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Semi-Analytical Solution for Eigenvalue Problems of Lattice Models with Boundary Conditions

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Synopsis

There exist closed-form expressions, for the limiting eigenvalues of an infinite k-periodic spatial lattice in any number of dimensions d. Additionally, there are semi-analytical extensions available for eigenvalues of such lattices of any given size n, which have free-free boundary conditions. These are based on the eigenvalues of tridiagonal k-Toeplitz matrices (representing chains and $d = 1$), and their tensor products or sums. The semi-analytical techniques for determining the eigenvalues of a lattice offer significant advantages over the direct numerical methods. The computational cost of these methods is significantly lower, with time complexity of $O(n)$ compared to $O(n^2)$ for direct numerical methods. Additionally, these methods provide higher accuracy for larger lattice sizes approaching the limiting case (i.e., $n > 100$). Another benefit of the semi-analytical approach is its numerical stability, which results from reducing the original eigenvalue problem of size nk to n eigenvalue problems each of size k. This reduction makes it feasible to use parallel computation when necessary. The accuracy of the semi-analytical method is compared to that of direct numerical methods by using special examples with high-condition numbers. If analytical methods for determining eigenvalues are unavailable, periodic boundary conditions are often used to reduce the size of numerical models that represent large systems. While such models converge to the limiting eigenvalues, closed-form solutions for these eigenvalues are highly useful. This highlights the importance of the closed-form solution for limiting eigenvalues. In addition, the fixed-fixed boundary conditions on a finite chain and their counterparts for periodic spatial lattices in higher dimensions ($d > 1$) are addressed using perturbations to tridiagonal k-Toeplitz matrices on their main diagonal. Semi-analytical methods for these cases are proposed by applying numerical methods only to update the few perturbed eigenvalues. An efficient extension is also presented for evaluating eigenvectors in the case of real eigenvalues, which is commonly required in physical systems.

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Semi-analytical solution for eigenvalue problems of lattice models with boundary conditions

A Thesis submitted for the degree of

MTech Research

by

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Abstract

Closed-form relations for limiting eigenvalues of an infinite k-periodic spatial lattice in any number of dimensions d, and its semi-analytical extensions for any given size n of the lattice with free-free boundary conditions, are known. These are based on the eigenvalues of tridiagonal k-Toeplitz matrices (representing chains and $d = 1$), and their tensor products or sums. These semi-analytical methods for eigenvalues incur drastically lower computing costs than the direct numerical methods i.e. $O(n)$ vs. $O(n^2)$ for the latter, and further they are more accurate for sufficiently large lattices approaching the limiting case ($n > 100$). This advantage in computing cost, accuracy, and numerical stability emerges as the original eigenvalue problem of nk in size is reduced to n eigenvalue problems each k in size, further making this approach very amenable to parallel computation when required. In this work, their errors in eigenvalues are compared with the errors of the direct numerical methods using special examples with high condition numbers. Secondly, in the absence of such analytical methods, one also resorts to periodic boundary conditions to limit the size of the numerical model representing a very large system. The convergence of numerical models with periodic boundary conditions to the limiting eigenvalues is highlighted, to emphasize the utility of the closed-form solution for the limiting eigenvalues. Thirdly, the fixed-fixed boundary conditions on a finite chain and their counterpart for periodic spatial lattices in higher dimensions ($d > 1$) are addressed using perturbations to tridiagonal k-Toeplitz matrices representing the first and last elements of the chain. Extensions of the semi-analytical methods for these cases by applying numerical methods only to update the few perturbed eigenvalues are proposed. An efficient extension for evaluating the eigenvectors in the case of real eigenvalues as required in most physical systems is also presented.

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Notations

M_k : k-toeplitz tridiagonal matrix

λ : Eigenvalue

I : Identity matrix

γ : Negative of the determinant of the k-toeplitz tridiagonal matrix

$A_{free-free}$: Adjacency matrix of the free-free lattice

$A_{periodic}$: Adjacency matrix lattice under periodic boundary condition

A_{fixed} : Adjacency matrix lattice under fixed boundary condition

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Chapter 1

Introduction: Methods for Eigenvalue Problems

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Chapter-outline

Numerical methods for the solution of eigenvalue problems are introduced, and we conclude with an outline of the thesis.

