An experimental approach to the NIEP using algebraic geometry

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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.

DS-SNIEP

- When we add the doubly stochastic restriction to the SNIEP (DS-SNIEP) we get that matrices we are pulling being doubly stochastic symmetric.
- For the eigenvalues, this guarantees all eigenvalues real and in the interval $[-1, 1]$.
- 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 nonnegative matrices and their spectra as a semialgebraic set in $\mathbb{R}^{n^2+n}$. The inequalities are

$$a_{ij} \geq 0 \text{ for all } i, j \in \{1, \ldots, n\}$$
$$E_k(A) - S_k(\sigma) = 0 \text{ for all } k \in \{1, \ldots, n\}$$

Question

What is wrong with the above semialgebraic set?

Embedding the NIEP cont.

- To overcome the fact that nonnegative matrices can have complex eigenvalues, we need to use the fact that the elementary symmetric functions maps complex conjugates to real numbers.
- Using this, we can make modified elementary symmetric functions based on the number of conjugate pairs.
- This gives that the solution to the NIEP is the projection of the union of $\lfloor (n-1)/2 \rfloor$ basic semialgebraic sets in $\mathbb{R}^{n^2+n}$

3x3 NIEP embedded semialgebraic set

If $\sigma = (\lambda_1, \lambda_2, \lambda_3)$ is real, then

$$\begin{aligned} a_{ij} \geq 0 \text{ for all } i, j \in \{1, 2, 3\} \\ E_1(A) - \lambda_1 - \lambda_2 - \lambda_3 = 0 \\ E_2(A) - \lambda_1\lambda_2 - \lambda_1\lambda_3 - \lambda_2\lambda_3 = 0 \\ E_3(A) - \lambda_1\lambda_2\lambda_3 = 0 \end{aligned}$$

or if $\sigma = (\lambda_1, \lambda_2 + i\lambda_3, \lambda_2 - i\lambda_3)$, then

$$\begin{aligned} a_{ij} \geq 0 \text{ for all } i, j \in \{1, 2, 3\} \\ E_1(A) - \lambda_1 - 2\lambda_2 = 0 \\ E_2(A) - 2\lambda_1\lambda_2 - \lambda_2^2 - \lambda_3^2 = 0 \\ E_3(A) - \lambda_1\lambda_2^2 - \lambda_1\lambda_3^2 = 0 \end{aligned}$$

SNIEP's and RNIEP's embedding as basic semialgebraic sets

For $A \in \mathrm{M}_n^+$ with spectra σ, the SNIEP is embedded as

$$\begin{aligned} a_{ij} &\geq 0 \text{ for all } i, j \in \{1, \dots, n\} \\ E_k(A) - S_k(\sigma) &= 0 \text{ for all } k \in \{1, \dots, n\} \\ a_{ij} - a_{ji} &= 0 \end{aligned}$$

The embedded SNIEP and RNIEP are basic semialgebraic sets in $\mathbb{R}^{n^2+n}$.

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 NIEP.

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 NIEP is solvable and the algorithm for solving it already exists. However...

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.

Semialgebraic sets for the NIEP up to $n = 4$

Theorem (Torre-Mayo et. al. Theorem 3)

Let $P(x) = x^n + \sum_{j=1}^{n}(-1)^j c_j x^{n-j}$ be a characteristic polynomial of degree $n \geq 3$ of a nonnegative matrix A. Then

$$0 \leq c_1$$

$$0 \leq (n-1)c_1^2 - 2nc_2$$

$$c_3 \geq \begin{cases} \frac{n-2}{n}\left(-c_1c_2 + \frac{n-1}{3n}\left(\left(c_1^2 - \frac{2n}{n-1}c_2\right)^{3/2} + c_1^3\right)\right) & \text{if } (n-1)(n-4)c_1^2 < 2(n-2)^2c_2, \\ \frac{(n-1)(n-3)}{3(n-2)^2}c_1^3 - c_1c_2 & \text{otherwise.} \end{cases}$$

Semialgebraic sets for the NIEP up to $n = 4$ cont.

In terms of the coefficients of the characteristic polynomial,

$$P(x) = x^n + \sum_{j=1}^{n} (-1)^j c_j x^{n-j},$$

the semialgebraic sets that make the NIEP are

- $n = 1: \quad P(x) = x - c_1$

$$c_1 \geq 0$$

- $n = 2: \quad P(x) = x^2 - c_1 + c_2$

$$c_1 \geq 0 \wedge c_1^2 - 4c_2 \geq 0$$

Semialgebraic sets for the NIEP up to $n = 4$ cont.

