Mathematical Connections through Eigenvalue Spacings

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Outline

Recall: Abbreviated Motivation

- Derived from *Finite Models for Arithmetical Quantum Chaos* by Dr. Audrey Terras
- Recall the motivation given last presentation

Motivation

In quantum mechanics, some energy systems are so complex that it becomes impossible to calculate all their energy levels. Physicists have discovered that the spectra of eigenvalues of various matrices, when normalized between 0 and 1, may model the behaviour of such energy systems (atomic spectra, for example).

The Tree of Quantum Chaos
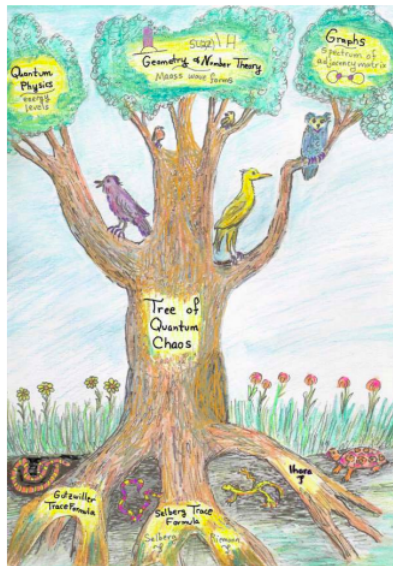
This tree is the motivator for Dr. Terras' research.

- **Three branches:** Quantum Physics, Geometry of Number Theory, and Graphs
- **Three roots:** Gutzwiller trace formula, Selberg trace formula, and Ihara zeta function

Dr. Terras' work involves studying spectra of numbers pertaining to these roots and branches in order to discover commonalities and new information about them. We will only consider this with the quantum physics and graphs branches.

Sophisticated Motivation

Sophisticated Motivation

To discover the "stochastic laws governing sequences having very different origins" (Oriol Bohigas and Marie-Joya Gionnoni)

- In particular, how may graph theory and quantum physics be interconnected, and what can they teach us about each other?

Quantum Physics-Graph Theory Intersection

In quantum physics, the energy levels of a physical system are *eigenvalues*. Because it is often impossible to know all these energy levels, we resort to using statistical theory of the energy levels to learn more about them.

The eigenvalues of the energy level operator are on an infinite dimensional vector space. In graph theory, we replace this operator with a finite analogue - the adjacency matrix/operator of a graph.

"Think of a graph as a system of masses connected by rubber bands. This is a reasonable model for a molecule"

Research Overview

Now that you have a more thorough understanding of the purpose of this research, I will walk you through new observations. First, let's review the research process.

Methodology Review:

1. Generate eigenvalues
   - Adjacency matrices of special graphs
   - Random matrices from probability distributions
   - And more!
2. Analyze spacings between eigenvalues
3. Make observations

Review of the n-gon example

- Generate an n-gon
- Create $n \times n$ adjacency matrix
  - Each row is a vertex from 1 to n
  - Each column is a vertex from 1 to n
  - Insert a 1 for every edge between 2 vertices and a 0 otherwise
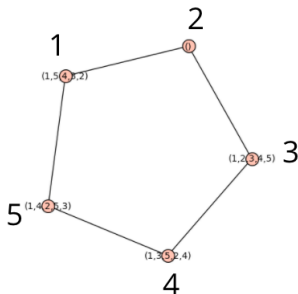
$$\begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

The n-gon Example

- Obtain eigenvalues from the adjacency matrix
- Sort eigenvalues from least to greatest, $\lambda_1 \ldots \lambda_n$ such that $\lambda_1 < \lambda_2 < \cdots < \lambda_n$
- Scale the eigenvalues to be between 0 and 1. This is important for comparing the eigenvalues between matrices; it makes it easier to find patterns

Normalization Equation

$$\forall i = 1, 2, \ldots, n, \quad \hat{\lambda}_i = \frac{\lambda_i - \lambda_1}{\lambda_n - \lambda_1}$$

- After normalizing, look at a histogram of the eigenvalues as well as statistical analysis.

