Eigenvalue Distribution of Pentadiagonal Doubly Stochastic Matrices

A Dissertation Report

Submitted in partial fulfilment of the

requirements for the award of the Degree of

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IN

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BY

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APPROVAL OF THE GUIDE(S)

This is to certify that the work presented in the dissertation report titled **"Eigenvalue Distribution of Pentadiagonal Doubly Stochastic Matrices"** in partial fulfillment of the requirement for the award of the Degree of Integrated Master of Science, Mathematics and Computing of Birla Institute of Technology, Mesra, Ranchi is an authentic work carried out under my supervision.

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CERTIFICATE OF APPROVAL

The dissertation titled **"Eigenvalue Distribution of Pentadiagonal Doubly Stochastic Matrices"** has been approved as a creditable study that was carried out and presented satisfactorily to warrant its acceptance as a prerequisite to the degree for which it was submitted. It is recognized that by granting this approval, the undersigned do not necessarily accept any conclusion or opinion expressed therein, but rather approve the project for which it was filed.

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I/we declare:

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b. This work has not been submitted to any other institute for a degree or diploma.

c. I followed the Institute's requirements for writing the dissertation.

d. I followed the Institute's ethical code of conduct.

e. Whenever I used materials from other sources (data, theoretical analysis, and text), I cited them in the thesis text and provided information in the references.

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Motivation

Over the past few decades, doubly stochastic matrices have attracted significant research interest. Initially studied in contexts such as language processing and card shuffling, their importance has expanded into numerous fields including Markov chains, theory of probability, statistical analysis, financial mathematics, algebraic structures, economic theory, engineering disciplines, computer sciences, genetic population studies and quantum information theory. Stochastic modeling - a key area in statistics, data science, and machine learning - adds further depth to their relevance.

Among the various properties of these matrices, their spectral characteristics have drawn particular attention. In particular, the distribution of eigenvalues across matrices of different sizes has proven to be a rich area of study. This thesis is structured into five sections:

- **Introduction:** This section includes essential definitions and theorems.
- **Literature Survey:** Here, We look at what others have done so far and where our work fits in.
- **Result and Discussion:** This is where we share what we found and what those findings mean.
- **Conclusion:** We wrap things up by highlighting the main takeaways and what could be done next.
- **References:** This part lists all the sources we used to build and support our thesis.

1. Introduction

Eigenvalues and Eigenvectors [3]

Definition 1.1. (Eigenvalue, Eigenvector, and Eigenpair): Let A be an $n \times n$ matrix. If a scalar $\lambda \in \mathbb{C}$ and a nonzero vector $x \in \mathbb{C}^n$ satisfy the relation $Ax = \lambda x$, then λ is called an **eigenvalue** of A, and x is called an **eigenvector** associated with λ. Together, (λ, x) form an **eigenpair** of A.

Definition 1.1.1. (Spectrum): The **spectrum** of a matrix $A \in M_n$ is defined as the set of all eigenvalues of A, and it is denoted by $\sigma(A)$.

Definition 1.2. (Characteristic Equation): For a square matrix A, the **characteristic polynomial** is given by $p_A(t) = \det(tI - A)$. The equation $p_A(t) = 0$ is called the **characteristic equation** of A.

Definition 1.3. (Algebraic Multiplicity): The **algebraic multiplicity** of an eigenvalue λ of A is the number of times λ appears as a root of the characteristic polynomial.

Definition 1.4. (Spectral Radius): The **spectral radius** of a matrix $A \in M_n$ is defined as the maximum absolute value among its eigenvalues, denoted by

$$\rho(A) = \max\{|\lambda| : \lambda \in \sigma(A)\}$$

Definition 1.5. (Eigenspace): The **eigenspace** of a matrix $A \in M_n$ corresponding to an eigenvalue $\lambda \in \sigma(A)$ is the set of all vectors $x \in \mathbb{C}^n$ satisfying $Ax = \lambda x$. Every nonzero vector in this set is an eigenvector of A for λ.

Definition 1.6. (Geometric Multiplicity): Let λ be an eigenvalue of a square matrix A. The **geometric multiplicity** of λ, written as $g(\lambda)$, is the dimension of the corresponding eigenspace—that is, the number of linearly independent eigenvectors associated with λ. This space is given by:

$$E_\lambda = \{x \in \mathbb{R}^n : (A - \lambda I)x = 0\}$$

Corollary 1.6.1.: For any eigenvalue λ, its geometric multiplicity is less than or equal to its algebraic multiplicity:

$$1 \leq g(\lambda) \leq a(\lambda)$$

where $a(\lambda)$ represents the algebraic multiplicity of λ.

Positive and Non-negative Matrices [3]

1.7. Inequalities and Generalities

a. Matrices and Their Entries

You are given two matrices:

- $A = [a_{ij}] \in M_{m,n}$ is matrix with m rows and n columns.
- $B = [b_{ij}] \in M_{m,n}$ is another matrix of the same size.

Both matrices have real entries, meaning the elements a_{ij} and b_{ij} are real numbers.

b. Entrywise Absolute Value

- The notation $|A| = [|a_{ij}|]$ means you take the absolute value of each individual element in the matrix A. So, each entry a_{ij} of matrix A is replaced with $|a_{ij}|$, the absolute value of that entry.

- **Example:** If $A = \begin{pmatrix} -1 & 2 \\ 3 & -4 \end{pmatrix}$, then $|A| = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$.

c. Nonnegative and Positive Matrices

- $A \geq 0$: This suggests that all entries in matrix A are zero or positive. In other words, for all i, j, $a_{ij} \geq 0$.
  - **Example:** If $A = \begin{pmatrix} 1 & 2 \\ 3 & 0 \end{pmatrix}$, then $A \geq 0$ because all the entries are nonnegative.
- $A > 0$: This means every element of the matrix A is strictly positive. For all i, j, $a_{ij} > 0$.
  - **Example:** If $A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$, then $A > 0$ because all the entries are positive.

d. Matrix Inequalities

- $A \geq B$: This means that $A - B \geq 0$, meaning when you subtract matrix B from matrix A, the result is a matrix where all entries are larger than or equal to zero.
  - **Example:** If $A = \begin{pmatrix} 3 & 4 \\ 5 & 6 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, then $A - B = \begin{pmatrix} 2 & 3 \\ 4 & 5 \end{pmatrix}$, which is nonnegative, so $A \geq B$.
- $A > B$: This states that $A - B > 0$, meaning when you subtract matrix B from matrix A, the result is a matrix where all entries are strictly greater than zero.
  - **Example:** If $A = \begin{pmatrix} 3 & 4 \\ 5 & 6 \end{pmatrix}$ and $B = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$, then $A - B = \begin{pmatrix} 2 & 3 \\ 4 & 5 \end{pmatrix}$, which is strictly positive, so $A > B$.

e. Reversed Inequalities

- The reversed relations $A \leq 0$ and $A < 0$ are defined similarly:
  - $A \leq 0$: Every element of A is less than or equal to zero.

– $A < 0$: Every element of A is strictly less than zero.

Definition 1.8. (Irreducible Matrix): A square matrix $A = [a_{ij}] \in \mathbb{R}^{n \times n}$ with non-negative entries is said to be **irreducible** if it cannot be transformed, by simultaneously permuting its rows and columns, into a block upper triangular matrix of the form:

$$A = \begin{pmatrix} B & C \\ 0 & D \end{pmatrix},$$

where B and D are square matrices and 0 is a zero block. If such a block form exists through permutation, the matrix is called **reducible**.

