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The noncompact portion of $Sp(4, R)$ via quaternions

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Abstract

This work provides a quaternionic representation for real symplectic matrices in dimension four, analogous to that for the orthogonal group. This is achieved by characterizing positive definite symplectic matrices via quaternions. It also provides a technique to compute the polar decomposition for $Sp(4, R)$ which requires no diagonalization, but relies only on the solution of a 2×2 linear system. This constructive technique to compute the 'non-compact portion' of $Sp(4, R)$ is then used to compute the smallest eigenvalue of the noise (covariance) matrix of the so-called Gaussian two-mode systems. Other applications where this non-compact portion is relevant are also discussed.

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1. Introduction

The most important groups in physics are, arguably, the rotation and the symplectic groups [2, 8]. In particular, the symplectic group is central to classical mechanics [16], to classical and quantum optics [2], quantum mechanics and quantum information processing [5]. Therefore, having as many parametrizations of these groups as possible is desirable.

In dimension four, there is a well-known parametrization of the orthogonal group via a pair of unit quaternions. This has innumerable applications in physics and engineering [15, 17]. For the symplectic group, $Sp(4, R)$, there seems to be none. Note, by the 'symplectic group', we refer to the real symplectic group, and *not the similarly labeled group* $Sp(n)$, which preserves the standard inner product on H^n (here H stands for the quaternions). The latter is, of course, already defined via quaternions. It is the intention of this note to provide such a quaternionic parametrization for $Sp(4, R)$.

The representation obtained here also achieves the following tasks of practical utility: (i) a test for positive definiteness of a symplectic, symmetric matrix which requires checking two simple inequalities; (ii) a parametrization of symplectic, positive definite matrices which can be used in applications; (iii) most importantly, an explicit procedure for obtaining the polar decomposition of a symplectic matrix, which requires no spectral calculations, but which instead requires the solution of a simple 2×2 linear system. This can be used, for instance, in applications where extracting the non-compact part of $Sp(4, R)$ is needed; (iv) an expression for the characteristic polynomial of a symplectic matrix, which can be used to find an explicit formula for the minimal eigenvalue of a positive definite, symplectic matrix (this is useful in applications such as quantifying the squeezing in Gaussian states).

For motivating the rest of the paper (in particular, the contents of the introductory section), we assume temporarily some familiarity with the algebra ismorphism between $H \otimes H$ (the tensor product of the quaternions, H, with itself) and the algebra of 4×4 real matrices, denoted $M_4(R)$ [7, 11, 14, 17–19, 21, 22]. See section 2 for more details. Using this algebra isomorphism, it would seem that to obtain a quaternion representation of an $X \in Sp(4, R)$ a logical approach would be to write out the conditions imposed on the quaternion representation of an $X \in M_4(R)$ by the relation

$$X^T J_4 X = J_4,$$

where J_4 is the defining matrix of the symplectic group (its quaternion representation is $1 \otimes j$). However, this produces an immensely complicated system of equations. Indeed, if one were to pursue this approach for the orthogonal group, i.e., write out the condition $X^T X = I$ in quaternion form, one does not recover the pair of unit quaternions representation unless one assumes *a priori* that the quaternions representing the matrix are decomposable, i.e., by an element $u \otimes v \in H \otimes H$. That this is not an assumption follows from the fact that the exponential map is onto $SO(4, R)$. However, the corresponding statement for $Sp(4, R)$ is incorrect.

To understand, the approach taken in this work, we note that the initial suggestion that one write out the quaternionic version of the condition $X^T J_4 X = J_4$ leads to something tractable, provided one imposes the additional restriction that the original X be also *real symmetric*. This is very useful since it is known that in the polar decomposition $X = UP$, of a symplectic X, both the orthogonal factor (U) and the positive definite factor (P) are symplectic as well (see [8, 16, 20] for instance). For a variety of reasons, it is more convenient to obtain quaternionic representations of symmetric and symplectic X and then further refine these to obtain quaternionic characterizations of positive definite and symplectic X. Characterizing symplectic, orthogonal matrices is simple. Combining the two one gets a quaternionic representation of symplectic matrices. This is stated in theorem 3.2.

There are, of course, other global factorizations of the symplectic group, such as the Euler (Cartan) and Iwasawa decompositions [2, 8–10, 24], which could have been used as starting points for finding a quaternionic representation. But we found the polar decomposition as the most useful, since the polar decomposition of a matrix has innumerable applications [12, 13].

It is appropriate at this point to record some history of the linear algebraic applications of the isomorphism between $H \otimes H$ and $M_4(R)$. This isomorphism is central to the theory of Clifford algebras [17]. However, it is only relatively recently been put into use for linear algebraic (especially numerical linear algebraic) purposes. To the best of our knowledge, the first instance seems to be the work of [14], where it was used in the study of linear maps preserving the Ky-Fan norm. Then in [11], this connection was used to obtain the Schur canonical form explicitly for real 4×4 skew-symmetric matrices. Next is the work of [7, 18, 19], wherein this connection was put to innovative use for solving eigenproblems of several classes of structured 4×4 matrices. Finally, in [21, 22], this isomorphism was used to explicitly calculate the exponentials of a wide variety of 4×4 matrices.

