u such that*
(i) If $a^*v \in \mathbb{R}$, then

$$(I - 2uu^*)a = \|a\|v, \tag{2.7}$$

(ii) If $a^*v \notin \mathbb{R}$, then

$$(I - 2uu^*)a = \frac{v^*a}{|v^*a|}\|a\|v. \tag{2.8}$$

Proof. We prove (i) and (ii) together by Lemma 2.2. Set

$$w = \begin{cases} v & \text{if } a^*v \in \mathbb{R} \\ \frac{v^*a}{|v^*a|}v & \text{if } a^*v \notin \mathbb{R} \end{cases},$$

then clearly $a^*w \in \mathbb{R}$ and $\|w\| = 1$. Let $\hat{u} = a - \|a\|w$, without loss of generality, we assume $\hat{u} \neq 0$. Let $u = \hat{u}/\|\hat{u}\|$, and let $\eta = \frac{a^*\hat{u}}{|u^*a|^2}$. Then, by Lemma 2.2, we have $(I - \eta uu^*)a = \|a\|w$. To finalize the proof, all we need is to show that $\eta = 2$:

Since $a^*\hat{u} = \|a\|^2 - \|a\|a^*w \in \mathbb{R}$, and $|u^*a|^2 = \frac{1}{\|\hat{u}\|^2}|\hat{u}^*a|^2 = \frac{1}{\|\hat{u}\|^2}(a^*\hat{u})^2$, we have

$$\eta = \frac{a^*\hat{u}}{|u^*a|^2} = \frac{\|\hat{u}\|^2}{a^*\hat{u}} = \frac{2\|a\|^2 - \|a\|(a^*w + w^*a)}{\|a\|^2 - \|a\|a^*w} = 2. \qquad \square$$

Figure 2 shows the comparison between the general reflector $H(\eta)$ and the Hermitian reflector H_2 for which the standard fix ([9, p. 243], represented in (2.8)) needs to be applied. The wall time (via `tic+toc`) as well as the reflection errors between the two reflectors are comparable. The measured time does not increase consistently as n increases mainly because it is so short that background operating system jobs can cause tiny but noticeable oscillations in the measurement. The plotted time and also the reflection error are the average of five runs of the same code on randomly generated vectors without repeat.

The construction time for H_2 appears slightly longer since it has an extra scaling (phase-rotation) of the target from v to $\frac{v^*a}{|v^*a|}v$, but such $O(n)$ cost is in general negligible. However, in some applications (such as signal processing and quantum computing), a phase-rotation of the target may lead to loss of information that can be difficult to recover. For these scenarios, the general reflector $H(\eta)$ without the need of a phase-rotation is to be preferred.

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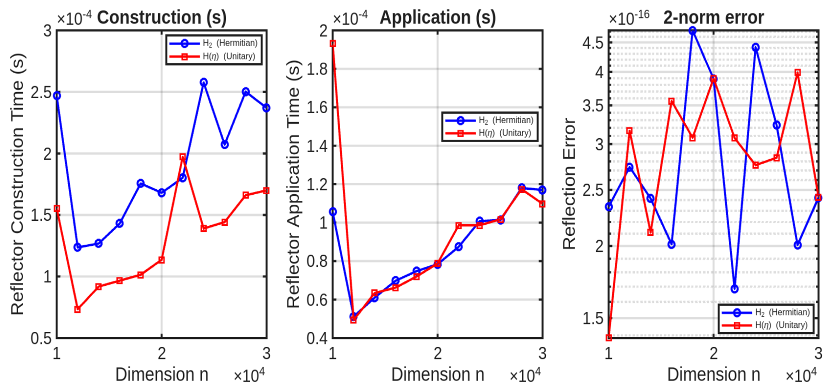