In other words:

- An **irreducible matrix** is one that is completely interconnected—there are no subsets of rows and columns that are isolated from the rest.
- A **reducible matrix** can be decomposed into smaller independent substructures.

Theorem 1.9. (Perron–Frobenius Theorem): Let $A \in M_n$ be a nonnegative and irreducible matrix, with $n \geq 2$. Then the following statements hold:

- **(a)** The spectral radius $\rho(A)$ is strictly positive.
- **(b)** The spectral radius $\rho(A)$ is a simple root of the characteristic polynomial—that is, it is an eigenvalue of algebraic multiplicity one.
- **(c)** There exists a unique positive vector $x = [x_i] \in \mathbb{R}^n$ such that $Ax = \rho(A)x$ and $\sum_{i=1}^{n} x_i = 1$.
- **(d)** There exists a unique positive row vector $y = [y_i] \in \mathbb{R}^n$ such that $y^T A = \rho(A) y^T$ and $\sum_{i=1}^{n} x_i y_i = 1$.

Definition 1.10. (Stochastic Matrix): A square matrix $P = [p_{ij}]$ is called a **stochastic matrix** if it satisfies the following conditions:

1. **Non-negative entries:** Every entry in the matrix must be non-negative. This condition ensures that each matrix element represents a probability, which cannot be negative.

2. **Column sums equal to 1:** The sum of the elements in each column must be equal to 1, i.e.

$$\sum_i p_{ij} = 1 \quad \text{for all } j.$$

- **Example:** $P = \begin{pmatrix} 0.5 & 0.2 \\ 0.5 & 0.8 \end{pmatrix}$.

Definition 1.11. (Doubly Stochastic Matrix): A **doubly stochastic matrix** is a special type of stochastic matrix with the additional property that both row sums and column sums equal 1.

1. **Non-negative entries:** Like a stochastic matrix, the entries in a doubly stochastic matrix are also non-negative.

2. **Row sums and column sums equal to 1:** In addition to the column sum condition of a stochastic matrix, the sum of the elements in each row must also equal 1:

$$\sum_j a_{ij} = 1 \quad \text{for all } i, \quad \text{and} \quad \sum_i a_{ij} = 1 \quad \text{for all } j.$$

- **Example:** $A = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}$.

2. Literature Survey

Fundamental Theoretical Framework

Definition 2.1. (Permutation Matrix): A matrix $P \in \mathbb{R}^{n \times n}$ is called a *permutation matrix* if it contains exactly one entry of 1 in each row and each column, with all other entries equal to 0. **Example (3×3 permutation matrix) :**

$$P = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Theorem 2.2. (Birkhoff–von Neumann Theorem): [1, 6, 9] Let $\mathcal{D}_n$ be the collection of all $n \times n$ doubly stochastic matrices, and $\mathcal{P}_n$ as the collection of all $n \times n$ permutation matrices. it follows:

> Every doubly stochastic matrix $A \in \mathcal{D}_n$ can be expressed as a convex combination of permutation matrices:
>
> $$A = \sum_{k=1}^{m} \lambda_k P_k,$$
>
> where each $P_k \in \mathcal{P}_n$, $\lambda_k \geq 0$, and $\sum_{k=1}^{m} \lambda_k = 1$.
>
> by **Carathéodory's theorem**, we have $m \leq n^2 - n + 1$.

Uniform Matrix Case (Special Worst Case): The uniform doubly stochastic matrix J_n (all entries $= 1/n$) requires all $n!$ permutation matrices in its decomposition:

$$J_n = \frac{1}{n!} \sum_{k=1}^{n!} P_k.$$

For e.g, $n = 5$, means $5! = 120$ permutation matrices requires (each with weight $1/120$).

Spectral Theory of Doubly Stochastic Matrices

Theorem 2.3. (Perron–Frobenius Theorem for Doubly Stochastic Matrices): [8] Let $A \in \mathbb{R}^{n\times n}$ be a doubly stochastic matrix. Then the following properties hold:

1. The spectral radius of A is $\lambda = 1$, and this eigenvalue appears with multiplicity at least one.
2. Every eigenvalue λ of A satisfies $|\lambda| \leq 1$.

Theorem 2.4. (Eigenvalue Localization): [6] For a matrix $A \in \mathbb{R}^{n\times n}$ that is doubly stochastic, its eigenvalues $\lambda \in \mathbb{C}$ are constrained as follows:

1. **In general:** All eigenvalues lie inside or on the unit circle, i.e., $|\lambda| \leq 1$.
2. **If A is symmetric:** Then all eigenvalues are real and lie in the interval $[-1, 1]$.
3. **If A is normal:** Then the eigenvalues lie within the convex hull of the nth roots of unity:

$$\lambda \in \operatorname{conv}\left\{e^{2\pi ik/n} : k = 0, 1, \ldots, n-1\right\}.$$

Conjecture 2.5. (Perfect–Mirsky): [7] Define Ω_n as the collection of all eigenvalues of $n \times n$ doubly stochastic matrices. Then the conjecture states:

$$\Omega_n = \bigcup_{k=1}^{n} \operatorname{conv}\left\{e^{2\pi ij/k} : j = 0, 1, \ldots, k-1\right\},$$

meaning Ω_n is the union of convex hulls of the kth roots of unity for all $k \leq n$.

This conjecture has been verified for $n = 2, 3, 4$, disproven for $n = 5$, and its status for $n \geq 12$ is still unresolved.

Theorem 2.6. [5] The set of eigenvalues of all 5×5 doubly stochastic matrices does not lie inside the union of convex hulls of kth roots of unity for $k = 1, \ldots, 5$. Some eigenvalues appear outside of the region. This shows that the Perfect–Mirsky conjecture does not hold for $n = 5$.

Geometric Aspects of Eigenvalue Distribution

Theorem 2.7. (Diamond Theorem): [2] The eigenvalues of any $n \times n$ doubly stochastic matrix are located within a diamond-shaped area:

$$\{\lambda \in \mathbb{C} : |\text{Re}(\lambda)| + |\text{Im}(\lambda)| \leq 1\}.$$

Theorem 2.8. (Marcus-Ree Theorem): [4] For $n \geq 3$, the eigenvalue region ω_n for $n \times n$ doubly stochastic matrices:

- is star-shaped with respect to 0,
- includes every convex combination of the k-th roots of unity where k $\leq$ n.

Special Structured Doubly Stochastic Matrices

Definition 2.9. (Pentadiagonal Matrix): A square matrix of size $n \times n$ is a *pentadiagonal matrix* where non-zero elements are restricted to the five diagonals: the main diagonal, the two diagonals directly above and below the main diagonal, and the two diagonals two places away from the main diagonal. Formally, a matrix $A = [a_{ij}]$ is pentadiagonal if:

$$a_{ij} \neq 0 \quad \text{only if} \quad |i - j| \leq 2.$$

Example (6×6 Pentadiagonal Matrix) :

$$A = \begin{bmatrix} a_1 & b_1 & c_1 & 0 & 0 & 0 \\ d_1 & a_2 & b_2 & c_2 & 0 & 0 \\ e_1 & d_2 & a_3 & b_3 & c_3 & 0 \\ 0 & e_2 & d_3 & a_4 & b_4 & c_4 \\ 0 & 0 & e_3 & d_4 & a_5 & b_5 \\ 0 & 0 & 0 & e_4 & d_5 & a_6 \end{bmatrix}$$

Definition 2.9.1. (Pentadiagonal Doubly Stochastic Matrix): A *pentadiagonal doubly stochastic matrix* is a square matrix $A = [a_{ij}]$ that meets the following criteria:

1. The matrix has a pentadiagonal structure, meaning nonzero entries are limited to the main diagonal and the two adjacent diagonals on each side.
2. All matrix elements are non-negative: $a_{ij} \geq 0$ for all i, j.
3. Every row and column sums to 1.