- $n = 3: \quad P(x) = x^3 - c_1x^2 + c_2x - c_3$

$$c_1 \geq 0 \ \wedge \ c_1^2 - 3c_2 \geq 0 \ \wedge \ 27c_3 + 9c_1c_2 - 2c_1^3 \geq 0 \ \wedge$$
$$-4c_1^3c_3 - c_1^2c_2^2 + 18c_1c_2c_3 + 4c_2^3 + 27c_3^2 \geq 0$$

- $n = 4: \quad P(x) = x^4 - c_1x^3 + c_2x^2 - c_3x + c_4$

$$c_1 \geq 0 \ \wedge \ 4c_3 + 4c_1c_2 - c_1^3 \geq 0 \ \wedge 8c_3 + 2c_1c_2 - c_1^3 \geq 0 \ \wedge$$
$$\left(-c_2 \geq 0 \vee -27c_1^3c_3 - 9c_1^2c_2^2 + 108c_1c_2c_3 + 32c_2^3 + 108c_3^2 \geq 0\right)$$

Semialgebraic sets as a tool for the NIEP

Some things to note about the semialgebraic approach:

- The perron condition (The largest eigenvalue in modulus is positive) is not necessary.
- Solving the RNIEP using these methods also gives a solution to the NIEP.
- Checking where 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,

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

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 DS-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

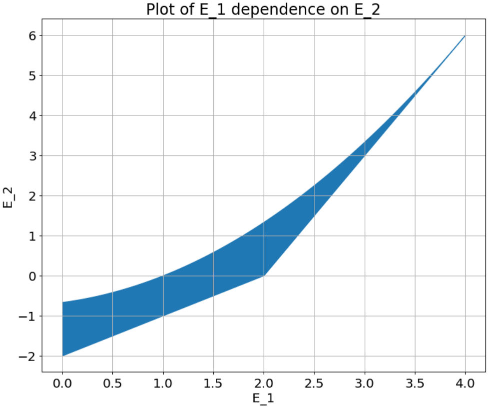


Figure 1: DS-SNIEP $n = 4$ E_1 dependence on E_2

Feasibility region 2d slices, E_1 dependence on E_3

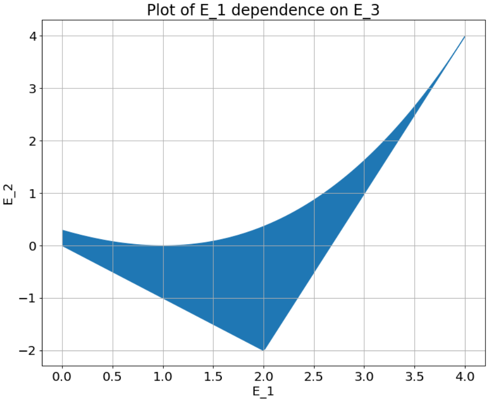


Figure 2: DS-SNIEP $n = 4$ E_1 dependence on E_3

Feasibility region 2d slices, E_2 dependence on E_3

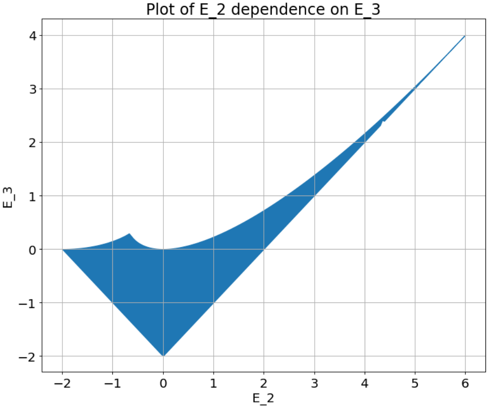
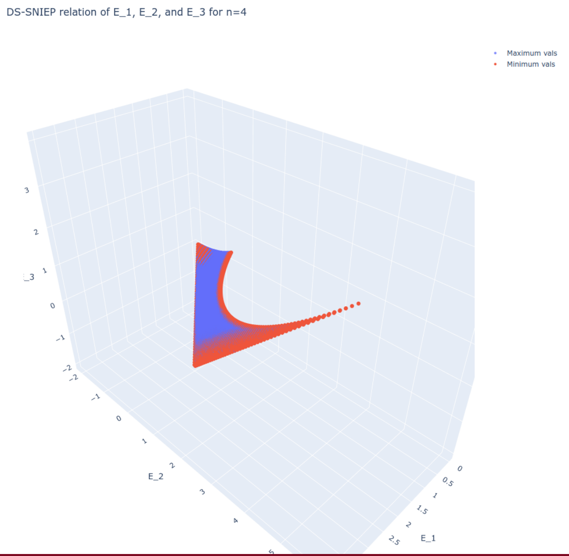


Figure 3: DS-SNIEP $n = 4$ E_2 dependence on E_3

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

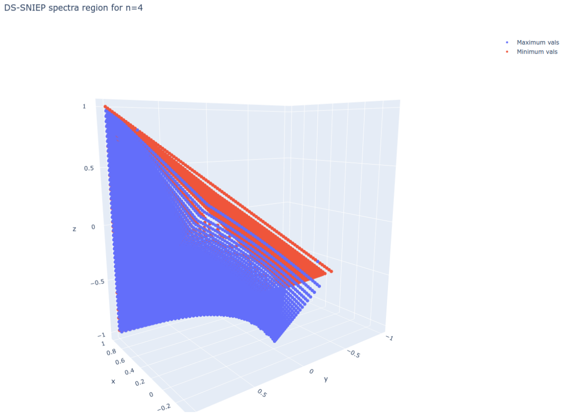


Figure 5: DS-SNIEP feasible spectral region

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.

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 NIEP forms a basic semialgebraic set with respect to its coefficients of the characteristic polynomial.
- This would reduce the worst case number of polynomials to n^2.

Improvements to the solver

- Write code to determine where the break-lines are in the region.
- Allow for the solver to take more types of NIEP sub-problems in.
- Better interpolation support.

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?