FIG. 2. *Comparisons of H_2 (from (2.8)) and $H(\eta)$ (from (2.5)) when $a^*v \notin \mathbb{R}$. The code is written in Matlab, where n varies in* `10000:2000:30000`. *Both a and v are chosen as random complex vectors in $\mathbb{C}^n$ and then normalized in 2-norm ($\|a\| = \|v\| = 1$). Application of the reflectors to a are both done via $O(n)$ operations as $a - cu(u^*a)$, where $c = 2$ or η. Neither approach constructs a full reflector matrix, only the two different u vectors are constructed, thus saving both computation time and memory.*

In addition to the non-Hermitian structure in $H(\eta)$, the part *(ii)* in Lemma 2.4 reveals another non-Hermitian structure: If we want the reflected vector for both *(i)* and *(ii)* to be solely $\|a\|v$, then we can express (2.8) as

$$\frac{a^*v}{|v^*a|}(I - 2uu^*)a = \|a\|v.$$

The "reflector" matrix is now $\frac{a^*v}{|v^*a|}(I - 2uu^*)$. This matrix has a special structure—it is a Hermitian matrix multiplied by a complex sign. Such a structure is termed *essentially Hermitian* in [14, p. 7]. If we associate the complex sign with a as $(I - 2uu^*)\frac{a^*v}{|v^*a|}a = \|a\|v$, then the standard Householder reflector $I - 2uu^*$ again works (since here the source vector a is phase-rotated correctly). This is expected since the complex sign exactly serves to remove the situation in which the standard Householder reflector fails.

This non-Hermitian structure $z(I - 2uu^*)$ where $|z| = 1$ differs from the structure $I - \eta uu^*$ represented by (2.5). Both structures are mostly Hermitian, and they become non-Hermitian only when $a^*v \notin \mathbb{R}$. Furthermore, since $z(I - 2uu^*) = I - \eta uu^*$ holds only when $z = 1$ and $\eta = 2$ (the trivial case), we know that the two structures are different. The $I - \eta uu^*$ where $|1 - \eta| = 1$ appears to introduce another *essentially Hermitian* structure, which differs from the existing structure defined by "a complex sign times a Hermitian matrix." However, from Lemma 2.3, we know $\eta = 1 + e^{i\beta}$; therefore, $I - \eta uu^* = I - uu^* - e^{i\beta}uu^*$; thus, the new structure is a hermitian matrix plus a standard *essentially Hermitian* matrix.

3. Extending Householder reflector for reflecting a block matrix. The previous section addressed reflecting one vector to another vector. A natural extension is to reflect multiple vectors simultaneously to their corresponding target vectors: Given matrices $X, Y \in \mathbb{C}^{n\times k}$, where $n \geq k \geq 1$, construct a 'reflector' A such that $AX = Y$. We study what conditions would allow such a "reflector" to exist and how to construct it when it exists.

The condition for the existence of a square matrix M such that $MX = Y$ is well-known: $\mathrm{null}(X) \subseteq \mathrm{null}(Y)$. This condition is both necessary and sufficient. If M is further required to be invertible, then the condition becomes the more stringent $\mathrm{null}(X) = \mathrm{null}(Y)$.

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The condition $X^*X = Y^*Y$ is sufficient for null$(X) =$ null(Y). Therefore, $X^*X = Y^*Y$ guarantees the existence of an invertible M such that $MX = Y$. Furthermore, since $X^*X = Y^*Y$ is a stronger condition than null$(X) =$ null(Y), it allows the M matrix to have additional properties beyond invertibility, such as being unitary or a reflector, both of which are studied in [4].

However, in [4], only a Hermitian reflector is studied. A second condition, $X^*Y = Y^*X$, is needed in addition to $X^*X = Y^*Y$ to ensure that the targeting problem has a solution that is a Hermitian reflector, as stated in Theorem 3.1.