Example (6×6 Pentadiagonal Doubly Stochastic Matrix):

$$P = \begin{bmatrix} 0.4 & 0.3 & 0.3 & 0 & 0 & 0 \\ 0.2 & 0.3 & 0.3 & 0.2 & 0 & 0 \\ 0.1 & 0.2 & 0.3 & 0.2 & 0.2 & 0 \\ 0 & 0.2 & 0.2 & 0.3 & 0.2 & 0.1 \\ 0 & 0 & 0.2 & 0.3 & 0.3 & 0.2 \\ 0 & 0 & 0 & 0.3 & 0.3 & 0.4 \end{bmatrix}$$

3. Results and Discussions

Over a century, several studies have been carried out related to the properties and distribution of eigenvalues of doubly stochastic matrices. In this study, we focus on a specific subset: **pentadiagonal doubly stochastic matrices** of orders up to 6. Our primary goal is to analyse how the eigenvalues of these matrices are distributed in the complex plane as we vary different combinations of permutation matrices. By plotting these eigenvalues, our aim is to visualize and better understand how their distribution changes with respect to different matrix structures.

3.1 For Order 3

A general **3×3 doubly stochastic matrix** is:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

As we know a **pentadiagonal matrix** is a matrix where nonzero elements are allowed only on the **main diagonal**, **two diagonals above**, and **two diagonals below** it. **So, a pentadiagonal doubly stochastic matrix of order 3 has similar structure as a general doubly stochastic matrix of order 3.**

According to the **Birkhoff's theorem**, every $n \times n$ doubly stochastic matrix can be expressed as a convex combination of permutation matrices of order n.

For the case of $n = 3$, maximum there can be $3! = 6$ permutation matrices.

In this study, Using MATLAB, we have randomly generated $2,00{,}000$ doubly stochastic matrices of order 3 of different convex combinations of these permutation matrices from 2 to 6. Since a penta-diagonal matrix of order 3 is same as a general doubly stochastic matrix of order 3, the eigenvalue distributions remain identical regardless of the specific combination of permutation matrices used.

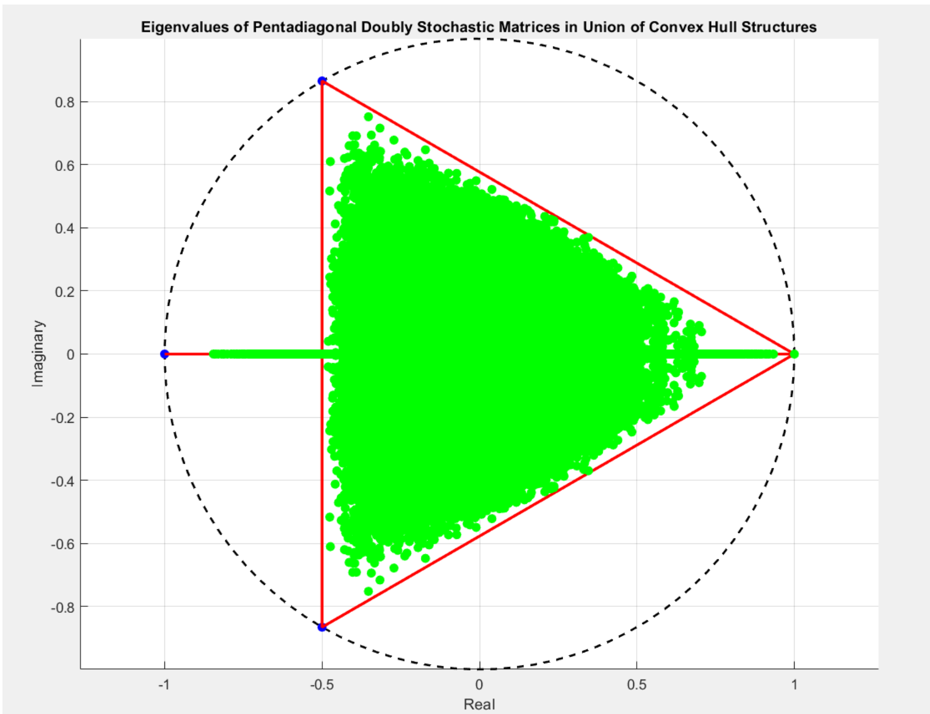

Figure 1: Distribution of Eigenvalues of 3×3 Doubly Stochastic Matrices.

Observation :- Let π_1, π_2, and π_3 denote the sets of 1^{st}, 2^{nd}, and 3^{rd} roots of unity, respectively. Each set lies on the complex unit circle:

- $\pi_1 = \{1\}$
- $\pi_2 = \{1, -1\}$
- $\pi_3 = \{1, \omega, \omega^2\}$ where $\omega = e^{2\pi i/3}$

Lets take the union of there convex hulls:

$$\omega_3 = \pi_1 \cup \pi_2 \cup \pi_3$$

The region ω_3 consists of:

- a point at 1,

- a line segment between 1 and -1,

- an equilateral triangle with vertices $1, \omega, \omega^2$ where $\omega = e^{2\pi i/3}$.

After plotting the eigenvalues of the doubly stochastic matrices of order 3 in the complex plane, we observed that **all eigenvalues lie strictly within the region $\boldsymbol{\omega_3}$**.
This suggests that the $\boldsymbol{\omega_3}$ act as a distribution boundary for the eigenvalues generated through different combinations of permutation matrices, satisfying the Perfect–Mirsky conjecture.

3.2 For Order 4

A general **4×4 penta-diagonal doubly stochastic matrix** is:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ 0 & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

According to the **Birkhoff's theorem**, every $n \times n$ doubly stochastic matrix can be expressed as a convex combination of permutation matrices of order n.
For the case of $n = 4$, maximum there can be $4! = 24$ permutation matrices.
But out of these 24, matrices having 'one' at (1,4) or (4,1) cannot generate a penta-diagonal doubly stochastic matrix.
So, out of 24, only 14 matrices are valid permutation matrices to generate a penta-diagonal doubly stochastic matrix.
Those are :-

$$P_1 = (1\ 3)(2\ 4), \quad P_2 = (1\ 3), \quad P_3 = (1\ 3\ 4\ 2), \quad P_4 = (1\ 3\ 2),$$

$$P_5 = (1\ 2\ 4\ 3), \quad P_6 = (1\ 2\ 3), \quad P_7 = (1\ 2)(3\ 4), \quad P_8 = (1\ 2),$$

$$P_9 = (2\ 4), \quad P_{10} = (2\ 4\ 3), \quad P_{11} = (2\ 3\ 4), \quad P_{12} = (2\ 3),$$

$$P_{13} = (3\ 4), \quad P_{14} = \text{identity}.$$

In this study, Using MATLAB, we have generated penta-diagonal doubly stochastic matrices of order 4 using convex combinations of valid permutation matrices in three phases:

i. Convex Combinations of Two Matrices (Pairs)

From 14 valid matrices, all possible ${}^{14}C_2 = 91$ pairs were considered. For each pair, 1,000 random convex combinations were generated, producing $91 \times 1{,}000 = 91{,}000$ matrices.

ii. Convex Combinations of Three Matrices (Triples)

All ${}^{14}C_3 = 364$ possible triples were examined. Each triple generated 1,000 random convex combinations, resulting in $364 \times 1{,}000 = 3,64{,}000$ matrices.

iii. General Combinations of Permutation Matrices (2 to 14)

We have randomly generated $2,00{,}000$ doubly stochastic matrices of order 4 of different convex combinations of these permutation matrices from 2 to 14.

