

## HYPERBOLIC RELAXATION OF $k$ -LOCALLY POSITIVE SEMIDEFINITE MATRICES\*

GRIGORIY BLEKHERMAN<sup>†</sup>, SANTANU S. DEY<sup>‡</sup>, KEVIN SHU<sup>†</sup>, AND SHENG DING SUN<sup>†</sup>

**Abstract.** A successful computational approach for solving large-scale positive semidefinite (PSD) programs is to enforce PSD-ness on only a collection of submatrices. For our study, we let  $\mathcal{S}^{n,k}$  be the convex cone of  $n \times n$  symmetric matrices where all  $k \times k$  principal submatrices are PSD. We call a matrix in this  $k$ -locally PSD. In order to compare  $\mathcal{S}^{n,k}$  to the cone of PSD matrices, we study eigenvalues of  $k$ -locally PSD matrices. The key insight in this paper is that there is a convex cone  $H(e_k^n)$  so that if  $X \in \mathcal{S}^{n,k}$ , then the vector of eigenvalues of  $X$  is contained in  $H(e_k^n)$ . The cone  $H(e_k^n)$  is the hyperbolicity cone of the elementary symmetric polynomial  $e_k^n$  (where  $e_k^n(x) = \sum_{S \subseteq [n]: |S|=k} \prod_{i \in S} x_i$ ) with respect to the all ones vector. Using this insight, we are able to improve previously known upper bounds on the Frobenius distance between matrices in  $\mathcal{S}^{n,k}$  and PSD matrices. We also study the quality of the convex relaxation  $H(e_k^n)$ . We first show that this relaxation is tight for the case of  $k = n - 1$ , that is, for every vector in  $H(e_{n-1}^n)$  there exists a matrix in  $\mathcal{S}^{n,n-1}$  whose eigenvalues are equal to the components of the vector. We then prove a structure theorem on nonsingular matrices in  $\mathcal{S}^{n,k}$  all of whose  $k \times k$  principal minors are zero, which we believe is of independent interest. This result shows that for  $1 < k < n - 1$  “large parts” of the boundary of  $H(e_k^n)$  do not intersect with the eigenvalues of matrices in  $\mathcal{S}^{n,k}$ .

**Key words.** hyperbolicity cone, positive semidefinite matrix, eigenvalue bounds

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### 1. Introduction.

**1.1.  $k$ -Locally positive semidefinite matrices.** Positive semidefinite (PSD) matrices are of fundamental interest in a wide variety of fields, ranging from optimization [31] to physics [8]. Formally, a symmetric matrix  $X \in \text{Sym}_n$  is PSD if and only if

$$u^\top X u \geq 0 \quad \forall u \in \mathbb{R}^n.$$

The property of being PSD is very strong and implies a large amount of structure in a matrix. For example, all the eigenvalues of a PSD matrix are non-negative. Another important property of a PSD matrix is that all its principal submatrices are also PSD. There are various conceivable converses to this fact which fail to hold; for instance, even if all of the proper submatrices of a matrix are PSD, it is still possible for the matrix to have a negative eigenvalue. Nevertheless, one might be interested in a partial converse: if enough submatrices of a matrix are PSD, we should expect that the matrix is “close” to being PSD, in some sense. Such a result would help explain a phenomenon observed in various recent computational experiments, where the constraint of a matrix being PSD is relaxed to that of some principal

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<sup>†</sup>School of Mathematics, Georgia Institute of Technology, Atlanta, GA 30332 USA (greg@math.gatech.edu, kshu8@gatech.edu, ssun313@gatech.edu).

<sup>‡</sup>School of Industrial and Systems Engineering, Georgia Institute of Technology, Atlanta, GA 30332 USA (santanu.dey@isye.gatech.edu).

submatrices being PSD. It has been empirically observed that the resulting relaxation has an optimal objective function value close to the optimal objective function of the original problem. See [17, 18, 28] for examples involving SDP relaxation of optimal electrical power flow problem and [2, 9, 23] for examples involving SDP relaxation of box quadratic programs.

To formally understand the relaxation of enforcing positive semidefiniteness on submatrices, we investigate a class of matrices, where we impose the conditions that all  $k \times k$  principal submatrices of an  $n \times n$  matrix are PSD. We will call such a matrix *k-locally PSD*. This terminology is meant to suggest that we only check the PSD conditions locally on some small parts of the matrix rather than globally. Let

$$(1.1) \quad \mathcal{S}^{n,k} := \{X \in \text{Sym}_n \mid \text{every } k \times k \text{ principal submatrix of } X \text{ is PSD}\}$$

be the set of  $k$ -locally PSD matrices. The set  $\mathcal{S}^{n,k}$  is a closed convex cone, and its dual cone is the set of symmetric matrices with factor width  $k$ , defined and studied in [6, 22, 11]. The set of symmetric matrices with factor width 2 is the set of scaled diagonally dominant matrices [6, 30], i.e., symmetric matrices  $A$  such that  $DAD$  is diagonally dominant for some positive diagonal matrix  $D$ . The paper [1] uses scaled diagonally dominant matrices for constructing inner approximation of the PSD cone for use in solving polynomial optimization problems. See [15, 25, 26] for related papers.

For  $X \in \text{Sym}_n$ , we let  $\lambda(X) = (\lambda_1(X), \dots, \lambda_n(X))$ , where  $\lambda_1(X) \leq \lambda_2(X) \leq \dots \leq \lambda_n(X)$  are the eigenvalues of  $X$  counting multiplicity. We say that a vector  $\lambda \in \mathbb{R}^n$  is a vector of eigenvalues of  $X$  if it can be obtained from  $\lambda(X)$  by permuting its coordinates.

*Our main goal is to understand properties of eigenvalues of k-locally PSD matrices.* In particular, we would like to understand how as  $k$  gets closer to  $n$ , the matrices in  $\mathcal{S}^{n,k}$  become closer to PSD matrices in terms of eigenvalues. This work extends (and improves) results in a recent paper [3] by identifying a relaxation of the set of eigenvalues of  $k$ -locally PSD matrices. This relaxation is based on the machinery of hyperbolic polynomials and hyperbolicity cones, which we discuss next.

**1.2. The hyperbolic relaxation.** In order to motivate the the machinery of hyperbolic polynomials and corresponding hyperbolicity cones (which we formally define later), let us first construct a natural relaxation of the set of eigenvalues of matrices in  $\mathcal{S}^{n,k}$ .

Given an  $n \times n$  matrix  $X$ , recall the definition of the characteristic polynomial of  $X$ :

$$p_X(t) = \det(X - tI) = \sum_{\ell=0}^n (-1)^{n-\ell} c_\ell^n(X) t^{n-\ell},$$

where

$$c_\ell^n(X) = \sum_{\substack{S \subseteq [n] \\ |S|=\ell}} \det(X|_S).$$

Here,  $X|_S$  is the principal submatrix of  $X$  obtained by restricting  $X$  to the rows and columns contained in  $S$ . Notice that if  $X \in \mathcal{S}^{n,k}$ , then for all  $S \subseteq [n]$  with  $|S| \leq k$ ,  $X|_S$  is PSD and, in particular,  $\det(X|_S) \geq 0$ . This implies that  $c_\ell^n(X) \geq 0$  for  $\ell \leq k$ .

Let us introduce the set

$$H(c_k^n) = \{X \in \text{Sym}_n : \forall \ell \leq k, c_\ell^n(X) \geq 0\}.$$

Our first observation is then that

$$(1.2) \quad \mathcal{S}^{n,k} \subseteq H(c_k^n).$$

The roots of  $p_X$  are precisely the negatives of the eigenvalues of  $X$ , so we have that

$$p_X(t) = \prod_{i=1}^n (\lambda_i - t) = \sum_{\ell=0}^n (-1)^{n-\ell} e_k^n(\lambda_1, \dots, \lambda_n) t^{n-\ell},$$

where  $\lambda_1, \lambda_2, \dots, \lambda_n$  are the eigenvalues of  $X$  in any order, counting multiplicity, and  $e_k^n \in \mathbb{R}[x_1, \dots, x_n]$  is the elementary symmetric polynomial

$$e_k^n(x) = \sum_{\substack{S \subseteq [n] \\ |S|=k}} \prod_{i \in S} x_i.$$

Comparing coefficients of the  $t^k$  terms, we see that for  $0 \leq k \leq n$ ,

$$c_k^n(X) = e_k^n(\lambda_1, \dots, \lambda_n).$$

Combining our previous observations, we see that  $X \in H(c_k^n)$  if and only if  $e_\ell^n(\lambda_1, \dots, \lambda_n) \geq 0$  for  $\ell \leq k$ .

We will define the set

$$H(e_k^n) = \{\lambda \in \mathbb{R}^n : \forall \ell \leq k, e_\ell^n(\lambda) \geq 0\}.$$

Combining these observations, we obtain the following.

**OBSERVATION 1.1.**  $\mathcal{S}^{n,k} \subseteq H(c_k^n)$ . Also,  $\lambda = (\lambda_1, \dots, \lambda_n)$  is a vector of eigenvalues of some  $X \in H(c_k^n)$  if and only if  $\lambda \in H(e_k^n)$ .

