PARAMETRIZATION OF THE MATRIX SYMPLECTIC GROUP AND APPLICATIONS*

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Abstract. The group of symplectic matrices is explicitly parameterized and this description is applied to solve two types of problems. First, we describe several sets of structured symplectic matrices, i.e., sets of symplectic matrices that simultaneously have another structure. We consider unitary symplectic matrices, positive definite symplectic matrices, entrywise positive symplectic matrices, totally nonegative symplectic matrices, and symplectic M-matrices. The special properties of the LU factorization of a symplectic matrix play a key role in the parametrization of these sets. The second class of problems we deal with is to describe those matrices that can be certain significant submatrices of a symplectic matrix, and to parameterize the symplectic matrices with a given matrix occurring as a submatrix in a given position. The results included in this work provide concrete tools for constructing symplectic matrices with special structures or particular submatrices that may be used, for instance, to create examples for testing numerical algorithms.

Key words. complementary bases, dense subsets of symplectic matrices, LU factorization, M-matrices, orthogonal, parametrization, positive matrices, positive definite, symplectic, submatrices of symplectic matrices, totally nonnegative, unitary

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1. Introduction. Let I_n denote the n-by-n identity matrix and J the $2n$-by-$2n$ matrix

$$J := \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}. \tag{1.1}$$

J is an orthogonal, skew-symmetric real matrix, so that $J^{-1} = J^T = -J$.

DEFINITION 1.1. *A $2n$-by-$2n$ matrix S with entries in $\mathbb{C}$ ($\mathbb{R}$) is called symplectic if $S^*JS = J$ ($S^TJS = J$).*

For the sake of brevity most of the results in this paper are presented only for complex symplectic matrices. They remain valid for real symplectic matrices by replacing every conjugate tranpose matrix, A^*, by the tranpose A^T. Notice also that the complex matrices satisfying $S^*JS = J$ are sometimes called conjugate symplectic matrices in the literature [10, 37].

The set of symplectic matrices forms a group. This group is very relevant both from a pure mathematical point of view [18], and from the point of view of applications. For instance, symplectic matrices play an important role in classical mechanics and Hamiltonian dynamical systems [1], in particular, in the theory of parametric resonance, a problem that have received recent attention from the matrix analysis community [23]. They are also used in electromagnetism [48]. Symplectic integrators

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are the preferred methods for the numerical solution of the differential equations appearing in these physical problems because they preserve the Hamiltonian structure [45, 46, 47], and in these integrators symplectic matrices arise. A natural extension of these methods is for solving linear Hamiltonian difference systems [9], and here symplectic matrices also occur. Moreover, eigenvalues and eigenvectors of symplectic matrices are important in applications like the discrete linear-quadratic regulator problem, discrete Kalman filtering, the solution of discrete-time algebraic Riccati equations, and certain large, sparse quadratic eigenvalue problems. See [33, 34, 41, 42] and the references therein. These applications have motivated the development of numerical structured algorithms for computing eigenvalues and eigenvectors of symplectic matrices–see [16] for a complete treatment of this topic and [5, 6, 17] for three interesting original references–, as well as for computing certain specific factorizations of symplectic matrices [7]. In general, these algorithms are potentially unstable (although they work very well for most symplectic matrices) and, therefore, a careful testing process is necessary to assess their practical numerical behaviour. These tests require to construct symplectic matrices with particular properties and the results presented in this work provide a variety of ways for performing this task.

The symplectic matrices are *implicitly* defined as solutions to a quadratic matrix equation. This definition is very convenient for checking if a matrix is symplectic and for proving certain properties of symplectic matrices, but, for instance, it is not convenient for constructing symplectic matrices. The implicit definition of the symplectic matrices makes it difficult to work with them in theory, and, also, in numerical algorithms. The main goal of this paper is to present an *explicit* description or parametrization of the group of symplectic matrices, i.e., to find the set of solutions of the matrix equation $S^*JS = J$. This description is based on two previous results: Proposition 2.36 in [40], a result whose theoretical relevance has not been fully appreciated, and the complementary bases theorem in [14, Theorem 3.1].

The classical parametrization of the symplectic group relies on the fact that every $2n$-by-$2n$ symplectic matrix is a product of at most $4n$ symplectic transvections [2]. See also [36] where a modern proof of this fact is presented. Symplectic transvections can be easily constructed, and so symplectic matrices. However, this parametrization does not allow us to know directly how the entries of a symplectic matrix are related to each other, to construct easily symplectic matrices with special structures, or to recognize if a certain matrix can be a submatrix of a symplectic matrix, which is the first step towards solving symplectic completion problems [28]. In addition, in numerical practice, multiplication by a symplectic matrix may be unstable and the computed product of several symplectic matrices may be far from being symplectic. A parametrization as a finite product of certain elementary unitary-symplectic matrices has been also developed for the unitary-symplectic group [43]. Another work in this line is [32].

A different parametrization of the matrix symplectic group as a finite product of elementary symplectic matrices can be inferred from [3], where the authors present a method to reduce every symplectic matrix to *butterfly form* by using symplectic similarities. Symplectic butterfly matrices are at the heart of the most efficient structure preserving algorithms for the symplectic eigenvalue problem [5, 16, 17]. The *butterfly form* is closely related to tridiagonal matrices, and $2n$-by-$2n$ symplectic butterfly matrices can be simply parameterized using $4n-1$ parameters. As a consequence, an arbitrary $2n$-by-$2n$ symplectic matrix can be parameterized as the product of $(n-1)$ symplectic Gauss matrices [16] and their inverses, (n^2-n) symplectic Givens matrices [16] and their inverses, $2(n-2)$ symplectic Householder matrices [16] and their inverses, one parameterized symplectic butterfly matrix, and, very rarely, some symplectic interchange matrices. The number of parameters in this parametrization is optimal because it coincides with the dimension of the symplectic group. This parametrization has the same drawbacks as the classical parametrization previously mentioned.

The parametrization of the symplectic group that we present describes the entries of the matrices and can be very useful in different contexts. In this work, we apply it to solve two types of problems: first, to parametrize sets of structured symplectic matrices, i.e., sets of symplectic matrices that also have another structure; second, to describe those matrices that can be certain significant submatrices of a symplectic matrix, and the parametrization of the symplectic matrices with a given matrix occurring as a submatrix in a given position. We will see that these parameterizations provide concrete tools for constructing matrices with special structures or fixed submatrices that may be used, for instance, to test numerical algorithms.

In the first class of problems, we describe the sets of unitary symplectic matrices, positive definite symplectic matrices, entrywise positive symplectic matrices, totally nonegative symplectic matrices, and symplectic M-matrices. Loosely speaking, one can say that these sets contain many nontrivial elements, except in the case of the set of totally nonnegative symplectic matrices, where we prove, in dimensions larger than two, that all its elements are diagonal and that there are no symplectic matrices that are totally positive or oscillatory. Our results can be used to easily generate symplectic matrices that have the additional structures previously mentioned, something that is not obvious from the definition of a symplectic matrix.

The structure of the matrix J in (1.1) makes it natural to consider any $2n$-by-$2n$ symplectic matrix in the partitioned form

$$S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}, \tag{1.2}$$

in which S_{11} is n-by-n. We shall use this partition throughout this work without explicitly referring to it. Therefore, unless otherwise stated, the reader should understand every 2-by-2 partitioned matrix appearing in the text with the dimensions of (1.2).

The partition in (1.2) is related to the second class of problems we consider. We call these problems *subparametrization problems*. In this context, we parametrize the set of symplectic matrices whose $(1,1)$-block has given rank (the same can be obviously done for any other block). As a consequence of this result, we show that any n-by-n matrix can be one of the blocks appearing in (1.2), and, if we fix a matrix A as one of these blocks, the set of symplectic matrices having A as the corresponding submatrix is explicitly parametrized. We will see that this problem is much simpler in the case one of the blocks is nonsingular. In fact, the set of symplectic matrices whose, say, $(1,1)$-block is nonsingular has a simple structure that makes it easy to work with it from several points of view. We also show that this set is an open dense subset of the group of symplectic matrices. These topological features imply that some properties of symplectic matrices can be proved first for the matrices whose $(1,1)$-block is nonsingular and then be extended to any symplectic matrix by a proper limiting argument. We will also parametrize the set of $2n$-by-n matrices that can be the first (or the last) n columns of a symplectic matrix, and the set of symplectic matrices whose first n columns are fixed. Also some results on principal submatrices of dimension larger than n of symplectic matrices are presented. It is interesting to remark that to study subparametrization problems with respect to the partition in (1.2) is related to intrinsic properties of symplectic geometry. For instance, it is well known that the columns of a $2n$-by-n matrix span a Lagrangian subspace if and only if this matrix is the submatrix containing the first n-columns of a symplectic matrix [18] (see also [19, Proposition 1.4]).

The paper is organized as follows: Section 2 contains basic and previous results that will be used in the rest of the paper. In Section 3 the explicit description of the symplectic group is presented. The special properties of the LU factorization of symplectic matrices are discussed in Section 4. This will be used in Section 5, where several sets of structured sympletic matrices are described. Subparametrization problems are studied in Section 6 and the brief Section 7 contains the conclusions.

2. Preliminaries. The set of all m-by-n matrices with entries in $\mathbb{F}$ ($\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$) is denoted by $M_{m,n}(\mathbb{F})$, and $M_{n,n}(\mathbb{F})$ is abbreviated to $M_n(\mathbb{F})$. We will use in some results MATLAB [39] notation for submatrices: $A(i : j, k : l)$ will denote the submatrix of A consisting of rows i through j and columns k through l; $A(i : j, :)$ will denote the submatrix of A consisting of rows i through j; and $A(:, k : l)$ will denote the submatrix of A consisting of columns k through l.

The following properties are very easily proved from Definition 1.1 and will be often used: the product of two symplectic matrices is also symplectic, and if S is symplectic then S^{-1} and S^* are symplectic. We will also need the following auxiliary lemma.

LEMMA 2.1. *Let $X, Z, G, Y, A, B, C \in M_n(\mathbb{C})$. Then*

1. *The matrix $\left[\begin{smallmatrix} I & 0 \\ X & I \end{smallmatrix}\right]$ is symplectic if and only if $X = X^*$.*
2. *The matrix $\left[\begin{smallmatrix} I & Z \\ 0 & I \end{smallmatrix}\right]$ is symplectic if and only if $Z = Z^*$.*
3. *The matrix $\left[\begin{smallmatrix} G & 0 \\ 0 & Y \end{smallmatrix}\right]$ is symplectic if and only if $Y = G^{-*}$.*
4. *The matrix $\left[\begin{smallmatrix} I & A \\ B & C \end{smallmatrix}\right]$ is symplectic if and only if $A = A^*$, $B = B^*$ and $C = I + BA$.*

Proof. The first three items follow trivially from Definition 1.1. Let us prove the fourth item. Let us denote $S \equiv \left[\begin{smallmatrix} I & A \\ B & C \end{smallmatrix}\right]$. If $A = A^*$, $B = B^*$, and $C = I + BA$ then,

$$S = \begin{bmatrix} I & A \\ B & I + BA \end{bmatrix} = \begin{bmatrix} I & 0 \\ B & I \end{bmatrix} \begin{bmatrix} I & A \\ 0 & I \end{bmatrix},$$

where the factors in the right hand side are both symplectic as a consequence of the first and second items. Thus S is symplectic. Now, we prove the converse. The equation $S^*JS = J$ implies $B = B^*$, $C = I + B^*A$, and $A^*C = C^*A$. Then $A^* + A^*BA = A + A^*BA$, which implies $A = A^*$. ◻

The next result is an n-by-n block LU factorization of a symplectic matrix. It appears in [40] and is the first key result on which many other results in this work are based. A proof is presented for completeness.