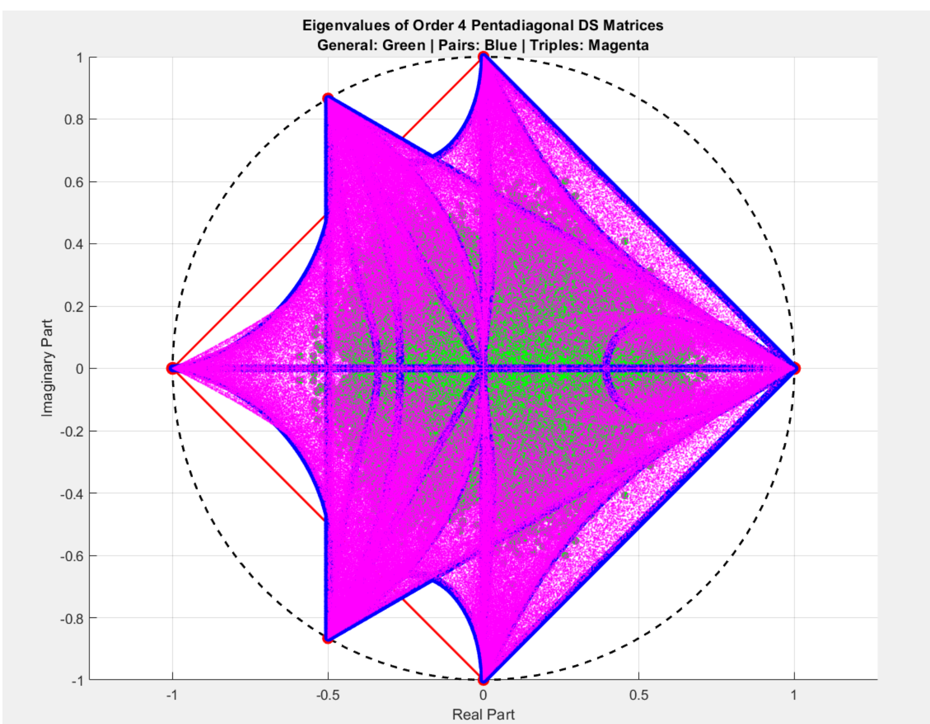

Figure 2: Distribution of Eigenvalues of 4×4 Penta-Diagonal Doubly Stochastic Matrices.

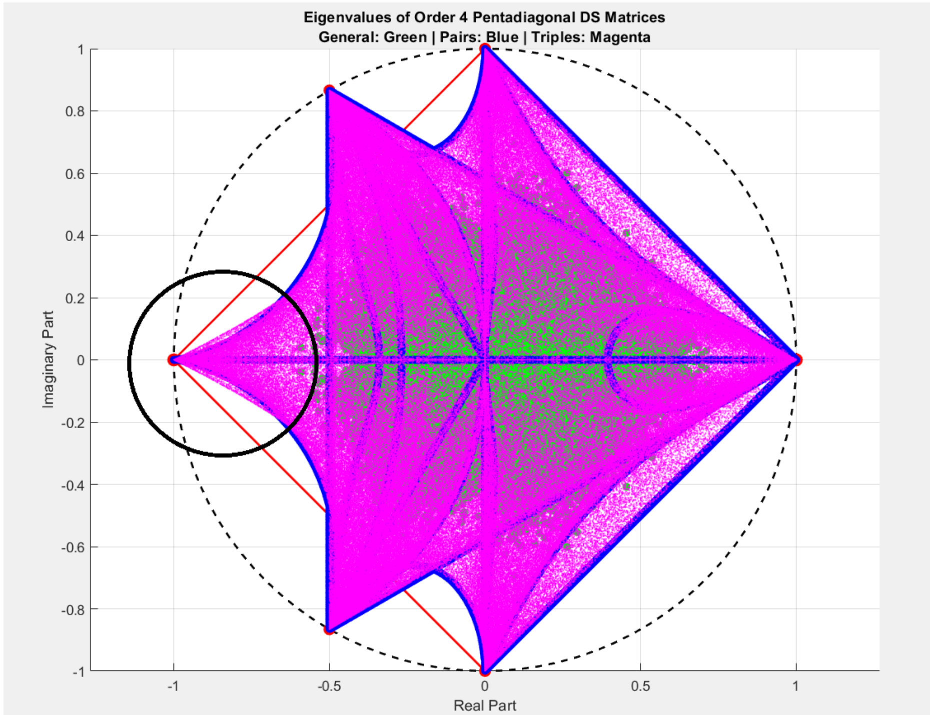

Figure 3: Black Circle shows the Exceptional areas in Fig 2.

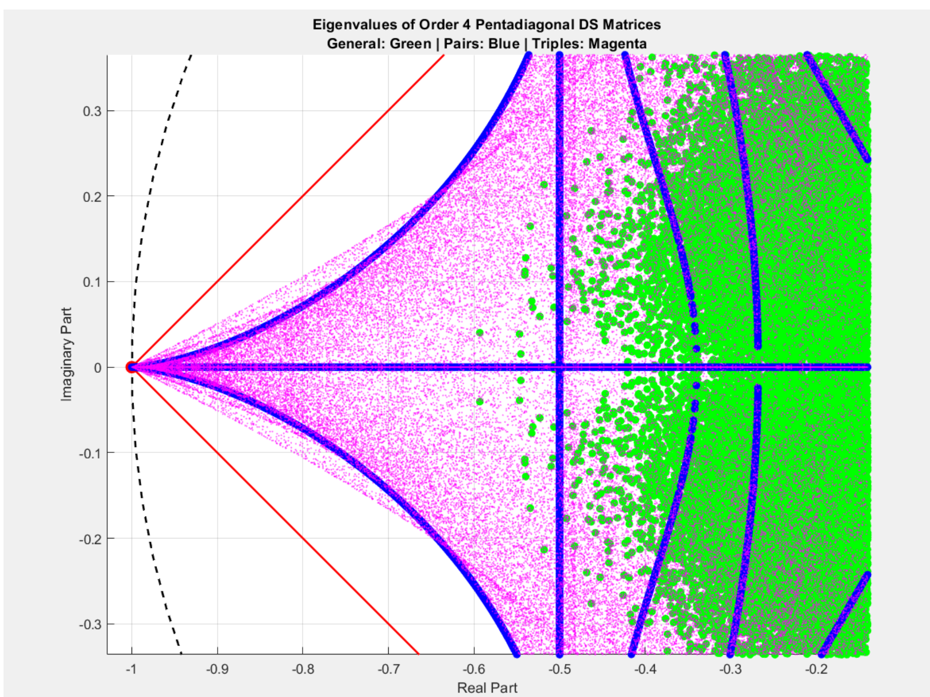

Figure 4: Zoomed in version of Fig 3.

