An experimental approach to the S-SNIEP using algebraic geometry

Benjamin J. Clark
Washington State University
April 2025

Table of Contents

NIEP

- Given a finite list $\Lambda = \{s_1, ..., s_n\}$ of complex numbers, the nonnegative inverse eigenvalue problem (NIEP) asks for necessary and sufficient conditions such that Λ is the spectrum of an n-by-n nonnegative matrix.
- A different formulation of the NIEP asks instead for necessary and sufficient conditions for a list of real numbers to be the coefficients of the characteristic polynomial of a nonnegative matrix.

NIEP current status

- The NIEP is solved for $n \leq 4$.
- The solutions for $n = 1, 2, 3$ are fairly easy to derive from conditions involving the trace, reality, moment (sums of powers of the eigenvalues), and Perron condition (the largest eigenvalue in modulus is nonnegative).
- Meehan in 1998 and Torre-Mayo et al. in 2005 both solved the $n = 4$ case. Both of them are more complicated.

RNIEP

A simplification of the NIEP is the real NIEP (RNIEP) where we are given a list of real numbers and asked for necessary and sufficient conditions for it to be the spectra of a nonnegative matrix.

RNIEP current status

- This problem is also only solved for $n \leq 4$.
- The solution for $n = 4$ however is substantially easier, only requiring the trace to be nonnegative and for a Perron root to exist.
- The trace/Perron conditions are known not to be sufficient for $n \geq 5$.

SNIEP

A further simplification of the NIEP is the symmetric NIEP (SNIEP) where we are given a list of real numbers and asked for necessary and sufficient conditions for it to be the spectra of a symmetric nonnegative matrix.

SNIEP current status, more of the same

- This problem is also only solved for $n \leq 4$.
- The solutions for $n \leq 4$ are equivalent to the RNIEP.
- This raises the question: are the RNIEP and SNIEP different?

SNIEP and RNIEP are different

Egleston, Lenker, and Narayan showed that

$$\left(1, \frac{71}{97}, -\frac{44}{97}, -\frac{54}{97}, -\frac{70}{97}\right)$$

is realizable in the RNIEP, but not in the SNIEP.

Stochastic restrictions

- A final common restriction to these problems is to force all the matrices that are picked from to be either singly or doubly stochastic.
- For some problems like the NIEP adding the stochastic restriction and solving that problem would be equivalent to solving the original problems.
- For other problems like the SNIEP we can't pull from both stochastic and symmetric matrices at the same time and still get the same solution set.

S-SNIEP

- When we add the stochastic restriction to the SNIEP (S-SNIEP) we get that matrices we are pulling being doubly stochastic symmetric.
- For the eigenvalues, this guarantees all eigenvalues real and in the interval $[-1, 1]$.
- However, with these seemingly nice restrictions, this problem is solved only for $n \leq 3$.

Semialgebraic set

Definition

Let $\mathbb{F}$ be a real closed field. A subset S of $\mathbb{F}^n$ is called a semialgebraic set if it is a finite union of a finite intersection of sets defined by the solutions of polynomial inequalities of the form

$$\{x \in \mathbb{F}^n : P(x) * 0\}$$

where $*$ could be $=$, $\geq$, $\leq$, $>$, or $<$.

A semialgebraic set is called basic if no unions are needed.

Elementary symmetric functions

Definition

The kth elementary symmetric function of n complex numbers $\sigma = (\lambda_1, \lambda_2, \ldots, \lambda_n)$, for $k \leq n$ is

$$S_k(\sigma) = \sum_{1 \leq i_1 < \cdots < i_k \leq n} \prod_{j=1}^{k} \lambda_{i_j}.$$

Elementary symmetric functions example

For $n = 2$ the elementary symmetric functions are

$$S_1(\lambda_1, \lambda_2) = \lambda_1 + \lambda_2$$
$$S_2(\lambda_1, \lambda_2) = \lambda_1 \lambda_2$$

For $n = 3$ the elementary symmetric functions are

$$S_1(\lambda_1, \lambda_2, \lambda_3) = \lambda_1 + \lambda_2 + \lambda_3$$
$$S_2(\lambda_1, \lambda_2, \lambda_3) = \lambda_1 \lambda_2 + \lambda_1 \lambda_3 + \lambda_2 \lambda_3$$
$$S_3(\lambda_1, \lambda_2, \lambda_3) = \lambda_1 \lambda_2 \lambda_3$$

Sums of the principal minors

Definition

A minor of a matrix A is the determinant of sub matrix of A. A minor is called principal if the picked rows and columns of the submatrix are the same.