The set  $H(e_k^n)$  will turn out to be the hyperbolicity cone of the polynomial  $e_k^n$  with respect to the all ones vector and in particular will turn out to be invariant to permutations of the coordinates and convex [10, 13]. We will refer to  $H(e_k^n)$  as the *hyperbolic relaxation* for the eigenvalues of  $\mathcal{S}^{n,k}$ . Similarly,  $H(c_k^n)$  will be the hyperbolicity cone of  $c_k^n$  with respect to the identity matrix. The cone  $H(c_k^n)$  is well known in the literature and is sometimes referred to as the  $(n-k)$ th Renegar derivative of the PSD cone [24].

By exploiting properties of these convex cones, we obtain bounds that indicate that if  $X \in \mathcal{S}^{n,k}$ , then in fact,  $X$  is close to being PSD in a number of different norms.

As an example, notice that  $e_n^n = \prod_{i=1}^n x_i$ , and  $H(e_n^n) = \mathbb{R}_+^n$ , the nonnegative orthant. Similarly,  $H(c_n^n)$  is the PSD cone, and we have that  $H(e_n^n)$  is exactly the set of possible eigenvalue vectors for matrices in  $H(c_n^n)$ .

This observation motivates us to ask the following related questions that tie in with our goal of understanding properties of  $\lambda(X)$  for  $X \in \mathcal{S}^{n,k}$ :

- Is it possible to obtain understanding of  $\{\lambda(X) \mid X \in \mathcal{S}^{n,k}\}$  in comparison to eigenvalues of PSD matrices by studying properties of  $H(e_k^n)$ ?
- How good is the approximation of the set  $\{\lambda(X) \mid X \in \mathcal{S}^{n,k}\}$  by  $H(e_k^n)$ ?

In this paper, we answer “yes” to the first question by improving on results in [3] via the hyperbolic relaxation of the set of eigenvalues of matrices in  $\mathcal{S}^{n,k}$ . This motivates us to delve further into the second question, and we verify various structural results that give a better understanding of relationship between the sets  $\{\lambda(X) \mid X \in \mathcal{S}^{n,k}\}$  and  $H(e_k^n)$ . One particularly interesting result that we would like to highlight is a structure theorem for matrices in  $\mathcal{S}^{n,k}$  all of whose principal  $k \times k$  minors vanish (Theorem 2.8). This theorem has relations to previous results in linear algebra: Theorem 13 in [29] and results of [21].

**1.3. Notation.** For a positive integer  $n$ , let  $[n] := \{1, \dots, n\}$ . Let  $\text{Sym}_n$  denote the vector space of  $n \times n$  symmetric matrices. Let  $\mathcal{S}^n$  denote the cone of PSD matrices inside of  $\text{Sym}_n$ . Note that  $\mathcal{S}^{n,n} = \mathcal{S}^n$ . If  $M \in \mathcal{S}^n$ , we write  $M \succeq 0$ . We use  $\mathcal{S}^{n,k}$  to refer to the  $k$ -locally PSD matrices, which are defined above in (1.1). We will refer to  $k$ -locally PSD matrices for convenience as locally PSD matrices if  $k$  is clear from context. An important example of a non-PSD matrix lying in  $\mathcal{S}^{n,k}$  is given by

$$(1.3) \quad G(n, k) = \frac{k}{k-1}I - \frac{1}{k-1}\bar{1}\bar{1}^\top.$$

Here,  $\bar{1}$  denotes the all ones vector of dimension  $n$ . All diagonal entries of  $G(n, k)$  are identically 1, and all off-diagonal entries are identically  $-\frac{1}{k-1}$ . Notice that all  $k \times k$  principal minors of  $G(n, k)$  vanish, but the matrix is nonsingular.

Given a matrix  $M \in \mathcal{S}^{n,k}$  and a diagonal matrix  $D$  with nonzero diagonal entries, observe that

$$DMD \in \mathcal{S}^{n,k}.$$

We say that the matrix  $DMD$  is *diagonally congruent* to  $M$ . By applying Sylvester’s law of inertia to any submatrix of  $M$ , the number of positive and negative eigenvalues is conserved for the same submatrix of a diagonally congruent matrix. In particular, a principal submatrix of a diagonally congruent matrix is singular if and only if the same submatrix is singular in the original matrix.

The rest of the paper is organized as follows: Section 2 lists all our main results, and section 3 concludes with some open questions. Then section 4 presents background results needed for proving the main results. The remaining sections present our proofs of the main results.

## 2. Main results.

**2.1. Bounds on minimum eigenvalues of matrices in  $\mathcal{S}^{n,k}$ .** The primary way we can measure the distance between a matrix in  $\mathcal{S}^{n,k}$  and the cone of PSD matrices is by considering the smallest eigenvalue of such a matrix. Certainly, if the minimum eigenvalue of a matrix is nonnegative, then the matrix is PSD, and we will say that a (suitably normalized) matrix is close to being PSD if its minimum eigenvalue is close to being nonnegative. We show that if  $k$  is sufficiently close to  $n$ , then the  $k$ -locally PSD matrices are close to the PSD matrices. Let  $\lambda_1(M)$  be the minimum eigenvalue of a matrix  $M \in \mathcal{S}^{n,k}$ .

Because  $\lambda_1$  is 1-homogeneous, i.e., if  $a \geq 0$ , then  $\lambda_1(aM) = a\lambda_1(M)$ , we should try to compare  $\lambda_1(M)$  for  $M \in \mathcal{S}^{n,k}$  to other 1-homogeneous (also called positively homogeneous) quantities on  $M$ .

Formally, let  $\mathcal{F}$  be the class of functions  $F : \text{Sym}_n \rightarrow \mathbb{R}$  so that  $F$  is a unitarily invariant matrix norm (thus, a norm depending entirely on the eigenvalues) or the trace function. Examples of unitarily invariant matrix norms are the Schatten  $p$ -norms,  $\|M\|_p = \sqrt[p]{\sum_{i=1}^n |\lambda_i(M)|^p}$  for  $p \geq 1$ . Note that the Frobenius norm is a

special case of the Schatten  $p$ -norm when  $p = 2$ . Also, recall that  $G(n, k)$  is defined in (1.3).

**THEOREM 2.1.** *Let  $k \in \{2, \dots, n\}$ . Let  $F \in \mathcal{F}$  and let  $\tilde{G}(n, k) = \frac{G(n, k)}{F(G(n, k))}$ . For any  $M \in \mathcal{S}^{n, k}$  with  $F(M) = 1$ , the minimum eigenvalue of  $M$  is at least as large as the minimum eigenvalue of  $\tilde{G}(n, k)$ , that is,*

$$\lambda_1(M) \geq \lambda_1(\tilde{G}(n, k)) \quad \forall M \in \mathcal{S}^{n, k} \quad \text{s.t.} \quad F(M) = 1.$$

*The bound on  $\lambda_1(M)$  is tight since  $\tilde{G}(n, k) \in \mathcal{S}^{n, k}$  achieves this bound.*

An immediate corollary of Theorem 2.1 in the case when  $F$  is the trace function is the following.

**COROLLARY 2.2.** *Let  $k \in \{2, \dots, n\}$ . For any  $M \in \mathcal{S}^{n, k}$  such that  $\text{Trace}(M) = 1$ , we have*

$$\lambda_1(M) \geq \frac{k - n}{n(k - 1)}.$$

The proof of Theorem 2.1 is a direct application of the fact that  $H(e_k^n)$  is a convex relaxation of the set of eigenvalues of matrices in  $\mathcal{S}^{n, k}$ . This allows us to write a convex relaxation of the optimization problem minimizing  $\lambda_1(M)$  over  $M \in \mathcal{S}^{n, k}$ . The optimal solution of this convex relaxation is the bound obtained in the above theorem.

*Remark 2.3.* The bound on  $\lambda_1(M)$  presented in Theorem 2.1 holds for  $M \in H(c_k^n)$ . Therefore, this bound can be used to provide upper bounds on the distance between the PSD cone and the Renegar derivative  $H(c_k^n)$  of the PSD cone.

We can use Theorem 2.1 to bound Frobenius distances of matrices in  $\mathcal{S}^{n, k}$  from those in  $\mathcal{S}^n$  (when we normalize the matrices using the Frobenius norm) as in the following result.

**COROLLARY 2.4.** *Let  $\overline{\text{dist}}(\mathcal{S}^{n, k}, \mathcal{S}^n) = \max_{A \in \mathcal{S}^{n, k}: \|A\|_F = 1} (\min_{G \in \mathcal{S}^n} \|A - G\|_F)$ . Then  $\overline{\text{dist}}(\mathcal{S}^{n, k}, \mathcal{S}^n) \leq \frac{(n-k)^{3/2}}{\sqrt{(n-k)^2 + (n-1)k^2}}$ .*

This corollary improves upon Theorem 2 in a previous paper [3]. Our new result has a better constant factor and applies to all regimes of  $k$  and  $n$ .

**2.2. Tightness of the relaxation  $H(e_k^n)$  for the set of eigenvalues of matrices in  $\mathcal{S}^{n, k}$ .** We have seen that the vector of eigenvalues of matrices in  $\mathcal{S}_k^n$  is precisely  $H(e_k^n)$  for  $n = k$ . We next show that this observation holds for two additional cases of  $k$ .