The rest of this manuscript is organized as follows. In the following section some notation and preliminary results on symplectic matrices, positive definite matrices and the algebra isomorphism between $H \otimes H$ and $M_4(R)$ are collected. The following section contains the technical results in this work. Theorem 3.1 provides the quaternion characterization of positive definite symplectic matrices central to this work. This is used in theorem 3.2 to provide a quaternion representation of $Sp(4, R)$. One technical tool in the proof of proposition 3.1 is that of squaring a symmetric, symplectic matrix. This is also a key ingredient in the proof of theorem 3.3. This latter theorem provides an explicit technique to calculate the polar decomposition of matrices in $Sp(4, R)$, which requires no diagonalization. This is summarized in an algorithm. Next a different perspective is provided on the paucity of symplectic, symmetric square roots of $X^T X$, for an $X \in Sp(4, R)$. As a byproduct an explicit formula for the characteristic polynomial of an $X \in Sp(4, R)$ is obtained. The following section considers applications to squeezing operations and to a key step in the computation of Lyapunov exponents of linear Hamiltonian dynamical systems. In particular, an explicit formula for the minimal eigenvalue of Gaussian covariance matrices is provided. The final section offers some conclusions.

2. Notation and preliminary observations

The following definitions, notations and results will be frequently met in this work:

- $M_4(R)$ (also denoted $gl(4, R)$) is the algebra of real 4×4 matrices.
- $J_{2n} = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}$. $Sp(2n, R)$ denotes the Lie group of symplectic matrices, i.e., those $2n \times 2n$ matrices, satisfying $X^T J_{2n} X = J_{2n}$. $sp(2n, R)$ is its Lie algebra, consisting of real Hamiltonian matrices.
- If $X \in Sp(2n, R)$, then $X^{-1} = -J_{2n} X^T J_{2n}$. Furthermore, if $X \in Sp(2n, R)$ then X^T is also in $Sp(2n, R)$.
- Essential use of the following theorem will be made in this work (see [8, 16, 20]):

  Proposition 2.1. *Let X be a real symplectic matrix, and let $X = UP$ be its polar decomposition, with P positive definite and U real orthogonal. Then P and U are also real symplectic.*

  Remark 2.1. An analogous statement holds for the polar decomposition of a symplectic X with orders of the factors switched. In other words, if $X = QV$ is the polar decomposition of a symplectic X, with Q positive definite and V orthogonal, then both Q and V are symplectic.

  See [20] for examples of other matrix groups for which an analogous statement holds. It is worth recalling here that P is the unique positive definite square root of the positive definite matrix $X^T X$.
- For a polynomial $P(x) = \sum_{i=0}^{n} a_i x^i$, of degree at most n, its reverse is the polynomial $P_{\text{rev}}(x) = \sum_{i=0}^{n} a_{n-i} x^i$. In this work we will use the fact that the characteristic polynomial of a symplectic matrix *equals its reverse* (see [20], for instance).

We next collect some definitions and results on real positive definite matrices. All details, together with extensions to the complex positive semidefinite case, may be found in [12, 13].

- **Definition 2.1.** *Let Y be a real positive definite matrix. A real square matrix Z satisfying $Y = Z^T Z$ is said to said to be a square root of Y.*

  Square roots of positive definite matrices are not unique. However, if Z_1 is a square root of Y then Z_2 is also a square root of Y iff there exists a real orthogonal matrix U such that $Z_2 = UZ_1$.

- Let Y be a real positive definite matrix. Then there exist real symmetric matrices H such that $Y = H^2$. Clearly any such H is a square root in the sense of definition 2.1.
- Let Y be a real positive definite matrix. Then there exists a unique real positive definite matrix P with $Y = P^2$. This P is an example of a real symmetric matrix whose square equals Y.

Next relevant definitions and results regarding quaternions and their connection to real matrices will be presented. Throughout H will be denoting the skew-field (the division algebra) of the *quaternions*, while P stands for the *purely imaginary* quaternions, tacitly identified with R^3.

$H \otimes H$ and $M_4(R)$: the algebra isomorphism between $H \otimes H$ and $gl(4, R)$, which is central to this work is the following [7, 17–19]:

- Associate to each product tensor $p \otimes q \in H \otimes H$, the matrix, $M_{p\otimes q}$, of the following linear map from H to itself (viewed as a linear map from R^4 to itself, by identifying R^4 with H via the basis $\{1, i, j, k\}$)

$$x \rightarrow px\bar{q}. \tag{2.1}$$

  Here, $\bar{q}$ is the conjugate of q. Extend this by linearity to all of $H \otimes H$. For instance the matrix of $2u_1 \otimes v_1 + 9u_2 \otimes v_2$ is $2M_{u_1\otimes v_1} + 9M_{u_2\otimes v_2}$.

  This yields an algebra isomorphism between $H \otimes H$ and $M_4(R)$. In particular, $J_4 = M_{1\otimes j}$.
- Define conjugation in $H \otimes H$ by first defining the conjugate of a decomposable tensor $a \otimes b$ as $\bar{a} \otimes \bar{b}$, and then extending this to all of $H \otimes H$ by linearity. Then $M_{\bar{a}\otimes\bar{b}} = (M_{a\otimes b})^T$, i.e., quaternionic conjugation's matrix analogue is matrix transposition.

  Thus, the most general element $X \in M_4(R)$ admits the quaternion representation $a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k + s \otimes 1 + 1 \otimes t$, with $a \in R$ and $p, q, r, s, t \in P$. Indeed, the first four summands are equal to their conjugate, while the remaining two are minus their conjugate. Thus, the summand $a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k$ is the symmetric part of X, while the summand $s \otimes 1 + 1 \otimes t$ is the anti-symmetric part of X.
- One can check by direct calculation, that all terms, except the $a(1 \otimes 1)$ term, have traceless matrix representations. Hence trace of X is $4a$. Expressions for p, q, r, s, t (which are linear in the entries of the matrix being represented) are easy to find [18]. For instance, if $Y = \frac{X+X^T}{2}$, then

$$q = \tfrac{1}{2}[(Y_{23} - Y_{14}), (Y_{11} - Y_{22} + Y_{33} - Y_{44}), (Y_{34} + Y_{12})].$$

3. Quaternion representations of $Sp(4, R)$

To develop a quaternionic representation of an $X \in Sp(4, R)$, we invoke proposition 2.1.