Observation :- Let π_1, π_2, π_3 and π_4 denote the sets of 1^{st}, 2^{nd}, 3^{rd} and 4^{th} roots of unity, respectively. Each set lies on the complex unit circle:

- $\pi_1 = \{1\}$
- $\pi_2 = \{1, -1\}$
- $\pi_3 = \{1, \omega, \omega^2\}$ where $\omega = e^{2\pi i/3}$
- $\pi_4 = \{1, i, -1, -i\}$ where $i = \sqrt{-1}$

Lets take the union of there convex hulls:

$$\omega_4 = \pi_1 \cup \pi_2 \cup \pi_3 \cup \pi_4$$

The region ω_4 consists of:

- a point at 1 (from π_1),

- a line segment between 1 and -1 (from π_2),

- an equilateral triangle with vertices $1, \omega, \omega^2$ where $\omega = e^{2\pi i/3}$,

- a square with vertices $1, -1, i, -i$ where $i = \sqrt{-1}$.

After plotting the eigenvalues of the doubly stochastic matrices of order 4 in the complex plane, we have observed that :

A. The eigenvalues of doubly stochastic matrices lie strictly within the ω_4, as guaranteed by the Perfect–Mirsky conjecture. Since pentadiagonal doubly stochastic matrices form a strict subset of all doubly stochastic matrices, certain portions near the boundary of the ω_4 remain unoccupied, resulting in a more restricted eigenvalue distribution.

B. Eigenvalues generated by pairs (in blue) form the complete boundary of the spectral region and the eigenvalues generated by triples (in magenta) and higher combinations (in green) lie strictly within the boundary.

In fact higher the combinations, more the eigenvalues concentrate towards the centre.

C. While result (B) holds generally, Figure 3 reveals a significant exception where eigenvalues generated by triples extends the boundary formed by pairs.

3.3 For Order 5

A general **5×5 penta-diagonal doubly stochastic matrix** is:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ 0 & a_{42} & a_{43} & a_{44} & a_{45} \\ 0 & 0 & a_{53} & a_{54} & a_{55} \end{bmatrix}$$

According to the **Birkhoff's theorem**, every $n \times n$ doubly stochastic matrix can be expressed as a convex combination of permutation matrices of order n.

For the case of $n = 5$, maximum there can be $5! = 120$ permutation matrices.

But out of these 120, matrices having 'one' at (1,4) or (1,5) or (2,5) or (4,1) or (5,1) or (5,2) cannot generate a penta-diagonal doubly stochastic matrix.

So, out of 120, only 31 matrices are valid permutation matrices to generate a penta-diagonal doubly stochastic matrix.

Those are :-

$P_1 = (1\ 3)(2\ 4)$, $P_2 = (1\ 3)(4\ 5)$, $P_3 = (1\ 3)$, $P_4 = (1\ 3\ 5\ 4\ 2)$

$P_5 = (1\ 3\ 4\ 2)$, $P_6 = (1\ 3\ 2\ 4\ 5)$, $P_7 = (1\ 3\ 2\ 4)$, $P_8 = (1\ 3\ 5)(2\ 4)$

$P_9 = (1\ 3\ 4\ 2)$, $P_{10} = (1\ 3\ 4)(2\ 5)$, $P_{11} = (1\ 3\ 4)$, $P_{12} = (1\ 3\ 5\ 2\ 4)$,

$P_{13} = (1\ 3\ 5\ 2)$, $P_{14} = (1\ 3\ 4\ 5\ 2)$ $P_{15} = (1\ 3\ 4\ 2\ 5)$, $P_{16} = (1\ 3\ 2\ 5\ 4)$,

$P_{17} = (1\ 3\ 2\ 4\ 5)$, $P_{18} = (2\ 4\ 5)$ $P_{19} = (2\ 4)$, $P_{20} = (2\ 4\ 5\ 3)$

$P_{21} = (2\ 4\ 3)$, $P_{22} = (2\ 3\ 5\ 4)$, $P_{23} = (2\ 3\ 4)$, $P_{24} = (2\ 3\ 4\ 5)$

$P_{25} = (2\ 3\ 4)$, $P_{26} = (3\ 5\ 4)$, $P_{27} = (3\ 5)$, $P_{28} = (3\ 4\ 5)$

$P_{29} = (3\ 4)$, $P_{30} = (4\ 5)$, $P_{31} =$ identity.

In this study, Using MATLAB, we have generated penta-diagonal doubly stochastic matrices of order 5 using convex combinations of valid permutation matrices in three phases:

i. Convex Combinations of Two Matrices (Pairs)

From 31 valid matrices, all possible ${}^{31}C_2 = 465$ pairs were considered. For each pair, 200 random convex combinations were generated, producing $465 \times 200 = 93{,}000$ matrices.

ii. Convex Combinations of Three Matrices (Triples)

All ${}^{31}C_3 = 4{,}495$ possible triples were examined. Each triple generated 100 random convex combination, resulting in $4{,}495 \times 100 = 4, 49{,}500$ matrices.

iii. General Combinations of Permutation Matrices (2 to 31)

We have randomly generated $2, 00{,}000$ doubly stochastic matrices of order 5 of different convex combinations of these permutation matrices from 2 to 31.

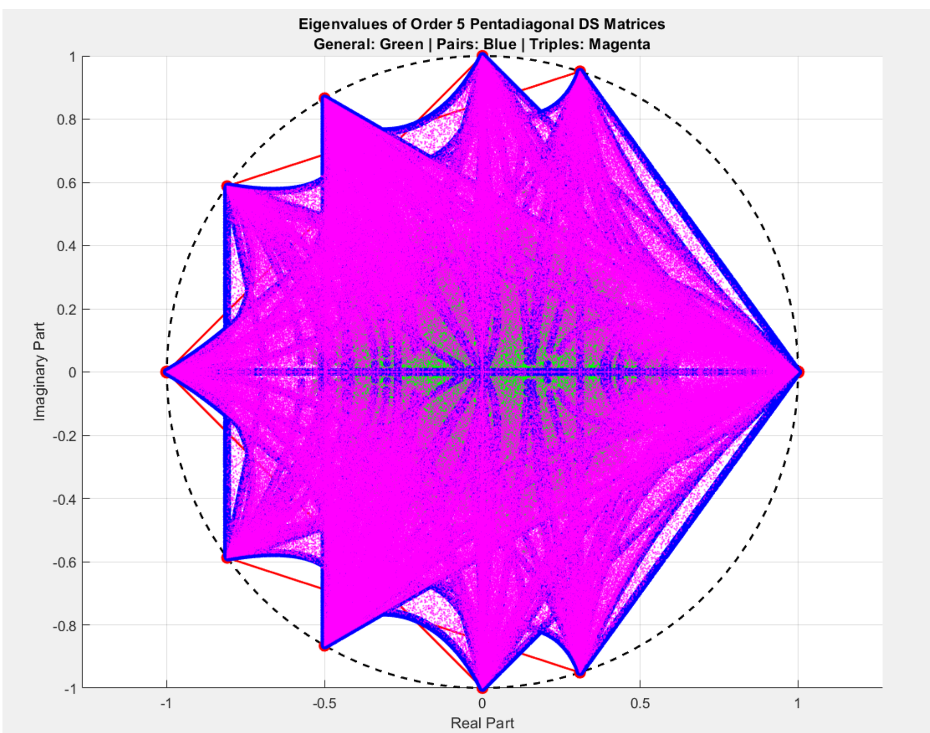

Figure 5: Distribution of Eigenvalues of 5×5 Penta-Diagonal Doubly Stochastic Matrices.