THEOREM 2.2. [40, Prop. 2.36] *Let $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C})$ be symplectic and S_{11} be nonsingular. Then*

$$S = \begin{bmatrix} I & 0 \\ S_{21}S_{11}^{-1} & I \end{bmatrix} \begin{bmatrix} S_{11} & 0 \\ 0 & S_{11}^{-*} \end{bmatrix} \begin{bmatrix} I & S_{11}^{-1}S_{12} \\ 0 & I \end{bmatrix}, \tag{2.1}$$

where the three factors are symplectic, equivalently, where $S_{21}S_{11}^{-1}$ and $S_{11}^{-1}S_{12}$ are Hermitian matrices.

Proof. The matrix

$$\left[\begin{array}{cc} S_{11}^{-1} & 0 \\ 0 & S_{11}^{*} \end{array}\right] S = \left[\begin{array}{cc} I & S_{11}^{-1} S_{12} \\ S_{11}^{*} S_{21} & S_{11}^{*} S_{22} \end{array}\right]$$

is symplectic because it is the product of two symplectic matrices. The fourth item of Lemma 2.1 implies that $S_{11}^{-1} S_{12}$ and $S_{11}^{*} S_{21}$ are Hermitian, and that $S_{11}^{*} S_{22} = I + S_{11}^{*} S_{21} S_{11}^{-1} S_{12}$. Notice that $S_{21} S_{11}^{-1} = S_{11}^{-*}(S_{11}^{*} S_{21}) S_{11}^{-1}$ is also Hermitian. Therefore, we have already proved that the three factors appearing in the right hand side of (2.1) are symplectic because the off-diagonal blocks in these factors are Hermitian. We still have to prove that equation (2.1) holds. From $S_{11}^{*} S_{22} = I + S_{11}^{*} S_{21} S_{11}^{-1} S_{12}$, we get $S_{11}^{-*} = S_{22} - S_{21} S_{11}^{-1} S_{12}$. The result follows from the identity

$$S = \left[\begin{array}{cc} I & 0 \\ S_{21} S_{11}^{-1} & I \end{array}\right] \left[\begin{array}{cc} S_{11} & 0 \\ 0 & S_{22} - S_{21} S_{11}^{-1} S_{12} \end{array}\right] \left[\begin{array}{cc} I & S_{11}^{-1} S_{12} \\ 0 & I \end{array}\right].$$

□

In the proof of Theorem 2.2, we have proved the next result on Schur complements in symplectic matrices.

COROLLARY 2.3. *Let* $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C})$ *be symplectic and* S_{11} *be nonsingular. Then the Schur complement of* S_{11} *is* S_{11}^{-*}*, i.e.,* $S_{11}^{-*} = S_{22} - S_{21} S_{11}^{-1} S_{12}$*.*

The symplectic matrices introduced in Definition 2.4 will appear in several results. They are traditional interchange matrices except for the fact that the sign of one of the rows (or columns) is changed to preserve the symplectic structure. They have been previously used in [4, 31].

DEFINITION 2.4. *Let* $1 \leq j \leq n$*. The symplectic interchange matrix* Π_j *is the* $2n$*-by-*$2n$ *matrix obtained by interchanging the columns* j *and* $j+n$ *of the* $2n$*-by-*$2n$ *identity matrix and multiplying the* j*th column of the resulting matrix by* -1*. The symplectic interchange matrix* $\widetilde{\Pi}_j$ *is the* $2n$*-by-*$2n$ *matrix obtained by interchanging the columns* j *and* $j+n$ *of the* $2n$*-by-*$2n$ *identity matrix and multiplying the* $(j+n)$*th column of the resulting matrix by* -1*. Notice that* $\Pi_j^T = \widetilde{\Pi}_j$*.*

Notice that Π_j ($\widetilde{\Pi}_j$) can be also obtained by interchanging the rows j and $j+n$ of the $2n$-by-$2n$ identity matrix and multiplying the $(j+n)$th (jth) row of the resulting matrix by -1.

Next, we state the second key result on which the rest of the results in this paper are based: the complementary bases theorem proved in [14]. To this purpose, we need to introduce the following notation: $|\alpha|$ denotes the cardinality of a set α. Moreover the binary variables p and q can take as values 1 or 2, and p' and q' denote, respectively, the complementary variables of p and q.

THEOREM 2.5. [14, Th. 3.1] *Let* $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C})$ *be symplectic. Suppose that rank*$(S_{pq}) = k$, $p, q \in \{1, 2\}$*, and that the rows (columns) of* S_{pq} *indexed by* α*,* $\alpha \subseteq \{1, \ldots, n\}$ *and* $|\alpha| = k$*, are linearly independent. Then the rows (columns) of* $S_{p'q}$ ($S_{pq'}$) *indexed by* α'*, the complement of* α*, together with the rows (columns)* α *of* S_{pq} *constitute a basis of* $\mathbb{C}^n$*, i.e., they constitute a nonsingular* n*-by-*n *matrix.*

The reader should notice that Theorem 2.5 was proved for matrices S satisfying $S^T J S = J$ and with entries in any field, but it remains valid for the matrices defined in Definition 1.1. This is commented after the proof of Corollary 3.2 in [14]. We will also use the following consequence of Theorem 2.5.

COROLLARY 2.6. *Let* $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C})$ *be symplectic and* S_{11} *be singular. Then there exist matrices* Q *and* Q' *that are products of at most* n *different symplectic* *interchange matrices such that $Q\,S$ and $S\,Q'$ are symplectic matrices with nonsingular $(1,1)$-block.*

Note that according to Theorem 2.5 the matrices Q and Q' in Corollary 2.6 may be not unique.

3. Parametrization of the set of symplectic matrices. The first result we present is Theorem 3.1 that parametrizes the set of symplectic matrices whose $(1,1)$-block is nonsingular. The same can be done for any other of the four blocks in the partition (1.2), because, by multiplying a symplectic matrix on the left, on the right, or on both sides by the matrix J, any of the blocks can be placed in the position $(1,1)$ and the matrix remains symplectic. This remark applies to many of the results in this paper.

THEOREM 3.1. *The set of $2n$-by-$2n$ complex symplectic matrices with nonsingular $(1,1)$-block is*

$$\mathcal{S}^{(1,1)} = \left\{ \begin{bmatrix} I & 0 \\ C & I \end{bmatrix} \begin{bmatrix} G & 0 \\ 0 & G^{-*} \end{bmatrix} \begin{bmatrix} I & E \\ 0 & I \end{bmatrix} : \begin{array}{c} G \in M_n(\mathbb{C}) \text{ nonsingular} \\ C = C^*\,,\; E = E^* \end{array} \right\}$$
$$= \left\{ \begin{bmatrix} G & GE \\ CG & G^{-*} + CGE \end{bmatrix} : \begin{array}{c} G \in M_n(\mathbb{C}) \text{ nonsingular} \\ C = C^*\,,\; E = E^* \end{array} \right\}.$$

Proof. According to Theorem 2.2 every symplectic matrix with nonsingular (1,1)-block can be written as

$$\begin{bmatrix} I & 0 \\ C & I \end{bmatrix} \begin{bmatrix} G & 0 \\ 0 & G^{-*} \end{bmatrix} \begin{bmatrix} I & E \\ 0 & I \end{bmatrix}, \quad \text{with} \quad C = C^*, \quad E = E^*. \tag{3.1}$$

Conversely, every matrix like the one in (3.1) is symplectic because it is a product of three symplectic matrices. See Lemma 2.1. ∎

REMARK 1. *Notice that the set $\mathcal{S}^{(1,1)}$ is parametrized in terms of the entries of G, C and E. In the case of real symplectic matrices these entries amount to $2n^2+n$ real parameters.*[1] *Note that for complex matrices the fact that the diagonal entries of C and E are real numbers prevents to parametrize $\mathcal{S}^{(1,1)}$ in terms of complex parameters, although it is obvious that it depends on $4n^2$ real parameters. To avoid such minor complications, from now on, we will only present the number of parameters for subsets of real symplectic matrices. The interested readers can count the parameters in the complex case from the descriptions we will introduce. Notice that $2n^2+n$ is precisely the dimension of the real symplectic group [18, Lemma 1.15], so the parametrization in Theorem 3.1 is optimal in this respect.*

Theorem 3.1 implies that every nonsingular n-by-n matrix is the $(1,1)$-block of a symplectic matrix. More precisely, given an arbitrary nonsingular n-by-n matrix G, the set of symplectic matrices whose $(1,1)$-block is G can be parametrized by the entries of the Hermitian matrices C and E appearing in Theorem 3.1. So, for real matrices this set depends on n^2+n parameters. Theorem 6.6 will show that every n-by-n matrix, singular or not, is the $(1,1)$-block of a symplectic matrix.

[1] Note that the n^2 entries of G are not totally free parameters because G is nonsingular. However, for instance, the whole set of nonsingular n-by-n matrices can be explicitly parameterized with n^2 parameters as $G = \Pi LU$, where Π is an arbitrary permutation matrix, L is an arbitrary lower triangular matrix with ones on the diagonal, and U is an arbitrary upper triangular matrix with nonzero diagonal entries. The nontrivial entries of L and U amount to n^2 free parameters. In this work, for simplicity, we will frequently use the entries of nonsingular matrices as free parameters of certain sets without writing explicitly these matrices in nonsingular form.

It is easy to construct examples of symplectic matrices whose four blocks are singular, therefore $\mathcal{S}^{(1,1)}$ is not the whole set of symplectic matrices $\mathcal{S}$. However, we will prove in Section 6.2 that $\mathcal{S}^{(1,1)}$ is a dense open subset in $\mathcal{S}$. Here, we are using on $\mathcal{S}$ the *subspace topology* induced by the usual topology in $M_{2n}(\mathbb{C})$, i.e., the topology associated with any norm defined on $M_{2n}(\mathbb{C})$. This means that a subset $\mathcal{G} \subset \mathcal{S}$ is open (closed) in $\mathcal{S}$ if $\mathcal{G}$ is the intersection of $\mathcal{S}$ and an open (closed) subset of $M_{2n}(\mathbb{C})$. The fact that $\mathcal{S}^{(1,1)}$ is dense and open in $\mathcal{S}$ implies that many properties of the set $\mathcal{S}$ can be obtained by proving first the corresponding property in $\mathcal{S}^{(1,1)}$ and then applying a proper limit argument. The advantage of this approach is that $\mathcal{S}^{(1,1)}$ admits the simple explicit parametrization presented in Theorem 3.1 and this makes simple to work in this set.