THEOREM 3.1. *[4]: Given $X, Y \in \mathbb{C}^{n\times k}$ where $n \geq k \geq 1$. There is a reflector of form $I - 2P$, where $P \in \mathbb{C}^{n\times n}$ is an orthogonal projector (i.e., $P^2 = P$, $P^* = P$), such that $(I - 2P)X = Y$ if and only if $X^*X = Y^*Y$ and $X^*Y = Y^*X$.*

The proof in [4] utilizes the Moore–Penrose pseudo-inverse for the construction of the projector P.

$$P = F(F^*F)^+F^* = FF^+, \qquad \text{where } F = Y - X. \tag{3.1}$$

By properties of a pseudo-inverse (e.g., [6]), we know P is an orthogonal projector. It is easy to verify $(I - 2P)^2 = I$, thus $I - 2P$ is a Hermitian unitary reflector. Moreover, P projects onto range(F), thus

$$PF = F \qquad \Longrightarrow \qquad PY - PX = Y - X. \tag{3.2}$$

Under the two conditions $X^*X = Y^*Y$ and $X^*Y = Y^*X$, we have

$$(X + Y)^*F = (X + Y)^*(Y - X) = Y^*Y - X^*X + X^*Y - Y^*X = 0. \tag{3.3}$$

Therefore, range$(X + Y) \perp$ range(F). By the definition of P, we get

$$P(X + Y) = F(F^*F)^+F^*(X + Y) = 0 \qquad \Longrightarrow \qquad PY = -PX. \tag{3.4}$$

Combining (3.2) with (3.4) leads to $-2PX = Y - X$, which directly satisfies the linear targeting goal $(I - 2P)X = Y$.

The standard Householder reflector has the unique structure $I - 2P$, where P is an orthogonal projector. This structure is intrinsic because the Householder reflector is a Hermitian unitary matrix. To see why, we can utilize an eigenvalue decomposition: For a general $n \times n$ Hermitian-unitary matrix H, its eigenvalues are either 1 or -1; assume it has k eigenvalues equal to 1, then its eigendecomposition is

$$H = V \begin{bmatrix} I_k & 0 \\ 0 & -I_{n-k} \end{bmatrix} V^*,$$

where the unitary matrix V contains the eigenvectors of H.

If we partition V as $V = [V_1, V_2]$, where $V_1 \in \mathbb{C}^{n\times k}$ contains the k eigenvectors associated with eigenvalues 1, then $V_1V_1^* + V_2V_2^* = I$, which leads to

$$H = V_1V_1^* - V_2V_2^* = I - 2V_2V_2^*.$$

This reveals the intrinsic Householder structure $I - 2P$, where $P = V_2V_2^*$ is an orthogonal projector.

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For the targeting problem in Theorem 3.1, the P is defined via (3.1). The standard Householder reflector $I - 2uu^*$ is a special case of (3.1).

However, for $I - 2P$ to fulfill the targeting goal $(I - 2P)X = Y$ under the condition that P is an orthogonal projector, the critical condition $X^*Y = Y^*X$ is needed. This is because the $(X + Y)^*F = 0$ in (3.3) holds only under this condition. But this symmetric condition $X^*Y = Y^*X$ is quite often not met, even when both X and Y are real. (Another example is for the case $X^* = X$ and $Y^* = Y$, noting that $XY = YX$ can easily fail since in general a matrix-matrix product is non-commutative.) Thus, requiring (3.4) to hold can significantly narrow the application scope of the reflector constructed under this condition. For example, the target $(I - 2P)X$ always fails to be Y whenever $X^*Y \neq Y^*X$.[2]

To construct a reflector that works for the larger class of matrices not satisfying the condition $X^*Y = Y^*X$, we must relax the Hermitian requirement on the reflector.

But generalizing the reflector from $I - \eta uu^*$ to $I - \eta UU^*$, where $\eta \in \mathbb{C}$ and $U^*U = I_k$ encounters immediate difficulty: a single parameter η is often insufficient to achieve $(I - \eta UU^*)X = Y$ for all vectors in X and Y simultaneously.

A practical solution is to further extend the η into a $k \times k$ matrix S, which extends ηUU^* to a special form of USU^*, as stated in Theorem 3.2.