**THEOREM 2.5.** *If  $k$  is one of  $1, n-1$ , or  $n$ , and  $x \in H(e_k^n)$ , then  $x$  is the vector of eigenvalues of some matrix in  $\mathcal{S}^{n, k}$ .*

Since  $H(e_k^n)$  is a convex set for all  $k$ , in particular, Theorem 2.5 implies that the set of possible vectors of eigenvalues for matrices in  $\mathcal{S}^{n, n-1}$  is convex, although there does not seem to be an easy way to see this directly. Therefore we have the following.

**COROLLARY 2.6.** *The set of all vectors of eigenvalues of matrices in  $\mathcal{S}^{n, n-1}$  is convex.*

On the other hand, we show that  $\{\lambda(X) \mid X \in \mathcal{S}^{n, k}\}$  is strictly contained in  $H(e_k^n)$  for  $1 < k < n-1$ , and thus we completely characterize the tightness of this hyperbolic relaxation.

In order to do so, we examine the boundary of the cone  $H(e_k^n)$  and obtain a result which is of independent interest. Recall that the boundary of  $H(e_k^n)$  is precisely the set of points in the hyperbolicity cone on which the polynomial  $e_k^n$  vanishes.

Recall that if  $M$  is a matrix and  $\lambda(M)$  is a vector of eigenvalues of  $M$ , we have that

$$e_k^n(\lambda(M)) = \sum_{S \subseteq [n]: |S|=k} \det(M|_S).$$

Because of this, we see that if  $e_k^n(\lambda(M)) = 0$  and  $M \in \mathcal{S}^{n,k}$ , then we have that  $\det(M|_S) = 0$  for all subsets  $S$  of size  $k$ . We formalize this notion.

**DEFINITION 2.7.** *We say that a matrix  $M$  is  $(n, k)$ -locally singular if it lies in  $\mathcal{S}^{n,k}$  and all of the  $k \times k$  minors of  $M$  are singular.*

We see that for  $M \in \mathcal{S}^{n,k}$ ,  $\lambda(M)$  is on the boundary of  $H(e_k^n)$  if and only if  $M$  is  $(n, k)$ -locally singular. Sometimes  $(n, k)$  is omitted and we say a matrix is locally singular if  $n$  and  $k$  are clear from context.

The simplest class of examples of locally singular matrices is the set of matrices of rank less than  $k$ . In particular, rank 1 PSD matrices will be locally singular for any  $n$  and  $k$ . A more interesting example of locally singular matrices is the  $G(n, k)$  matrices defined in (1.3). Not only are these matrices locally singular, but they are also nonsingular. From this example we can construct an  $n$ -dimensional space of locally singular matrices by taking an arbitrary invertible diagonal matrix  $D$  and considering

$$DG(n, k)D \in \mathcal{S}^{n,k},$$

that is, the set of matrices that are *diagonally congruent* to  $G(n, k)$ .

It follows from Sylvester's law of inertia, applied to the various submatrices of  $G(n, k)$ , that any matrix diagonally congruent to  $G(n, k)$  is in fact locally singular and nonsingular.

On the other hand, it is worth performing a quick dimension counting heuristic to estimate how many possible matrices satisfy these conditions: Each submatrix that is constrained to be singular imposes a single polynomial equation on the possible solution set. If  $n - 1 > k > 2$ , then we see that the number of equations is  $\binom{n}{k}$ , which is in fact greater than the dimension of the space of  $n \times n$  symmetric matrices, which is  $\binom{n}{2}$ . This indicates that solutions to this type of system should be somewhat "uncommon." Therefore, it is perhaps not surprising that in the cases when  $n - 1 > k > 2$ , we are able to show that all of the locally singular matrices in  $\mathcal{S}^{n,k}$ , which are not singular, are diagonally congruent to  $G(n, k)$ .

The following theorem formalizes this idea. Both the statement and the proof of this theorem seem closely related to Theorem 13 in [29]. More generally, the theorem can be viewed as giving semialgebraic relations between the various principal minors of a symmetric matrix. A complete characterization of the algebraic relations between the principal minors of a symmetric matrix was given in [21].

**THEOREM 2.8.** *Let  $n - 1 > k > 2$  or  $(n, k) = (4, 2)$ . Suppose that  $M \in \mathcal{S}^{n,k}$ ,  $M$  is  $(n, k)$ -locally singular, and  $M$  is invertible. Then  $M$  must be diagonally congruent to  $G(n, k)$ .*

Note that this immediately implies that there are points on the boundary of  $H(e_k^n)$  which are not the eigenvalues of any matrix in  $\mathcal{S}^{n,k}$ : since  $G(n, k)$  has only one negative eigenvalue, any matrix diagonally congruent to  $G(n, k)$  has at most one

negative eigenvalue, and there are points on the boundary of  $H(e_k^n)$  with as many as  $n - k$  negative entries and no zero entries.

When  $k = 2$  and  $n = 4$ , locally singular matrices in  $\mathcal{S}^{4,2}$  are diagonally congruent to a symmetric matrix with diagonal entries identically one and  $\pm 1$  off-diagonal entries. We can numerically check that a such matrix has at most one negative eigenvalue. Thus by Cauchy's interlacing theorem, for any  $n > 4$  and  $k = 2$ , any locally singular matrix in  $\mathcal{S}^{n,2}$  can have at most  $n - 3$  negative eigenvalues, whereas the boundary of  $H(e_2^n)$  contains points with as many as  $n - 2$  negative eigenvalues. Thus we get the following corollary.

**COROLLARY 2.9.** *If  $n - 1 > k \geq 2$ , then the set of possible eigenvalue vectors for matrices in  $\mathcal{S}^{n,k}$  is strictly contained in  $H(e_k^n)$ .*

**2.3. Eigenvalues of matrices in  $\mathcal{S}^{4,2}$  whose eigenvalues lie on the boundary of  $H(e_2^4)$ .** Theorem 2.8 implies that if  $X$  is a nonsingular matrix in  $\mathcal{S}^{n,k}$  whose eigenvalues lie on the boundary of  $H(e_k^n)$ , then  $X$  is in fact diagonally congruent to the matrix  $G(n, k)$ . Because  $G(n, k)$  has only one negative eigenvalue, Sylvester's law of inertia [14] implies that a matrix of this form has at most one negative eigenvalue.

The next lemma is a converse to the previous observation when  $n = 4$  and  $k = 2$ .

**LEMMA 2.10.** *If  $\lambda \in H(e_2^4)$  so that  $e_2^4(\lambda) = 0$  and  $\lambda$  has at most one negative eigenvalue, then  $\lambda$  is a vector of eigenvalues for a matrix which is diagonally congruent to  $G(4, 2)$ .*

The idea of the proof is to use a characterization of the coefficients of real-rooted polynomials to reduce the problem to proving that there exist real-rooted polynomials having certain properties. These properties can be described entirely in terms of polynomial inequalities, so we can use algorithms for quantifier elimination over real closed fields to solve this problem. We do not know of a proof of this result that does not rely on computational methods.

**3. Conclusions and open questions.** The key insight in this paper is the observation that  $H(e_k^n)$ , i.e., the hyperbolicity cone of the elementary symmetric polynomial  $e_k^n$ , is a convex relaxation of the set of the eigenvalues of matrices in  $\mathcal{S}^{n,k}$ . Using this insight, we are able to improve upper bounds on the distance of the matrices in  $\mathcal{S}^{n,k}$  from PSD matrices  $\mathcal{S}^n$  given in [3]. The next question that was considered is how good is the relaxation  $H(e_k^n)$ : We first show that this relaxation (apart from the trivial case of  $k = n$ ) is tight for the case of  $k = n - 1$ . Indeed, in this case, we are able to show that  $H(e_{n-1}^n)$  is exactly the set of eigenvalues of matrices in  $\mathcal{S}^{n,n-1}$ . However, in general we prove that if  $\lambda(M)$  belongs to the boundary of  $H(e_k^n)$  and  $M \in \mathcal{S}^{n,k}$ , then either  $M$  is nonsingular or  $M$  is diagonally congruent to  $G(n, k)$ . Since there are points on the boundary of  $H(e_k^n)$  with as many as  $n - k$  negative entries and no zero entries, this shows that “large parts” of the boundary of  $H(e_k^n)$  do not intersect with the eigenvalues of matrices in  $\mathcal{S}^{n,k}$ .

There are many interesting open questions. As discussed above, we have shown that the set of eigenvalues of matrices in  $\mathcal{S}^{n,n-1}$  is convex. It was recently shown in [19] that the set of eigenvalue vectors of matrices in  $\mathcal{S}^{4,2}$  is not convex, but it is still an open question for all other values of  $k < n - 1$ . Another question vis-à-vis the structure theorem is to classify singular matrices in  $\mathcal{S}^{n,k}$  that lie on the boundary of  $H(e_k^n)$ . Finally, instead of enforcing PSD-ness on all submatrices, we can enforce PSD-ness of a smaller set of submatrices. Are there similar relaxations like  $H(e_k^n)$  for specially structured collections of submatrices?