Let $X = UP$ be the polar decomposition of X. Since U is symplectic and orthogonal it must, in fact, be special orthogonal. Obtaining the quaternionic representation of such a matrix is easy [7]. It is given by $q = u \otimes v$, with u, v unit quaternions with the further restriction that $vj = jv$. Hence, $v = v_0 + v_2 j$, with $v_0^2 + v_2^2 = 1$.

We now obtain a quaternionic representation of P:

Theorem 3.1. *Let X be a 4×4 symplectic matrix, with nonzero trace, which is also symmetric. Then it admits the quaternion representation $X = a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k$, with $aq = r \times p$, $p \cdot q = 0 = r \cdot q$, and a satisfying the constraint $a^2 - p \cdot p + q \cdot q - r \cdot r = 1$. If $a = \frac{1}{4}\mathrm{Tr}(X) \neq 0$, then X is symplectic iff $aq = r \times p$ and $a^2 - p \cdot p + q \cdot q - r \cdot r = 1$. Such* *an X is positive definite in addition, iff (i)* $a > 0$ *and (ii)* $2a^2 - 2(q \cdot q) + 1 > 0$. *In particular, a symmetric, symplectic matrix with* $a > 0, q = 0$ *is always positive definite.*

Proof. The proof proceeds by equating the quaternion expansion of $X^T J_4 X$ to that of J_4, namely, with $1 \otimes j$. Since for any X, the matrix $X^T J_{2n} X$ is always skew-symmetric, one needs to only calculate, only those terms of the form $s \otimes 1$ and $1 \otimes t$, with $s, t \in P$. The remaining will automatically be zero. Specifically, the expansion of $X^t J_4 X$ is

$$(a^2 - p \cdot p + q \cdot q - r \cdot r)(1 \otimes j) + (2r \times p - 2aq) \otimes 1 + (2p \cdot q)1 \otimes i + (2r \cdot q)1 \otimes k.$$

Hence, the stated conditions for symplecticity follow. Note that the vanishing of the second term yields the condition $aq = r \times p$. Thus, if $a \neq 0$, then $q = \frac{r \times p}{a}$ and this, of course, ensures the conditions $p \cdot q = 0 = r \cdot q$.

Now X is positive definite, in addition, iff all coefficients a_i of X's characteristic polynomial $p(x) = x^4 - a_3 x^3 + a_2 x^2 - a_1(x) + a_0$ are positive (this follows from Descartes rule of signs, for instance).

Since X is symplectic, $p(x)$ equals its reverse. So $a_3 = a_1 = 4a, a_0 = 1$. Now, $a_2 = \frac{1}{2}[(\mathrm{Tr}(X))^2 - \mathrm{Tr}(X^2)]$. But, from the expansion of X, it follows that the $1 \otimes 1$ term in X^2 is $a^2 + p \cdot p + q \cdot q + r \cdot r$. So, using $1 = a^2 + q \cdot q - p \cdot p - r \cdot r$, we see that $a_2 = 2(2a^2 - 2(q \cdot q) + 1)$. Hence the result follows. □

Remark 3.1. From the above theorem, we have a simple test to check if a real symmetric matrix is symplectic and positive definite. Note, in particular, that only two inequalities have to be verified for positive definiteness, in contrast to the general situation. These conditions also yield an inequality free parametrization of such matrices, as follows. Pick two vectors $\alpha, \beta \in R^3$. Define θ via $\tan(2\theta) = \frac{2\alpha^T \beta}{\beta^T \beta - \alpha^T \alpha}$. Define $\gamma_1 = \sqrt{\alpha^T \alpha \cos^2(\theta) + \beta^T \beta \sin^2(\theta) - \alpha^T \beta \sin(2\theta)}$, $\gamma_2 = \sqrt{\alpha^T \alpha \sin^2(\theta) + \beta^T \beta \cos^2(\theta) + \alpha^T \beta \sin(2\theta)}$. Set $c_i = \cosh(\gamma_i), s_i = \sinh(\gamma_i)$. Finally, define $w_1 = (\alpha_1 \cos(\theta) - \beta_1 \sin(\theta), \alpha_2 \cos(\theta) - \beta_2 \sin(\theta), \alpha_3 \cos(\theta) - \beta_3 \sin(\theta)]$, $w_2 = [\alpha_1 \sin(\theta) + \beta_1 \cos(\theta), \alpha_2 \sin(\theta) + \beta_2 \cos(\theta), \alpha_3 \sin(\theta) + \beta_3 \cos(\theta)]$. Then the parametrization of symplectic, positive-definite matrices is $X = c_1 c_2 (1 \otimes 1) + p \otimes i + \frac{r \times p}{c_1 c_2} \otimes j + r \otimes k$, with $p = \frac{c_2 s_1 \cos(\theta)}{\gamma_1} w_1 + \frac{c_1 s_2 \sin(\theta)}{\gamma_2} w_2$ and $r = \frac{c_1 s_2 \sin(\theta)}{\gamma_2} w_2 - \frac{c_2 s_1 \sin(\theta)}{\gamma_1} w_1$. It is important to note that this is only a parametrization, and does not provide the positive definite factor of the polar decomposition of a *given* symplectic matrix.