1.1 Summary of Numerical Methods for Eigenvalue Problems

An eigenvalue problem can be written as

$$Ax = \lambda x \tag{1.1}$$

Here A is a square matrix, $A \in C^{m \times m}$, $\lambda \in C$ and $x \in C^m$. λ is one of the eigenvalue of A and x is the eigenvector of A corresponding to the eigenvalue λ.

The characteristic polynomial of a square matrix can be defined as

$$det(A - \lambda I) = 0 \tag{1.2}$$

λ, the eigenvalues of the square matrix A, are given by the solutions of the characteristic polynomial. Since the polynomial root-finding problem is ill-conditioned, we can't find eigenvalues using the polynomial root-finding approach. So any eigenvalue solver must be iterative.

Theorem[1]: *For any $m \geq 5$, there is a polynomial $p(z)$ of degree m with rational coefficients that has real root $p(r) = 0$ with the property that r can't be written using any expression involving rational numbers, addition, subtraction, multiplication, division, and kth roots.*

There are different types of eigenvalue algorithms. The power iteration algorithm finds the largest eigenvalue of the matrix and is only applicable to real symmetric matrices. Both inverse iteration and rayleigh quotient iteration work based on the initial guess and that eigenvalue will be found which is closest to the initial guess. Whereas the QR algorithm and simultaneous iteration give the eigenspectra of the square matrix.

1.1.1 Power methods (Power Iteration, Inverse Power, and Rayleigh Quotient Iterations)

Power Iteration Algorithm

The power Iteration [2] algorithm gives the largest eigenvalue of the matrix and the corresponding eigenvector. Power Iteration is limited to real symmetric matrices.

Algorithm 1 Power Iteration Algorithm

Require: Some vector $v^{(0)}$ with$||v^{(0)}||$ =1
  for $k = 1, 2...$ **do**
    $w \leftarrow Av^{(k-1)}$
    $v^{(k)} \leftarrow w/||w||$
    $\lambda^{(k)} \leftarrow (v^{(k)})^T Av^{(k)}$
  end for

Convergence Relation for Power Iteration [1]

The initial eigenvector, $v^{(0)}$ be the linear combination of the orthonormal eigenvectors q_i.

$$v^{(0)} = a_1 q_1 + a_2 q_2 + ... + a_m q_m \tag{1.3}$$

$v^{(k)}$ is the multiple of $Av^{(0)}$, So we can write,

$$\begin{aligned} v^{(k)} &= c_k A^k v^{(0)} \\ &= c_k(a_1\lambda_1^k q_1 + a_2\lambda_2^k q_2 + ... + a_m\lambda_m^k q_m) \\ &= c_k\lambda_1^k(a_1 q_1 + a_2(\lambda_2/\lambda_1)^k q_2 + ... + a_m(\lambda_m/\lambda_1)^k q_m) \end{aligned} \tag{1.4}$$

From the above equation, we reach the following conclusion[1].

Suppose $|\lambda_1| > |\lambda_2| \geq ..... \geq |\lambda_m| \geq 0$ and $q_1^T v^{(0)} \neq 0$. Then Power Iteration algorithm satisfies the following relation

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$$||v^{(k)} - \pm q_1|| = O(\left|\frac{\lambda_2}{\lambda_1}\right|^k) \tag{1.5}$$

$$|\lambda^{(k)} - \lambda_1| = O(\left|\frac{\lambda_2}{\lambda_1}\right|^{2k}) \tag{1.6}$$

When $|\lambda_2|$ is closer to $|\lambda_1|$, the convergence of the power iteration is slow and when $|\lambda_1| >> |\lambda_2|$, power iteration converge very fast.

Inverse Iteration with Shift

In inverse iteration [3], an initial guess for the eigenvalue is given and that eigenvalue will be found which is closest to the initial guess. This algorithm is only applicable to real symmetric matrices.