The n-gon Example

- Analyze
  - ▸ Create histograms of normalized eigenvalues
  - ▸ Look at statistics
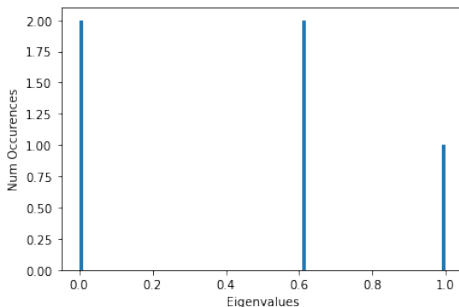 - ▸ Look for patterns and significance

Figure: Histogram of normalized eigenvalues for adjacency matrix of 5-gon

Statistics

- **Average:** Indicates left/right skew of eigenvalues
- **Standard Deviation:** Indicates distance of eigenvalues from the average

$$\frac{\sqrt{\sum_{i=1}^{n-1} \left(\lambda_i - \bar{\lambda} \right)^2}}{n}$$

- For **centralization**, replace $\bar{\lambda}$ with $\frac{1}{2}$. This detects distance from the center, rather than distance from the average.

Statistics

- Detect large spacings between successive lines

$$\frac{\sqrt{\sum_{i=1}^{n-1}\left(\lambda_i - \lambda_{i+1}\right)^2}}{n}$$

- Detect large spacings between all lines

$$\frac{\sqrt{\sum_{1<i<j<n}\left(\lambda_i - \lambda_j\right)^2}}{\binom{n}{2}}$$

Observations: Symmetry Groups

Idea

Eigenvalues of 'special' matrices, such as adjacency matrices of n-gons, have unique properties that eigenvalues from random matrices don't. Dr. Terras notes that symmetry groups have a large effect on energy levels.

Symmetry of n-gons

- n-gons are polygons with rotational symmetry of $\frac{360}{n}$ degrees.
- The eigenvalues of n-gons also have a clear symmetry. The normalized eigenvalues always have an average very close to 0.5.
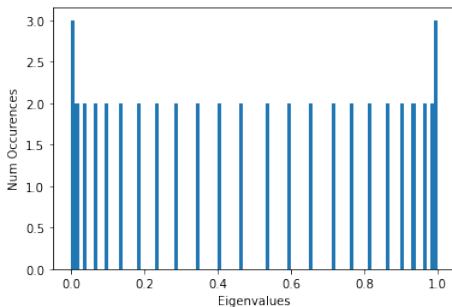

Figure: Histogram of normalized eigenvalues from adjacency matrix of 50-gon

Contrast: Random 'adjacency' matrices

Recall: A random adjacency matrix, chosen with binomial distribution

- Each entry in the 50x50 matrix is chosen independently to be 0 or 1, and the probability that 1 is chosen is the success rate p.
- Then, the matrix is made symmetric by setting each entry $a_{i,j} = a_{j,i}$, and the diagonal entries are set to 0.
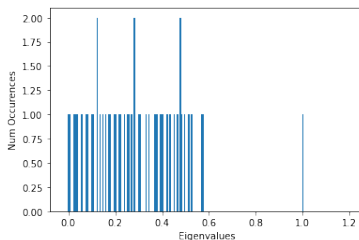- Simulates a 'random' molecule

Figure: Histogram of normalized eigenvalues for random adjacency matrix, $p = 0.25$

Contrast: Random 'adjacency' matrices

- The average is very low, at 0.15884.
- The spacings between lines about 0.001, which is very low. This indicated that most lines are clumped right around the average.
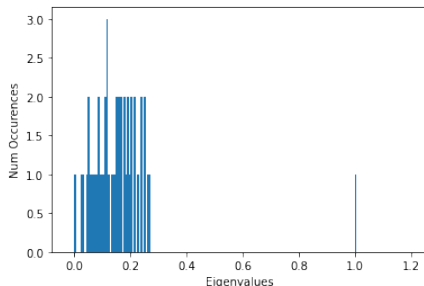

Figure: Histogram of normalized eigenvalues for random adjacency matrix, $p = 0.75$

Background: Normal Distribution

Standard Normal Distribution

- $\mu = 0$, $\sigma = 1$. Symmetrically distributed, with values clustered near the mean.
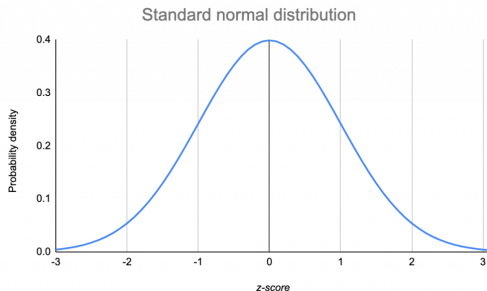- Area under the curve must be 1.