From here we get the quaternionic representation of a symplectic X, which we record for completeness.

Theorem 3.2. *Let X be an element of* $Sp(4, R)$. *Then there exist* $a, v_0, v_2 \in R$, $p, q, r \in P$, *and a unit quaternion u satisfying the constraints* $a^2 - p \cdot p + q \cdot q - r \cdot r = 1, q = \frac{r \times p}{a}$, $a > 0, 2a^2 - 2q \cdot q + 1 > 0$ *and* $v_o^2 + v_2^2 = 1$, *such that X admits the following quaternion representation* $X = [u \otimes (v_0 + v_2 j)][a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k]$.

We now turn to the issue of computing these quaternions from the entries of X. Assuming the positive definite portion of the representation is available, the calculation of the factor $[u \otimes (v_0 + v_2 j)]$ is amenable to the any technique which will yield the quaternion representation of a matrix in $SO(4, R)$. This ought to be folklore, but surprisingly the only explicit record of this that we were able to find is in [4].

Next, consider computing the positive definite factor. It is the unique positive definite square root of $X^T X$. We will see below that there is a very explicit method for finding it, which reveals some facts which are of interest in their own right. Specifically, recall from section 2, that any positive definite matrix is the square of a real symmetric matrix. The real symmetric matrix is not unique, but one of these is the unique positive definite square root of the positive definite matrix in question. Now, when the positive matrix is $X^T X$, $X \in Sp(4, R)$, we know that the unique positive definite square root is also symplectic. Furthermore, being positive definite its trace is positive. So, instead of looking at all possible real symmetric matrices whose square is $X^T X$, one needs to inspect only those which are symplectic and have positive trace, in addition. One then finds the pleasant conclusion that there are only few such candidates.

Theorem 3.3. *Let $X \in Sp(4, R)$. Then there are at most two (and, at least one) matrices H which satisfy (i) $H^2 = X^T X$; (ii) H is real symmetric and symplectic; and (iii) $Trace(H) > 0$. One of these is precisely the unique positive definite square root of $X^T X$, and thus the positive definite factor in the polar decomposition of X. Furthermore, H can be found explicitly via the solution of a simple linear system.*

Proof. Let $X \in Sp(4, R)$. Then so is X^T and hence $X^T X \in Sp(4, R)$. Let $b1 \otimes 1 + c \otimes i + d \otimes j + e \otimes k$ be its quaternion representation. Note, as $X^T X$ is positive definite, $b > 0$, while c, d, e are pure quaternions. Let H be a real symmetric, symplectic matrix with nonzero trace satisfying $H^2 = X^T X$. Suppose $H = a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k$. Then equating H^2 to $X^T X$ yields the system of equations

$$\begin{aligned} b &= a^2 + p \cdot p + q \cdot q + r \cdot r \\ c &= 2ap + 2q \times r \\ d &= 2aq + 2r \times p \\ e &= 2ar + 2p \times q. \end{aligned} \tag{3.1}$$

□

In addition, as H is symplectic, this system is augmented by conditions (i) $a > 0$; (ii) $q = \frac{r \times p}{a}$; (iii) $1 = a^2 + q \cdot q - p \cdot p - r \cdot r$.

The second equation in the system equation (3.1), together with $aq = r \times p$, yields $q = \frac{d}{4a}$.

At this point it is convenient to divide the argument into two cases. The case $q \neq 0$ and the case $q = 0$. Note (as $a \neq 0$) these are equivalent to the cases $d \neq 0$ and $d = 0$ respectively.

The case $d \neq 0$. Using, $1 = a^2 - q \cdot q + p \cdot p - r \cdot r$, we find $\frac{b+1}{2} = a^2 + q \cdot q = a^2 + \frac{d \cdot d}{16a^2}$. This yields a quadratic for a^2, namely

$$a^4 - \frac{b+1}{2} a^2 + \frac{d \cdot d}{16} = 0. \tag{3.2}$$

Note that the discriminant of the above equation is $\frac{(b+1)^2}{4} - \frac{d \cdot d}{4}$, which is easily seen to be positive. Further, since its coefficients change sign both these roots are positive. One of these roots must correspond to the positive definite square root of $X^T X$, while the other cannot (due to uniqueness). In view of the requirement $2a^2 - 2q \cdot q + 1 > 0$, for positive definiteness, it is easily seen that the larger of these two roots is the one to pick. This yields a and hence q.

To find r and p, one inserts the expression $q = \frac{r \times p}{a}$ into the equations for c and e to find

$$\begin{aligned} c &= 2ap + \frac{2}{a}[(r \cdot r)p - (p \cdot r)r] \\ e &= 2ar + \frac{2}{a}[(p \cdot p)r - (p \cdot r)p]. \end{aligned} \tag{3.3}$$

This would yield a linear system for the unknowns p, r in terms of the knowns c and e provided we can express $p \cdot p, r \cdot r, p \cdot r$ in terms of e, c. To achieve this, first note that

$$c \cdot c = 4a^2 p \cdot p + 4\|q \times r\|^2 + 8a^2 p \cdot (q \times r)$$
$$e \cdot e = 4a^2 r \cdot r + 4\|p \times q\|^2 + 8a^2 r \cdot (p \times q).$$

Hence,

$$c \cdot c - e \cdot e = 4a^2 p \cdot p - 4a^2 r \cdot r + 4\|q \times r\|^2 - 4\|p \times q\|^2.$$

Next, since $\|q \times r\|^2 = (q \cdot q)(r \cdot r)$ and $\|p \times q\|^2 = (p \cdot p)(q \cdot q)$, one gets

$$p \cdot p - r \cdot r = \frac{c \cdot c - e \cdot e}{4a^2 - 4q \cdot q}.$$

Using $\frac{b+1}{2} = a^2 + q \cdot q = 1 + p \cdot p + r \cdot r$, we find $p \cdot p + r \cdot r = \frac{b-1}{2}$. So, one gets a linear system for $p \cdot p$ and $r \cdot r$, in terms of already determined quantities. To find $p \cdot r$, we note that since $a^2 - q \cdot q \neq 0$, one gets $p \cdot r = \frac{c \cdot e}{4(a^2 - q \cdot q)}$.