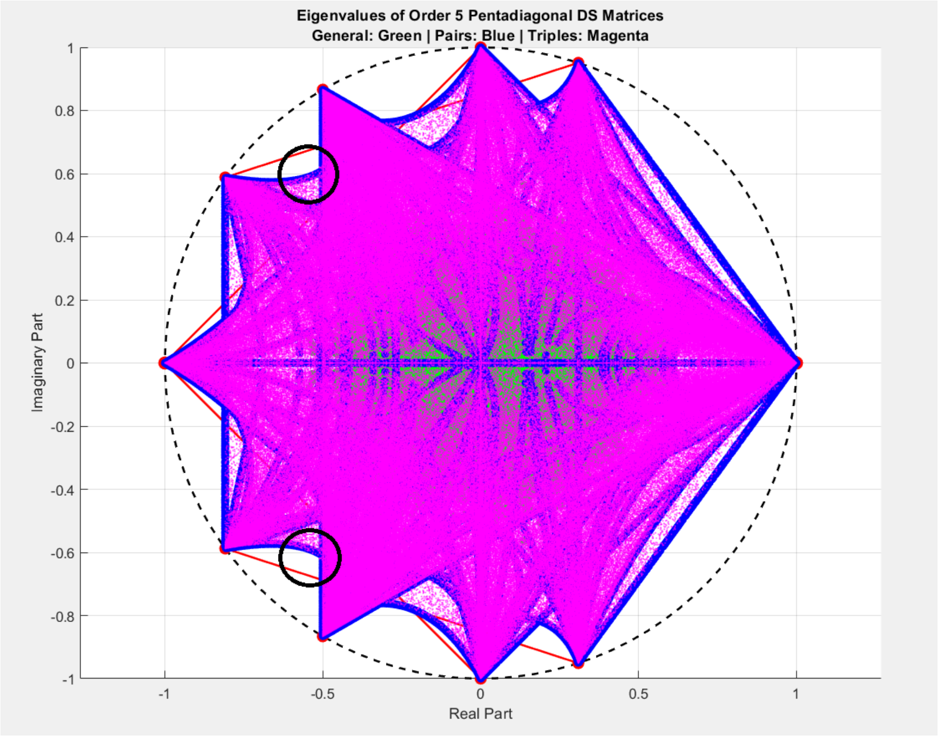

Figure 6: Black Circles shows the Exceptional areas in Fig 5.

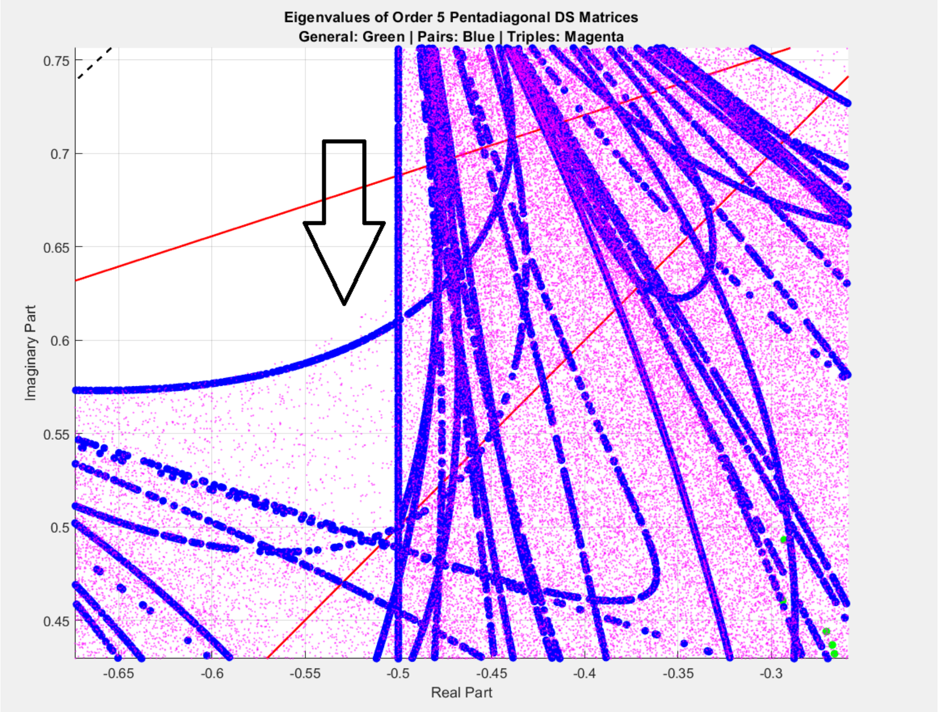

Figure 7: Zoomed in version of Fig 6 (above the real axis).

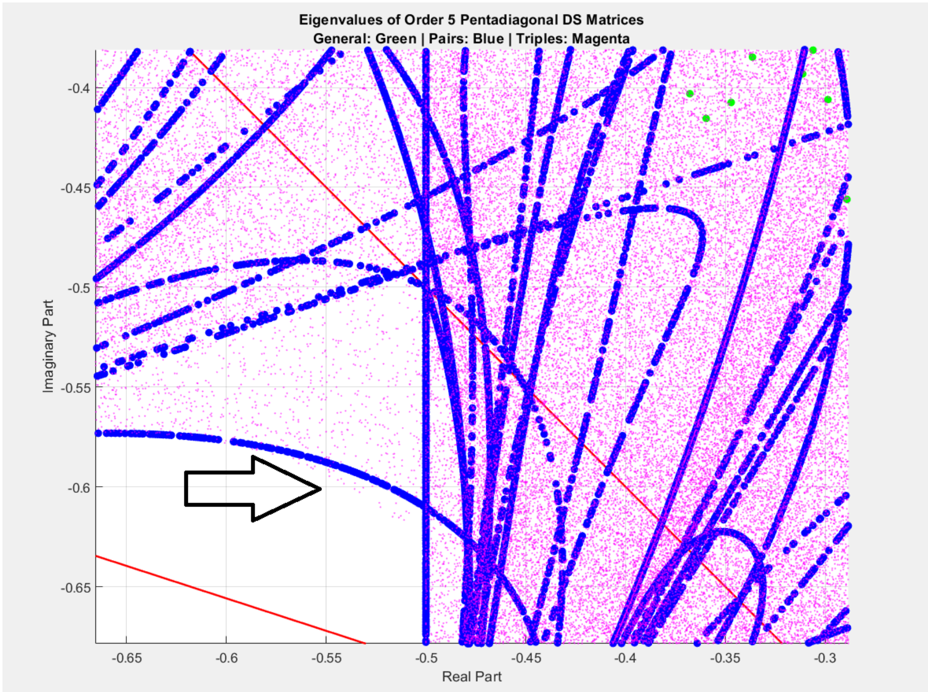

Figure 8: Zoomed in version of Fig 6 (below the real axis).

