DOUBLY STRUCTURED SETS OF SYMPLECTIC MATRICES

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Symplectic Matrices

$$J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix} \quad \text{where} \quad I_n \quad n \times n \text{ identity matrix}$$

Definition: $S \in \mathbb{R}^{2n \times 2n}$ is symplectic if $S^T J S = J$

We will consider often the partition of symplectic S

$$S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \quad \text{with} \quad S_{ij} \in \mathbb{R}^{n \times n}$$

The symplectic group is important in theory and applications (Hamiltonian mechanics, parametric resonance, electromagnetism, symplectic integrators, discrete control problems, Kalman filtering,....)

The problem to be solved

Symplectic matrices are **implicitly defined** as solutions of the nonlinear matrix equation $S^T J S = J$

This is useful for **checking** if a matrix is symplectic, **but not for constructing** symplectic matrices.

This characterization makes difficult to work with them, both in theory and in structured numerical algorithms.

OUR GOAL: To present an **explicit description (parametrization)** of the group of symplectic matrices, i.e., to find the set of solutions of

$$S^T J S = J \text{ where } S \text{ unknown}$$

and to apply this parametrization to construct symplectic matrices that have extra structures.

Outline of the talk

1. Previous results
2. Parametrization
3. Brief Summary on subparametrization problems
4. Description of doubly structured sets (symplectic and other property):
    - LU factorizations of symplectic
    - Orthogonal symplectic
    - Positive definite symplectic
    - Positive elementwise symplectic
    - TN, TP, oscillatory symplectic
    - Symplectic M-Matrices
5. Conclusions and Open problems

Previous I: A result by Mehrmann (SIMAX, 1988)

Theorem: Let $S = \left[\begin{smallmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{smallmatrix}\right]$ be symplectic with S_{11} non-singular. Then

$$S = \begin{bmatrix} I & 0 \\ S_{21}S_{11}^{-1} & I \end{bmatrix} \begin{bmatrix} S_{11} & 0 \\ 0 & S_{11}^{-T} \end{bmatrix} \begin{bmatrix} I & S_{11}^{-1}S_{12} \\ 0 & I \end{bmatrix}$$

where

1. The three factors are symplectic.

2. $S_{21}S_{11}^{-1}$ and $S_{11}^{-1}S_{12}$ are symmetric.

Let us combine this with three trivial facts...

Parametrization with nonsingular (1,1)-block

1. $\begin{bmatrix} I & 0 \\ X & I \end{bmatrix}$ is symplectic if and only if $X = X^T$.
2. $\begin{bmatrix} G & 0 \\ 0 & Y \end{bmatrix}$ is symplectic if and only if $Y = G^{-T}$.
3. Products and transposes of symplectic are symplectic.

Theorem: The set of symplectic matrices with non-singular S_{11} is

$$\mathcal{S}^{(1,1)} = \left\{ \underbrace{\begin{bmatrix} G & GE \\ CG & G^{-T} + CGE \end{bmatrix}}_{\begin{bmatrix} I & 0 \\ C & I \end{bmatrix} \begin{bmatrix} G & 0 \\ 0 & G^{-T} \end{bmatrix} \begin{bmatrix} I & E \\ 0 & I \end{bmatrix}} : \begin{array}{c} G \text{ nonsingular} \\ C = C^T,\ E = E^T \end{array} \right\}$$

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$2n^2 + n$ free parameters in this parametrization. This is precisely the dimension of the symplectic group.

What happens if S_{11} is singular?

Definition: Symplectic interchange matrices

$$\Pi_j = \begin{array}{c c} & \begin{array}{ccccc ccccc} & & j & & & & & j+n & & \end{array} \\ \begin{array}{c} \\ \\ j \\ \\ \\ \\ \\ j+n \\ \\ \\ \end{array} & \left[\begin{array}{ccccc|ccccc} 1 & & & & & & & & & \\ & \ddots & & & & & & & & \\ & & 0 & & & & & 1 & & \\ & & & \ddots & & & & & & \\ & & & & 1 & & & 0 & & \\ \hline & & & & & 1 & & & & \\ & & & & & & \ddots & & & \\ & & -1 & & & & & 0 & & \\ & & & & & & & & \ddots & \\ & & & & & & & & & 1 \end{array}\right] \end{array} \in \mathbb{R}^{2n\times 2n}$$

Theorem (FD, Johnson, LAA 2006): If $S \in \mathbb{R}^{2n\times 2n}$ is symplectic with singular (11)-block then there exist matrices Q and Q' that are products of at most n symplectic interchange matrices such that:

$Q\,S$ and $S\,Q'$ are symplectic with nonsingular $(1,1)$ block.