Inserting these values for $p \cdot p$, $p \cdot r$ and $r \cdot r$ into equations (3.3) yields a linear system for the vectors p and r,

$$c = \alpha p + \beta r, \qquad e = \beta p + \gamma r \tag{3.4}$$

with $\alpha = 2a + \frac{b-1}{2a} + \frac{e \cdot e - c \cdot c}{a(4a^2 - 4q \cdot q)}$, $\beta = -\frac{c \cdot e}{4a^2 - 4q \cdot q}$, $\gamma = 2a + \frac{2p \cdot p}{a} = 2a + \frac{b-1}{2a} + \frac{c \cdot c - e \cdot e}{a(4a^2 - 4q \cdot q)}$.

The system equation (3.4) is invertible as the Cauchy–Schwarz inequality reveals that the quantity $\alpha\gamma - \beta^2$ is at least $4a^2$.

Thus, we have found H.

The case $d = 0$. Now equation (3.2), when $d = 0$, has two roots, namely $\frac{b+1}{4}$ (which is strictly positive) and 0. Thus, by picking $a = \frac{\sqrt{b+1}}{2}$, $q = 0$, $p = \frac{c}{\sqrt{b+1}}$ and $r = \frac{e}{\sqrt{b+1}}$, we find the only H which is symplectic, real symmetric, with positive trace and which satisfies $H^2 = X^T X$. Thus, by uniqueness, H must be the unique positive definite square root of $X^T X$.

We summarize the above discussion into an algorithm for finding the polar decomposition of an $X \in Sp(4, R)$:

Algorithm 3.1.

- *(1) Compute directly $X^T X$.*
- *(2) Compute the quaternion representation of $X^T X$. This is guaranteed to be of the form $b(1 \otimes 1) + c \otimes i + d \otimes j + e \otimes k$ (with $b \in R, c, d, e \in P$) since $X^T X$ is symmetric. Furthermore, these quantities are linear in the entries of $X^T X$.*
- *(3) Let H be a matrix which has positive trace, real symmetric and symplectic, and which satisfies $H^2 = X^T X$. One such H is the positive definite factor in the polar decomposition of X. Let H, which is symmetric, have quaternion representation $a(1 \otimes 1) + p \otimes i + q \otimes j + r \otimes k$ (with $a \in R$, $p \cdot q \cdot r \in P$). Steps 4–6 show how to compute a, p, q, r.*
- *(4) If $d = 0$, then compute $a = \frac{\sqrt{b+1}}{2}$, $q = 0$, $p = \frac{c}{\sqrt{b+1}}$ and $r = \frac{e}{\sqrt{b+1}}$. This is guaranteed to be the positive factor in the polar decomposition of X.*
- *(5) If $d \neq 0$, then let a be the positive square root of the larger of the two strictly positive roots of the quadratic $x^2 - \frac{b+1}{2}x + \frac{d \cdot d}{16} = 0$. Define $q = \frac{d}{4a}$. Find p, r by solving the linear system of equations (3.4).*
- *(6) This yields H as the unique positive definite square root of $X^T X$ and thus the symmetric part of the polar decomposition of X.*

- *(7) Next compute XH^{-1}, by using $H^{-1} = \begin{pmatrix} D^T & -B^T \\ -C^T & A^T \end{pmatrix}$, if $H = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$. The matrix XH^{-1} is symplectic and orthogonal, and thus will admit the quaternion representation $u \otimes (v_0 + v_2 j)$, with u a unit quaternion and $v_0^2 + v_2^2 = 1$.*
- *(8) To compute u, v_0, v_2 use the algorithm described in, e.g., [4].*

Remark 3.2. If one is interested in computing the other polar decomposition, described in remark 2.1, then one has to replace $X^T X$ by XX^T in step 1, and replace XH^{-1} by $H^{-1}X$ in step 7.

We give a different perspective on the 'paucity' of symplectic, symmetric square roots of $X^T X$ when $d \neq 0$.

Thus, suppose that H is a real symmetric, symplectic matrix with nonzero trace satisfying $H^2 = X^T X$, and suppose $\tilde{H}$ is another. Then, since $H, \tilde{H}$ are square roots of $X^T X$ (in the sense of definition 2.1), there exists a real orthogonal matrix U with $\tilde{H} = HU$. Clearly U must be symplectic too. Further, the conditions $\tilde{H}^2 = H^2$ and that $\tilde{H}$ be real symmetric are both equivalent to

$$UH = HU^T.$$

So, considering H as fixed we examine which symplectic orthogonal U lead to $UH = HU^T$. An elaborate calculation of UH and HU^T, the details of which are omitted, reveals that the only candidates for $U = u \otimes v$ are $1 \otimes 1, -1 \otimes 1, \frac{q}{\|q\|} \otimes j$ or $-\frac{q}{\|q\|} \otimes j$. Thus, there are precisely four symplectic, real symmetric square roots of $X^T X$ of which two have positive trace, and the remaining two have negative trace. If H has positive trace, then it is easy to see (e.g., by inspecting the $1 \otimes 1$ term in $\tilde{H}$) that of the remaining three candidates only the one corresponding to $U = \frac{q}{\|q\|} \otimes j$ can also have positive trace.