Observation :- Let π_1, π_2, π_3, π_4 and π_5 denote the sets of 1^{st}, 2^{nd}, 3^{rd}, 4^{th} and 5^{th}roots of unity, respectively. Each set lies on the complex unit circle:

- $\pi_1 = \{1\}$
- $\pi_2 = \{1, -1\}$
- $\pi_3 = \{1, \omega, \omega^2\}$ where $\omega = e^{2\pi i/3}$
- $\pi_4 = \{1, i, -1, -i\}$ where $i = \sqrt{-1}$
- $\pi_5 = \left\{1, e^{2\pi i/5}, e^{4\pi i/5}, e^{6\pi i/5}, e^{8\pi i/5}\right\}$

Lets take the union of there convex hulls:

$$\omega_5 = \pi_1 \cup \pi_2 \cup \pi_3 \cup \pi_4 \cup \pi_5$$

The region ω_5 consists of:

- a point at 1 (from π_1),

- a line segment between 1 and -1 (from π_2),

- an equilateral triangle with vertices $1, \omega, \omega^2$ where $\omega = e^{2\pi i/3}$,

- a square with vertices $1, -1, i, -i$ where $i = \sqrt{-1}$,

- a regular pentagon with vertices $\{1, e^{2\pi i/5}, e^{4\pi i/5}, e^{6\pi i/5}, e^{8\pi i/5}\}$.

After plotting the eigenvalues of the doubly stochastic matrices of order 5 in the complex plane, we have observed that :

A. The eigenvalues of doubly stochastic matrices lie strictly within the ω_5 (with some exceptions for order 5), as guaranteed by the Perfect–Mirsky conjecture. Since pentadiagonal doubly stochastic matrices form a strict subset of all doubly stochastic matrices, certain portions near the boundary of the ω_5 remain unoccupied, resulting in a more restricted eigenvalue distribution.

B. Eigenvalues generated by pairs (in blue) form the complete boundary of the spectral region and the eigenvalues generated by triples (in magenta) and higher combinations (in green) lie strictly within the boundary.

In fact higher the combinations, more the eigenvalues concentrate towards the centre.

C. While result (B) holds generally, Figure 6 reveals a significant exception where some eigenvalues generated by triples extends the boundary formed by pairs.

3.4 For Order 6

A general **6×6 penta-diagonal doubly stochastic matrix** is:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & a_{24} & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} & 0 \\ 0 & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ 0 & 0 & a_{53} & a_{54} & a_{55} & a_{56} \\ 0 & 0 & 0 & a_{64} & a_{65} & a_{66} \end{bmatrix}$$

According to the **Birkhoff's theorem**, every $n \times n$ doubly stochastic matrix can be expressed as a convex combination of permutation matrices of order n.

For the case of $n = 6$, maximum there can be $6! = 720$ permutation matrices.

But out of these 720, matrices having ‘one’ at (1,4) or (1,5) or (1,6) or (2,5) or (2,6) or (3,6) or (4,1) or (5,1) or (5,2) or (6,1) or (6,2) or (6,3) cannot generate a penta-diagonal doubly stochastic matrix.

So, out of 720, only 73 matrices are valid permutation matrices to generate a penta-diagonal doubly stochastic matrix.

Those are :-

$P_1 : (1\ 3)(2\ 4)(5\ 6)$	$P_2 : (1\ 3)(2\ 4)$	$P_3 : (1\ 3)(4\ 6)(5)$
$P_4 : (1\ 3)(4\ 6)$	$P_5 : (1\ 3)(4\ 5\ 6)$	$P_6 : (1\ 3)(4\ 5)$
$P_7 : (1\ 3)(4)(5\ 6)$	$P_8 : (1\ 3)$	$P_9 : (1\ 3\ 5)(2)(4\ 6)$
$P_{10} : (1\ 3\ 5)(4\ 6)$	$P_{11} : (1\ 3\ 5\ 4\ 2)(6)$	$P_{12} : (1\ 3\ 5\ 4\ 2)$
$P_{13} : (1\ 3\ 2)(4\ 6)(5)$	$P_{14} = (1\ 3\ 2)(4\ 6)$	$P_{15} = (1\ 3\ 2)(4\ 5\ 6)$
$P_{16} = (1\ 3\ 2)(4\ 5)$	$P_{17} = (1\ 3\ 2)(4)(5\ 6)$	$P_{18} = (1\ 3\ 2)$
$P_{19} = (1\ 3)(2\ 4\ 6)(5)$	$P_{20} = (1\ 3)(2\ 4\ 6)$	$P_{21} = (1\ 3)(2\ 4)(5\ 6)$
$P_{22} = (1\ 3)(2\ 4)$	$P_{23} = (1\ 3)(2\ 5\ 6)(4)$	$P_{24} = (1\ 3)(2\ 5\ 6)$
$P_{25} = (1\ 3)(2\ 5)(4\ 6)$	$P_{26} = (1\ 3)(2\ 5)$	$P_{27} = (1\ 3)(2\ 6\ 5)(4)$
$P_{28} = (1\ 3)(2\ 6\ 5)$	$P_{29} = (1\ 3\ 5)(2)(4\ 6)$	$P_{30} = (1\ 3\ 5)(4\ 6)$
$P_{31} = (1\ 3\ 5\ 4\ 2)(6)$	$P_{32} = (1\ 3\ 5\ 4\ 2)$	$P_{33} = (1\ 3\ 2)(4\ 6)(5)$
$P_{34} = (1\ 3\ 2)(4\ 6)$	$P_{35} = (1\ 3\ 2)(4\ 5\ 6)$	$P_{36} = (1\ 3\ 2)(4\ 5)$
$P_{37} = (1\ 3\ 2)(4)(5\ 6)$	$P_{38} = (1\ 3\ 2)$	$P_{39} = (1\ 3)(2\ 4\ 6)(5)$
$P_{40} = (1\ 3)(2\ 4\ 6)$	$P_{41} = (1\ 3)(2\ 4)(5\ 6)$	$P_{42} = (1\ 3)(2\ 4)$
$P_{43} = (1)(2\ 4)(3\ 5)$	$P_{44} = (1)(2\ 4)(3)(5\ 6)$	$P_{45} = (1)(2\ 4)$
$P_{46} = (1)(2\ 4\ 6)(3\ 5)$	$P_{47} = (1)(2\ 4\ 6)$	$P_{48} = (1)(2\ 4)(3\ 5\ 6)$
$P_{49} = (1)(2\ 4)(3\ 5)$	$P_{50} = (1)(2\ 5\ 6)(3\ 4)$	$P_{51} = (1)(2\ 5\ 6)$
$P_{52} = (1)(2\ 5)(3\ 4\ 6)$	$P_{53} = (1)(2\ 5)(3\ 4)$	$P_{54} = (1)(2\ 6\ 5)(3\ 4)$
$P_{55} = (1)(2\ 6\ 5)$	$P_{56} = (1)(2\ 6)(3\ 4\ 5)$	$P_{57} = (1)(2\ 6)(3\ 4)$

$P_{58} = (1)(2\ 5\ 6\ 4\ 3)$ $\quad P_{59} = (1)(2\ 5\ 6\ 4)$ $\quad P_{60} = (1)(2)(3\ 5)(4\ 6)$

$P_{61} = (1)(2)(3\ 5)$ $\quad P_{62} = (1)(2)(3\ 5\ 6\ 4)$ $\quad P_{63} = (1)(2)(3\ 5\ 6)$

$P_{64} = (1)(2)(3\ 4\ 6)(5)$ $\quad P_{65} = (1)(2)(3\ 4\ 6)$ $\quad P_{66} = (1)(2)(3\ 4)(5\ 6)$

$P_{67} = (1)(2)(3\ 4)$ $\quad P_{68} : (1)(2)(3)(4\ 6)(5)$ $\quad P_{69} = (1)(2)(3)(4\ 6)$

$P_{70} = (1)(2)(3)(4\ 5\ 6)$ $\quad P_{71} = (1)(2)(3)(4\ 5)$ $\quad P_{72} = (1)(2)(3)(4)(5\ 6)$

$P_{73} =$ identity.