THEOREM 3.2. *: Given $X, Y \in \mathbb{C}^{n\times k}$ where $n \geq k \geq 1$. There is a unitary matrix of form $I - USU^*$, where $U \in \mathbb{C}^{n\times k}$ has orthonormal columns and $S \in \mathbb{C}^{k\times k}$, such that $(I - USU^*)X = Y$ if and only if $X^*X = Y^*Y$.*

The $(\Longrightarrow)$ part is obvious: if $(I - USU^*)X = Y$ and $I - USU^*$ is unitary, then $Y^*Y = X^*(I - USU^*)^*(I - USU^*)X = X^*X$.

For the $(\Longleftarrow)$ part we need to construct the U and S such that three conditions are satisfied: (i) $U^*U = I_k$, (ii) $I - USU^*$ is unitary, and (iii) $(I - USU^*)X = Y$.

The $I - USU^*$ being unitary means $(I - US^*U^*)(I - USU^*) = I$, which is equivalent to $S + S^* = S^*S$.

Let a QR decomposition of $X - Y$ be $UR = X - Y$, where $U^*U = I_k$. For $(I - USU^*)X = Y$ to hold, we need $USU^*X = X - Y = UR$, which requires $SU^*X = R$.

If U^*X is invertible, then $S = R(U^*X)^{-1}$; and the constructed U and S instantly satisfy $(I - USU^*)X = Y$. Furthermore, $S + S^* = R(U^*X)^{-1} + (X^*U)^{-1}R^*$ and $S^*S = (X^*U)^{-1}R^*R(U^*X)^{-1}$, we have

$$\begin{aligned} & S + S^* = S^*S \\ \Longleftrightarrow\ & X^*UR + R^*U^*X = R^*R \\ \Longleftrightarrow\ & X^*(X - Y) + (X - Y)^*X = (X - Y)^*(X - Y) \\ \Longleftrightarrow\ & 2X^*X - X^*Y - Y^*X = X^*X - X^*Y - Y^*X + Y^*Y. \end{aligned}$$

The last equation is exactly satisfied under the norm-preserving condition $X^*X = Y^*Y$. Therefore, the constructed U and S make $I - USU^*$ unitary and fulfill the target $(I - USU^*)X = Y$.

[2]Even if X and Y are two vectors, our earlier discussions showed that $I - 2P$ cannot work when X^*Y is not real, which is the 1-dimensional case of $X^*Y \neq Y^*X$. In other words, the failure of the constructed Hermitian reflector is caused by the loss of symmetry in X^*Y.

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The downside of the above approach is that it depends on U^*X being invertible, which is not required for Theorem 3.2 to hold. We remark that a different approach used to prove Theorem 3.3 will naturally provide a complete proof of Theorem 3.2.

One may wonder if the above approach can be enhanced by using the pseudo-inverse of U^*X, similar to the one used in Theorem 3.1 for the symmetric case, so that it does not depend on U^*X being invertible and can provide a complete proof of Theorem 3.2. Unfortunately, the answer is only a partial yes. Pseudo-inverses can help prove $(I-USU^*)X = Y$ in general, but not enough to guarantee that $I-USU^*$ is unitary. We state the weakened result in the following proposition.

Proposition 3.1. *: Given $X, Y \in \mathbb{C}^{n\times k}$ where $n \geq k \geq 1$, assume $X^*X = Y^*Y$. There is a matrix of form $I - USU^*$, where $U \in \mathbb{C}^{n\times k}$ has orthonormal columns and $S \in \mathbb{C}^{k\times k}$, such that $(I - USU^*)X = Y$.*

Proof. Let $X - Y = UR$ be the QR decomposition of $X - Y$, where $U^*U = I_k$. Define $T = U^*X$ and $N = U^*(X - Y)$.

Similar to the technique used in Theorem 3.1, we construct the S matrix via $S = NT^+$.

We first show that $\ker(T) \subseteq \ker(N)$ holds under the condition $X^*X = Y^*Y$: For any $v \in \ker(T)$, $Tv = U^*Xv = 0$, thus $Xv \perp \operatorname{range}(U)$. From the QR decomposition, we know $\operatorname{range}(X - Y) \subseteq \operatorname{range}(U)$, therefore $(X - Y)^*Xv = 0$. This leads to $X^*Xv = Y^*Xv$.