The next theorem describes explicitly the whole set of symplectic matrices.

THEOREM 3.2. *The set of* $2n$*-by-*$2n$ *complex symplectic matrices is*

$$\mathcal{S} = \left\{ Q \begin{bmatrix} I & 0 \\ C & I \end{bmatrix} \begin{bmatrix} G & 0 \\ 0 & G^{-*} \end{bmatrix} \begin{bmatrix} I & E \\ 0 & I \end{bmatrix} : \begin{array}{c} G \in M_n(\mathbb{C}) \text{ nonsingular} \\ C = C^*\ ,\ E = E^* \\ Q \text{ a product of symplectic interchanges} \end{array} \right\}$$

$$= \left\{ Q \begin{bmatrix} G & GE \\ CG & G^{-*} + CGE \end{bmatrix} : \begin{array}{c} G \in M_n(\mathbb{C}) \text{ nonsingular} \\ C = C^*\ ,\ E = E^* \\ Q \text{ a product of symplectic interchanges} \end{array} \right\}.$$

The symplectic unitary matrix Q is a product of at most n different symplectic interchange matrices. The matrix Q may also be placed on the right side of the product.

Proof. The result follows by combining Corollary 2.6 and Theorem 3.1. ☐

A different explicit description of the set $\mathcal{S}$ will be discussed in Remark 2 in Subsection 6.1. Theorem 3.2 is not a strict parametrization, because given a symplectic matrix S, several matrices Q may exist that allow us to express S in the form appearing above for different sets of parameters.

4. The LU factorization of a symplectic matrix. The existence of the LU factorization of a symplectic matrix is completely determined by properties of its $(1,1)$-block. Moreover, the LU factors of a symplectic matrix have a very special structure that will play a key role in Section 5, where sets of symplectic matrices with additional structures are studied. Some of these additional structures imply further properties on the LU factors that allow us to describe explicitly relevant subsets of symplectic matrices. In this paper, we adopt the usual convention that in the LU factorization of a matrix, $A = LU$, the L factor is *unit* lower triangular and the U factor is upper triangular. The next theorem presents the most important properties of the LU factorization of a symplectic matrix.

THEOREM 4.1. *Let* $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C})$ *be symplectic. Then*

1. *If S has an LU factorization then the factorization is unique.*
2. *S has LU factorization if and only if S_{11} and S_{11}^{-*} have LU factorizations.*
3. *S has LU factorization if and only if S_{11} is nonsingular and has LU and UL factorizations.*
4. *S has LU factorization if and only if* $\det S_{11}(1:k,1:k) \cdot \det S_{11}(k:n,k:n) \neq 0$ *for* $k = 1,\ldots,n$.
5. *If* $S_{11} = L_{11}U_{11}$ *and* $S_{11}^{-*} = L_{22}U_{22}$ *are LU factorizations, then the LU factorization of S is*

$$S = \begin{bmatrix} L_{11} & 0 \\ S_{21}U_{11}^{-1} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & L_{11}^{-1}S_{12} \\ 0 & U_{22} \end{bmatrix} \tag{4.1}$$

6. *The LU factors of S are symplectic if and only if S_{11} is diagonal and nonsingular.*

Proof. **1.** Symplectic matrices are nonsingular and the LU factorization of a nonsingular matrix is unique when it exists [24, Theorem 3.2.1].
2. If S has LU factorization, $S = LU$, then the factorization is unique. Therefore, all the leading principal minors of S are nonzero [25, Ch. 9]. This implies that S_{11} is nonsingular and that (2.1) holds. By combining (2.1) with $S = LU$, one gets

$$\begin{bmatrix} S_{11} & 0 \\ 0 & S_{11}^{-*} \end{bmatrix} = \left(\begin{bmatrix} I & 0 \\ -S_{21}S_{11}^{-1} & I \end{bmatrix} L \right) \left(U \begin{bmatrix} I & -S_{11}^{-1}S_{12} \\ 0 & I \end{bmatrix} \right) \equiv \widetilde{L}\widetilde{U}.$$

This means that $\widetilde{L}\widetilde{U}$ is the LU factorization of $\left[\begin{smallmatrix} S_{11} & 0 \\ 0 & S_{11}^{-*} \end{smallmatrix}\right]$. Let us write the previous equation as

$$\begin{bmatrix} S_{11} & 0 \\ 0 & S_{11}^{-*} \end{bmatrix} = \begin{bmatrix} \widetilde{L}_{11} & 0 \\ \widetilde{L}_{21} & \widetilde{L}_{22} \end{bmatrix} \begin{bmatrix} \widetilde{U}_{11} & \widetilde{U}_{12} \\ 0 & \widetilde{U}_{22} \end{bmatrix}.$$

Then, it is straightforward to see that $\widetilde{L}_{21} = \widetilde{U}_{12} = 0$, $S_{11} = \widetilde{L}_{11}\widetilde{U}_{11}$, and $S_{11}^{-*} = \widetilde{L}_{22}\widetilde{U}_{22}$. This proves S_{11} and S_{11}^{-*} have LU factorizations.

Conversely, if S_{11} and S_{11}^{-*} have the LU factorizations $S_{11} = L_{11}U_{11}$ and $S_{11}^{-*} = L_{22}U_{22}$ then we obtain from (2.1) that

$$S = \begin{bmatrix} L_{11} & 0 \\ S_{21}U_{11}^{-1} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & L_{11}^{-1}S_{12} \\ 0 & U_{22} \end{bmatrix}$$

is the LU factorization of S. This also proves item **5.**
3. Simply notice that if S_{11} is nonsingular then $S_{11}^{-*} = L_{22}U_{22}$ if and only if $S_{11} = L_{22}^{-*}U_{22}^{-*}$, i.e., S_{11}^{-*} has LU factorization if and only if S_{11} has UL factorization.
4. It follows from the fact that S_{11}^{-*} has LU factorization if and only if $\det S_{11}^{-*}(1 : k, 1 : k) \neq 0$, for $k = 1, \ldots, n$. This is equivalent to $\det S_{11}(k : n, k : n) \neq 0$, for $k = 1, \ldots, n$, taking into account the well known expressions for the minors of the inverse [26, Sec 0.8.4] and that S_{11} is nonsingular.
5. It was proved in the proof of **2.**.
6. If S_{11} is diagonal and nonsingular then in (4.1) $L_{11} = L_{22} = I$, $U_{11} = S_{11}$, and $U_{22} = S_{11}^{-*}$. So, the L factor of S is $\left[\begin{smallmatrix} I & 0 \\ S_{21}S_{11}^{-1} & I \end{smallmatrix}\right]$, which is the first factor in (2.1) and, therefore, it is symplectic. The U factor is $\left[\begin{smallmatrix} S_{11} & S_{12} \\ 0 & S_{11}^{-*} \end{smallmatrix}\right]$, which is the product of the second and third factor in (2.1) and, therefore, symplectic.

Conversely, if the LU factors of S are symplectic then the matrices $L = \left[\begin{smallmatrix} L_{11} & 0 \\ S_{21}U_{11}^{-1} & L_{22} \end{smallmatrix}\right]$ and $U = \left[\begin{smallmatrix} U_{11} & L_{11}^{-1}S_{12} \\ 0 & U_{22} \end{smallmatrix}\right]$ in (4.1) are symplectic. The fact that U is symplectic implies that U_{11} is nonsingular then the block factorization (2.1) holds for U with the $(2, 1)$-block equal to zero. Therefore, $U_{22} = U_{11}^{-*}$. But U_{22} is upper triangular and U_{11}^{-*} lower triangular, hence U_{11} is diagonal. A similar argument on L implies that $L_{22} = L_{11}^{-*}$, hence $L_{11} = I$. This shows that $S_{11} = U_{11}$ is diagonal. ☐

We have seen that, except in the very particular case that S_{11} is diagonal and nonsingular, the LU factors of a symplectic matrix do not inherit the symplectic structure. If one insists on preserving this structure then block LU factorizations have to be considered. Apart from the block LU factorization appearing in Theorem 2.2, we have these other two block LU-like factorizations[2].

[2] Notice that the factorizations in Theorem 4.2 are not block LU factorizations in the sense defined in [25, p. 246] because they do not have identity matrices on the diagonal blocks of the L matrices.

THEOREM 4.2. *Let* $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C})$ *be symplectic. Then*

1. *If* S_{11} *is nonsingular and has the LU factorization* $S_{11} = L_{11}U_{11}$ *then*

$$S = \begin{bmatrix} L_{11} & 0 \\ S_{21}U_{11}^{-1} & L_{11}^{-*} \end{bmatrix} \begin{bmatrix} U_{11} & L_{11}^{-1}S_{12} \\ 0 & U_{11}^{-*} \end{bmatrix},$$

and both factors are symplectic.

2. *If* S_{11}^{-*} *has the LU factorization* $S_{11}^{-*} = L_{22}U_{22}$ *then*

$$S = \begin{bmatrix} L_{22}^{-*} & 0 \\ S_{21}U_{22}^{*} & L_{22} \end{bmatrix} \begin{bmatrix} U_{22}^{-*} & L_{22}^{*}S_{12} \\ 0 & U_{22} \end{bmatrix},$$

and both factors are symplectic.

Proof. Both results follow straightforwardly from (2.1). □

5. Structured sets of symplectic matrices. This section is devoted to the study of five subsets of symplectic matrices: unitary symplectic matrices, positive definite symplectic matrices, entrywise positive symplectic matrices, totally nonnegative symplectic matrices, and symplectic M-matrices.

5.1. Unitary symplectic matrices. The results presented in this section for complex unitary symplectic matrices remain valid for real orthogonal symplectic matrices by replacing conjugate transpose ($*$) by transpose (T), and *unitary* by *orthogonal* matrices.

The intersection between the unitary and the symplectic groups is treated in general references, as for instance [18]. In addition, a parametrization of this group in terms of finite products of certain elementary symplectic-unitary matrices is described in [43]. We present in this section an alternative description by blocks of the unitary-symplectic matrices in terms of unitary and Hermitian matrices.