Algorithm 2 Inverse Iteration Algorithm

Require: Some vector $v^{(0)}$ with$||v^{(0)}||$ =1
  for $k = 1, 2...$ **do**
    solve $(A - \mu I)w = v^{(k-1)}$ for w
    $v^{(k)} \leftarrow w/||w||$
    $\lambda^{(k)} \leftarrow (v^{(k)})^T A v^{(k)}$
  end for

$\lambda^{(k)}$ and $v^{(k)}$ are the eigenvalue and eigenvector calculated using inverse iteration.

Convergence Relation for Inverse Iteration

The initial eigenvector, $v^{(0)}$ be the linear combination of the orthonormal eigenvectors q_i.

$$v^{(0)} = a_1 q_1 + a_2 q_2 + ... + a_m q_m \tag{1.7}$$

$v^{(k)}$ is the multiple of $(A - \mu I)v^{(0)}$, So we can write,

$$\begin{aligned} v^{(k)} &= c_k (A - \mu I)^k v^{(0)} \\ &= c_k [a_1 (\lambda_1 - \mu)^k q_1 + a_2 (\lambda_2 - \mu)^k q_2 + ... + a_m (\lambda_m - \mu)^k q_m] \\ &= c_k (\lambda_1 - \mu)^k [a_1 q_1 + a_2 \frac{(\lambda_2 - \mu)^k}{(\lambda_1 - \mu)^k} q_2 + ... + a_m \frac{(\lambda_m - \mu)^k}{(\lambda_1 - \mu)^k} q_m] \end{aligned} \tag{1.8}$$

From the above equation, we reach the following conclusion.

Suppose λ_J is the closest eigenvalue to μ and λ_K is the second closest, that is $|\mu - \lambda_J| < |\mu - \lambda_K| \leq |\mu - \lambda_j|$ for each $j \neq J$. Suppose ${q_J}^T v^{(0)} \neq 0$, then Inverse Iteration satisfy the following relation [1].

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$$||v^{(k)} - \pm q_1|| = O(\left|\frac{\mu - \lambda_J}{\mu - \lambda_K}\right|^k) \tag{1.9}$$

$$|\lambda^{(k)} - \lambda_J| = O(\left|\frac{\mu - \lambda_J}{\mu - \lambda_K}\right|^{2k}) \tag{1.10}$$

Rayleigh Quotient Iteration

Rayleigh Quotient, $r(x)$ of a vector x is defined (with respect to A) by the given below equation [4].

$$r(x) = \frac{x^T A x}{x^T x} \tag{1.11}$$

Rayleigh Quotient algorithm [5] extends the idea of inverse iteration by using the Rayleigh Quotient and is limited to real symmetric matrices.

Algorithm 3 Rayleigh Quotient Algorithm

Require: Some vector $v^{(0)}$ with $||v^{(0)}|| = 1$ and $\lambda^{(0)} = v^{(0)^T} A v^{(0)}$ = corresponding Rayleigh Quotient.
for $k = 1, 2...$ **do**
solve $(A - \lambda^{(k-1)} I)w = v^{(k-1)}$ for w
$v^{(k)} \leftarrow w/||w||$
$\lambda^{(k)} \leftarrow (v^{(k)})^T A v^{(k)}$
end for

Convergence Relation for Rayleigh Quotient Iteration

The convergence equation of the Rayleigh Quotient algorithm is given below [1].

$$||v^{(k+1)} - \pm q_J|| = O(||v^{(k)} - \pm q_J||^3) \tag{1.12}$$

$$|\lambda^{(k+1)} - \lambda_J| = O(|\lambda^{(k)} - \lambda_J|^3) \tag{1.13}$$

1.1.2 QR Algorithm

QR algorithm [6] gives the eigenspectra of the square matrix, A. It combines both the power method, the Rayleigh quotient iteration, and the QR factorization [7].

Unshifted QR Algorithm

This algorithm [8] converges to upper triangular if A is arbitrary, and diagonal if A is hermitian.

Output: Upper triangular R having the same eigenvalues of A.