Since $X^*X = Y^*Y$, we get $Y^*Yv = Y^*Xv$, which means $(X - Y)v \perp \operatorname{range}(Y)$. Then, by the Pythagorean theorem, $\|Xv\|^2 = \|Yv\|^2 + \|(X - Y)v\|^2$. But $X^*X = Y^*Y$ also means $\|Xv\|^2 = \|Yv\|^2$, therefore, $(X - Y)v = 0$. Thus, $Nv = U^*(X - Y)v = 0$, so $v \in \ker(N)$. This proves $\ker(T) \subseteq \ker(N)$, therefore, $\operatorname{range}(N^*) \subseteq \operatorname{range}(T^*)$.

Since T^+T is an orthogonal projector onto $\operatorname{range}(T^*) = \operatorname{range}(T^+T)$, we have $T^+TN^* = N^*$, this gives $N = NT^+T$. Therefore, $ST = NT^+T = N$. And because UU^* is an orthogonal projector onto $\operatorname{range}(X-Y)$, we have $UU^*(X - Y) = X - Y$. Therefore,

$$ST = N \implies SU^*X = U^*(X - Y) \implies USU^*X = UU^*(X - Y) = X - Y.$$

This establishes $(I - USU^*)X = Y$. ∎

The above construction cannot guarantee the matrix $I - USU^*$ to be unitary because the latter will need $S + S^* = S^*S$, which simplifies to the condition $S = TT^+S$ after plugging in the above quantities. But in general ,$S = TT^+S$ does hold when T is singular.

Without the symmetric condition $X^*Y = Y^*X$, using a pseudo-inverse does not guarantee $I - USU^*$ to be unitary. In comparison, the proof in [4] of Theorem 3.1 shows that the unitary of the $I - 2P$ is trivially guaranteed by $P = FF^+$ in (3.1) being an orthogonal projector. The weakened result in Property 3.1 even after using a pseudo-inverse shows that $X^*Y \neq Y^*X$ generates more intricacies over the case where $X^*Y = Y^*X$ holds.

Next, we explore a way to keep the $I - 2P$ structure that is typical in a Householder reflector. This approach requires placing the possible non-Hermitian structure directly in P. It means the P is no longer an orthogonal projector, but we will see that there is still an orthogonal projector hidden in the term represented by $2P$.

Theorem 3.3. *Given $X, Y \in \mathbb{C}^{n\times k}$, where $n \geq k \geq 1$ There is a matrix $P \in \mathbb{C}^{n\times n}$ with $\operatorname{rank}(P) \leq k$ such that $I - 2P$ is unitary and $(I - 2P)X = Y$ if and only if $X^*X = Y^*Y$.*

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Proof. The ($\Longrightarrow$) part is obvious since $(I-2P)X = Y$ and $I-2P$ being unitary lead to $X^*X = X^*(I-2P)^*(I-2P)X = Y^*Y$.

For the ($\Longleftarrow$) part: Let a QR decomposition of $X-Y$ be $UR = X-Y$, where $U^*U = I_k$ and R is upper triangular of size $k \times k$. Define $T = U^*X$, $M = U^*Y$. We first show that $T^*T = M^*M$ under the condition $X^*X = Y^*Y$.

Since UU^* is an orthogonal projector onto range$(X-Y)$, we have $UU^*(X-Y) = X-Y$. Thus,

$$\begin{aligned} T^*T - M^*M &= X^*UU^*X - Y^*UU^*Y \\ &= X^*UU^*(X-Y) + (X^*-Y^*)UU^*Y \\ &= X^*(X-Y) + (X-Y)^*Y \\ &= X^*X - X^*Y + X^*Y - Y^*Y = 0. \end{aligned}$$

Since $T^*T = M^*M$, a simple argument based on SVD of T and M shows that T and M share the same right singular subspace and singular values. Thus,there exists a unitary $Q \in \mathbb{C}^{k\times k}$ such that $M = QT$.