#### 4. Preliminaries.

##### 4.1. Introduction to hyperbolic polynomials and hyperbolicity cones.

Hyperbolic multivariate polynomials are a rich collection of polynomials with connections to convex optimization, combinatorics, and theoretical computer science. We give a brief description of the important properties of hyperbolic polynomials here. We say that a polynomial  $p \in \mathbb{R}[x_1, \dots, x_n]$  is *hyperbolic* with respect to a fixed vector  $v$  if  $p(v) > 0$ , and for any fixed  $x \in \mathbb{R}^n$ , the univariate polynomial  $p(x - tv) \in \mathbb{R}[t]$  has only real roots. An important example of this comes from the determinant of symmetric matrices,  $\det(X) \in \mathbb{R}[x_{ij} : i \leq j]$ , which is hyperbolic with respect to the identity matrix, by the spectral theorem. Another example which is critical for our purposes is the elementary symmetric polynomial  $e_k^n(x)$ , defined as

$$e_k^n(x) = \sum_{S \subseteq [n] : |S|=k} \prod_{i \in S} x_i.$$

This polynomial is hyperbolic with respect to  $\vec{1}$ , the all ones vector.

Let  $V(p) \subset \mathbb{R}^n$  be the set of zeros of the polynomial  $p$ . Let  $p$  be hyperbolic with respect to  $v \in \mathbb{R}^n$ . The closed hyperbolicity cone of polynomial  $p$  with respect to  $v$  is the closure of the connected component of  $\mathbb{R}^n \setminus V(p)$  containing  $v$  [10, 13, 24]. We will denote it by  $H_v(p)$ . When  $p$  is the determinant or sum of certain principal subdeterminants of a symmetric matrix, we will abbreviate  $H(p) = H_I(p)$ , where  $I$  is the identity matrix.

The hyperbolicity cone of elementary symmetric polynomial  $e_k^n(x)$  with respect to  $\vec{1}$  will be denoted by  $H(e_k^n)$ . A simple algebraic characterization of  $H(e_k^n)$  is given by (see, for example, [33])

$$H(e_k^n) = \{x \in \mathbb{R}^n : e_l^n(x) \geq 0 \ \forall 1 \leq l \leq k\}.$$

It is also known that  $H(e_k^n)$  is spectrahedral [7] for all  $1 \leq k \leq n$ , i.e., an affine slice of a higher dimensional PSD cone.

The key fact for our purposes is Proposition 1 in [24] originally proved by Gårding in [10].

**LEMMA 4.1.** *If  $p$  is hyperbolic with respect to  $v$ , then  $H_v(p)$  is convex, and its boundary is precisely  $H_v(p) \cap V(p)$ .*

**4.2. Linear algebra.** We use the following standard results in the paper. Proofs can be found in [14].

**THEOREM 4.2** (Schur–Horn theorem). *Let  $d, \lambda \in \mathbb{R}^n$  such that  $d_i \geq d_{i+1}$  and  $\lambda_i \geq \lambda_{i+1}$ ,  $i \in [n-1]$ . There is a symmetric matrix with diagonal values  $d$  and eigenvalues  $\lambda$  if and only if*

- $\sum_{i=1}^j d_i \leq \sum_{i=1}^j \lambda_i$  for all  $j \in [n-1]$ ,
- $\sum_{i=1}^n d_i = \sum_{i=1}^n \lambda_i$ .

Note that the original theorem in [14] proves the existence of a real symmetric matrix (not just Hermitian) that achieves the desired eigenvalues and diagonal entries.

We next present the famous Cauchy's interlacing theorem.

**THEOREM 4.3** (Cauchy's interlacing theorem). *Consider an  $n \times n$  symmetric matrix  $A$ , and let  $A|_J$  be any of its  $k \times k$  principal submatrices. Then for all  $1 \leq i \leq k$ ,*

$$\lambda_{n-k+i}(A) \leq \lambda_i(A|_J) \leq \lambda_i(A).$$



We also present the symmetric case of Jacobi's complementary minors formula. The proof for general case can be found in [20]

**THEOREM 4.4** (Jacobi's complementary minors formula, symmetric case). *Let  $M$  be an invertible  $n \times n$  matrix and  $\emptyset \subsetneq S \subsetneq [n]$ .*

$$(4.1) \quad \det(M|_S) = \det(M) \det(M^{-1}|_{S^c}).$$

This theorem states that the minor of  $M$  corresponding to a subset  $S$  can be written in terms of the minor of  $M^{-1}$  with respect to the complement  $S^c$ . In the simplest case when  $|S| = n - 1$ , this is simply Cramer's rule for the diagonal entries of the inverse matrix.

## 5. Proof of Theorem 2.1 and Corollary 2.4.

**5.1. Proof of Theorem 2.1.** For the remainder of this section, fix  $n > k \geq 2$  and an  $F \in \mathcal{F}$ . Let  $f$  be the function so that  $f(\lambda(M)) = F(M)$  for each  $M \in \text{Sym}_n$ .

In order to prove the theorem, we would like to verify an appropriate lower bound on  $z^*$  defined as

$$\begin{aligned} z^* := \text{minimize } & \lambda_1(M) \\ \text{s.t. } & f(\lambda(M)) = 1, \\ & M \in \mathcal{S}^{n,k}, \end{aligned}$$

where  $\lambda_1(M)$  is the smallest eigenvalue of  $M$ .

In order to provide a lower bound on  $z^*$ , we (i) apply the hyperbolic relaxation for the eigenvalues of  $\mathcal{S}^{n,k}$  to replace  $\{\lambda(M) \mid M \in \mathcal{S}^{n,k}\}$  with  $H(e_k^n)$  and (ii) replace  $f(\lambda(M)) = 1$  by  $f(\lambda(M)) \leq 1$  to obtain the following convex optimization problem:

$$(5.1) \quad \begin{aligned} z^l := \text{minimize } & \lambda_1 \\ \text{s.t. } & \lambda_1 \leq \lambda_i \quad \forall i \in \{2, \dots, n\}, \\ & f(\lambda) \leq 1, \\ & (\lambda_1, \lambda_2, \dots, \lambda_n) \in H(e_k^n). \end{aligned}$$

It is straightforward to verify that the set  $\{\lambda \mid f(\lambda) \leq 1, \lambda \in H(e_k^n)\}$  is compact. Thus  $z^l$  is finite, and at least one optimal solution exists. Also note that since (5.1) is a convex program which is symmetric with regard to variables  $\lambda_2, \dots, \lambda_n$ , it is straightforward to verify that there exists an optimal solution where  $\lambda_2 = \dots = \lambda_n$ . Therefore, we arrive at the following two-variable optimization problem:

$$(5.2) \quad \begin{aligned} z^l := \text{minimize } & \lambda_1 \\ \text{s.t. } & \lambda_1 \leq \lambda_2, \\ & f(\lambda_1, \lambda_2, \dots, \lambda_2) \leq 1, \\ & (\lambda_1, \lambda_2, \dots, \lambda_2) \in H(e_k^n). \end{aligned}$$

Next observe that if we remove the constraint  $(\lambda_1, \lambda_2, \dots, \lambda_2) \in H(e_k^n)$  from (5.2), then the following hold:

- If  $f$  corresponds to a norm, then one optimal solution of the resulting problem is of the form  $(a, 0, \dots, 0)$  where  $a < 0$ , which is infeasible for (5.2) since it does not satisfy the constraint  $(\lambda_1, \lambda_2, \dots, \lambda_n) \in H(e_k^n)$ . Thus, there must be at least one optimal solution of (5.2) belonging to the boundary of  $H(e_k^n)$ .
- If  $f$  corresponds to the trace function, then the optimal solution of the resulting problem is unbounded. Thus, again we can conclude that the optimal solution of (5.2) belongs to the boundary of  $H(e_k^n)$ .

A simple computation shows that for  $(\lambda_1, \lambda_2, \dots, \lambda_2)$  to be on the boundary of  $H(e_k^n)$ , we have  $\lambda_1 = -\frac{n-k}{k}\lambda_2$ . Thus, we obtain that  $z^l = -\frac{1}{f(-1, \frac{k}{n-k}, \dots, \frac{k}{n-k})}$ . Since  $f$  is 1-homogeneous, it is easy to verify that  $\lambda_1(\tilde{G}(n, k)) = -\frac{1}{f(-1, \frac{k}{n-k}, \dots, \frac{k}{n-k})}$ , which completes the proof of the theorem.

**5.2. Proof of Corollary 2.4.** Let  $A \in \mathcal{S}^{n,k}$  with  $\|A\|_F = 1$ . If  $A$  is PSD, then the distance is zero, so we assume  $A$  has at least one negative eigenvalue. By Cauchy's interlacing theorem (Theorem 4.3),  $A$  has at most  $n - k$  negative eigenvalues. So  $\text{dist}(A, \mathcal{S}_+^n) \leq |\lambda_1(A)|\sqrt{n - k}$ . By Theorem 2.1 we have that  $|\lambda_1(A)| \leq \frac{1}{\sqrt{1+(n-1)\frac{k^2}{(n-k)^2}}}$ , which completes the proof.

**6. Proof of Theorem 2.5.** When  $k = n$  the statement is clear, since  $x \in H(e_n^n)$  if and only if  $x \geq 0$ , and it is the eigenvalues of  $\text{diag}(x)$  which is PSD. When  $k = 1$ , let  $x \in H(e_1^n) = \{y : \sum_{i=1}^n y_i \geq 0\}$ . By the Schur–Horn theorem (Theorem 4.2), there exists a symmetric matrix  $M_0$  with identically zero diagonal entries and eigenvalues  $x - \frac{\sum_{i=1}^n x_i}{n}$ . Thus,  $M_0 + \frac{\sum_{i=1}^n x_i}{n}I$  has eigenvalues  $x$  and is in  $\mathcal{S}^{n,1}$ , since all of its diagonal entries are nonnegative.