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Algorithm 4 Unshifted QR Algorithm

for $k = 1, 2...$ **do**
  $A^{(0)} \leftarrow A$
  $A^{(k-1)} \leftarrow Q^{(k)}R^{(k)}$
  $A^{(k)} \leftarrow R^{(k)}Q^{(k)}$
  $\underline{Q^{(k)}} \leftarrow Q^{(1)}Q^{(2)}....Q^{(k)}$
  $\underline{R^{(k)}} \leftarrow R^{(k)}R^{(k-1)}....R^{(1)}$
end for

The eigenvalues of matrix A are diagonal elements of matrix R.

Convergence Relation for Unshifted QR Algorithm [1]

Let the QR algorithm be applied to a real symmetric matrix A whose eigenvalues satisfy $\lambda_1 > \lambda_2 > .... > \lambda_n$ and whose corresponding eigenvector matrix Q has all non-singular leading principal minors. Then as $k \to \infty$, $A^{(k)}$ converges linearly with constant $max_k|\lambda_{k+1}|/|\lambda_k|$ to $diag(\lambda_1, ...\lambda_n)$, and $\underline{Q^{(k)}}$ converges at the same rate to Q.

$$|a_{j,j}^{(k)} - \lambda_j| = O(C^{(k)}) \tag{1.14}$$

$$|q_j^{(k)} - \pm q_j| = O(C^{(k)}) \tag{1.15}$$

For each j with $1 \leq j \leq n$, where $C < 1$ is the constant $max_k|\lambda_{k+1}|/|\lambda_k|$.

Practical QR Algorithm

The convergence of the unshifted QR algorithm can be painfully slow. So we need shifted QR algorithm[9].

Output: Upper triangular R having the eigenvalues of A.

Algorithm 5 Practical QR Algorithm

Require: $A^{(0)}$. ▷ $(Q^{(0)})^T A^{(0)} Q^{(0)} = A$, $A^{(0)}$ is a tridiagonalization of A
for $k = 1, 2...$ **do**
  Pick a shift μ^k ▷ e.g: choose $\mu^k = A_{m,m}^{k-1}$
  $Q^{(k)}R^{(k)} \leftarrow A^{(k-1)} - \mu^k I$
  $A^{(k-1)} \leftarrow Q^{(k)}R^{(k)}$ ▷ QR factorization of $A^{(k-1)} - \mu^k I$
  $A^{(k)} = R^{(k)}Q^{(k)} + \mu^k I$ ▷ Recombine factors in reverse order
  If any off-diagonal $A_{j,j+1}$ close to zero: set $A_{j,j+1} = A_{j+1,j} = 0$, $A = \begin{bmatrix} A1 & 0 \\ 0 & A2 \end{bmatrix}$
  $\underline{R^{(k)}} \leftarrow R^{(k)}R^{(k-1)}....R^{(1)}$
end for
Apply the QR algorithm on $A1$ and $A2$.

Since the eigenvalues of the upper triangular matrix are its diagonal entries, the

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eigenvalues of matrix A are diagonal entries of R. The shifted QR algorithm converges in cubic rate [10].

1.1.3 Simultaneous Iteration

Simultaneous Iteration [11] is a generalized version of the power method. This method finds an invariant subspace corresponding to the first few dominant eigenvalues.

Output: orthogonal Q spanning the eigenspace of A.

Algorithm 6 Simultaneous Iteration Algorithm

Require: Pick $Q^{(0)} \in R^{m \times n}$ with orthonormal columns
  for $k = 1, 2...$ **do**
    $Z \leftarrow AQ^{(k-1)}$
    $Q^{(k)}R^{(k)} \leftarrow Z$ ▷ Reduced QR factorization of Z
  end for

Like the unshifted QR algorithm, simultaneous iteration also converges at a linear rate [12].

1.2 Outline of the Thesis

In chapter-2, the earlier work on the limiting sets of eigenvalues of the tridiagonal k-Toeplitz matrices and their approximations for the finite size of the matrix are discussed.

In chapter-3, the relevant boundary conditions of lattices, and the corresponding perturbations required in the entries of the tridiagonal k-Toeplitz matrix are explained. A specific example of tight-binding models used in physical sciences is presented for motivation.