The omitted elaborate calculation of UH is also useful for finding an explicit expression for the characteristic polynomial of a symplectic X. Write $X = UP = \alpha(1 \otimes 1) + \beta \otimes p + \gamma \otimes j + \delta \otimes k + s \otimes 1 + 1 \otimes t$, where α is scalar and the $\beta, \gamma, \delta, s, t$ are pure quaternions.

Since its characteristic polynomial $P_X(x)$ equals its reverse, it is of the form $P_X(x) = x^4 + a_3 x^3 + a_2 x^2 + a_3 x + 1$. Furthermore, $a_3 = -\mathrm{Tr}(X)$ and $a_2 = \frac{1}{2}((\mathrm{Tr}(X))^2 - \mathrm{Tr}(X^2))$.

Clearly, then

$$a_3 = -4\alpha = -4(au_0 v_0 + (\mathrm{Im}\, u \cdot q)v_2). \tag{3.5}$$

To find a_2 one needs the trace of X^2. *A useful observation here is that for this one does not need to calculate X^2.* Once X has been found the trace of X^2 is simply $4(\alpha^2 + \beta \cdot \beta + \gamma \cdot \gamma + \delta \cdot \delta - s \cdot s - t \cdot t)$.

Now an explicit calculation (which makes repeated use of the fact that u, v are unit quaternions) reveals $\alpha^2 + \beta \cdot \beta + \gamma \cdot \gamma + \delta \cdot \delta - s \cdot s - t \cdot t$ is the expression $(v_0^2 - v_2^2)\left[q \cdot q + (u_0^2 - \|\mathrm{Im}\, u\|^2)a^2 - 2(\mathrm{Im}\, u \cdot q)^2\right] + p \cdot p + r \cdot r - 2[(\mathrm{Im}\, u \cdot p)^2 + (\mathrm{Im}\, u \cdot r)^2] + 8au_0 v_0 v_2(\mathrm{Im}\, u \cdot q)$.

Hence the expression for a_2 is

$$\begin{aligned} a_2 = {} & 8a^2 u_0^2 v_0^2 + 8v_2^2(\mathrm{Im}\, u \cdot q)^2 + 2(v_2^2 - v_0^2)\left[q \cdot q + (u_0^2 - \|\mathrm{Im}\, u\|^2)a^2 - 2(\mathrm{Im}\, u \cdot q)^2\right] \\ & - 2(p \cdot p + r \cdot r) + 4[(\mathrm{Im}\, u \cdot p)^2 + (\mathrm{Im}\, u \cdot r)^2]. \end{aligned} \tag{3.6}$$

The above calculations can be summarized in

Theorem 3.4. *Let $X \in Sp(4, R)$ be represented by quaternions as in theorem 3.2. Then its characteristic polynomial is expressible as $P_X(x) = x^4 + a_3 x^3 + a_2 x^2 + a_3 x + 1$, with a_3 and a_2 given by equation (3.5) and equation (3.6) respectively.*

4. Applications

In this section we consider potential applications of the previous sections.

We first note some immediate applications to the study of squeezing operations in quantum optics. Let us begin with a brief overview of squeezing mostly adapted from the treatment in [1–3, 23]. Given an n-mode continuous variable system evolving according to a Hamiltonian which is quadratic in the position ($\hat{q}$) and momentum ($\hat{p}$) operators, its density matrix evolves according to

$$\rho \rightarrow U(S)\rho U^{-1}(S).$$

Here S stands for the symplectic matrix representing the evolution of the corresponding classical system and $U(S)$ stands for the metaplectic representation of S. Note $U(S)$ acts on an infinite-dimensional Hilbert space and S acts on R^{2n}.

Next, let $\psi = (\hat{q}_1, \ldots, \hat{q}_n, \hat{p}_1, \ldots, \hat{p}_n)$. The noise or variance matrix of the quantum system in state ρ is a $2n \times 2n$ real matrix consisting of the second-order moments of the anti-commutators of the components of ψ. More specifically $V_{ij} = \frac{1}{2}\,\mathrm{Tr}(\rho(\psi_i\psi_j + \psi_j\psi_i))$, where ψ_k is the kth entry of ψ, $k = 1, \ldots, 2n$. Here one assumes, without loss of generality, that $\mathrm{Tr}(\rho\psi_k) = 0, k = 1, \ldots, 2n$. Note that some authors differ by a factor of two in their definition of the entries of V. The diagonal entries of V are commonly called quadrature noise.

V is a real symmetric positive definite matrix satisfying the further constraint that $V + \frac{i}{2}J_{2n}$ is positive semidefinite. This constraint is an expression of the uncertainty relations.

For our purposes it is significant that, while ρ experiences an infinite-dimensional evolution (specified by $U(S)$), the associated transformation of V itself is finite-dimensional given by

$$V \rightarrow SVS^T.$$

Now the state of the quantum system is said to be squeezed if there is an $U \in U(n)$ such that there is a diagonal entry of UVU^T which is strictly less than $\frac{1}{2}$. See [1], for instance, for an operational interpretation of this criterion. Here $U(n)$ stands for $2n \times 2n$ real symplectic, *orthogonal* matrices. The notation is justified due to the fact that this group of matrices is isomorphic to the group of $n \times n$ unitary matrices. The work of [23] provides an elegant test for characterizing whether ρ is squeezed or not. As per this test, ρ is squeezed iff the least eigenvalue, $l(V)$, of V is strictly less than $\frac{1}{2}$. This is the so-called $U(n)$-invariant criterion for squeezing.