It is well-known that the set of $2n$-by-$2n$ unitary symplectic matrices is [44, p. 14]

$$\mathcal{S}^U = \left\{ \begin{bmatrix} Q_1 & Q_2 \\ -Q_2 & Q_1 \end{bmatrix} : \begin{array}{c} Q_1^*Q_1 + Q_2^*Q_2 = I \\ Q_1^*Q_2 - Q_2^*Q_1 = 0 \end{array} \right\}. \tag{5.1}$$

This result is easily proved because if S is simultaneously symplectic and unitary then $JS = SJ$. This implies the block structure appearing in (5.1). The conditions on Q_1 and Q_2 follow from imposing $S^*S = I$ (or equivalently $S^*JS = J$) to the matrix $S = \left[\begin{smallmatrix} Q_1 & Q_2 \\ -Q_2 & Q_1 \end{smallmatrix}\right]$. However, (5.1) is not an explicit description of the set $\mathcal{S}^U$ because the n-by-n matrices Q_1 and Q_2 are defined through a system of quadratic equations. In Theorem 5.1 we describe explicitly $\mathcal{S}^U$ in terms of n-by-n Hermitian and unitary matrices, and of products of at most n symplectic interchange matrices of dimension $2n$-by-$2n$. A related result that allows us to generate unitary symplectic matrices according to the Haar measure was presented in [35].

THEOREM 5.1. *The set of* $2n$*-by-*$2n$ *unitary symplectic matrices is*

$$\mathcal{S}^U = \left\{ Q \begin{bmatrix} (I+C^2)^{-1/2}U & -C(I+C^2)^{-1/2}U \\ C(I+C^2)^{-1/2}U & (I+C^2)^{-1/2}U \end{bmatrix} : \begin{array}{c} U \in M_n(\mathbb{C}) \text{ unitary} \\ C = C^* \in M_n(\mathbb{C}) \\ Q \text{ a product of symplectic interchanges} \end{array} \right\},$$

where the symplectic unitary matrix Q is a product of at most n different symplectic interchange matrices and $(I+C^2)^{1/2}$ denotes the unique positive definite square root of $I+C^2$. Besides, if U is unitary and C is Hermitian then

$$\begin{bmatrix} (I+C^2)^{-1/2}U & -C(I+C^2)^{-1/2}U \\ C(I+C^2)^{-1/2}U & (I+C^2)^{-1/2}U \end{bmatrix} = \begin{bmatrix} I & 0 \\ C & I \end{bmatrix} \begin{bmatrix} (I+C^2)^{-1/2} & 0 \\ 0 & (I+C^2)^{1/2} \end{bmatrix} \begin{bmatrix} I & -C \\ 0 & I \end{bmatrix} \begin{bmatrix} U & 0 \\ 0 & U \end{bmatrix}. \quad (5.2)$$

Proof. According to Theorem 3.2 we have to prove that every unitary symplectic matrix with nonsingular $(1,1)$-block can be written as (5.2), and, conversely, that every matrix of the form (5.2) is unitary and symplectic. This latter fact can be easily proved by checking that every matrix S of the form (5.2) satisfies $S^*S = I$ and $S^*JS = J$ (or notice that the matrix in (5.2) is the product of three symplectic matrices by Lemma 2.1, and, therefore, is symplectic).

To prove that every unitary symplectic matrix with nonsingular $(1,1)$-block is of the form (5.2), let us remember that Theorem 3.1 states that every symplectic matrix with nonsingular $(1,1)$-block can be expressed as

$$S = \begin{bmatrix} G & GE \\ CG & G^{-*}+CGE \end{bmatrix}, \quad (5.3)$$

with G nonsingular and $C = C^*$, $E = E^*$. The equation $S^*S = I$ is equivalent to

$$\begin{aligned} (1,1)-\text{block} &\quad G^*G + G^*C^2G = I & (5.4)\\ (2,1)-(1,2)-\text{blocks} &\quad EG^*G + G^{-1}CG + EG^*C^2G = 0 & (5.5)\\ (2,2)-\text{block} &\quad EG^*GE + (G^{-*}+CGE)^*(G^{-*}+CGE) = I. & (5.6) \end{aligned}$$

The equation (5.4) implies

$$I = G^*(I+C^2)G = ((I+C^2)^{1/2}G)^*((I+C^2)^{1/2}G),$$

therefore

$$G = (I+C^2)^{-1/2}U \quad \text{with } U \text{ unitary.} \quad (5.7)$$

Notice that equation (5.5) can be written as $E(G^*G + G^*C^2G) + G^{-1}CG = 0$, and with (5.4), we get

$$E = -G^{-1}CG.$$

This result can be combined with (5.7) to get

$$E = -U^*CU. \quad (5.8)$$

Equation (5.6) is directly satisfied by G and E given by (5.7) and (5.8). So, the Hermitian matrix C and the unitary matrix U remain as free parameters. The result is proved by substituting (5.7) and (5.8) in (5.3). □

As in Theorem 3.2, the description presented in Theorem 5.1 is not a strict parametrization because given a unitary symplectic matrix S, several matrices Q may exist that allow us to express S in the form appearing in Theorem 5.1. However, it is a strict parametrization in the case of unitary symplectic matrices whose $(1,1)$-block is nonsingular, because then Q is not present, and, given S, there exists only one pair of matrices C and U to represent S as in Theorem 5.1.

5.2. Positive definite symplectic matrices. Theorem 5.2 presents the most relevant properties of positive definite symplectic matrices. Item 5 was proved in a much more general setting in [38, Sec. 3]. We include the proof of this item for completeness.

THEOREM 5.2. *Let* $S = \left[\begin{smallmatrix} S_{11} & S_{21}^* \\ S_{21} & S_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C})$ *be Hermitian and symplectic. Then*

1. *S is positive definite if and only if S_{11} is positive definite.*
2. *The set of positive definite symplectic matrices is*

$$\mathcal{S}^{PD} = \left\{ \begin{bmatrix} I & 0 \\ C & I \end{bmatrix} \begin{bmatrix} G & 0 \\ 0 & G^{-1} \end{bmatrix} \begin{bmatrix} I & C \\ 0 & I \end{bmatrix} : \begin{array}{c} G \in M_n(\mathbb{C}) \text{ positive definite} \\ C = C^* \end{array} \right\}$$
$$= \left\{ \begin{bmatrix} G & GC \\ CG & G^{-1} + CGC \end{bmatrix} : \begin{array}{c} G \in M_n(\mathbb{C}) \text{ positive definite} \\ C = C^* \end{array} \right\}.$$

3. *For real symplectic matrices the set $\mathcal{S}^{PD}$ depends on n^2+n parameters.*[3] *For complex matrices, see Remark 1.*
4. *If S is positive definite and $S_{11} = L_{11}L_{11}^*$ is the Cholesky factorization of S_{11} then $S = HH^*$, in which*

$$H = \begin{bmatrix} L_{11} & 0 \\ S_{21}L_{11}^{-*} & L_{11}^{-*} \end{bmatrix}$$

is symplectic.

5. *If S is positive definite then the unique positive definite square root of S is symplectic.*

Proof. **1.** If S is positive definite then all its principal submatrices are positive definite. Hence, S_{11} is positive definite. Conversely, if S_{11} is positive definite then it is nonsingular, and $S_{11}^{-*} = S_{11}^{-1}$ is also positive definite. The factorization (2.1) can be written in this case as:

$$S = \begin{bmatrix} I & 0 \\ S_{21}S_{11}^{-1} & I \end{bmatrix} \begin{bmatrix} S_{11} & 0 \\ 0 & S_{11}^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ S_{21}S_{11}^{-1} & I \end{bmatrix}^*, \tag{5.9}$$

which implies that S is positive definite because $\left[\begin{smallmatrix} S_{11} & \\ & S_{11}^{-1} \end{smallmatrix}\right]$ is positive definite.

2. According to (5.9), every positive definite symplectic matrix can be written as

$$\begin{bmatrix} I & 0 \\ C & I \end{bmatrix} \begin{bmatrix} G & 0 \\ 0 & G^{-1} \end{bmatrix} \begin{bmatrix} I & C \\ 0 & I \end{bmatrix}, \tag{5.10}$$

with G positive definitive and C Hermitian. To prove the converse, simply notice that any matrix as in (5.10) is symplectic, because it is the product of three symplectic matrices, and is positive definite because it is congruent to the positive definite matrix $\left[\begin{smallmatrix} G & \\ & G^{-1} \end{smallmatrix}\right]$.

3. In item 2., G contributes with $(n^2+n)/2$ parameters and the same holds for C.

4. It follows from (5.9) by taking into account that in (5.9) the three factors are symplectic.

5. Let $S^{1/2}$ be the unique positive definite square root of S. Notice that $S = S^{1/2}S^{1/2}$ implies that $S^{-1} = (S^{1/2})^{-1}(S^{1/2})^{-1}$, so the positive definite square root of S^{-1}

[3] Every n-by-n positive definite matrix can be written as $G = LL^*$, with L lower triangular with positive entries on the diagonal. Therefore, the whole set of n-by-n positive definite matrices can be explicitly described using as free parameters the $(n^2+n)/2$ nontrivial entries of L.

is $(S^{-1})^{1/2} = (S^{1/2})^{-1}$. Let us denote this matrix simply by $S^{-1/2}$. Notice that $SJS = J$ because S is symplectic and Hermitian. Then $S = JS^{-1}J^* = (JS^{-1/2}J^*)^2$. The matrix $JS^{-1/2}J^*$ is positive definite. This means that $S^{1/2} = JS^{-1/2}J^*$ and $S^{1/2}JS^{1/2} = J$, i.e., $S^{1/2}$ is symplectic. ∎

An alternative proof of the last item in Theorem 5.2 relies in the special structure of the singular value decomposition of a symplectic matrix, see [50, Theorem 2]. This result easily implies that if S is symplectic and positive definite then $S = U\,\mathrm{diag}(\Sigma, \Sigma^{-1})U^*$, where U is unitary symplectic and Σ is diagonal with all its diagonal entries larger than or equal to one. Therefore, $S^{1/2} = U\,\mathrm{diag}(\Sigma^{1/2}, \Sigma^{-1/2})U^*$ and this matrix is symplectic since the three factors are symplectic.

5.3. Entrywise positive symplectic matrices. The purpose of this section is to show that there exist real symplectic matrices whose entries are all strictly positive. This is in contrast to real orthogonal matrices, because it is clear that there are no orthogonal matrices of dimension larger than one with all the entries strictly positive. We will also show how to generate entrywise positive symplectic matrices. These results are simple consequences of the parametrization in Theorem 3.1. Given a matrix A, we write $A > 0$ if all the entries of A are positive. According to Theorem 3.1, entrywise positive symplectic matrices can be constructed through the following three steps:

1. Select arbitrary real n-by-n matrices $G > 0$, $C = C^T > 0$, and $\widetilde{E} = \widetilde{E}^T > 0$ such that G is nonsingular.
2. Select a number $\alpha > 0$ such that $\alpha CG\widetilde{E} + G^{-T} > 0$. Obviously α may be any positive number such that $\alpha > \max_{ij} \left(-(G^{-T})_{ij}/(CG\widetilde{E})_{ij} \right)$.
3. Define $E = \alpha\widetilde{E}$.

Then the matrix

$$\begin{bmatrix} G & GE \\ CG & G^{-T} + CGE \end{bmatrix}$$

is symplectic with all the entries positive.