In chapter-4, the direct numerical methods and the above semi-analytical solutions are compared to highlight that the latter is not only more efficient but also more accurate for the tridiagonal k-Toeplitz matrices (i.e. a chain with free-free boundary).

In chapter-5, the closed-form expressions for the characteristic polynomials, of a perturbed tridiagonal k-Toeplitz matrix are derived, for different boundary conditions i.e. entries of the first two rows and the last two rows may have to be perturbed representing the boundary condition on the chain. We show that a general solution for the roots of these characteristic polynomials is intractable, unlike the free-free chain in the previous chapter. Hence we suggest a few methods for identifying and updating only the perturbed eigenvalues of the free-free chain due to the boundary conditions applied. In the case of a lattice, the corresponding perturbations apply to all the chains required to construct the lattice.

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In chapter-6, the numerical results of these approaches, and also the convergence of periodic boundary conditions typically used in numerical models, to the limiting eigenvalues are presented. These highlight the utility of the semi-analytical methods proposed.

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Chapter 2

Introduction to Semi-Analytical Solution for Eigenvalues of Tridiagonal k-Toeplitz Matrices

Chapter-outline

The earlier work on the limiting sets of eigenvalues of the tridiagonal k-Toeplitz matrices, and its approximations for a finite size of the matrix are presented.

Tridiagonal k-Toeplitz matrices are special tridiagonal matrices whose tridiagonal elements in the first k rows repeat after k rows [13]. They are of the form

$$M_k = \begin{bmatrix} a1 & x1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ y1 & a2 & x2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & y2 & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & a_k & x_k & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_k & a_1 & x_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & y_1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & y_{k-2} & a_{k-1} & x_{k-1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & y_{k-1} & a_k \end{bmatrix} \tag{2.1}$$

With periodicity constraint $M_k(i,i) = a_{(i_{mod}k)}$, $M_k(i,i+1) = x_{(i_{mod}k)}$ and $M_k(i+1,i) = y_{(i_{mod}k)}$. Here x_j,y_j, and a_j are complex numbers. Since polynomial root finding is an ill-conditioned problem, any eigenvalue solver must be iterative. The computational cost

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of finding eigenvalues of a matrix by built-in Python or Matlab functions is $o((nk)^2)$, where nk is the size of the matrix. Here k is the period and n is the number of blocks of the k-Toeplitz tridiagonal matrix.

In this section, we present a less computationally costly method [14] compared to builtin iterative methods [15], to find the eigenvalues of the k-Toeplitz tridiagonal matrix.

2.1 Characteristic Polynomial of Tridiagonal k-Toeplitz Matrix and Three-Term Recurrence Relation

Our objective in this section is to get a three-term recurrence relation of the characteristic polynomial of the matrix M_k of dimension $nk \times nk$, in terms of characteristic polynomials of matrices of dimensions $(n-1)k \times (n-1)k$ and $(n-2)k \times (n-2)k$.

Characteristic equation of matrix M_k can be written as $|M_k - \lambda I| = 0$ and let $-\lambda = z$, then

$$M_k - \lambda I = \begin{bmatrix} z+a1 & x1 & 0 & 0 & 0 \\ y1 & z+a2 & x2 & 0 & 0 \\ 0 & y2 & z+a3 & x3 & 0 \\ 0 & 0 & y3 & \ddots & \ddots \\ 0 & 0 & 0 & \ddots & \ddots \end{bmatrix} \tag{2.2}$$

Let $p_n(z)$ denote the characteristic polynomial of the matrix M_k of dimension $nk \times nk (n = 1, 2, \cdots)$ and $q_n(z)$ be the characteristic polynomial of the first principal submatrix of M_k eliminating first row and first column, which is of dimension $(nk-1) \times (nk-1)$. Similarly, let $r_n(z)$ be the characteristic polynomial of the second principal submatrix obtained by eliminating the first two rows and first two columns, and $x_j y_j = u_j$. Then we have,

$$p_n(z) = (z + a_1) q_n(z) - u_1 r_n(z) \tag{2.3}$$

In the matrix form, we have,

$$\begin{bmatrix} p_n(z) \\ q_n(z) \end{bmatrix} = \begin{bmatrix} z+a_1 & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} q_n(z) \\ r_n(z) \end{bmatrix}, \tag{2.4}$$