Now let  $k = n - 1$ . First, we reduce to the case when  $x$  is on the boundary of  $H(e_{n-1}^n)$ . To do that, we note that if  $x$  is any point in  $H(e_{n-1}^n)$ , then for some  $t > 0$ ,  $x - t\vec{1}$  will lie on the boundary of the cone. If  $x - t\vec{1}$  is a vector of eigenvalues of a matrix  $M$  in  $\mathcal{S}^{n,n-1}$ , then  $x$  is a vector of eigenvalues of  $M + tI$ , also in  $\mathcal{S}^{n,n-1}$ .

**LEMMA 6.1.** *If  $x \in H(e_{n-1}^n)$  and  $x$  has a negative entry, then all other entries of  $x$  are strictly positive.*

*Proof.* By Theorem 1.1 in [27], we have that  $x \in H(e_{n-1}^n)$  if and only if

$$X = \text{diag}(x_1, \dots, x_{n-1}) + x_n \vec{1}_{n-1} \vec{1}_{n-1}^\top \succeq 0.$$

Here, we use  $\vec{1}_{n-1}$  to denote the all ones vector in  $n - 1$  dimensions for emphasis.

By permuting the coordinates, we can assume that  $x_n$  is an entry so that  $x_n < 0$ . Then, we have that the diagonal entries of  $X$  are nonnegative, so for  $i \neq n$ ,

$$x_i + x_n \geq 0.$$

So,  $x_i \geq -x_n > 0$ , concluding the theorem.  $\square$

Thus, if  $x$  lies on the boundary, we will consider two cases: either all entries of  $x$  are nonnegative, or exactly one entry of  $x$  is negative and others are positive. If all entries of  $x$  are nonnegative, then there is a PSD matrix whose vector of eigenvalues is  $x$  and, in particular, a matrix in  $\mathcal{S}^{n,n-1}$  with these eigenvalues.

If  $x$  lies on the boundary and exactly one entry of  $x$  is negative, then consider

$$e_{n-1}^n(x) = \sum_{i \in [n]} \prod_{j \in [n] \setminus i} x_j = \left( \prod_{j \in [n]} x_j \right) \sum_{i \in [n]} \frac{1}{x_i} = 0,$$

which is well defined since in the previous lemma, we showed that all entries of  $x$  are nonzero. Thus,  $\sum_{i \in [n]} \frac{1}{x_i} = 0$ .

Now, we can apply the Schur–Horn theorem (Theorem 4.2), which implies that there is a matrix  $L$  whose diagonal entries are all zeros and whose eigenvalues are  $\{\frac{1}{x_i}\}$ . In particular,  $L$  is invertible, so let  $M = L^{-1}$ . Since all of the diagonal entries

of  $L$  are 0, all of the  $(n-1) \times (n-1)$  minors of  $M$  are zero by Cramer's rule for the diagonal entries of the inverse matrix. Also note that  $x$  has  $(n-1)$  positive entries, so by eigenvalue interlacing, all of the  $(n-1) \times (n-1)$  minors of  $M$  have at most 1 nonpositive eigenvalue. Now, simply by noting that they all have 0 as an eigenvalue, this in particular implies that all  $(n-1) \times (n-1)$  minors of  $M$  have nonnegative eigenvalues and hence are PSD. Thus,  $M$  is a matrix in  $\mathcal{S}^{n,n-1}$  with the desired eigenvalues.

## 7. Proof of the structure theorem for $\mathcal{S}^{n,k}$ .

**7.1. Proof roadmap.** Given a matrix in  $\mathcal{S}^{n,k}$ , which is nonsingular and locally singular—we will abbreviate by saying that  $M$  is an *NLS* matrix.

We show Theorem 2.8 in three steps. We first prove base cases  $n-k=2$  and  $k=3$  and then we use double induction on  $n-k$  and  $k$  to prove the statement for general  $k$ . For the base case  $n-k=2$ , there is a very interesting step of taking the inverse of a given NLS matrix and using some facts about the structure of the inverse matrix.

The inductive step for this argument relies on some observations about Schur complements. The Schur complement of a symmetric matrix  $M$  with respect to a nonzero diagonal entry  $M_{ii}$  is defined to be the  $(n-1) \times (n-1)$  matrix

$$M \setminus \{i\} = M|_{[n] \setminus \{i\}} - \frac{1}{M_{ii}} \tilde{M}_i \tilde{M}_i^\top,$$

where  $\tilde{M}_i$  is obtained from the  $i$ th column of  $M$  after removing the  $i$ th entry.

Now, we recall some facts for matrices  $M$  with strictly positive diagonal entries [32].

- **Schur complements preserve PSD-ness.**  $M$  is PSD if and only if  $M \setminus \{i\}$  is PSD.
- **Schur complements preserve singularity.**  $M$  is nonsingular if and only if  $M \setminus \{i\}$  is nonsingular.
- **Schur complements commute with taking submatrices.** If  $i \notin S$ , then  $(M \setminus \{i\})|_S = (M|_{S \cup \{i\}}) \setminus \{i\}$ .

The previous three properties imply the following: a matrix in  $\mathcal{S}^{n,k}$  is NLS if and only if for each  $i \in [n]$ ,  $M \setminus \{i\}$  is in  $\mathcal{S}^{n-1,k-1}$  and NLS.

**7.2. Structure theorem when  $k = n-2$ .** Let  $M$  be a matrix in  $\mathcal{S}^{n,n-2}$ , which is NLS. Observe that NLS matrices in  $\mathcal{S}^{n,n-2}$  must have strictly positive diagonal entries. If any diagonal entry is zero, then since  $2 \times 2$  minors of  $M$  are nonnegative, an entire row and column of  $M$  are filled with zeros, and then  $M$  is singular, which is a contradiction.

As a base case when  $n=4$ , consider an NLS matrix  $M \in \mathcal{S}^{4,2}$ . We can perform a diagonal congruence transformation to obtain a matrix  $\tilde{M}$  such that all of the diagonal entries of  $\tilde{M}$  are 1, and since all  $2 \times 2$  minors of  $M$  are zero, we see that all off-diagonal entries of  $\tilde{M}$  are  $\pm 1$ . There are 6 off-diagonal entries, so there are 64 distinct possibilities for locally singular matrices, up to diagonal congruence. All of these 64 matrices are either singular or congruent to  $G(4,2)$ , which can be checked using direct computation.

**LEMMA 7.1.** *Let  $M \in \mathcal{S}^{n,n-2}$  be an NLS matrix. Then the following hold:*

1.  $\det(M) < 0$ .
2. All  $(n-1) \times (n-1)$  principal minors of  $M$  are strictly negative.
3. All  $(n-3) \times (n-3)$  principal minors of  $M$  are strictly positive.

*Proof.* We prove these facts by inducting on  $n$ , with the base case  $\mathcal{S}^{4,2}$  following from direct checking of the 64 cases above. For the inductive step we take the Schur complement of an NLS matrix  $M$  with respect to a diagonal entry. Observe that a diagonal entry of the Schur complement cannot be zero.

Otherwise the whole row of the Schur complement must be zero as all  $2 \times 2$  minors are nonnegative, and this is a contradiction since  $M$  is nonsingular, and Schur complements preserve nonsingularity. Since taking Schur complements with respect to a positive diagonal entry preserves the property of being NLS, preserves the signs of determinants, and commutes with the operation of taking submatrices, all three above statements follow by induction.  $\square$

Now we are ready to prove the main theorem of this section.

**THEOREM 7.2.** *Let  $M \in \mathcal{S}^{n,n-2}$  be an NLS matrix. Then  $M$  is diagonally congruent to  $G(n, n-2)$ .*

*Proof.* Let  $M \in \mathcal{S}^{n,n-2}$  be an NLS matrix, and consider the inverse matrix  $M^{-1}$ . Using Lemma 7.1 and Theorem 4.4 and what we know about principal minors of  $M$ , we have the following:

1. All diagonal entries of  $M^{-1}$  are strictly positive.
2. All  $2 \times 2$  principal minors of  $M^{-1}$  are zero.
3. All  $3 \times 3$  principal minors of  $M^{-1}$  are strictly negative.

Observe that (1) and (2) together imply that all off-diagonal entries of  $M^{-1}$  are nonzero. We conjugate  $M^{-1}$  by a diagonal matrix  $D$  given by  $D_{11} = -1/\sqrt{(M^{-1})_{11}}$  and  $D_{ii} = \text{sgn}(M_{1i})/\sqrt{(M^{-1})_{ii}}$ , to obtain matrix  $T$  with 1's on the diagonal and  $-1$ 's in first row and column other than the  $(1, 1)$  entry. By Theorem 4.4, all  $2 \times 2$  principal minors of  $T$  are zero, so its off-diagonal entries must be  $\pm 1$ .

Now for all distinct  $i, j \neq 1$ , we consider the principal submatrix with rows and columns indexed by  $\{1, i, j\}$ . It has form  $\begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & x \\ -1 & x & 1 \end{pmatrix}$ , where  $x$  is either 1 or  $-1$ . Since this submatrix has negative determinant, we must have  $x = -1$ . Thus  $T$  is  $G(n, 2)$ , and  $M^{-1}$  is diagonally congruent to  $G(n, 2)$ .