What we need is a P such that $(I-2P)X = Y$, which means

$$2PX = X - Y = UU^*(X-Y) = U(T-M).$$

For this to hold, we can choose

$$P = \frac{1}{2}U(U^* - QU^*).$$

Clearly, rank$(P) \leq k$, and it is straightforward to verify that

$$2PX = U(U^* - QU^*)X = U(T - QT) = U(T-M) = X - Y \quad\Longrightarrow\quad (I-2P)X = Y.$$

Notice that

$$2P = U(I_k - Q)U^*.$$

Let $S = I_k - Q$, then $I - 2P = I - USU^*$. This matrix being unitary is equivalent to $S + S^* = S^*S$, the latter is easy to verify since Q is unitary:

$$S + S^* = I_k - Q + I_k - Q^* = (I_k - Q^*)(I_k - Q) = S^*S. \qquad \square$$

The proof for Theorem 3.3 also gives a complete proof of Theorem 3.2 without needing any extra condition: The constructed U and S in the proof of Theorem 3.3 can serve as the sought matrices in Theorem 3.2.

Observe that the $I-2P$ matrix in Theorem 3.3 essentially contains a subtraction from I by two matrices instead of one: $I - 2P = I - (UU^* - UQU^*)$. It reveals another way to extend the $I-2P$ structure in the standard Householder matrix where P is an orthogonal projector: When X^*Y is not Hermitian, the $2P$ needs to be separated into two matrices as $P_1 + P_2$, where $P_1 = UU^*$ is still an orthogonal projector; however, $P_2 = -UQU^*$, which loses symmetry caused by $X^*Y \neq Y^*X$. The P_2 may not even be an oblique projector, but such structure deviation from an orthogonal projector is necessary in order to address the lost symmetry in X^*Y.

Comparing with the $I - uu^* - e^{i\beta}uu^*$ matrix mentioned at the end of Section 2, we see that $I - P_1 - P_2 = I - UU^* + UQU^*$ turns out to be a direct generalization of the former matrix.

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Finally, we study the case where matrices X and Y may be rank deficient. This is another intricacy that does not exist when reflecting a single vector. The results in Theorems 3.2 and 3.3 can be strengthened in the rank deficient case.

Observe that the S matrix in Theorem 3.2 is of size $k \times k$, and the rank of P in Theorem 3.3 is upper bounded by k. But when the block matrices $X, Y \in \mathbb{C}^{n\times k}$ are rank deficient, it is possible to reduce the size of S and the rank of P. The deciding factor is $\mathrm{rank}(X-Y)$: If $\mathrm{rank}(X-Y) < k$, then the size of S and the rank of P can be reduced from k to $\mathrm{rank}(X-Y)$.

We first strengthen Theorem 3.3 in Theorem 3.4.

THEOREM 3.4. *: Given $X, Y \in \mathbb{C}^{n\times k}$ where $n \geq k \geq 1$. Let $p = \mathrm{rank}(X-Y)$. There is a matrix $P \in \mathbb{C}^{n\times n}$ with $\mathrm{rank}(P) \leq p$ such that $I - 2P$ is unitary and $(I-2P)X = Y$ if and only if $X^*X = Y^*Y$.*

Proof. The proof is essentially the same as that for Theorem 3.3. One only needs to observe that the QR decomposition of $X - Y$ can be replaced by a thin QR decomposition: When $UR = X - Y$ is the thin QR decomposition of $X - Y$, the U has p orthonormal columns, where $p = \mathrm{rank}(X-Y) \leq k$. All the remaining steps in the proof of Theorem 3.3 can go through without any problem. The $T = U^*X$ and $M = U^*Y$ are now of size $p \times k$, and the Q matrix for $M = QT$ is of size $p \times p$. The needed P matrix is

$$P = \frac{1}{2}U(I_p - Q)U^*.$$

Thus, $\mathrm{rank}(P) \leq p \leq k$. ∎

Similarly, the S matrix in Theorem 3.2 can be reduced to size $p \times p$ as well because the same proof for Theorem 3.4 with $S = I_p - Q$ can be applied to establish the corresponding result. We summarize it in Theorem 3.5. Since one of the *if and only if* directions based on $X^*X = Y^*Y$ is trivial, in Theorem 3.5, we only state the nontrivial direction and make another *if and only if* equivalence based on the key deciding factor $\mathrm{rank}(X-Y)$.