The group of symplectic matrices

Theorem: The group of symplectic matrices is

$$\mathcal{S} = \left\{ Q \begin{bmatrix} G & GE \\ CG & G^{-T} + CGE \end{bmatrix} : \begin{array}{c} G \text{ nonsingular} \\ C = C^T \,,\; E = E^T \\ Q \text{ product of symplectic interchanges} \end{array} \right\}$$

REMARK: Given a symplectic matrix, Q may be not unique, then the previous description is not a *rigurous parametrization*. The nonuniqueness of Q can be useful for numerical purposes.

Subparametrization Problems (I)

1. Parametrization of symplectic matrices with $\mathrm{rank}(S_{11}) = k$. This set depends on $2n^2 + n - \frac{(n-k)^2+(n-k)}{2}$ parameters.

SIMILAR FOR ANY OTHER BLOCK

2. Any matrix can be S_{11} of a symplectic. If S_{11} is fixed and has $\mathrm{rank}(S_{11}) = k$ the set of symplectic matrices compatible can be parametrized and depends on $\frac{n^2+n}{2} + \frac{k^2+k}{2} + n(n-k)$ parameters.

3. $\mathcal{S}^{(1,1)}$ is a dense open subset of $\mathcal{S}$ and secuences can be explicitly constructed.

Subparametrization Problems (II)

4. Parametrization of the set of $2n \times n$ matrices that can be $\begin{bmatrix} S_{11} \\ S_{21} \end{bmatrix}$ of a symplectic.

5. Parametrization of the set of symplectic matrices with given $\begin{bmatrix} S_{11} \\ S_{21} \end{bmatrix}$. This is an affine subspace in $\mathbb{R}^{2n \times 2n}$ of dimension $\frac{n^2+n}{2}$.

6. Any $A \in \mathbb{R}^{(n+1)\times(n+1)}$ can be $S(1:n+1, 1:n+1)$ of a symplectic S except by the fact that $a_{n+1,n+1}$ is determined by the other entries.

and more...

LU factorizations of Symplectic Matrices (I)

Theorem: Let $S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}$ be symplectic. Then

1. S has LU factorization if and only if

S_{11} and S_{11}^{-T} have LU factorizations.

2. S has LU factorization if and only if

S_{11} is nonsingular and has LU and UL factorizations.

3. S has LU factorization if and only if

$$\det S_{11}(1:k, 1:k)\ \det S_{11}(k:n, k:n) \neq 0 \qquad k = 1:n$$

to be continued....

LU factorizations of Symplectic Matrices (II)

4. If $S_{11} = L_{11}U_{11}$ and $S_{11}^{-T} = L_{22}U_{22}$ are LU factorizations, then the LU factorization of S is

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

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

Symplectic LU-like factorization

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

upper triang.   lower triang.

Symplectic Orthogonal Matrices

Theorem: The set of $2n$-by-$2n$ orthogonal symplectic matrices is

$$\mathcal{S}^O = \left\{ Q \begin{bmatrix} (I+C^2)^{-1/2}U & -C(I+C^2)^{-1/2}U \\ C(I+C^2)^{-1/2}U & (I+C^2)^{-1/2}U \end{bmatrix} : \begin{array}{c} U \text{ orthogonal} \\ C = C^T \\ Q \text{ product of symplectic interchanges} \end{array} \right\}$$

Idea of the proof: Impose $S^T S = I$ on

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

with G nonsingular, $C = C^T$, $E = E^T$.

Symplectic Positive Definite (PD) Matrices

Theorem: Let $S = \left[\begin{smallmatrix} S_{11} & S_{21}^T \\ S_{21} & S_{22} \end{smallmatrix}\right]$ be symmetric and symplectic. Then

1. S is PD if and only if S_{11} is PD.

2. The set of PD symplectic matrices is

$$\mathcal{S}^{\mathrm{PD}} = \left\{ \begin{bmatrix} G & GC \\ CG & G^{-1} + CGC \end{bmatrix} : \begin{array}{c} G \text{ positive definite} \\ C = C^T \end{array} \right\}$$

$\mathcal{S}^{\mathrm{PD}}$ depends on $n^2 + n$ parameters.