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$$\begin{bmatrix} p_n(z) \\ q_n(z) \end{bmatrix} = \begin{bmatrix} z+a_1 & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \dots \begin{bmatrix} z+a_k & -u_k \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ q_{n-1}(z) \end{bmatrix} \tag{2.5}$$

With the initial condition,

$$\begin{bmatrix} p_1(z) \\ q_1(z) \end{bmatrix} = \begin{bmatrix} z+a_1 & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \dots \begin{bmatrix} z+a_{k-1} & -u_{k-1} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_k \\ 1 \end{bmatrix} \tag{2.6}$$

Note that when $k = 1$, $q(z)$ and $r(z)$ will reduce to $p_{n-1}(z)$ and $p_{n-2}(z)$ without any loss of generality of the above. Similarly $r(z)$ will reduce to $p_{n-1}(z)$ in the case of $k = 2$. Let us denote,

$$U(i) = \begin{bmatrix} z+a_i & -u_i \\ 1 & 0 \end{bmatrix} \tag{2.7}$$

Also let $U_k = \prod_{i=1}^{k} U(i)$. Entries of U_k are polynomials in z, and for generality, we can denote them as,

$$U_k = \begin{bmatrix} A(z) & B(z) \\ C(z) & D(z) \end{bmatrix}, \tag{2.8}$$

$$\begin{bmatrix} p_n(z) \\ q_n(z) \end{bmatrix} = \begin{bmatrix} A(z) & B(z) \\ C(z) & D(z) \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ q_{n-1}(z) \end{bmatrix}. \tag{2.9}$$

where $A(z)$, $B(z)$, $C(z)$ and $D(z)$ are some polynomials of degree at most k.
From 2.6, we can derive Proposition 1, which is given below.

Proposition 1 : The characteristic polynomial of a tridiagonal k-Toeplitz matrix p_n satisfies the following recurrence relation, where k is the period and nk is the dimension of the matrix,

$$p_{n+1}(z) = Q_k(z)p_n(z) + \gamma p_{n-1}(z) \tag{2.10}$$

Here $Q_k = A(z) + D(z)$ is a polynomial of degree k, and $\gamma = -\prod_{i=1}^{k} u_i$

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$$p_{n+1}(z) = trace(U_k)p_n(z) - det(U_k)p_{n-1}(z) \tag{2.11}$$

We have $trace(U_k) = A(z) + D(z)$ and $det(U_k) = \prod_{i=1}^{k} u_i$. This proves the proposition with $Q_k(z) = trace(U_k)$ and $\gamma = -det(U_k)$.

2.1.1 Existence of a Limiting Set and the Nature of Convergence of Roots

Let $\zeta = \frac{p_1(z) - Q_k(z)}{\sqrt{\gamma}}$. Then we can write,

$$\lambda = \frac{-Q_k(z)}{\sqrt{\gamma}} \tag{2.12}$$

where λ is the eigenvalue of the $n \times n$ matrix given below.

$$\begin{bmatrix} \zeta & -1 & 0 & 0 & \dots & 0 \\ 1 & 0 & -1 & 0 & \dots & 0 \\ 0 & 1 & 0 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & \dots & 0 & 0 \end{bmatrix}_{n \times n} \tag{2.13}$$

Let $L_n(\zeta, \lambda)$ be the characteristic polynomial for the above matrix and $T_n(\lambda)$ be the characteristic polynomial for a skew-symmetric matrix given below,

$$\begin{bmatrix} 0 & -1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & -1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & -1 & 0 & \dots & 0 \\ 0 & \dots & \ddots & \vdots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{bmatrix}_{n \times n} \tag{2.14}$$

Using the above equations, We get

$$L_n(\zeta, \lambda) = \zeta T_n + T_{n-1} \tag{2.15}$$

When $L_n(\zeta, \lambda) = 0$,

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$$t_+^{2n+2} + \zeta t_+^{2n+1} + (-1)^{n+1}[\zeta t_+ - 1] = 0 \tag{2.16}$$

where $t_+ = \frac{-\lambda+\sqrt{\lambda^2+4}}{2}$

By applying Rouche's theorem on 2.16, we will get except two, all the other limiting zeros of $L_n(\zeta, \lambda)$ converge to the unit circle. So this represents among the solutions of $L_n(\zeta, \lambda)$, up to a maximum of 2k points that may lie outside the continuous curves.