The previous procedure does not generate all the possible entrywise positive symplectic matrices because, for instance, given $G > 0$, nonpositive matrices C such that $CG > 0$ may be easily constructed. This shows that to describe explicitly the whole set of entrywise positive symplectic matrices is difficult.

5.4. Totally nonnegative symplectic matrices. The matrices with all minors nonnegative (positive) are called *totally nonnegative (TN)* (*totally positive (TP)*). They appear in a wide area of problems [20, 21] and many numerical linear algebra tasks can be very accurately performed on nonsingular TN matrices when they are properly parametrized [29, 30]. If a matrix A is TN and A^k is TP for some positive integer k then A is called *oscillatory.* TN matrices are matrices with real entries, therefore in this section we will only consider *real* symplectic matrices.

It is obvious that there exist TN symplectic matrices because the identity is TN and symplectic. The existence of oscillatory or TP symplectic matrices is not evident. Let us begin by considering this existence problem. We start by describing the set of 2-by-2 TN symplectic matrices.

THEOREM 5.3. *The matrix $S \in M_2(\mathbb{R})$ is symplectic and TP (TN) if and only if $\det S = 1$ and $s_{ij} > 0$ ($s_{ij} \geq 0$) for all (i,j). Additionally, $S \in M_2(\mathbb{R})$ is symplectic and TN but not TP if and only if $s_{ij} \geq 0$ for all (i,j), $s_{22} = 1/s_{11}$, and $s_{12}s_{21} = 0$.*

Proof. The proof is straightforward. We sketch the main ideas. A real 2-by-2 matrix is symplectic if and only if its determinant is 1. Besides, a real 2-by-2 matrix is TP (TN) if and only if all its entries and its determinant are positive (nonnegative). For the last part, notice that if a 2-by-2 TN symplectic matrix is not TP then at least one of its entries is zero. But the diagonal entries are necessarily different from zero because, otherwise, $\det S = -a_{12}a_{21} \leq 0$. □

Therefore the set of 2-by-2 TP symplectic matrices depends on three parameters and can be easily described, because if three arbitrary positive values are chosen for s_{11}, s_{12} and s_{21} then s_{22} is obtained from $\det S = 1$ as $s_{22} = (1+s_{12}s_{21})/s_{11}$. However, Theorem 5.4 shows that this is the end of the story, in the sense that for dimensions larger than 2 there are no TP symplectic matrices, nor oscillatory symplectic matrices.

THEOREM 5.4. *Let $S \in M_{2n}(\mathbb{R})$, with $n > 1$, be symplectic. Then S is neither TP, nor oscillatory.*

Proof. Let us assume that S is TP and we will get a contradiction. If S is TP then S has an LU factorization, $S = LU$, whose factors are *triangular totally positive* (ΔTP) matrices [11]. This means that all the "non-trivial" minors of L and U are positive, where we understand by "trivial" minors of a lower (upper) triangular matrix those minors that are zero for every lower (upper) triangular matrix with the same dimension [11, 15]. Besides, if S is symplectic then (4.1) is the LU factorization of S, and L_{22} and U_{22} are both ΔTP because they are submatrices of ΔTP matrices. Notice that in this case $S_{11}^{-T} = L_{22}U_{22}$, with T (transpose) instead of $*$ (conjugate transpose) because we are dealing with real matrices. This implies that S_{11}^{-T} is TP [15, p. 700], so S_{11}^{-1} is TP. On the other hand S_{11} is TP because it is a submatrix of the TP matrix S. Then, the well-known adjoint formula [26, Sec. 0.8.2] for the elements of the inverse guarantees that all the entries of S_{11}^{-1} are different from zero and the sign of $(S_{11}^{-1})_{ij}$ is $(-1)^{i+j}$. Thus S_{11}^{-1} has negative entries if $n > 1$. This is in contradiction with S_{11}^{-1} being TP.

Proceed again by contradiction for the oscillatory case. If S is oscillatory then S^k is TP for some positive integer k. This is impossible if $n > 1$ because S^k is a product of symplectic matrices, and, therefore, it is symplectic. □

The last task of this section is to describe the set of $2n$-by-$2n$ TN symplectic matrices. For $n > 1$, this is simply the set of symplectic diagonal matrices with positive diagonal entries. We need the simple Lemma 5.5 to prove this result in Theorem 5.6. Lemma 5.5 appears implicitly in [29, p. 4], but we do not know an explicit statement of it.

LEMMA 5.5. *Let A be a p-by-p nonsingular TN matrix. (i) If $a_{i1} = 0$ for some $i > 1$ then $a_{l1} = 0$ for $l = i, \ldots, p$; and (ii) if $a_{1j} = 0$ for some $j > 1$ then $a_{1l} = 0$ for $l = j, \ldots, p$.*

Proof. We only need to prove (i) because (ii) follows from applying (i) to A^T. A is nonsingular, thus there exists at least one nonzero element in its ith row. Let $a_{ik} \neq 0$, $k > 1$, be such an element. Let us consider the minors $\det \left[\begin{smallmatrix} a_{i1} & a_{ik} \\ a_{l1} & a_{lk} \end{smallmatrix}\right] = -a_{l1}a_{ik} \geq 0$ for $l = i+1, \ldots, p$. The entries of A are nonnegative, therefore these inequalities imply $a_{l1} = 0$ for $l = i+1, \ldots, p$. □

THEOREM 5.6. *The set of $2n$-by-$2n$, $n > 1$, TN symplectic matrices is*

$$\mathcal{S}^{TN} = \left\{ \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix} : D = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}, \ \lambda_i > 0 \ \textit{for} \ i = 1, \ldots, n \right\}.$$

Proof. It is obvious that every matrix $\left[\begin{smallmatrix} D & \\ & D^{-1}\end{smallmatrix}\right]$ with D positive diagonal is symplectic and TN. It remains to prove that every TN symplectic matrix is a matrix of this type. Let $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22}\end{smallmatrix}\right]$ be TN and symplectic then: (i) S is TN and nonsingular; (ii) S has a unique LU factorization whose factors are also TN [12, 15, 22]; (iii) this LU factorization is given by (4.1), and, therefore, L_{22} and U_{22} are TN; and (iv) S_{11} is TN and nonsingular, and, therefore, $(S_{11}^{-1})_{ij} \leq 0$ whenever $i+j$ is an odd number. This last inequality is a consequence of the classical adjoint formula for the elements of the inverse. Property (iii) implies that $S_{11}^{-T} = L_{22}U_{22}$ is TN. Thus, from (iv),

$$(S_{11}^{-T})_{ij} = 0 \quad \text{if } \ i+j \ \text{ is an odd number.} \tag{5.11}$$

In particular, $(S_{11}^{-T})_{12} = (S_{11}^{-T})_{21} = 0$ and by Lemma 5.5, $(S_{11}^{-T})_{1l} = (S_{11}^{-T})_{l1} = 0$ for $l = 2, \ldots, n$. This implies that $S_{11}^{-T}(2:n, 2:n)$ is nonsingular. By (5.11), $(S_{11}^{-T})_{k,k+1} = (S_{11}^{-T})_{k+1,k} = 0$ for all k, so Lemma 5.5 can be successively applied on the TN nonsingular matrices $(S_{11}^{-T})(k:n, k:n)$, $k = 2, \ldots, n$, to prove that S_{11}^{-T} is diagonal. We have proved that

$$S_{11} = D \quad \text{and} \quad S_{11}^{-T} = D^{-1},$$

with D positive diagonal. This means, in the notation of (4.1), that $L_{11} = L_{22} = I$, $U_{11} = D$, and $U_{22} = D^{-1}$, and the LU factorization of $S \equiv LU$ is

$$S = \begin{bmatrix} I & 0 \\ S_{21}D^{-1} & I \end{bmatrix} \begin{bmatrix} D & S_{12} \\ 0 & D^{-1} \end{bmatrix}.$$

According to (2.1), $S_{21}D^{-1}$ and $D^{-1}S_{12}$ are symmetric matrices. This can be combined with Lemma 5.5 applied successively to the TN nonsingular matrices $L(k: 2n, k: 2n)$ and $U(k: 2n, k: 2n)$, for $k = 1, \ldots, n$, to show that $S_{12} = S_{21} = 0$. □

5.5. Symplectic M-matrices. M-matrices occur very often in a wide variety of areas including finite difference methods for partial differential equations, economics, probability and statistics [8, Ch. 6]. In this section we want to find the set of matrices that are simultaneously symplectic and an M-matrix. Therefore we consider only nonsingular M-matrices. Many equivalent definitions of an M-matrix exist. We adopt the following one [27, p. 113].

DEFINITION 5.7. *$A \in M_n(\mathbb{R})$ is an M-Matrix if $a_{ij} \leq 0$ for $i \neq j$ and* $\mathrm{Re}(\lambda) > 0$ *for every eigenvalue λ of A.*

As in Section 5.4, we will consider in this section symplectic matrices with real entries because M-Matrices have real entries.

The proof of Theorem 5.8 below has the same flavor as the proof of Theorem 5.6. It is again based on the special properties of the LU factors of M-Matrices. The condition that the matrix HDK is diagonal, appearing in Theorem 5.8, is not explicit and it may seem awkward at a first glance but Lemma 5.9 will show that the sign structures of H, K, and D make it extremely simple to choose matrices H and K such that HDK is diagonal for any positive diagonal matrix D.

THEOREM 5.8. *The set of* $2n$*-by-*$2n$ *symplectic M-matrices is*

$$\mathcal{S}^M = \left\{ \begin{bmatrix} I & 0 \\ H & I \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix} \begin{bmatrix} I & K \\ 0 & I \end{bmatrix} : \begin{array}{c} D \in M_n(\mathbb{R}) \textit{ positive diagonal} \\ H = H^T \leq 0 \\ K = K^T \leq 0 \\ HDK \textit{ diagonal} \end{array} \right\}$$

$$= \left\{ \begin{bmatrix} D & DK \\ HD & D^{-1} + HDK \end{bmatrix} : \begin{array}{c} D \in M_n(\mathbb{R}) \textit{ positive diagonal} \\ H = H^T \leq 0 \\ K = K^T \leq 0 \\ HDK \textit{ diagonal} \end{array} \right\},$$

where the inequalities $H \leq 0$ *and* $K \leq 0$ *mean that* $h_{ij} \leq 0$ *and* $k_{ij} \leq 0$ *for all* i, j.

Proof. In the first place we will prove that any matrix of the form

$$\begin{bmatrix} I & 0 \\ H & I \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix} \begin{bmatrix} I & K \\ 0 & I \end{bmatrix} = \begin{bmatrix} D & DK \\ HD & D^{-1} + HDK \end{bmatrix}, \tag{5.12}$$

with D positive diagonal, $H = H^T \leq 0$, $K = K^T \leq 0$, and HDK diagonal, is symplectic and an M-matrix. The matrix in (5.12) is the product of three symplectic matrices, see Lemma 2.1, therefore it is symplectic. Note also that the product of the last two factors in the left hand side of equation (5.12) is an upper triangular matrix whose diagonal is $\mathrm{diag}(D, D^{-1})$, so this product is the U factor of the LU factorization of the matrix in the right hand side of (5.12). This implies that the leading principal minors of this matrix are positive because they are products of entries of D and D^{-1} [25, Eq. (9.1), p. 161]. Besides, the matrix in (5.12) has nonpositive off-diagonal entries and, therefore, it is an M-matrix by [27, Theorem 2.5.3, p.114-115].