There are some immediate applications of the results of the previous sections of this work to this subject.

- First, one can parametrize all squeezing operations for two-mode systems. From the polar decomposition it is clear that all such operations for n-mode systems are precisely the collection of $2n \times 2n$ positive definite symplectic matrices, *denoted* $\Pi(n)$ in [2, 3]. Indeed, if $S = UP$ is the polar decomposition of S, then $SVS^T = UPVP^TU^T$. As U is orthogonal, the eigenvalues of SVS^T are equal to those of PVP^T. Thus, only elements of $\Pi(n)$ can change $l(V)$, i.e., produce squeezing. In this regard, note that a parametrization of the equivalence classes of $\Pi(2)$, under $U(2)$ conjugation, is given in [3]. However, the squeezing effect on a quantum state of two elements of $\Pi(2)$ belonging to the same $U(2)$ conjugacy class, will, in general, be different, cf [3]. While pre-multiplication of an element of $\Pi(2)$ by an element of $U(2)$ does not change $l(V)$, conjugation by an element of $U(2)$ can. Indeed, if $\tilde{S} = UPU^T$, with $U \in U(n)$, $P \in \Pi(n)$, then $\tilde{S}V\tilde{S}^T = UPU^TVUPU^T$. Hence, the eigenvalues of $\tilde{S}V\tilde{S}^T$ are not, in general related to those of PVP^T. Thus, the parametrization in remark 3.1, which is not a parametrization of a $U(2)$ orbit, is relevant for this application.

- Next given a specific $S \in Sp(2n, R)$, corresponding to a specific quantum evolution, one can attempt to extract the 'amount of squeezing' in it. This is precisely performing the polar decomposition of S. Algorithm 3.1 does this for $n = 2$. Explicitly one computes P and then the least eigenvalue of PVP^T, where V is the noise matrix corresponding to $\rho(0)$, the initial density matrix.
- A third application to the same topic is to actually compute $l(V)$, for classes of noise matrices. The characterization of positive definite symplectic matrices in theorem 3.1 allows us to do this in closed form for the so-called Gaussian noise matrices. Following [2], these are noise matrices, V, which satisfy the further condition that $2V \in Sp(2n, R)$. All such matrices, except $\frac{I}{2}$, are squeezed. First, given a physically realizable noise matrix, theorem 3.1 lets one determine if it is Gaussian, when $n = 2$, because it detects if $2V$ is symplectic and positive definite. Next, putting $u = v = 1$ in the expression for the characteristic polynomial given by theorem 3.4 yields a polynomial whose roots can be explicitly computed. For reasons of brevity we do not list these roots, but we note that it is not merely the fact that the characteristic polynomial is quartic, but the fact that $q = \frac{r\times p}{a}$ which facilitates this explicit determination.

  This leads to the following expression for the minimal eigenvalue, $l(V)$. There are three cases to consider.

  – First suppose that $r \times p \neq 0$. Then, if $p\cdot p + r\cdot r - \sqrt{(p\cdot p + r\cdot r)^2 - \|r\times p\|^2} \geqslant \frac{2\|r\times p\|^2}{a^2}$, one finds
  $$2l(V) = a - \frac{\|r\times p\|}{a} - \sqrt{p\cdot p + r\cdot r + 2\sqrt{(p\cdot p)(r\cdot r) + (p\cdot r)^2}}.$$
  – If $r\times p \neq 0$ and $\frac{2\|r\times p\|^2}{a^2} \geqslant p\cdot p + r\cdot r - \sqrt{(p\cdot p + r\cdot r)^2 - \|r\times p\|^2}$, then
  $$2l(V) = a + \frac{\|r\times p\|}{a} - \sqrt{(p\cdot p + r\cdot r) - 2\sqrt{(p\cdot p)(r\cdot r) + (r\cdot p)^2}}.$$
  – Finally, if $r\times p = 0$, one gets
  $$2l(V) = a - (p\cdot p + r\cdot r) = \sqrt{1 + p\cdot p + r\cdot r} - (p\cdot p + r\cdot r).$$

  Note the condition $q = 0$ (forced by $r\times p = 0$) does not preclude $V + \frac{\mathrm{i}}{2}J_4$ from being positive semidefinite, inasmuch as the vector q does not involve the $(1, 3)$ and the $(2, 4)$ entries of V.

  A similar analysis can be performed for the effect of a squeezing transformation on other noise matrices. In general, if S represents an active squeezing operation and V is the noise matrix of a state, then SVS^T will only be positive definite, but not symplectic. Nevertheless, its smallest eigenvalue can be explicitly computed, using quaternions. Since this expression is cumbersome, we omit the details. Of course if V is also Gaussian, then the above analysis can be used verbatim for this purpose.

The next application we discuss is the work of [10] on a *key step* in the computation of Lyapunov exponents for linear Hamiltonian dynamical systems.