***Theorem**: The limiting roots of polynomials in the three-term recurrence relation $p_{n+1}(z) = Q_k(z)p_n(z) + \gamma p_{n-1}(z)$ with z, γ in C, is a subset of $[z : Q_k(z) = 2i\sqrt{\gamma}sin\theta] \cup [z : Q_k(z) = \frac{\gamma}{p(z)} - p(z)]$, where $p(z) = p_1(z) - Q_k(z)$.*

2.1.2 Chebyshev Approximation

We can approximate zeros of $L_n(\zeta, \lambda)$ by the roots of T_n for finite large n. As the roots of T_n are distributed on the imaginary line just as the real roots of Chebyshev polynomials of the second kind, we call this Chebyshev approximation. The nk roots are the solution of z in the following equation, where λ_i with $i = 1, 2...n$ are the roots of T_n.

$$Q_k(z) = -\sqrt{\gamma}\lambda_i \tag{2.17}$$

Our nk eigenvalue problem can be converted into n number of k eigenvalue problem as in equation 2.17.

The computational complexity for the eigenvalue computation by this method is $O(nk^2)$.

2.1.3 Chebyshev-Taylor Approximation

Applying Taylor series approximation to 2.15 ,

$$Q_k(z^{'}) = -\sqrt{\gamma}\frac{\lambda_i T_n^{'}(\lambda_i) + \zeta\lambda_j T_{n-1}^{'}(\lambda_j)}{T_n^{'}(\lambda_i) + \zeta T_{n-1}^{'}(\lambda_j)} \tag{2.18}$$

Let λ_i and λ_j be the roots of T_n and T_{n-1} respectively that are closest to each other. Given $T_n(\lambda_i) = T_{n-1}(\lambda_j) = 0$, $T_n^{'}(\lambda_i)$ and $T_{n-1}^{'}(\lambda_j)$ are the first order derivative of T_n and T_{n-1} at λ_i and λ_j respectively.

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$$\lambda = \frac{\lambda_i T_n^{'}(\lambda_i) + \zeta \lambda_j T_{n-1}^{'}(\lambda_j)}{T_n^{'}(\lambda_i) + \zeta T_{n-1}^{'}(\lambda_j)} \tag{2.19}$$

This approximation is denoted as the Chebyshev-Taylor approximation. The computational cost to find the eigenvalues of the k-Toeplitz tridiagonal matrix by this approximation is $O(nk^3)$.

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Chapter 3

Boundary Conditions on Lattices, and Applications

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Chapter-outline

The relevant boundary conditions of lattices, and the corresponding perturbations required in the entries of the tridiagonal k-Toeplitz matrix are explained. A specific example of tight-binding models used in physical sciences is presented for motivation.

Adjacency matrices of atomic chains [16] in which only nearest neighbor interactions are present and all other interactions are negligible can be represented by the tridiagonal k-toeplitz matrices and their perturbations. In this section, we are going to introduce free-free boundary conditions, fixed-fixed boundary conditions, and periodic boundary conditions and discuss the applications of each of them.