In the second part of the proof, we will see that every symplectic M-matrix can be written as in (5.12). Let $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right]$ be a symplectic M-matrix then: (i) S_{11} is an M-matrix [27, p. 114]; (ii) S_{11} is nonsingular and $S_{11}^{-1} \geq 0$ componentwise [27, Theorem 2.5.3]; (iii) S has a unique LU factorization and both factors are M-matrices [27, p. 117]; and, (iv) the LU factorization of $S = LU$ is given by (4.1). Thus

$$S_{11}^{-T} = L_{22} U_{22} \geq 0, \tag{5.13}$$

and L_{22} and U_{22} are M-matrices because they are principal submatrices of the M-matrices L and U. This means, in particular, that the diagonal entries of L_{22} and U_{22} are positive while the off-diagonal entries are non-positive. If this information is combined with (5.13), we get in MATLAB notation: $L_{22}(2:n,1) = 0$ and $U_{22}(1,2:n) = 0$; then $L_{22}(3:n,2) = 0$ and $U_{22}(2,3:n) = 0$; ... ;$L_{22}(n,n-1) = 0$ and $U_{22}(n-1,n) = 0$. We have proved that L_{22}, U_{22}, and S_{11}^{-T} are diagonal positive matrices. Let us denote

$$S_{11} = D \quad \text{and} \quad S_{11}^{-T} = D^{-1},$$

with D positive diagonal. This means, in the notation of (4.1), that $L_{11} = L_{22} = I$, $U_{11} = D$, and $U_{22} = D^{-1}$, and the LU factorization of $S \equiv LU$ is

$$S = \begin{bmatrix} I & 0 \\ S_{21}D^{-1} & I \end{bmatrix} \begin{bmatrix} D & S_{12} \\ 0 & D^{-1} \end{bmatrix} = \begin{bmatrix} I & 0 \\ S_{21}D^{-1} & I \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix} \begin{bmatrix} I & D^{-1}S_{12} \\ 0 & I \end{bmatrix},$$

where, according to (2.1), $S_{21}D^{-1}$ and $D^{-1}S_{12}$ are symmetric matrices, and $S_{21}D^{-1} \leq 0$ and $D^{-1}S_{12} \leq 0$ because the LU factors of S are M-matrices. Therefore, we have proved that every symplectic M-matrix S can be expressed as:

$$S = \begin{bmatrix} I & 0 \\ H & I \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix} \begin{bmatrix} I & K \\ 0 & I \end{bmatrix} = \begin{bmatrix} D & DK \\ HD & D^{-1} + HDK \end{bmatrix},$$

with D positive diagonal, $H = H^T \leq 0$ and $K = K^T \leq 0$. Notice that the off-diagonal elements of $D^{-1} + HDK$ are less than or equal to zero because S is an M-matrix, but, on the other hand, $D^{-1} + HDK \geq 0$. This implies that HDK is diagonal. ☐

LEMMA 5.9. *Let D, H, and K be n-by-n real matrices such that D is positive diagonal, $H = H^T \leq 0$, and $K = K^T \leq 0$. Then*

1. *HDK is diagonal if and only if HK is diagonal.*
2. *HK is diagonal if and only if for every (i, j) such that $h_{ij} = h_{ji} \neq 0$, $k_{il} = k_{li} = 0$ for $l \neq j$, and $k_{jp} = k_{pj} = 0$ for $p \neq i$.*

Notice that item 2. implies that for every pair $h_{ij} = h_{ji} \neq 0$ the only elements that can be different from zero in the rows i and j and in the columns i and j of K are precisely $k_{ij} = k_{ji}$.

The proof of this Lemma is trivial. The important point with respect to Theorem 5.8 is that once arbitrary matrices D, positive diagonal, and $H = H^T \leq 0$ are chosen, a set of zero entries of K is easily fixed, and those entries of K that are not in this set can be arbitrarily chosen with only the constraint $K = K^T \leq 0$. Obviously, it is possible to choose H, D and K arbitrary diagonal matrices with the required sign constraints. It is also possible to choose $H = H^T \leq 0$ completely arbitrary, however, loosely speaking, the nonzero off-diagonal entries of H impose many zeros on K by Lemma 5.9. Let us illustrate this with a simple example.

EXAMPLE 1. *Let us assume that an arbitrary positive diagonal matrix D has been chosen, and $H = H^T \leq 0$ is such that*

$$H = \begin{bmatrix} 0 & \times & 0 \\ \times & 0 & \times \\ 0 & \times & 0 \end{bmatrix},$$

where $\times$ denotes a negative entry. Then neccesarily $K = 0$. Note that Lemma 5.9 and $h_{12} = h_{21} \neq 0$ imply that all the entries in the rows 1 and 2 and the columns 1 and 2 of K are zero except perhaps $k_{12} = k_{21}$. But $k_{12} = k_{21}$ are also zero because $h_{23} = h_{32} \neq 0$. This also implies that k_{33} is zero and so $K = 0$. This example extends easily to prove that $K = 0$ if H is an irreducible tridiagonal matrix.

6. Subparametrization problems and consequences. Several results in this section are stated for the $(1, 1)$-block of a symplectic matrix. The reader should notice that similar results hold for any other of the four blocks in the partition (1.2), because by multiplying a symplectic matrix on the left, on the right, or on both sides by the matrix J any of the blocks can be placed in the position $(1, 1)$ and the matrix remains symplectic. A similar remark holds for the results we present for the first n columns of a symplectic $2n$-by-$2n$ matrix.

6.1. Symplectic matrices with $(1, 1)$-block of given rank. This section extends Theorem 3.1 to symplectic matrices whose $(1, 1)$-block has a given rank that is different from n. The result we present, Theorem 6.2, is different from Theorem 3.2 because symplectic interchanges among different blocks in the partition (1.2) are not allowed. The results in this section are based on the following simple lemma, whose trivial proof is omitted.

LEMMA 6.1. *The set of n-by-n complex matrices with rank k is*

$$M_n^k(\mathbb{C}) = \left\{ P \begin{bmatrix} X_1 \\ F\,X_1 \end{bmatrix} : \begin{array}{c} X_1 \in M_{k,n}(\mathbb{C})\,,\; F \in M_{n-k,k}(\mathbb{C}) \\ \operatorname{rank}(X_1) = k \\ P \in M_n(\mathbb{C}) \textit{ permutation matrix} \end{array} \right\}.$$

A counterpart of Lemma 6.1 by "columns" is obviously possible if the permutation matrix is placed on the right. The explicit description of the set $M_n^k(\mathbb{C})$ presented in Lemma 6.1 is not a "rigurous" parametrization because given an n-by-n matrix A with $\operatorname{rank}(A) = k$, there may exist several permutation matrices P such that A can be expressed as $P\left[\begin{smallmatrix} X_1 \\ F X_1 \end{smallmatrix}\right]$. This is a fact similar to that appearing in Theorem 3.2. However, if this indeterminacy in the permutation is ignored, the description in Lemma 6.1 is optimal because the number of free parameters,[4] i.e., the number of entries of X_1 and F, is $2kn - k^2$. This is precisely the dimension of the manifold of matrices with rank at most k [13, Lemma 3.3]. Another relevant fact to be remarked here is that given A with $\operatorname{rank}(A) = k$, once the permutation matrix P is chosen, there are only one matrix X_1 and only one matrix F such that $A = P\left[\begin{smallmatrix} X_1 \\ F X_1 \end{smallmatrix}\right]$.

The main result in this section is Theorem 6.2, which reduces to Theorem 3.1 if $\operatorname{rank}(S_{11}) = n$ and $P = I_n$.

THEOREM 6.2. *The set of $2n$-by-$2n$ symplectic matrices $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right]$, where $S_{11} \in M_n(\mathbb{C})$ and $\operatorname{rank}(S_{11}) = k$ is*

$$\mathcal{S}_k^{(1,1)} = \left\{ \left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c|c} X_1 & X_1 E \\ C_{21}\,X_1 & X^{-*}(k+1:n,:) + C_{21}\,X_1\,E \\ \hline [C_{11}\; C_{21}^*]\,X & X^{-*}(1:k,:) + [C_{11}\; C_{21}^*]\,X\,E \\ -X_2 & -X_2 E \end{array}\right] : \right.$$
$$\left. \begin{array}{c} X_1 \in M_{k,n}(\mathbb{C})\;,\; P \in M_n(\mathbb{C}) \textit{ permutation matrix} \\ X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \in M_n(\mathbb{C}) \textit{ nonsingular}\,,\; \begin{bmatrix} C_{11} & C_{21}^* \\ C_{21} & 0 \end{bmatrix} \in M_n(\mathbb{C}) \textit{ Hermitian} \\ E = E^* \in M_n(\mathbb{C}) \end{array} \right\}.$$

Notice that $C_{11} \in M_k(\mathbb{C})$ follows from $\left[\begin{smallmatrix} X_1 \\ C_{21} X_1 \end{smallmatrix}\right] \in M_n(\mathbb{C})$, and that this theorem holds true for $k = 0$ if we consider that X_1, C_{11}, C_{21} are empty matrices, $P = I_n$, $X = X_2$, and the $(1,1)$-block $\left[\begin{smallmatrix} X_1 \\ C_{21} X_1 \end{smallmatrix}\right] = 0 \in M_n(\mathbb{C})$.

REMARK 2. Notice that Theorem 6.2 provides the following explicit description of the group $\mathcal{S}$ of symplectic matrices: $\mathcal{S} = \bigcup_{k=0}^{n} \mathcal{S}_k^{(1,1)}$. This description is different from the one presented in Theorem 3.2, because the permutation Q in Theorem 3.2 interchanges rows between different blocks. However, both descriptions are based on the same ideas: Theorems 2.2 and 2.5. Notice that a counterpart of Theorem 6.2 with the permutation P on the right is also possible.