Definition

For a given matrix A, denote $E_k(A)$ to be the sums of the principal minors of size k of A.

Coefficients of the characteristic polynomial

For a given matrix A let

$$p_A(t) = t^n + (-1)a_1 t^{n-1} + \cdots + (-1)^{n-1} a_{n-1} t + (-1)^n a_n$$

be its characteristic polynomial, then

$$a_k = E_k(A) = S_k(\sigma(A)).$$

Embedding the NIEP as a semialgebraic set

Let $A \in \mathrm{M}_n^+$ with spectra σ. Using the equality between $E_k(A)$ and $S_k(\sigma)$ we can embed stochastic symmetric matrices and their spectra as a semialgebraic set in $\mathbb{R}^{n^2+n}$. The inequalities are

$$\begin{aligned} a_{ij} &\geq 0 \\ a_{ij} - a_{ji} &= 0 \\ 1 - \sum_{k=1}^{n} a_{ik} &= 0 \\ E_i(A) - S_i(\sigma) &= 0 \end{aligned}$$

for all $i, j \in \{1, \ldots, n\}$.

3x3 S-SNIEP embedded semialgebraic set example

Let

$$A = \begin{bmatrix} a_1 & a_2 & a_3 \\ a_2 & a_4 & a_5 \\ a_3 & a_5 & a_6 \end{bmatrix},$$

then the semialgebraic set is

$$\begin{aligned} a_i &\geq 0 \text{ for } i \in \{1,2,3,4,5,6\} \\ a_1 + a_2 + a_3 &= 1 \\ a_2 + a_4 + a_5 &= 1 \\ a_3 + a_5 + a_6 &= 1 \\ a_1 + a_4 + a_6 &= 1 + \lambda_2 + \lambda_3 \\ a_1 a_4 + a_1 a_6 + a_4 a_6 - a_2^2 - a_3^2 - a_5^2 &= \lambda_2 \lambda_3 + \lambda_2 + \lambda_3 \\ a_1 a_4 a_6 + 2 a_2 a_3 a_5 - a_1 a_5^2 - a_2^2 a_6 - a_3^2 a_4 &= \lambda_2 \lambda_3 \end{aligned}$$

Notes on the idea

1. We can use the linear equality conditions to reduce the number of variables.
2. Because the matrix is stochastic we can ignore the $E_n(A) = S_n(\sigma)$ equation.

3x3 S-SNIEP embedded semialgebraic set example simplified

Let

$$A = \begin{bmatrix} 1-a_1-a_2 & a_1 & a_2 \\ a_1 & 1-a_1-a_3 & a_3 \\ a_2 & a_3 & 1-a_2-a_3 \end{bmatrix},$$

then the semialgebraic set is

$$a_i \geq 0 \text{ for } i \in \{1,2,3\}$$
$$3-2a_1-2a_2-2a_3 = 1+\lambda_2+\lambda_3$$
$$3a_1a_2+3a_1a_3+3a_2a_3-4a_1-4a_2-4a_3+3 = \lambda_2\lambda_3+\lambda_2+\lambda_3$$

Project your way to a solution

- One of the most important properties of a semialgebraic set is that they are closed under projection. This is known as the Tarski–Seidenberg theorem.
- This means that if you can find a semialgebraic set in an embedded space, then we know there exists a semialgebraic set in the projected space.
- The reality condition and a finite union/intersection of polynomial inequalities solves the S-SNIEP.

Cylindrical algebraic decomposition

- Collin's algorithm or Cylindrical algebraic decomposition is the algorithm for computing the projections of a semialgebraic set.
- It is a major improvement upon Tarski-Seidenberg's result by giving a straight forward approach to computing the projection.
- This means that the S-SNIEP is solvable and the algorithm for solving it already exists.