Figure: Standard Normal Distribution Curve

The Wigner Semi-Circle

- In the 1950's, physicist and mathematician Eugene Wigner noted that energy levels could be modeled with large real symmetric matrices whose entries are chosen with normal distribution.
- The histogram of one of these matrices forms what is called the **Wigner Semi-Circle**
- The histogram of 200 50x50 real symmetric matrices from my project depicts this semi-circle!

200 Real 50x50 Symmetric Matrices

1. For 50x50 matrix, each entry is populated using standard normal distribution
2. The matrix is made symmetric by setting all $a_{i,j} = a_{j,i}$
3. The eigenvalues from this matrix are added to a master list, and this process is repeated 200 times (for 200 matrices)
4. Finally, ALL eigenvalues from these 200 matrices are normalized and plotted on a histogram
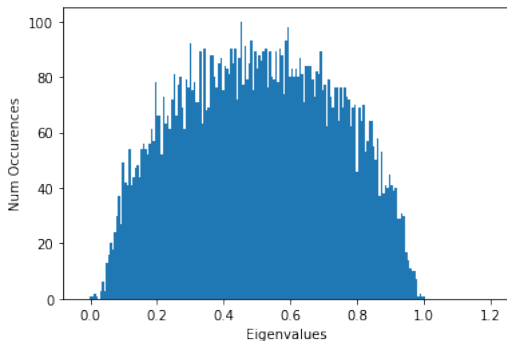
The Wigner Semi-Circle

Figure: Histogram of normalized eigenvalues from 200 real, symmetric, 50x50 matrices, populated using normal distribution

The average is 0.49328. What do you think would happen if we increase the amount of matrices?

Background: Uniform Distribution

What happens when we recreate 200 real, symmetric 50x50 matrices, but use uniform distribution instead?

- Uniform Distribution chooses any number between a certain continuous range. For this project, it's [0, 1].
- Any number in the range is equally probable.

Essentially, create the 200 matrices in the same way, except now we just populate entries independently with *uniform distribution*.
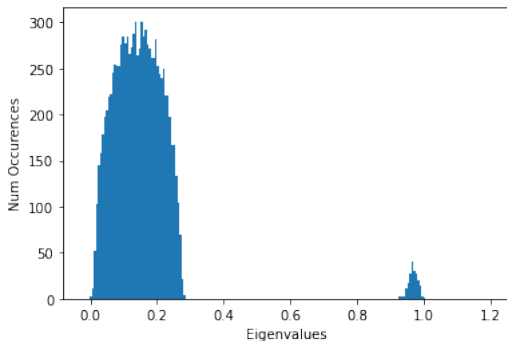
Contrast: Uniform Distribution

Figure: Histogram of normalized eigenvalues from 200 real, symmetric, 50x50 matrices populated using uniform distribution

The average is 0.15772. Very off-center!

Significance of Wigner Semi-Circle

- Refuting Wigner's initial conjecture, the Wigner Semi-Circle shows no similarity to observed distribution in atomic spectra
- The Wigner Semi-Circle actually has similarity to a distribution in graph and number theory, the Sato-Tate distribution!

Future Work

Finding connections between all the roots and branches of the tree of quantum chaos is a huge undertaking that mathematicians have been working on for a long time.

Takeaway thoughts:

- What other symmetry groups are out there, and what can they tell us about energy levels? (matrices from star graphs, etc.)
- Idea: taking easy-to-model energy levels and turning them into graphs, then studying their eigenvalue distributions and comparing them to other eigenvalue distributions
- Someday being skilled enough to venture into the roots of the tree

Thank you! –Resources
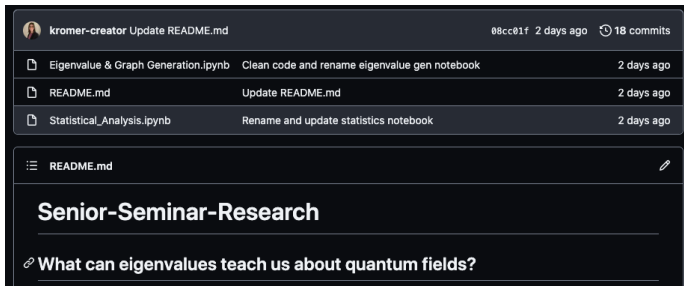
- All of my code, as well as a link to my Google drive with data can be viewed on my Senior Seminar Github repository: `https://github.com/kromer-creator/Senior-Seminar-Research`
- The paper *Finite Models for Arithmetical Quantum Chaos* by Audrey Terras can be accessed here: `https://mathweb.ucsd.edu/~aterras/newchaos.pdf`