Finally, notice that inverting a matrix sends diagonally congruent matrices to diagonally congruent matrices and that for  $n \geq 4$ ,

$$G(n, 2)^{-1} = \frac{n-3}{2(n-2)} G(n, n-2). \quad \square$$

Thus, we have shown that  $M$  is diagonally congruent to  $G(n, n-2)$ , as desired.

**7.3. Structure theorem for  $k = 3$ .** In this section we prove the structure theorem for  $k = 3$ .

**THEOREM 7.3.** *Let  $M \in \mathcal{S}^{n,3}$  with  $n \geq 5$  be an NLS matrix. Then  $M$  is diagonally congruent to  $G(n, 3)$ .*

Our proof proceeds by induction on  $n$ . As a base case, note that the result holds for  $\mathcal{S}^{5,3}$  by Theorem 7.2.

To finish the induction we need the following lemma.

**LEMMA 7.4.** *If  $M$  is a nonsingular symmetric matrix, then either one of its  $(n-1) \times (n-1)$  principal minors is nonzero, or one of its  $(n-2) \times (n-2)$  principal minors is nonzero.*

*Proof.* Let  $M$  be a nonsingular matrix, and consider  $M^{-1}$ . If all of the principal  $(n-1) \times (n-1)$  minors of  $M$  are zero, then by Theorem 4.4 all of the diagonal entries

of  $M^{-1}$  are 0. If, in addition, all  $(n-2) \times (n-2)$  principal minors of  $M$  are zero, then all  $2 \times 2$  minors of  $M^{-1}$  are zero, and then  $M^{-1}$  is the zero matrix, which is a contradiction.  $\square$

Now for an inductive hypothesis, assume that for  $5 \leq m < n$ , any NLS  $M \in \mathcal{S}^{m,3}$  is diagonally congruent to  $G(m, 3)$ . Fix  $n$ , and let  $M \in \mathcal{S}^{n,3}$  be any NLS matrix. If the submatrix of  $M$  given by Lemma 7.4 has size at least 5, then it must be diagonally congruent to  $G(n-1, 3)$  or  $G(n-2, 3)$  due to the inductive hypothesis. We divide the remaining proof into three cases:

1.  $n \geq 6$ , and there exists an  $(n-1) \times (n-1)$  submatrix of  $M$  that is diagonally congruent to  $G(n-1, 3)$ . Then after permutation and suitable diagonal congruence we may assume

$$M = \left( \begin{array}{c|c} G(n-1, 3) & v \\ \hline v^\top & 1 \end{array} \right)$$

for some vector  $v \in \mathbb{R}^{n-1}$ .

Let  $M'$  be any  $5 \times 5$  principal submatrix of  $M$  which includes index  $n$ . Then  $M'$  must have the form

$$M' = \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & v_1 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & -\frac{1}{2} & v_2 \\ -\frac{1}{2} & -\frac{1}{2} & 1 & -\frac{1}{2} & v_3 \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 1 & v_4 \\ v_1 & v_2 & v_3 & v_4 & 1 \end{pmatrix}.$$

If we look at the  $3 \times 3$  submatrix corresponding to entries  $\{i, j, 5\}$ , we get

$$\begin{pmatrix} 1 & -\frac{1}{2} & v_i \\ -\frac{1}{2} & 1 & v_j \\ v_i & v_j & 1 \end{pmatrix}.$$

The determinant of this matrix is

$$(7.1) \quad \frac{3}{4} - v_i^2 - v_i v_j - v_j^2.$$

Because all  $3 \times 3$  submatrices of  $M'$  are singular, this determinant must equal 0 for all  $i, j \in \{1, 2, 3, 4\}$ . Notice that this is a quadratic equation in  $v_i$  and  $v_j$ . If we fix a value for  $v_1$ , then (7.1) implies that the remaining three  $v_i$  can take on at most 2 other values (which only depend on  $v_1$ ). By the pigeonhole principle, at least two of these  $v_i$  must be equal. After permuting entries we may assume  $v_2 = v_3$ . Plugging this into (7.1), we see that either  $v_2 = v_3 = \frac{1}{2}$  or  $v_2 = v_3 = -\frac{1}{2}$ . In the first case we may conjugate  $M'$  by  $\text{diag}(1, 1, 1, 1, -1)$ . Therefore we may assume  $v_2 = v_3 = -\frac{1}{2}$ .

Now, we can consider (7.1) for the cases when  $i = 2$  and  $j = 1$  or  $i = 2$  and  $j = 4$ . Because we assume  $v_2 = -\frac{1}{2}$ , (7.1) implies that

$$\frac{3}{4} - v_2^2 - v_1 v_2 - v_1^2 = -(v_1 - 1) \left( v_1 + \frac{1}{2} \right)$$

and

$$\frac{3}{4} - v_2^2 - v_2 v_4 - v_4^2 = -(v_4 - 1) \left( v_4 + \frac{1}{2} \right).$$

We then get that both  $v_1$  and  $v_4$  are either 1 or  $-\frac{1}{2}$ . They cannot both be 1; otherwise the equation fails for  $i = 1, j = 4$ . Therefore at least one of them must be  $-\frac{1}{2}$ , and after permuting entries we may assume  $v_1 = -\frac{1}{2}$ .

Summarizing the above, we see that  $M'$  can only take on two values up to diagonal congruence and permutation: either  $M' = G(5, 3)$ , or

$$M' = \begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & 1 & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 1 & 1 \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 1 & 1 \end{pmatrix}.$$

Now, because this holds for all  $5 \times 5$  submatrices of  $M$ , it is clear that  $v$  must have the properties that all entries of  $v$  are either  $-\frac{1}{2}$  or 1 and that at most one entry of  $v$  can be 1. If the  $i$ th entry of  $v$  is 1, then notice that rows  $i$  and row  $n$  of  $M$  are the same, meaning that  $M$  is singular, a contradiction. We conclude that all entries of  $v$  are  $-\frac{1}{2}$ , and we have shown that  $M$  is diagonally congruent to  $G(n, 3)$ .

2.  $n \geq 7$ , and there exists an  $(n-2) \times (n-2)$  submatrix of  $M$  which is nonsingular. By induction, this implies that this submatrix is diagonally congruent to  $G(n-2, 3)$ . Then after permutation and suitable diagonal congruence we may assume

$$M = \begin{pmatrix} G(n-2, 3) & v & w \\ v^\top & 1 & x \\ w^\top & x & 1 \end{pmatrix}.$$

If either  $v$  or  $w$  has all entries  $-\frac{1}{2}$ , then  $M$  has an  $(n-1) \times (n-1)$  principal submatrix equal to  $G((n-1), 3)$ , and we are back to the previous case.

Upon considering any  $5 \times 5$  principal submatrix of  $M$  that has exactly one index from  $\{n-1, n\}$ , and using observations from the previous case, we may assume  $v$  and  $w$  to both have exactly one entry that is 1, with the remaining entries being  $-\frac{1}{2}$ , and  $x$  is some scalar number. There are two cases of interest:  $v$  and  $w$  have the 1 entry either in the same position or in different positions.

If they are both in the same place, then without loss of generality, let us assume that they are in position  $(n-2)$ . Now, if we look at the  $3 \times 3$  block corresponding to entries  $\{n-2, n-1, n\}$ , then we will see the  $3 \times 3$  matrix

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & x \\ 1 & x & 1 \end{pmatrix}.$$

The determinant of this matrix is  $-(x-1)^2$ . We can see that if this matrix is singular, then  $x$  must in fact be equal to 1, and so we see that the last 3 rows of  $M$  are all the same, implying  $M$  is singular. Now, suppose that  $v$  and  $w$  have these 1 entries in two different positions. Then we see that there is a  $3 \times 3$  submatrix of the form

$$\begin{pmatrix} 1 & 1 & -\frac{1}{2} \\ 1 & 1 & x \\ -\frac{1}{2} & x & 1 \end{pmatrix}.$$

The determinant of this matrix is  $1 + x - x^2 - \frac{1}{4} - 1 = -(x + \frac{1}{2})^2$ , and we must then have  $x = -\frac{1}{2}$ . In this case, we see that the  $(n-2)$  and  $(n-3)$  rows of  $M$  are equal, and so  $M$  is singular. In other words, if  $M \in \mathcal{S}^{n,3}$  is locally singular, and  $M$  is nonsingular, and some  $(n-2) \times (n-2)$  minor of  $M$  is diagonally congruent to  $G(n-2, 3)$ , then  $M$  is diagonally congruent to  $G(n, 3)$ .

3.  $n = 6$ , and all  $(n-1) \times (n-1)$  principal minors of  $M$  are zero. Then using Theorem 4.4, all diagonal entries of  $M^{-1}$  are zero. Since  $M \in \mathcal{S}^{6,3}$  is NLS, again using Theorem 4.4, we also see that all  $3 \times 3$  minors of  $M^{-1}$  are zero. Any  $3 \times 3$  submatrix of  $M^{-1}$  must be of the form

$$\begin{bmatrix} 0 & a & b \\ a & 0 & c \\ b & c & 0 \end{bmatrix},$$

which has determinant  $2abc$ . Since the determinant must be 0, this means that there cannot be any  $3 \times 3$  submatrix of  $M^{-1}$  where all off-diagonal entries are nonzero. Now we define an edge coloring on  $K_6$ , the complete graph with 6 vertices, as follows. An edge  $(i, j)$  is colored red if  $(M^{-1})_{ij} = 0$  and blue otherwise. Our previous result shows that there cannot be any blue triangles in this colored graph. Therefore, using the fact that the Ramsey number  $R(3, 3)$  is at most 6 [12], there must exist a red triangle.