3. Every PD symplectic matrix $S = HH^T$ with H symplectic.

4. The unique PD square root of S is symplectic, but not the Cholesky factor.

Symplectic Matrices with positive entries

Set of symplectic matrices with nonsingular S_{11}

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

This allows us to generate symplectic matrices with positive entries (contrast with orthogonal matrices).

START by choosing arbitrary $G > 0$, $C > 0$, and $\widetilde{E} > 0$ with positive entries. So $CG\widetilde{E} > 0$.

THEN, a number $\alpha > 0$ is chosen such that

$$\alpha CG\widetilde{E} + G^{-T} > 0.$$

FINALLY: $E \equiv \alpha \widetilde{E}$

Totally Nonnegative (TN) Symplectic Matrices (I)

DEFINITIONS:

Matrices with all minors nonnegative (positive) are called TN (totally positive TP) matrices.

If A is TN and A^k TP for some positive integer k then A is called OSCILLATORY.

Applications in mechanical oscillatory problems

Totally Nonnegative (TN) Symplectic Matrices (II)

I is symplectic and TN.

Are there symplectic TP matrices?
Are there symplectic oscillatory matrices?

What is the set of symplectic TN matrices?

Theorem (the 2×2 case): $S \in \mathbb{R}^{2\times 2}$ is symplectic and TP if and only if $\det S = 1$ and $s_{ij} > 0$ for all (i, j).

If any three positive entries s_{11}, s_{12}, s_{21} are chosen then the remaining entry a_{22} is obtained from $\det S = 1$ as $s_{22} = (1 + s_{12}s_{21})/s_{11}$.

Totally Nonnegative (TN) Symplectic Matrices (III)

Theorem: Let $S \in \mathbb{R}^{2n\times 2n}$ with $n > 1$ be symplectic. Then

1. S is not TP.
2. S is not oscillatory.

Sketch of the Proof: LU factorization of S is

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

If S TP then S_{11} is TP and the LU factors of S are triangular TP. Therefore L_{22} and U_{22} are triangular TP and S_{11}^{-T} is TP.

CONTRADICTION!!, S_{11} TP implies that S_{11}^{-T} has negative entries.

Totally Nonnegative (TN) Symplectic Matrices (IV)

Theorem: The set of $2n \times 2n$ $(n > 1)$ symplectic and TN matrices is

$$\mathcal{S}^{\mathsf{TN}} = \left\{ \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix} : D = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \lambda_i > 0 \right\}$$

Symplectic M-Matrices (I)

Definition: $A \in \mathbb{R}^{n\times n}$ is a M-Matrix if $a_{ij} \leq 0$ for $i \neq j$ and $\mathrm{Re}(\lambda) > 0$ for every eigenvalue λ of A.

Theorem: The set of $2n \times 2n$ symplectic M-Matrices is

$$\mathcal{S}^{\mathrm{M}} = \left\{ \begin{bmatrix} D & DK \\ HD & D^{-1} + HDK \end{bmatrix} : \begin{array}{c} D \text{ positive diagonal} \\ H = H^T \leq 0 \\ K = K^T \leq 0 \\ HDK \text{ diagonal} \end{array} \right\}$$

Symplectic M-Matrices (II)

Given an arbitrary $H = H^T \leq 0$, the matrices $K = K^T \leq 0$ such that HDK is *diagonal* can be easily determined. For instance if $h_{12} = h_{21} \neq 0$:

$$H = \begin{bmatrix} & x & & & \\ x & & & & \\ & & & & \\ & & & & \\ & & & & \end{bmatrix} \longrightarrow K = \begin{bmatrix} 0 & ? & 0 & 0 & 0 \\ ? & 0 & 0 & 0 & 0 \\ 0 & 0 & & & \\ 0 & 0 & & & \\ 0 & 0 & & & \end{bmatrix}$$

The **?** that remain in K after this process is repeated for all entries $h_{ij} = h_{ji} \neq 0$, are free parameters in $K = K^T \leq 0$ for a given H.

Conclusions and Open Problems

- An explicit description of the group of symplectic matrices has been introduced.
- It allows us to characterize very easily several structured sets of symplectic matrices.
- How to extend this approach to other structured sets? Rank structured symplectic matrices?
- Perturbation theory with respect the symplectic parameters? Interesting properties?
- How to compute the parametrization in a stable an efficient way if we are given the entries of a symplectic matrix?
- Have these symplectic parameters an intrinsic meaning?