THEOREM 3.5. *: Given $X, Y \in \mathbb{C}^{n\times k}$ where $n \geq k \geq 1$ and $X^*X = Y^*Y$. Let $p \leq k$. There is a unitary matrix of form $I - USU^*$, where $U \in \mathbb{C}^{n\times p}$ has orthonormal columns and $S \in \mathbb{C}^{p\times p}$, such that $(I - USU^*)X = Y$ if and only if $\mathrm{rank}(X-Y) \leq p$.*

Proof. The ($\Longleftarrow$) part essentially follows from the proof of Theorem 3.4, and the ($\Longrightarrow$) part follows directly from $X - Y = USU^*X$. ∎

The size reduction of S and U is more significant when $p = \mathrm{rank}(X-Y)$ is much smaller than k. For example, if X is very rank deficient, i.e., $\mathrm{rank}(X) = r \ll k$, and if in addition $\mathrm{range}(X) = \mathrm{range}(Y)$, which is sufficient to ensure $\mathrm{rank}(X-Y) \leq r$, then the S matrix only needs to be of size $r \times r$. In numerical computations, such size reduction in S and U can be highly preferred since it can reduce both memory requirement and computational cost.

4. The $I - (P_1 + P_2)$ structure for a targeting problem without the norm-preserving requirement. The standard Householder reflector is an Hermitian unitary matrix that has the intrinsic structure $I - 2P$, where P is an orthogonal projector. This unique structure makes the Householder reflector norm-preserving.

Our earlier studies are for the cases in which the Hermitian matrix $2P$ needs to be extended to be non-Hermitian, such as the μP in (2.3) or the USU^* in Theorem 3.2. These have the subtraction-by-one-matrix

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structure of $I - M$ for a certain matrix M, similar to $I - 2P$. While in Theorem 3.3, we encountered the subtraction-by-two-matrices structure $I - (P_1 + P_2)$.

Interestingly, the special structure $I - (P_1 + P_2)$ turns out to be useful also for a different type of targeting problem (e.g., from [7]), in which the norm-preserving condition $X^*X = Y^*Y$ is not required. The unique features of such a targeting problem are (i) X^*Y is known to be positive definite and (ii) the matrix A for $AX = Y$ is required to be positive definite.

For this targeting problem, we construct $A = I - (P_1 + P_2)$, where P_1 is an orthogonal projector, but P_2 needs to have certain definiteness (thus Hermitian) in order to satisfy the requirement of A being positive definite.

THEOREM 4.1. *Given $X, Y \in \mathbb{C}^{n\times k}$, where $n \geq k \geq 1$ and X^*Y is positive definite. There is a positive definite matrix of form $I - P_1 - P_2$, where P_1 is an orthogonal projector and P_2 is negative semidefinite, such that $(I - P_1 - P_2)X = Y$.*

Proof. The X^*Y being positive definite means that $X^*Y = (X^*Y)^* = Y^*X$ and that both X and Y have full rank k. Therefore, $Y(Y^*X)^{-1}Y^*$ is a rank-k Hermitian positive semidefinite matrix. Let $P = Y(Y^*X)^{-1}Y^*$, then clearly P maps X into Y. However, the constructed P is only positive semidefinite but not definite if $n > k$.

Note that the orthogonal projector $I - X(X^*X)^{-1}X^*$ is also positive semidefinite and satisfies $(I - X(X^*X)^{-1}X^*)X = 0$.