In other words, there must exist an identically zero  $3 \times 3$  submatrix within  $M^{-1}$ . After permuting rows and columns we may assume its index to be  $\{1, 2, 3\}$ . Now consider the submatrix of  $M^{-1}$  indexed by  $\{1, 2, 3, 4, 5\}$ . The span of first three rows is at most two dimensional, so this submatrix is singular. Using Theorem 4.4 we get  $M_{66} = 0$ . But this is a contradiction since all diagonal entries of  $M$  must be nonzero.

**7.4. Structure theorem in general.** We have shown the structure theorem in the cases when  $k = 3$  or  $n - k = 2$ . Now we use induction to prove the general case.

**THEOREM 7.5.** *Fix integers  $n \geq 5$  and  $3 \leq k \leq n - 2$ . Let  $M \in \mathcal{S}^{n,k}$  be NLS. Then  $M$  is diagonally congruent to  $G(n, k)$ .*

*Proof.* We will use induction. The base cases are when  $k = 3$  or  $k = n - 2$ , and they are already proven. These include all cases when  $n = 5$  or  $n = 6$ .

For induction, fix  $n \geq 7$  and  $3 < k < n - 2$ . Assume the theorem statement holds for  $(n-1, k)$  and  $(n-1, k-1)$ . Let  $M \in \mathcal{S}^{n,k}$  be NLS. The Schur complement of  $M$  with respect to any diagonal entry is NLS in  $\mathcal{S}^{n-1, k-1}$  and is therefore diagonally congruent to  $G(n-1, k-1)$ . Because all  $(n-2) \times (n-2)$  principal submatrices of  $G(n-1, k-1)$  are nonsingular for  $k < n-1$ , all of the  $(n-2) \times (n-2)$  minors of the Schur complement of  $M$  are nonsingular. This implies that all of  $(n-1) \times (n-1)$  minors of  $M$  are nonsingular, since Schur complements preserve the property of being singular.

Thus, if we consider any  $(n-1) \times (n-1)$  principal submatrix of  $M$ , we see that it is NLS in  $\mathcal{S}^{n-1, k}$ , and by our inductive hypothesis, all  $(n-1) \times (n-1)$  submatrices of  $M$  are diagonally congruent to  $G(n-1, k)$ . This in particular shows that all entries of  $M$  must be nonzero, and all diagonal entries strictly positive.

Let  $D'$  be a nonsingular diagonal matrix so that  $DM|_{\{1, \dots, n-1\}} D = G(n-1, k)$ . Since we may freely choose between  $D'$  and  $-D'$ , without loss of generality we may

assume  $D'_{11}$  is negative. Let  $c = \frac{\text{sgn}(M_{1n})}{\sqrt{M_{nn}}}$  (where  $\text{sgn}(x)$  is  $-1$  if  $x$  is negative,  $1$  if  $x$  is positive, and  $\text{sgn}(0) = 0$ ). We then have

$$\begin{bmatrix} D' & 0 \\ 0 & c \end{bmatrix} M \begin{bmatrix} D' & 0 \\ 0 & c \end{bmatrix} = M' = \begin{bmatrix} G(n-1, k) & v \\ v^\top & 1 \end{bmatrix}$$

for some vector  $v$ , and we know  $v_1 < 0$ . Our goal now is to show that all entries of  $v$  must be  $-\frac{1}{k-1}$ , and  $M$  is therefore diagonally congruent to  $G(n, k)$ .

Consider any size  $n-1$  principal submatrix of  $M'$  containing columns 1 and  $n$ . It is diagonally congruent to  $G(n-1, k)$ , so there exists diagonal matrix  $D = \text{diag}(d_1, \dots, d_n)$  such that

$$D \begin{bmatrix} G(n-2, k) & \hat{v} \\ \hat{v}^\top & 1 \end{bmatrix} D = G(n-1, k),$$

where  $\hat{v}$  is obtained from  $v$  by truncating one entry other than the first coordinate, and  $\hat{v}_1 < 0$ . We may also choose  $d_1 > 0$ . Now comparing diagonal entries of both sides we get  $d_i^2 = 1$  for all  $i$ . Now for all  $i > 1$  the  $(1, i)$  entry on both sides is negative, so  $d_i d_1 > 0$  for all  $i > 1$ . This shows in fact  $D = I$ , and all entries of  $\hat{v}$  are  $-\frac{1}{k-1}$ . Now varying over all possible choices of principal submatrices containing columns 1 and  $n$ , we see all entries of  $v$  must be  $-\frac{1}{k-1}$ . This concludes the proof.  $\square$

**8. Eigenvalues of locally singular matrices in  $\mathcal{S}^{4,2}$ .** In the previous section, we found that all locally singular matrices in  $\mathcal{S}^{4,2}$  are either singular or congruent to  $G(n, k)$ . In this section, we consider the eigenvalues of NLS matrices in  $\mathcal{S}^{4,2}$ .

In general, we may ask the following question: what are the possible eigenvalues of a matrix of the form  $DG(n, k)D$ , where  $D$  is a nonsingular diagonal matrix? We know that  $DG(n, k)D$  is locally singular and in  $\mathcal{S}^{n,k}$ , which implies that its eigenvalues lie on the boundary of  $H(e_k^n)$ .

Furthermore, by Sylvester's law of inertia, for any nonsingular diagonal matrix  $D$ ,  $DG(n, k)D$  has exactly one negative eigenvalue, and the remainder are positive. Hence, if  $\lambda$  is the eigenvalue vector of a  $DG(n, k)D$ , then  $\lambda$  has exactly one negative entry. We conjecture that this is in fact sufficient for  $\lambda$  to be the vector of eigenvalues for an NLS matrix in  $\mathcal{S}^{n,k}$ .

**CONJECTURE 8.1.** *If  $\lambda \in H(e_k^n)$ ,  $e_k^n(\lambda) = 0$ , and  $\lambda$  has at most 1 negative entry, then  $\lambda$  is a vector of eigenvalues for  $DG(n, k)D$  for some diagonal matrix  $D$ .*

As evidence for this conjecture, we will give a computational proof of the following theorem.

**THEOREM 8.2.** *If  $\lambda \in H(e_2^4)$  lies on the boundary of the hyperbolicity cone of  $e_2^4$  and  $\lambda$  has exactly 1 negative entry, then  $\lambda$  is an eigenvalue vector of some matrix in  $\mathcal{S}^{4,2}$ .*

We prove this by converting the question into a question about real-rooted polynomials. We should think of these as being the characteristic polynomials of certain types of symmetric matrices, and these characteristic polynomials completely characterize their eigenvalues. We defer the proofs of these characterizations to the appendix.

We say that a univariate polynomial of degree 4,  $p = a_0 + a_1x + a_2x^2 + a_3x^3 + x^4$ , has *good roots* if it is real rooted,  $a_0 < 0$ ,  $a_2 = 0$ , and  $a_3 \leq 0$ .

**LEMMA 8.3.** *A real-rooted polynomial  $p$  has good roots if and only if  $p$  has no zero roots and exactly one negative root and the roots of  $p$  lie on the boundary of  $H(e_2^4)$ .*



We then say that a polynomial  $p = a_0 + a_1x + a_2x^2 + a_3x^3 + x^4$  is *almost-nonnegative rooted* if there is some  $k \in \mathbb{R}$  so that the polynomial  $q = \frac{a_0}{-16} + \frac{a_1}{-4}x + kx^2 + a_3x^3 + x^4$  has nonnegative real roots.

LEMMA 8.4.  *$p$  is almost-nonnegative rooted if and only if there is some nonsingular diagonal matrix  $D$  so that  $p$  is the characteristic polynomial of  $DG(4, 2)D$ .*

Now, Theorem 8.2 is easily seen to be equivalent to the following lemma.

LEMMA 8.5. *A polynomial  $p$  has good roots if and only if it is almost-nonnegative rooted.*

We will prove Lemma 8.5 precisely in the appendix but sketch the ideas here. In principle, Lemma 8.5 is a statement in the first order theory of real closed fields. That is, it can be expressed entirely in terms of universal and existential quantifiers applied to real polynomial inequalities. Such questions are well known to be answerable algorithmically through quantifier elimination techniques. The first such algorithm for deciding such statements was found by Tarski and Seidenberg [5], and further developments in this field can be found, for example, in [5]. We used the quantifier elimination methods in Mathematica [16] to solve this problem.

The main technical difficulty in applying these quantifier elimination methods is reducing the number of variables needed to express the inequalities so that the problem becomes tractable on a computer. For this purpose, we prove a number of polynomial inequalities in the coefficients of a degree 4 univariate polynomial which imply both good-rootedness and almost-real-rootedness in the appendix. Once these polynomial inequalities have been proven, the problem can be directly solved by a computer.

**Appendix A. Proofs of results in section 8.** We first prove the characterization of the eigenvalues of matrices diagonally congruent to  $G(4, 2)$  in terms of characteristic polynomials.

*Proof of Lemma 8.3.* Suppose that  $p(x) = (x - r_1)(x - r_2)(x - r_3)(x - r_4)$  so that the roots of  $p$  are  $r_1, r_2, r_3, r_4$ .