Doubly exponential means computers don't help

- Cylindrical algebraic decomposition has a doubly exponential computing time.
- Computing the solution to the NIEP for $n = 2$ took less than 1 second. I stopped my attempt for computing the solution to the NIEP for $n = 3$ after 13 hours. The software claimed to be approximately 2% done.
- The first result that would be interesting would be, $n = 4$ and the first new result would be $n = 5$. So even with massive parallelization, computers won't be able to brute force the problem.
- Another problem with CAD is that the solution set is obtuse. The way CAD solves the space is by cutting it into interesting regions, then lifting those. This leads to unsimplified outputs that are difficult to read.

2x2 Solution

In the 2x2 case our matrix is given as

$$A = \begin{bmatrix} 1-a & a \\ a & 1-a \end{bmatrix}.$$

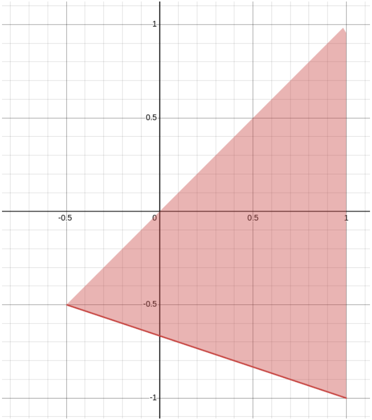
The eigenvalues are easily calculated to be 1 and $1-2a$. Since a can vary between 0 and 1 we get the solution that the spectra, $(1, \lambda)$, must satisfy $1+\lambda \geq 0$.

3x3 Solution

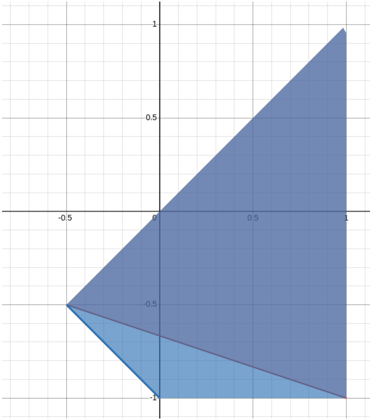
In the 3x3 case the spectra is of the form $(1, \lambda_2, \lambda_3)$ and we can assume that $\lambda_2 \geq \lambda_3$. With this setup, our solution becomes

$$2 + \lambda_2 + 3\lambda_3 \geq 0,$$
$$1 \geq \lambda_2 \geq \lambda_3 \geq -1.$$

3x3 solution picture



(a) S-SNIEP $n = 3$ solution



(b) SNIEP $n = 3$ solution

Semialgebraic sets as a tool for the NIEP

Why use semialgebraic sets on the NIEP:

- In my mind, the heart of the NIEP is to give clear conditions for a list to be realizable.
- These semialgebraic sets give a direct solution using polynomial inequalities.
- Checking whether a given list is realizable can be done in linear time with respect to the number of polynomial inequalities.

How to numerically build the boundary polynomials?

- We can think of the semialgebraic set for the coefficients of the characteristic polynomial as a n dimensional feasibility region defined by n^2 bounded and constrained parameters.
- With this, we can turn the problem into a series of optimization problems of the form,

$$\min E_j \quad \text{subject to}$$
$$E_i = c_i \text{ for } i \in \{1, \ldots, j-1\}$$

where the c_i values are within the feasibility region defined by $E_1, \ldots, E_{j-1}$.

Approach applied to the DS-SNIEP

- As mentioned above, the S-SNIEP is still open for $n \geq 4$.
- Since the matrices we are working with are stochastic and symmetric, we know that the perron root will be 1 and that the rest of the eigenvalues will be real. This allows us to plot the feasibility region in 3d.