Let $A = P + I - X(X^*X)^{-1}X^*$, then A is at least positive semidefinite. Now we show by contradiction that A must be positive definite: If A is not positive definite, then there is an eigenvector v of A associated with an eigenvalue 0, i.e., $Av = 0$ with $v \neq 0$.

Express this v into two parts as $v = v_1 + v_2$, where $v_1 \in \text{range}(X)$ and $v_2 \in \text{range}^{\perp}(X)$, i.e., $v_1 = Xw$ for some $w \in \mathbb{C}^k$, and $v_2^*X = 0$. Then,

$$\begin{aligned} Av = (P + I - X(X^*X)^{-1}X^*)(v_1 + v_2) = Pv + v_2 = 0, \\ v^*Av = 0 \iff v^*Pv = -v_2^*v_2 = -\|v_2\|^2 \leq 0. \end{aligned}$$

Since P is positive semidefinite, $v^*Pv = -\|v_2\|^2$ is possible only when $v_2 = 0$. Therefore, $v = v_1 = Xw \in \text{range}(X)$. Since $v^*Pv = v^*Y(Y^*X)^{-1}Y^*v = 0$, but $(Y^*X)^{-1}$ is positive definite, we must have $Y^*v = Y^*Xw = 0$. Since Y^*X is positive definite, this leads to $w = 0$. Therefore, $v = Xw = 0$, which contradicts $v \neq 0$. Therefore, $A = I - X(X^*X)^{-1}X^* + P$ is positive definite. The requested matrices are $P_1 = X(X^*X)^{-1}X^*$, which is an orthogonal projector, and $P_2 = -P = -Y(Y^*X)^{-1}Y^*$, which is negative semidefinite. ∎

Remark: For the targeting problem under the condition that X^*Y is positive definite, there are infinitely many positive definite matrices A that can fulfill $AX = Y$. In fact, the matrix of form $A = Y(Y^*X)^{-1}Y^* + c(I - X(X^*X)^{-1}X^*)$ is positive definite for any scalar $c > 0$, it readily fulfills the target $AX = Y$. The vast non-uniqueness of A is an interesting feature of such type of targeting problem without a norm-preserving requirement. The structure in the general A appears to be different from $I - (P_1 + P_2)$; however, the nonzero c can be factored out and moved to the target as

$$(I - X(X^*X)^{-1}X^* + \frac{1}{c}Y(Y^*X)^{-1}Y^*)X = \frac{1}{c}Y.$$

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This equivalent formulation reveals that even the general matrix for this specific SPD targeting problem has the $I - (P_1 + P_2)$ structure, where one of the P_1 and P_2 is an orthogonal projector.

5. Conclusions. For two vectors x, y with $\|x\| = \|y\|$, the standard Householder reflector $H = I - 2uu^*$ cannot satisfy $Hx = y$ if $x^*y \notin \mathbb{R}$. In Section 2, we extended the Householder reflector into $H = I - \eta uu^*$ for some appropriate η, so that the "reflection" $Hx = y$ can hold for all x and y without a phase rotation of y. In Lemma 2.3, we derived that the magic number 2 in the standard Householder reflector appears implicitly in $I - \eta uu^*$ when $\eta \neq 2$.

In Section 3, we generalized the Householder reflector to solve the the norm-preserving linear targeting problem $HX = Y$ for $X, Y \in \mathbb{C}^{n\times k}$, where $\|X\| = \|Y\|$ and $k \geq 1$. We extended the methodology from [4] to achieve targeting for a wider class of matrices X and Y that do not satisfy the symmetry condition $X^*Y = Y^*X$. We developed two extensions: $H = I - USU^*$, where $U^*U = I_p$ with $p \leq k$, and $S \in \mathbb{C}^{p\times p}$ is generally not Hermitian; and $H = I - P_1 - P_2$, where P_1 and P_2 are low-rank matrices but only P_1 is required to be an orthogonal projector. Intriguingly, the $I - P_1 - P_2$ structure also arises in a distinct SPD targeting problem $AX = Y$ where norm preservation $\|X\| = \|Y\|$ is not required, as discussed in Section 4.

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