Note that the condition that  $a_2 \geq 0, a_3 \leq 0$  is equivalent to the condition that  $e_2^4(r_1, r_2, r_3, r_4), e_1^4(r_1, r_2, r_3, r_4) \geq 0$ . These inequalities are equivalent to the condition that  $(r_1, r_2, r_3, r_4) \in H(e_2^4)$  [13]. Once we know that  $(r_1, r_2, r_3, r_4) \in H(e_2^4)$ ,  $a_2 = e_2^4(r_1, r_2, r_3, r_4) = 0$  is equivalent to the condition that  $(r_1, r_2, r_3, r_4)$  lies on the boundary of the hyperbolicity cone.

Every  $(r_1, r_2, r_3, r_4) \in H(e_2^4)$  has at most 2 negative entries, and if there were exactly 2 negative entries, then  $r_1r_2r_3r_4 > 0$  (it cannot be the case that there are two negative entries and a zero entry by interlacing). Therefore, the condition that  $a_0 < 0$  is equivalent to there being at most 1 negative entry in  $(r_1, r_2, r_3, r_4)$ .  $\square$

*Proof of Lemma 8.4.* The characteristic polynomial of the matrix  $DG(4, 2)D$  is, by definition,

$$p(\lambda) = \det(DG(4, 2)D - I\lambda) = \sum_{i=0}^4 \sum_{S \subseteq [n], |S|=i} (-1)^i \det((DG(4, 2)D)|_S) \lambda^{4-i}.$$

Now, note that because  $D$  is diagonal,

$$\det((DG(4, 2)D)|_S) = \det(D|_S)^2 \det(G(4, 2)|_S).$$

Also, because  $G(n, k)$  is symmetric with respect to permutations of the coordinates,  $\det(G(n, k)|_S)$  only depends on the size of  $S$ . So, we have that

$$p(\lambda) = \sum_{i=0}^4 \det(G(4, 2)|_{[i]}) \sum_{S \subseteq [n], |S|=i} (-1)^i \det((D)^2|_S) \lambda^{4-i}.$$

Now, we simply compute

$$\begin{aligned} \det(G(4, 2)|_{\{1\}}) &= 1, \\ \det(G(4, 2)|_{\{1,2\}}) &= 0, \\ \det(G(4, 2)|_{\{1,2,3\}}) &= -4, \\ \det(G(4, 2)|_{\{1,2,3,4\}}) &= -16. \end{aligned}$$

Now, consider the polynomial

$$q(\lambda) = \sum_{i=0}^4 \sum_{S \subseteq [n], |S|=i} (-1)^i \det((D)^2|_S) \lambda^i = b_0 + b_1 \lambda + b_2 \lambda^2 + b_3 \lambda^3 + \lambda^4.$$

This is equal to the characteristic polynomial of the matrix  $D^2$ . As  $D^2$  is a diagonal matrix with nonnegative real entries, its eigenvalues are nonnegative. Moreover, if  $q$  is a polynomial with nonnegative real roots, then there is a diagonal matrix  $D$  so that  $q$  is its characteristic polynomial.

Finally, note that from our above characterization of the coefficients of  $p$ ,

$$p(\lambda) = -16b_0 + -4b_1\lambda + b_3\lambda^3 + \lambda^4.$$

On the other hand, if  $p$  has almost-nonnegative roots, then we can construct the desired  $D$  from the roots of  $q$ ; then  $DG(n, k)D$  will have the desired eigenvalues.  $\square$

We now prove a number of polynomial inequalities which are equivalent to the good-rooted and almost-real-rooted conditions.

LEMMA A.1.  $p = a_0 + a_1x - x^3 + x^4$  has good roots if and only if  $a_0 < 0$  and

$$-4a_1^3 - 27a_1^4 - 6a_1^2a_0 - 27a_0^2 - 192a_1a_0^2 + 256a_0^3 \geq 0.$$

*Proof.* This polynomial  $-4a_1^3 - 27a_1^4 - 6a_1^2a_0 - 27a_0^2 - 192a_1a_0^2 + 256a_0^3$  is the discriminant of  $p$ , which is nonnegative if and only if the number of real roots of  $p$  is a multiple of 4 or  $p$  has a double root.

If  $p$  has 4 nonreal roots, say  $r_1, r_2, r_3, r_4$ , then they must come in conjugate pairs, so that, say,  $r_1 = \bar{r}_2$  and  $r_3 = \bar{r}_4$ , which would imply that then

$$a_0 = r_1r_2r_3r_4 = |r_1|^2|r_3|^2$$

is nonnegative, a contradiction.

Similarly, if  $p$  has a double root, say  $r_3 = r_4$ , and a pair of complex conjugate roots, say  $r_1 = \bar{r}_2$ , then we see that

$$a_0 = r_3^2|r_1|^2 \geq 0,$$

which is a contradiction.  $\square$

LEMMA A.2.  $p = a_0 + a_1x - x^3 + x^4$  has almost-nonnegative roots if and only if  $a_0 < 0$ ,  $a_1 < 0$ , and there is  $k > 0$  so that the following 4 inequalities are satisfied:

$$\left( -\frac{27a_1^4}{256} - \frac{9a_1^3k}{32} + \frac{a_1^3}{16} - \frac{9}{16}a_1^2a_0k + \frac{3a_1^2a_0}{128} - \frac{a_1^2k^3}{4} + \frac{a_1^2k^2}{16} + \frac{3a_1a_0^2}{16} - \frac{5}{4}a_1a_0k^2 + \frac{9a_1a_0k}{32} - \frac{a_0^3}{16} - \frac{a_0^2k^2}{2} + \frac{9a_0^2k}{16} - \frac{27a_0^2}{256} - a_0k^4 + \frac{a_0k^3}{4} \right) \geq 0,$$

$$\left( \frac{27a_1^4}{256} + \frac{9a_1^3k}{32} + \frac{a_1^3}{8} + \frac{45}{128}a_1^2a_0k - \frac{9a_1^2a_0}{128} + \frac{a_1^2k^3}{4} + \frac{45a_1^2k^2}{16} + a_1^2k + \frac{37a_1^2}{8} - \frac{9a_1a_0^2}{128} + \frac{11}{16}a_1a_0k^2 - \frac{43a_1a_0k}{32} - \frac{53a_1a_0}{32} + 9a_1k^3 + \frac{27a_1k}{2} - 3a_1 + \frac{a_0^3}{64} + \frac{3a_0^2k^2}{16} + \frac{23a_0^2k}{128} + \frac{77a_0^2}{256} + \frac{a_0k^4}{2} + \frac{27a_0k^3}{8} - 3a_0k^2 + \frac{3a_0k}{8} - \frac{3a_0}{8} + 8k^5 - 2k^4 + 16k^3 - 4k^2 \right) \leq 0,$$

$$\left( -\frac{3a_1^3}{16} + \frac{3a_1^2a_0}{64} - \frac{19a_1^2k^2}{16} - a_1^2k - \frac{17a_1^2}{16} + \frac{11a_1a_0k}{32} + \frac{17a_1a_0}{32} - \frac{9a_1k^3}{2} - a_1k^2 + 3a_1k - \frac{15a_1}{2} - \frac{3a_0^2k}{32} - \frac{17a_0^2}{256} - \frac{5a_0k^3}{4} + \frac{9a_0k^2}{8} - \frac{11a_0k}{8} + \frac{21a_0}{8} - 4k^5 + k^4 - 16k^3 + 33k^2 - 38k + 9 \right) \geq 0,$$

$$\left( -\frac{3a_1^2}{16} - 3a_1k + \frac{5a_1}{2} + \frac{3a_0k}{8} - \frac{5a_0}{8} + 2k^3 - 11k^2 + 12k - 7 \right) \leq 0.$$

*Proof.* The classical results that we need about real-rooted univariate polynomials, such as the Newton identities and the Hermite–Sylvester conditions, can be found at [4, section 3.1].

If we have the sign conditions on the coefficients,  $a_0 < 0$ ,  $a_1 < 0$ ,  $k > 0$ , then the polynomial  $q = \frac{a_0}{16} + \frac{a_1}{4}x + kx^2 - x^3 + x^4$  has coefficients which alternate in sign. If  $q$  is real rooted, then we can apply Descartes' rule of signs to conclude that  $q$  has nonnegative real roots.

The remaining inequalities cut out the space of real-rooted polynomials. This follows from the Hermite–Sylvester criterion for the polynomial having real roots. It states that if we let  $m_k = \sum_{i=1}^4 r_i^k$ , where  $r_1, r_2, r_3, r_4$  are the roots of  $q$ , then  $p$  has nonnegative real roots if and only if the  $4 \times 4$  matrix  $M$  given by

$$M_{ij} = m_{i+j}$$

is PSD.

We can then use the Newton identities to determine the  $m_k$  in terms of  $a_0$ ,  $a_1$ , and  $k$ .

Once  $M$  has been computed, the 4 polynomials above are the 4 coefficients of the characteristic polynomial of  $M$ .  $M$  being PSD is equivalent to these 4 polynomials alternating in sign, which results in the four inequalities listed.  $\square$

*Proof of Lemma 8.5.* We want to show that for all  $a_0$  and  $a_1$  satisfying the conditions of Lemma A.1, there exists  $k$  satisfying the conditions of Lemma A.2.

We are now at the point where we can directly apply any quantifier elimination algorithm to solve this problem, say the one included in Mathematica [16]. The results of this computation show that the lemma holds.  $\square$

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