Proof of Theorem 6.2. First, we prove that every matrix of the form

$$\left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c|c} X_1 & X_1 E \\ C_{21}\,X_1 & X^{-*}(k+1:n,:) + C_{21}\,X_1\,E \\ \hline [C_{11}\; C_{21}^*]\,X & X^{-*}(1:k,:) + [C_{11}\; C_{21}^*]\,X\,E \\ -X_2 & -X_2 E \end{array}\right], \tag{6.1}$$

[4] Analogously to the footnote 1, the kn entries of X_1 are not totally free parameters due to the rank condition on X_1. But the whole set of k-by-n matrices with rank k can be explicitly parameterized in terms of nk parameters as $X_1 = \Pi L U \Pi'$, where L is an arbitrary k-by-k lower triangular matrix with ones on the diagonal, U is an arbitrary k-by-n upper triangular matrix with nonzero diagonal entries, and Π and Π' are arbitrary permutation matrices.

with the properties mentioned in Theorem 6.2 is symplectic and the rank of its $(1,1)$-block is k. This latter fact is obvious. To prove that the matrix in (6.1) is symplectic notice that

$$\widetilde{\Pi}_n \cdots \widetilde{\Pi}_{k+1} \left[\begin{array}{c|c} X_1 & X_1 E \\ C_{21}\, X_1 & X^{-*}(k+1:n,:) + C_{21}\, X_1\, E \\ \hline [C_{11}\ C_{21}^*]\, X & X^{-*}(1:k,:) + [C_{11}\ C_{21}^*]\, X\, E \\ -X_2 & -X_2 E \end{array}\right] =$$

$$\left[\begin{array}{c|c} X & X\, E \\ \hline \begin{bmatrix} C_{11} & C_{21}^* \\ C_{21} & 0 \end{bmatrix} X & X^{-*} + \begin{bmatrix} C_{11} & C_{21}^* \\ C_{21} & 0 \end{bmatrix} X\, E \end{array}\right],$$

where $\widetilde{\Pi}_j$ are the symplectic interchange matrices introduced in Definition 2.4. The matrix in the right hand side of the previous equation is symplectic by Theorem 3.1, therefore the second factor in (6.1) is also symplectic because $\widetilde{\Pi}_n \cdots \widetilde{\Pi}_{k+1}$ is symplectic. Combining this with the fact that $S = \left[\begin{smallmatrix} P & 0 \\ 0 & P \end{smallmatrix}\right]$ is symplectic, we get that any matrix as the one in (6.1) is symplectic.

Now, let us prove that every symplectic matrix $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right]$ with $\operatorname{rank}(S_{11}) = k$ can be expressed as (6.1). By Lemma 6.1 $S_{11} = P\left[\begin{smallmatrix} X_1 \\ C_{21} X_1 \end{smallmatrix}\right]$, where $X_1 \in M_{k,n}(\mathbb{C})$ and $\operatorname{rank}(X_1) = k$. Thus, we can partition

$$\left[\begin{array}{c|c} P^T & 0 \\ \hline 0 & P^T \end{array}\right] S = \left[\begin{array}{c|c} X_1 & Y_1 \\ C_{21}X_1 & Y_2 \\ \hline Z_1 & K_1 \\ -X_2 & -K_2 \end{array}\right]. \tag{6.2}$$

Theorem 2.5 guarantees that the n-by-n matrix $\left[\begin{smallmatrix} X_1 \\ X_2 \end{smallmatrix}\right]$ is nonsingular. Thus the symplectic matrix

$$\widetilde{\Pi}_n \cdots \widetilde{\Pi}_{k+1} \left[\begin{array}{c|c} P^T & 0 \\ \hline 0 & P^T \end{array}\right] S = \left[\begin{array}{c|c} X_1 & Y_1 \\ X_2 & K_2 \\ \hline Z_1 & K_1 \\ C_{21}X_1 & Y_2 \end{array}\right]$$

has its $(1,1)$-block nonsingular and has the structure described in Theorem 3.1, i.e.,

$$\widetilde{\Pi}_n \cdots \widetilde{\Pi}_{k+1} \left[\begin{array}{c|c} P^T & 0 \\ \hline 0 & P^T \end{array}\right] S = \left[\begin{array}{c|c} \begin{matrix} X_1 \\ X_2 \end{matrix} & \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} E \\ \hline C \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} & \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}^{-*} + C \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} E \end{array}\right], \tag{6.3}$$

with $C = \left[\begin{smallmatrix} C_{11} & C_{21}^* \\ C_{21} & 0 \end{smallmatrix}\right]$. The structure (6.1) appears when S is found from equation (6.3). ☐

Corollary 6.3. *The set of $2n$-by-$2n$ real symplectic matrices whose $(1,1)$-block has rank k depends on*

$$2n^2 + n - \frac{(n-k)^2 + (n-k)}{2}$$

real parameters. For complex matrices, see Remark 1.

Proof. This is just the sum of free entries in $X = \left[\begin{smallmatrix} X_1 \\ X_2 \end{smallmatrix}\right]$, C_{11}, C_{21} and E. ☐

6.2. $\mathcal{S}^{(1,1)}$ is a dense open subset of $\mathcal{S}$. As announced in Section 3, the set $\mathcal{S}^{(1,1)}$ of symplectic matrices whose $(1,1)$-block is nonsingular is a dense open subset in the group of symplectic matrices, $\mathcal{S}$, when we consider in $\mathcal{S}$ the subspace topology induced by the usual topology on $M_{2n}(\mathbb{C})$. The purpose of this section is to prove this result. Although it can be accomplished through general properties of algebraic manifolds, we follow here a different way based on the explicit description presented in Theorem 6.2. We begin with the technical Lemma 6.4 that shows how to generate a sequence of symplectic matrices whose $(1,1)$-block is nonsingular and whose limit is a given symplectic matrix S.

LEMMA 6.4. *Let $S \in M_{2n}(\mathbb{C})$ be a symplectic matrix whose $(1,1)$-block has rank k, and let us express S according to Theorem 6.2 as follows*

$$S = \left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c|c} X_1 & X_1 E \\ C_{21}\, X_1 & X^{-*}(k+1:n,:) + C_{21}\, X_1\, E \\ \hline [C_{11}\ C_{21}^*]\, X & X^{-*}(1:k,:) + [C_{11}\ C_{21}^*]\, X\, E \\ -X_2 & -X_2 E \end{array}\right],$$

where $X_1 \in M_{k,n}(\mathbb{C})$, $P \in M_n(\mathbb{C})$ is a permutation matrix, $X = \left[\begin{smallmatrix} X_1 \\ X_2 \end{smallmatrix}\right] \in M_n(\mathbb{C})$ is nonsingular, and $\left[\begin{smallmatrix} C_{11} & C_{21}^* \\ C_{21} & 0 \end{smallmatrix}\right]$ and E are n-by-n Hermitian matrices. Let $\{C_{22}^{(q)}\}_{q=1}^{\infty} \subset M_{n-k}(\mathbb{C})$ be any sequence of nonsingular Hermitian matrices such that $\lim_{q\to\infty} C_{22}^{(q)} = 0$. Then the sequence

$$S^{(q)} = \left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c|c} \begin{bmatrix} I_k & 0 \\ C_{21} & C_{22}^{(q)} \end{bmatrix} X & \begin{bmatrix} 0 & 0 \\ 0 & I_{n-k} \end{bmatrix} X^{-*} + \begin{bmatrix} I_k & 0 \\ C_{21} & C_{22}^{(q)} \end{bmatrix} X\, E \\ \hline \begin{bmatrix} C_{11} & C_{21}^* \\ 0 & -I_{n-k} \end{bmatrix} X & \begin{bmatrix} I_k & 0 \\ 0 & 0 \end{bmatrix} X^{-*} + \begin{bmatrix} C_{11} & C_{21}^* \\ 0 & -I_{n-k} \end{bmatrix} X\, E \end{array}\right],$$

satisfies

1. *$S^{(q)}$ is symplectic for all $q \in \{1, 2, \ldots\}$.*
2. *The $(1,1)$-block of $S^{(q)}$ is nonsingular for all $q \in \{1, 2, \ldots\}$.*
3. *$\lim_{q\to\infty} S^{(q)} = S$.*

This lemma holds true for $k = 0$ under the same considerations for which Theorem 6.2 does.

REMARK 3. It is very easy to create sequences $\{C_{22}^{(q)}\}_{q=1}^{\infty} \subset M_{n-k}(\mathbb{C})$ as those appearing in Lemma 6.4. For instance $C_{22}^{(q)} = \operatorname{diag}(1/q, \ldots, 1/q)$ is one of them.

Proof of Lemma 6.4. It is straightforward to check that the $(1,1)$-block of $S^{(q)}$ is nonsingular for all q and that $\lim_{q\to\infty} S^{(q)} = S$. To prove that $S^{(q)}$ is symplectic for all q notice that

$$\widetilde{\Pi}_n \cdots \widetilde{\Pi}_{k+1} \left[\begin{array}{c|c} P^T & 0 \\ \hline 0 & P^T \end{array}\right] S^{(q)} = \left[\begin{array}{c|c} X & X\, E \\ \hline \begin{bmatrix} C_{11} & C_{21}^* \\ C_{21} & C_{22}^{(q)} \end{bmatrix} X & X^{-*} + \begin{bmatrix} C_{11} & C_{21}^* \\ C_{21} & C_{22}^{(q)} \end{bmatrix} X\, E \end{array}\right].$$

The right-hand side of the previous equation is symplectic by Theorem 3.1, and $\widetilde{\Pi}_n \cdots \widetilde{\Pi}_{k+1}$ and $\left[\begin{smallmatrix} P^T & 0 \\ 0 & P^T \end{smallmatrix}\right]$ are obviously symplectic, therefore $S^{(q)}$ is symplectic. □

Now, we prove the main result in this section.

THEOREM 6.5. *$\mathcal{S}^{(1,1)}$ is a dense open subset of $\mathcal{S}$ when we consider in $\mathcal{S}$ the subspace topology induced by the usual topology on $M_{2n}(\mathbb{C})$.*

Proof. Lemma 6.4 implies that every symplectic matrix whose $(1,1)$-block is singular is the limit of a sequence of symplectic matrices with nonsingular $(1,1)$-blocks. Therefore $\mathcal{S}^{(1,1)}$ is dense in $\mathcal{S}$. Now, let us prove that $\mathcal{S}^{(1,1)}$ is open in

$\mathcal{S}$. Let $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right] \in \mathcal{S}^{(1,1)}$, $S' = \left[\begin{smallmatrix} S'_{11} & S'_{12} \\ S'_{21} & S'_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C})$ with S'_{11} singular, and σ_n be the smallest singular value of S_{11}. Let $\|A\|_2$ be the spectral norm of the matrix A. Then, it is well-known that $\|S - S'\|_2 \geq \|S_{11} - S'_{11}\|_2 \geq \sigma_n$ [49]. So, $\mathcal{C} = \{R = \left[\begin{smallmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{smallmatrix}\right] \in M_{2n}(\mathbb{C}) \,:\, \|S - R\|_2 < \sigma_n\}$ is an open set in $M_{2n}(\mathbb{C})$ with R_{11} nonsingular. By definition of the subspace topology, $\mathcal{S} \cap \mathcal{C}$ is open in $\mathcal{S}$, besides $S \in \mathcal{S} \cap \mathcal{C}$, and $\mathcal{S} \cap \mathcal{C} \subset \mathcal{S}^{(1,1)}$. This means that S is an interior point of $\mathcal{S}^{(1,1)}$, which proves that $\mathcal{S}^{(1,1)}$ is open in $\mathcal{S}$. $\square$

6.3. The $(1,1)$-blocks of symplectic matrices and the set of symplectic matrices with fixed $(1,1)$-block. Theorem 6.2 allows us to answer the following two questions: (i) what matrices can be the $(1,1)$-block of a symplectic matrix?; (ii) if the $(1,1)$-block of a symplectic matrix is fixed, what is the set of symplectic matrices that have this $(1,1)$-block?