Specifically, let $\psi = (q_1, \ldots, q_n, p_1, \ldots, p_n)$ be the state of a classical system with n degrees of freedom. Here q_i and p_i are the canonical position and conjugate momentum coordinates. Let H be a quadratic form in the components of ψ, and let S be the $2n \times 2n$ real symmetric matrix representing this quadratic form. The evolution of the system is prescribed by

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = -\{H, \psi\},$$

where {, } stands for the Poisson bracket. Then, as H is quadratic, the state ψ satisfies

$$\psi(t) = M(t)\psi(0),$$

where $M(t) = \mathrm{e}^{tJ_{2n}S}$ is a symplectic matrix. Now form the matrix $\Lambda = \lim_{t\to\infty}(MM^T)^{\frac{1}{2t}}$. The Lyapunov exponents are the eigenvalues of Λ. Note one can just as well work with M^TM. MM^T satisfies $\frac{\mathrm{d}MM^T}{\mathrm{d}t} = J_{2n}SMM^T - MM^TSJ_{2n}$.

The authors now make the observation that every symplectic matrix can be written in the form

$$M = \mathrm{e}^{J_{2n}S_a}\,\mathrm{e}^{J_{2n}S_b},$$

where S_a is a symmetric matrix which anti-commutes with J_{2n}, while S_b is a symmetric matrix which commutes with J_{2n}. Now both $J_{2n}S_a$ and $J_{2n}S_b$ are Hamiltonian matrices. The condition that S_a anti-commutes with J_{2n} renders $J_{2n}S_a$ also symmetric, as is easily verified. Similarly $J_{2n}S_b$ is also anti-symmetric. But then $\mathrm{e}^{J_{2n}S_a}$ is simultaneously symplectic and positive definite, while $\mathrm{e}^{J_{2n}S_b}$ is symplectic and orthogonal. Thus, this is precisely the polar decomposition of M (though the authors do not mention this explicitly).

From here it follows that $MM^T = \mathrm{e}^{2J_{2n}S_a}$. The authors argue that it is better to work directly with $\mathrm{e}^{2J_{2n}S_a}$, for the purposes of computing Lyapunov exponents. For instance, $\mathrm{e}^{2J_{2n}S_a}$ has fewer parameters than M. The authors study the $n = 1$ case. They represent $\mathrm{e}^{2J_{2n}S_a}$ parametrically and then relate the Lyapunov exponents to these parameters. They then derive, for certain Hamiltonians, nonlinear differential equations for these parameters from the differential equation for MM^T above.

One can use the results of the previous sections for the $n = 2$ case. First, one can represent $\mathrm{e}^{2J_{2n}S_a}$ parametrically by using remark 3.1. Then using the method in the squeezing example before, derive explicitly the eigenvalues of $\mathrm{e}^{2J_{2n}S_a}$ as *closed form* expressions in these parameters. This yields formulae for the Lyapunov exponents in terms of these parameters. Then one could derive a system of coupled nonlinear differential equations for the six parameters. The derivation of these differential equations, which is very much dependent on the quadratic Hamiltonian, is beyond the scope of this work. It will, of course, be significantly more nonlinear than the $n = 1$ case.

In view of this, an alternative (depending on the Hamiltonian of the system) would be to solve the linear differential equation for $M(t)$ directly and then compute its polar decomposition using algorithm 3.1. This would yield Λ, whose eigenvalues can be found analogously to the application to squeezing discussed before in this section. For instance, if $J_{2n}S$ is either symmetric or skew-symmetric, then it is possible to solve for $M(t)$ in closed form.

Note that, since Hamiltonian matrices are not normal, $J_{2n}S_a$ and $J_{2n}S_b$ are not the symmetric and skew-symmetric parts of, $tJ_{2n}S$, the logarithm of $M(t)$. Thus, in other applications which require the non-compact part *of a specific* symplectic M, one has to resort to algorithm 3.1.

It is easy to see that any representation of the non-compact part of the symplectic group may be analogously used to compute Lyapunov exponents of linear Hamiltonian dynamical systems. In [9], the author proposes the use of the Iwasawa decomposition to compute this non-compact part. Since the Iwasawa decomposition involves more factors than the polar decomposition, it seems more economical to use the latter decomposition.

5. Conclusions

This work provides a quaternionic representation for the symplectic group $Sp(4, R)$. One of the principal applications is that, in attempting to provide explicit formulae for this representation, one obtains a very simple and explicit technique for finding the polar decomposition of matrices in $Sp(4, R)$. Since the positive definite factor in this decomposition is one representation of the non-compact part of the symplectic group, this circumstance can be used to address applications where this factor is relevant [1–3, 9, 10, 23]. There are other applications which we did not dwell upon here. Using the representation here one can constructively obtain the Euler–Cartan decomposition of $Sp(4, R)$ (see [2] for the definition of this decomposition). Likewise the so-called symplectic Procrustes problem, i.e., the problem of finding $U \in U(2)$, given $X_1, X_2 \in Sp(4, R)$, such that the Frobenius norm of $X_2 - UX_1$ is minimized, is explicitly solvable using algorithm 3.1.

Finding similar quaternionic representations of matrix groups preserving other bilinear forms in dimension four is an interesting question. It remains to see whether these lead to as elegant a set of expressions, such as those for the symplectic group. Indeed, it is no exaggeration to say that a pivotal role in the results here is played by the fact that the q term, in theorem 3.2, is essentially the cross product of the r and p terms. It seems implausible that a similar geometric simplification occurs for other bilinear forms. Extending such representations to higher dimensional symplectic matrices is also open. Quaternionic representations are, of course, limited to dimension four, just as there is no similar extension of the pair of unit quaternions representation to higher dimensional orthogonal groups. However, one can hope that in conjunction with either numerical techniques for the symplectic group [6], or methods of Clifford algebras [17], these results can be extended to higher dimensions. However, since the fact that q is essentially the cross-product of r and p was crucial, it seems unlikely that Clifford algebra based representations would be as amenable to calculating the polar decomposition in closed form in higher dimensions.

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