Feasibility region 2d slices, E_1 dependence on E_2

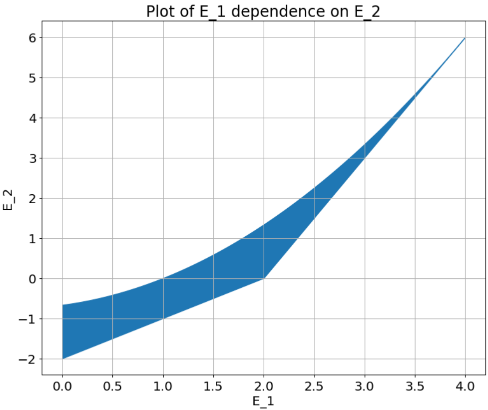


Figure 2: DS-SNIEP $n = 4$ E_1 dependence on E_2

Feasibility region 2d slices, E_1 dependence on E_3

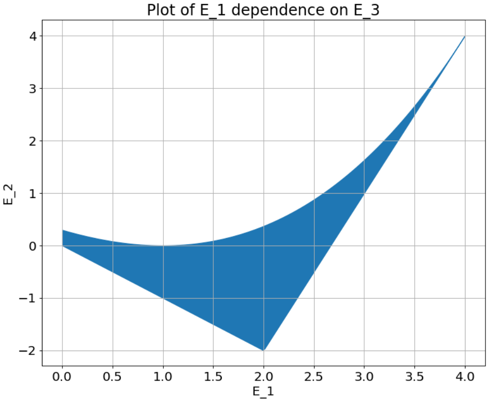


Figure 3: DS-SNIEP $n = 4$ E_1 dependence on E_3

Feasibility region 2d slices, E_2 dependence on E_3

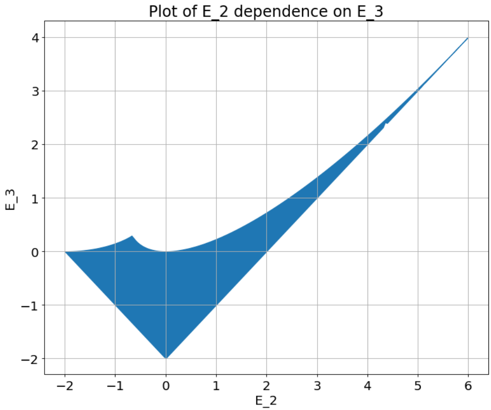
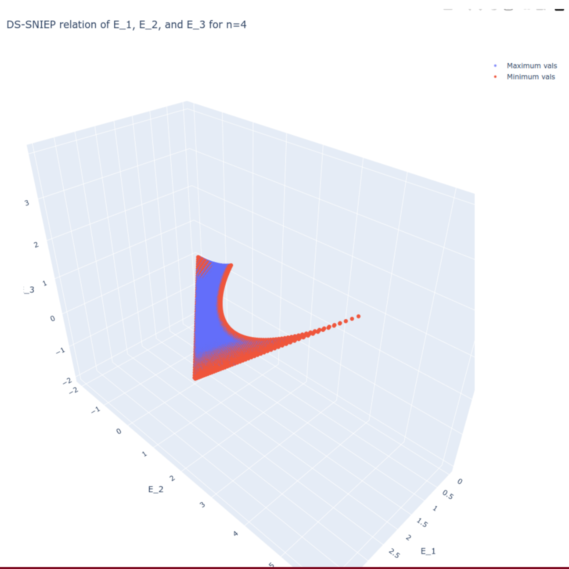


Figure 4: DS-SNIEP $n = 4$ E_2 dependence on E_3

Feasibility region of E_3



Turn that region to the spectra

- The optimization process has the added benefit of returning the matrix that was found for each optimized point.
- Using this, we can turn this region of feasibility for the characteristic polynomials into a region of feasibility of the spectra.

Turn that region to the spectra

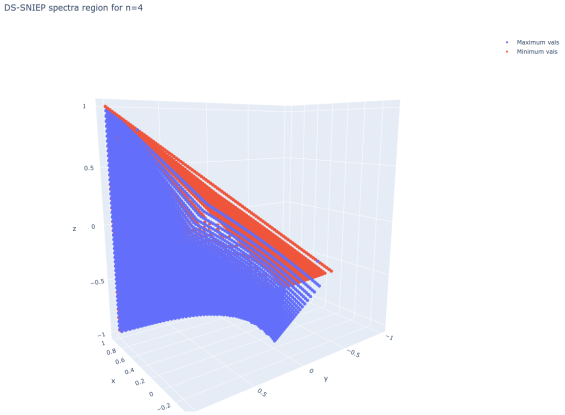


Figure 6: S-SNIEP feasible spectral region

Bringing the numerical region to a conjecture

- Given the points on the boundary of a feasibility region. We can interpolate those points to build conjectures on solutions to these spectra problems.
- Two major drawbacks with this approach are the difficulty in finding the appropriate piecewise break points in higher dimensions and the numerical instability that arise from higher order optimizations.