In this study, Using MATLAB, we have generated penta-diagonal doubly stochastic matrices of order 6 using convex combinations of valid permutation matrices in three phases:

i. Convex Combinations of Two Matrices (Pairs)

From 73 valid matrices, all possible ${}^{73}C_2 = 2{,}628$ pairs were considered. For each pair, 50 random convex combinations were generated, producing $2{,}628 \times 50 = 1, 31{,}400$ matrices.

ii. Convex Combinations of Three Matrices (Triples)

All ${}^{73}C_3 = 62{,}196$ possible triples were examined. Each triple generated 10 random convex combination, resulting in $62{,}196 \times 10 = 6, 21{,}960$ matrices.

iii. General Combinations of Permutation Matrices (2 to 73)

we have randomly generated $2, 00{,}000$ doubly stochastic matrices of order 6 of different convex combinations of these permutation matrices from 2 to 73.

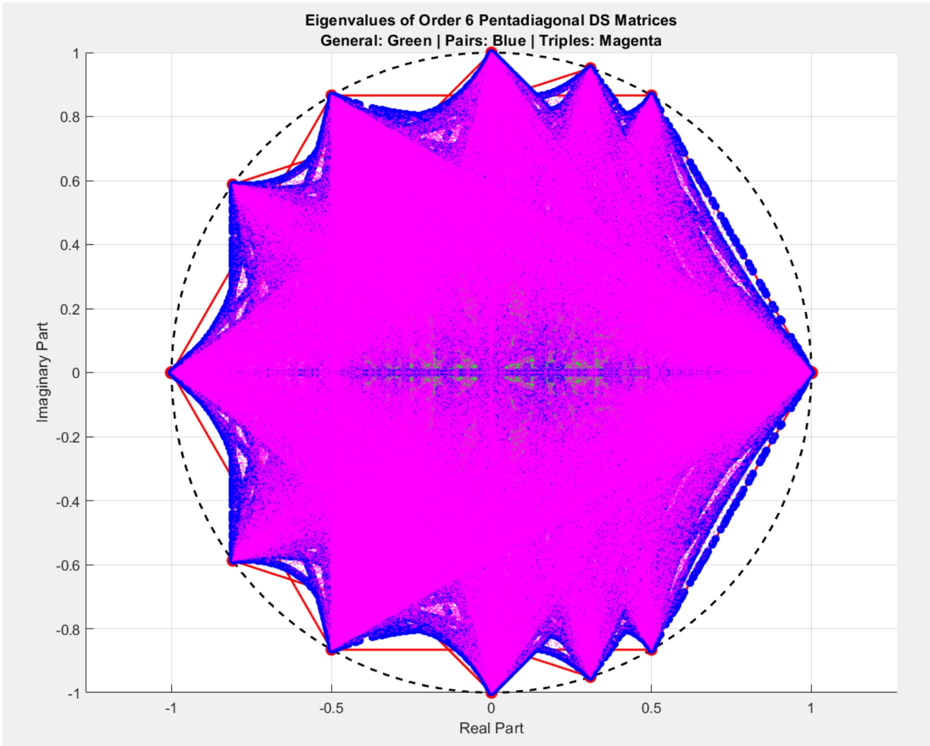

Figure 9: Distribution of Eigenvalues of 6×6 Penta-Diagonal Doubly Stochastic Matrices.

Observation :- Let π_1, π_2, π_3, π_4, π_5 and π_6 denote the sets of 1^{st}, 2^{nd}, 3^{rd}, 4^{th}, 5^{th} and 6^{th} roots of unity, respectively. Each set lies on the complex unit circle:

- $\pi_1 = \{1\}$
- $\pi_2 = \{1, -1\}$
- $\pi_3 = \left\{1, e^{2\pi i/3}, e^{4\pi i/3}\right\}$
- $\pi_4 = \left\{1, e^{\pi i/2}, e^{\pi i}, e^{3\pi i/2}\right\}$
- $\pi_5 = \left\{1, e^{2\pi i/5}, e^{4\pi i/5}, e^{6\pi i/5}, e^{8\pi i/5}\right\}$
- $\pi_6 = \left\{1, e^{2\pi i/6}, e^{4\pi i/6}, e^{6\pi i/6}, e^{8\pi i/6}, e^{10\pi i/6}\right\}$

Lets take the union of there convex hulls:

$$\omega_6 = \pi_1 \cup \pi_2 \cup \pi_3 \cup \pi_4 \cup \pi_5 \cup \pi_6$$

The region ω_6 consists of:

- a point at 1 (from π_1),

- a line segment between 1 and -1 (from π_2),

- an equilateral triangle with vertices $1, \omega, \omega^2$ where $\omega = e^{2\pi i/3}$,

- a square with vertices $1, -1, i, -i$ where $i = \sqrt{-1}$,

- a regular pentagon with vertices $\{1, e^{2\pi i/5}, e^{4\pi i/5}, e^{6\pi i/5}, e^{8\pi i/5}\}$,

- a regular hexagon with vertices $\{1, e^{2\pi i/6}, e^{4\pi i/6}, e^{6\pi i/6}, e^{8\pi i/6}, e^{10\pi i/6}\}$.

After plotting the eigenvalues of the doubly stochastic matrices of order 6 in the complex plane, we have observed that :

A. The eigenvalues of doubly stochastic matrices lie strictly within the ω_6, as guaranteed by the Perfect–Mirsky conjecture. Since pentadiagonal doubly stochastic matrices form a strict subset of all doubly stochastic matrices, certain portions near the boundary of the ω_6 remain unoccupied, resulting in a more restricted eigenvalue distribution.

B. Eigenvalues generated by pairs (in blue) form the complete boundary of the spectral region and the eigenvalues generated by triples (in magenta) and higher combinations (in green) lie strictly within the boundary.

In fact higher the combinations, more the eigenvalues concentrate towards the centre.

C. NO EXCEPTION arises for result (B) in order 6 and this pattern may continue for order ≥ 7.

4. Conclusion

4.1 Conclusion

This study explored the spectral behavior of penta-diagonal doubly stochastic matrices constructed from various convex combinations of permutation matrices. By analyzing the eigenvalue distributions across different matrix orders, a consistent and fascinating pattern emerged. For matrices of order n = 3 to 6, all eigenvalues were found to lie strictly within their respective spectral regions, denoted by ω_n.

For order n $\geq$ 4, a deeper examination revealed that matrices formed by pairwise combinations of permutation matrices that follow pentadiagonal pattern consistently generate the outer boundary of the spectral region. In contrast, eigenvalues arising from higher-order combinations—triples and beyond—remain strictly enclosed within this boundary, concentrating toward the centre as number of combinations of permutation matrices increases.

Interestingly, while this behavior generally held true across all observed cases, notable exceptions were identified for matrices of orders 4 and 5. In these instances, certain triples of permutation matrices produced eigenvalues that extended beyond the spectral boundary established by pairwise combinations. However, this anomaly disappears in higher dimensions: for order 6 and maybe beyond, the spectral boundary defined by pairwise combinations appears to be stable and exhaustive, with no violations observed.

These findings not only show a clear relationship between the structure of permutation matrices and the spectral characteristics of the resulting doubly stochastic matrices but also hint at deeper geometric and algebraic regularities that govern these systems. This work creates opportunities for future research and a better understanding of how eigenvalues behave in more complex stochastic systems.

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