THEOREM 6.6.

1. *Every n-by-n complex matrix is the $(1,1)$-block of a symplectic matrix.*
2. *Let G be an arbitrary n-by-n complex matrix with rank k. If G is expressed as $G = P\left[\begin{smallmatrix} X_1 \\ C_{21} X_1 \end{smallmatrix}\right]$, where P is an n-by-n permutation matrix, $X_1 \in M_{k,n}(\mathbb{C})$, and* $\operatorname{rank}(X_1) = k$, *then the set of symplectic matrices whose $(1,1)$-block is G is*

$$\mathcal{S}_G = \left\{ \left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c|c} X_1 & X_1 E \\ C_{21}\, X_1 & X^{-*}(k+1:n,:) + C_{21}\, X_1\, E \\ \hline [C_{11}\ C_{21}^*]\, X & X^{-*}(1:k,:) + [C_{11}\ C_{21}^*]\, X\, E \\ -X_2 & -X_2 E \end{array}\right] : \right.$$
$$\left. \begin{array}{c} X_2 \in M_{n-k,n}(\mathbb{C}) \ \text{ such that } \ X = \left[\begin{array}{c} X_1 \\ X_2 \end{array}\right] \in M_n(\mathbb{C}) \ \text{ is nonsingular,} \\ C_{11} = C_{11}^* \in M_k(\mathbb{C}) \ , \ E = E^* \in M_n(\mathbb{C}) \end{array} \right\}. \tag{6.4}$$

The set $\mathcal{S}_G$ for real matrices depends on

$$\frac{n^2+n}{2} + \frac{k^2+k}{2} + (n-k)\,n$$

parameters. For the complex case, see Remark 1.

Proof. Let G be any n-by-n matrix with rank k. Then one can express $G = P\left[\begin{smallmatrix} X_1 \\ C_{21} X_1 \end{smallmatrix}\right]$ by Lemma 6.1. Theorem 6.2 shows how to construct symplectic matrices whose $(1,1)$-block is G by choosing arbitrary matrices $X_2 \in M_{n-k,n}(\mathbb{C})$ such that $\left[\begin{smallmatrix} X_1 \\ X_2 \end{smallmatrix}\right]$ is nonsingular, $C_{11} = C_{11}^* \in M_k(\mathbb{C})$, and $E = E^* \in M_n(\mathbb{C})$. This proves that every n-by-n matrix is the $(1,1)$-block of a symplectic matrix. All the matrices in the set (6.4) have G as its $(1,1)$-block and they are symplectic by Theorem 6.2. Besides, it is clear from the fact that P and $\left[\begin{smallmatrix} X_1 \\ X_2 \end{smallmatrix}\right]$ are nonsingular that different selections of X_2, C_{11}, and E produce different symplectic matrices with $(1,1)$-block equal to G, i.e., the $(n^2+n)/2 + (k^2+k)/2 + (n-k)\,n$ entries of X_2, C_{11}, and E are not redundant parameters. The final step is to prove that every symplectic matrix whose $(1,1)$-block is G can be expressed as in (6.4). This can be done by the argument presented after (6.2). $\square$

6.4. The first n columns of symplectic matrices and the set of symplectic matrices whose first n columns are fixed. Theorem 6.2 also allows us to answer the following two questions: (i) what $2n$-by-n matrices can be the first n columns of a $2n$-by-$2n$ symplectic matrix?; (ii) if the n first columns of a symplectic matrix are fixed, what is the set of symplectic matrices that have these first n

columns? We would like to remark that in [19, Proposition 1.4] the following answer to the first question was presented: a $2n$-by-n matrix $\left[\begin{smallmatrix} S_{11} \\ S_{21} \end{smallmatrix}\right]$ contains the n first columns of a $2n$-by-$2n$ symplectic matrix if and only if $[S_{11}^* S_{21}^*]\, J \left[\begin{smallmatrix} S_{11} \\ S_{21} \end{smallmatrix}\right] = 0$, i.e., if and only if the columns of $\left[\begin{smallmatrix} S_{11} \\ S_{21} \end{smallmatrix}\right]$ span a Lagrangian subspace. This nice characterization, however, is not explicit because it characterizes all possible $\left[\begin{smallmatrix} S_{11} \\ S_{21} \end{smallmatrix}\right]$ as the set of solutions of a quadratic matrix equation. The first goal in this section is to present an explicit description of this set that allows us to generate easily its elements.

THEOREM 6.7. *The set of $2n$-by-n matrices $\left[\begin{smallmatrix} S_{11} \\ S_{21} \end{smallmatrix}\right]$ with $\operatorname{rank}(S_{11}) = k$ that are the first n columns of a $2n$-by-$2n$ symplectic matrix is*

$$\mathcal{S}_k^{ncol} = \left\{ \left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c} X_1 \\ C_{21}\, X_1 \\ \hline [C_{11}\; C_{21}^*]\, X \\ -X_2 \end{array}\right] : \begin{array}{c} X_1 \in M_{k,n}(\mathbb{C}) \;,\; P \in M_n(\mathbb{C}) \textit{ permutation matrix} \\ X = \left[\begin{array}{c} X_1 \\ X_2 \end{array}\right] \in M_n(\mathbb{C}) \textit{ nonsingular} \;,\; \left[\begin{array}{cc} C_{11} & C_{21}^* \\ C_{21} & 0 \end{array}\right] \in M_n(\mathbb{C}) \textit{ Hermitian} \end{array} \right\}.$$

For real matrices, this set depends on $(3n^2+n)/2 - ((n-k)^2 + (n-k))/2$ parameters. In the complex case, see Remark 1.

Proof. It is a direct consequence of Theorem 6.2.□

The second result in this section reveals an interesting structure for the set of symplectic matrices whose first n columns are fixed. In the case of real symplectic matrices this set is an *affine subspace* of $M_{2n}(\mathbb{R})$, i.e., a fixed symplectic matrix plus a vector subspace of $M_{2n}(\mathbb{R})$. It should be noticed, however, that the matrices in this subspace are not symplectic.

THEOREM 6.8. *Let $S_1 \in M_{2n,n}(\mathbb{C})$ be a matrix that contains the n first columns of a $2n$-by-$2n$ symplectic matrix. Let us express S_1 according to Theorem 6.7 as*

$$S_1 = \left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c} X_1 \\ C_{21}\, X_1 \\ \hline [C_{11}\; C_{21}^*]\, X \\ -X_2 \end{array}\right],$$

where $X = \left[\begin{smallmatrix} X_1 \\ X_2 \end{smallmatrix}\right]$, C_{11}, C_{21}, and P have the properties appearing in Theorem 6.7. Using the elements of S_1, we define the symplectic matrix

$$Z_0 = \left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c|c} X_1 & 0 \\ C_{21}\, X_1 & X^{-*}(k+1:n,:) \\ \hline [C_{11}\; C_{21}^*]\, X & X^{-*}(1:k,:) \\ -X_2 & 0 \end{array}\right], \tag{6.5}$$

and the set

$$\mathcal{V} = \left\{ \left[\begin{array}{c|c} P & 0 \\ \hline 0 & P \end{array}\right] \left[\begin{array}{c|c} 0 & X_1 \\ 0 & C_{21}\, X_1 \\ \hline 0 & [C_{11}\; C_{21}^*]\, X \\ 0 & -X_2 \end{array}\right] \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & E \end{array}\right] : E = E^* \in M_n(\mathbb{C}) \right\}.$$

Then,

1. *The set of symplectic matrices whose n first columns are S_1 is*

$$\mathcal{S}_{S_1} = \{Z_0 + V \,:\, V \in \mathcal{V}\}\,.$$

2. *In the real case $\mathcal{S}_{S_1}$ depends on $(n^2+n)/2$ parameters, that are the entries of E. For complex matrices, see Remark 1.*
3. *For real matrices $\mathcal{V}$ is a linear subspace of $M_{2n}(\mathbb{R})$.*

Proof. This theorem is a straightforward consequence of Theorems 6.2 and 6.7. Notice that the fact that Z_0 is symplectic follows from Theorem 6.2 by taking $E = 0$. □

6.5. Leading principal submatrices of symplectic matrices of dimension greater than n. Theorem 6.6 guarantees that, if $p \leq n$, any p-by-p matrix is the leading principal submatrix $S(1:p, 1:p)$ of a $2n$-by-$2n$ symplectic matrix S. A natural question in this context is if this property can be extended to leading principal submatrices of dimension greater than n. Notice for instance that for real matrices the number of entries of an $(n+1)$-by-$(n+1)$ leading principal submatrix is less than $2n^2+n$, i.e., the dimension of the group of $2n$-by-$2n$ symplectic matrices, whenever $n > 1$. Therefore one might think that any $(n+1)$-by-$(n+1)$ matrix can be the leading principal submatrix $S(1:(n+1), 1:(n+1))$ of a $2n$-by-$2n$ symplectic matrix. However, the next theorem shows that this is not the case. We focus on real matrices.

THEOREM 6.9. *Any $(n+1)$-by-$(n+1)$ real matrix A with $A(1:n, 1:n)$ nonsingular can be the leading submatrix $S(1:(n+1), 1:(n+1))$ of a real $2n$-by-$2n$ symplectic matrix S, except for the fact that the entry $A(n+1, n+1)$ is determined by the others.*

Proof. This is a consequence of the parametrization in Theorem 3.1. Let us use the notation in that theorem. Let $G = A(1:n, 1:n)$. Then the first column of E is simply $E(:,1) = G^{-1}A(1:n, n+1)$ and the first row of C is $C(1,:) = A(n+1, 1:n)G^{-1}$. Therefore $A(n+1, n+1) = G^{-*}(1,1) + C(1,:)GE(:,1)$ is fixed by the remaining entries of A. □

Notice that the situation for complex matrices is more complicated because it is no longer true that always the first column of E is $E(:,1) = G^{-1}A(1:n, n+1)$ and the first row of C is $C(1,:) = A(n+1, 1:n)G^{-1}$, because $E(1,1)$ and $C(1,1)$ are real numbers (E and C are Hermitian). Thus, it is not so simple to select a leading $(n+1)$-by-$(n+1)$ principal submatrix of a symplectic matrix.

7. Conclusions. Two explicit parameterizations of the group of symplectic matrices have been presented in Theorems 3.2 and 6.2. These results are applied to parameterize the sets of certain symplectic matrices that have additional structures, and to parameterize the sets of symplectic matrices with certain fixed blocks. These parameterizations provide concrete tools for constructing general symplectic matrices, structured symplectic matrices, and symplectic matrices with fixed blocks. These matrices may be used for instance for testing numerical algorithms.

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