Conjectured solution

Conjecture

The list $1, \lambda_2, \lambda_3, \lambda_4$ *where* $\lambda_4 \leq \lambda_3 \leq \lambda_2 \leq 1$ *is the spectra of a stochastic symmetric matrix if and only if*

$$
\begin{aligned}
1 + \lambda_2 + \lambda_3 + \lambda_4 &\geq 0 \\
(1 + \lambda_3)(1 + \lambda_4) + (\lambda_2 + \lambda_3)(\lambda_2 + \lambda_4) &\geq 0
\end{aligned}
$$

Sufficient direction

The parameterized matrices

$$\begin{bmatrix} 0 & 1-\alpha & 0 & \alpha \\ 1-\alpha & 0 & \alpha & 0 \\ 0 & \alpha & \beta & 1-\alpha-\beta \\ \alpha & 0 & 1-\alpha-\beta & \beta \end{bmatrix}$$

and

$$\begin{bmatrix} 0 & 1-\alpha-\beta & \beta & \alpha \\ 1-\alpha-\beta & 0 & \alpha & \beta \\ \beta & \alpha & 0 & 1-\alpha-\beta \\ \alpha & \beta & 1-\alpha-\beta & 0 \end{bmatrix}.$$

give the feasibility region.

Necessary direction

1. The idea with the necessary direction is to build the feasibility region using a parameterized form of the eigenvectors.
2. To do this note that because the matrices are stochastic we first have the eigenvector for the 1 eigenvalue is $[1/2,\ 1/2,\ 1/2,\ 1/2]^\top$.
3. Also note that all the other eigenvalues must have mixed sign entries.

Soules Vectors

The Soules vectors

$$v_2 = \begin{bmatrix} 1/2 \\ 1/2 \\ -1/2 \\ -1/2 \end{bmatrix}, \quad v_3 = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix}, \quad v_4 = \begin{bmatrix} 0 \\ 0 \\ 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}.$$

form a basis for where the eigenvectors of λ_2, λ_3, and λ_4 can live.

Necessary direction conjecture

Conjecture

Any spectra, $1, \lambda_2, \lambda_3, \lambda_4$ where $\lambda_4 \leq \lambda_3 \leq \lambda_2 \leq 1$, that can be realized by a 4x4 symmetric stochastic matrix can have its first two eigenvectors be

$$\begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix} \text{ and } \begin{bmatrix} 1/2 \\ 1/2 \\ -1/2 \\ -1/2 \end{bmatrix}$$

If the above conjecture is true, we are done. Since we have a proof of how using those two eigenvectors for eigenvalues 1 and λ_2 captures the conjectured region.

Theoretical improvements to the semialgebraic set.

- A major question with semialgebraic sets is how many polynomials and of what degree do we need them.
- The worst case of the projection operation is 2^n polynomials per variable projected and per polynomial in the initial constraints.
- My conjecture is that the S-SNIEP forms a basic semialgebraic set.
- This would reduce the worst case number of polynomials to n^2.

Improvements to the solver

- Write now the solver is optimizing over the matrix region, which gives $\binom{n+1}{2}$ variables. Using the knowledge of eigenbasis the number of variables could be reduced to

$$(n-1)^2 - (n-1) - \binom{n-1}{2}.$$

For $n = 5$ this takes it from 10 down to 6 variables.

- The solver is performing a rudimentary grid search, it would be a major improvement to allow for flexibility in where points are picked.

Interesting paper/book

[1] Johnson, Marijuán, Paparella and Pisonero.
The NIEP.
Operator Theory, Operator Algebras, and Matrix Theory

[2] Kamron Saniee.
A Simple Expression for Multivariate Lagrange Interpolation.
SIAM Undergraduate Research Online

[3] Bochnak, Coste, and Roy.
Real Algebraic Geometry.
Springer-Verlag Berlin.

Questions?