3.0.1 Free-Free Boundary Condition

The free-free boundary condition is the same as the case where there is no boundary condition. So, in free-free boundary conditions, the adjacency matrix of the chain can be represented by a tridiagonal k-Toeplitz matrix [16]. The eigenvalues of the chain with free-free boundary conditions can be calculated using Chebyshev or Chebyshev-Taylor

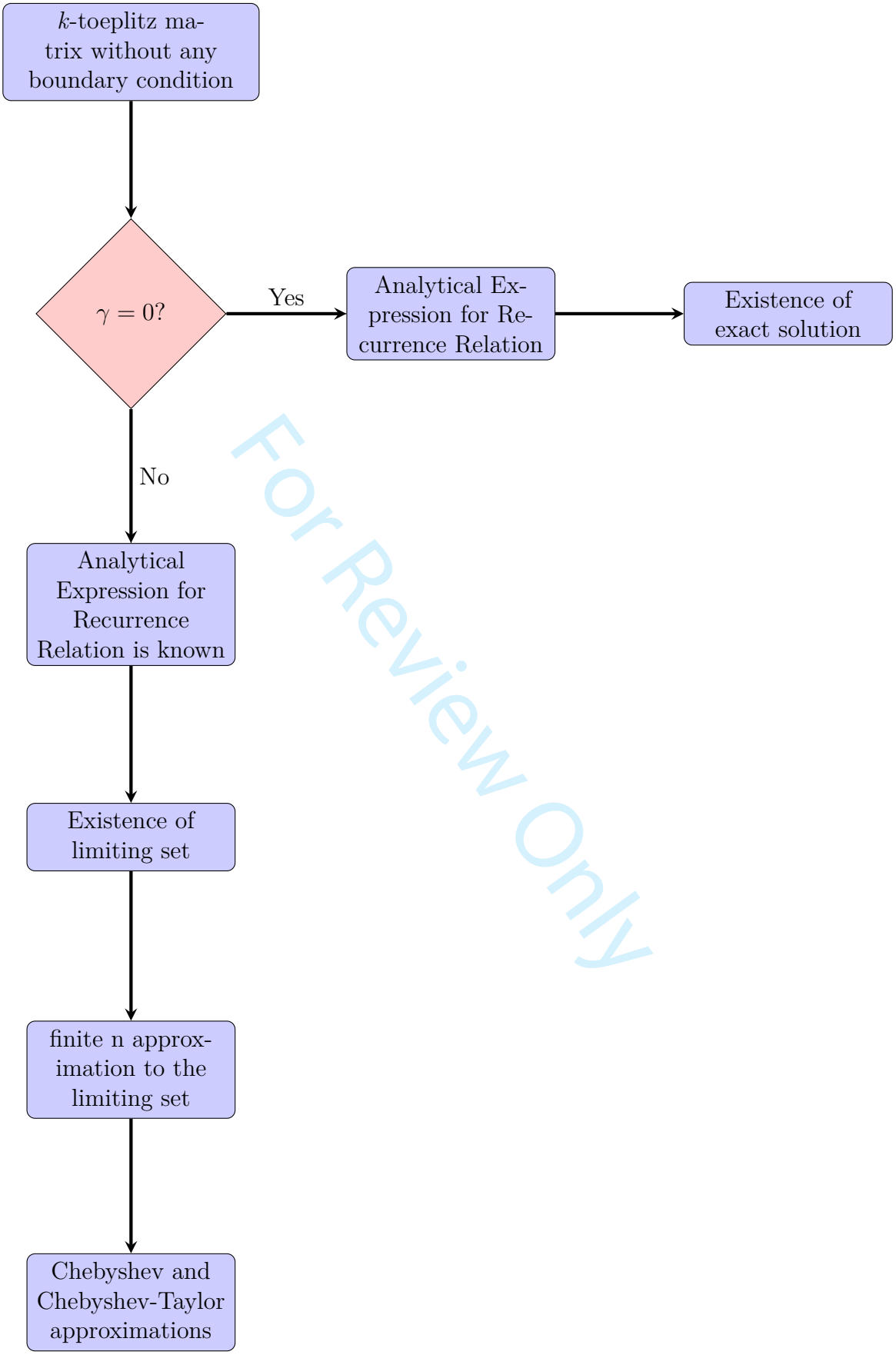

Figure 3.1: The above flowchart illustrates the methods used for eigenvalue computation of tridiagonal k-Toeplitz matrices.

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approximations.

$$A_{free-free} = \begin{bmatrix} a1 & x1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ y1 & a2 & x2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & y2 & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & a_k & x_k & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_k & a_1 & x_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & y_1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & y_{k-2} & a_{k-1} & x_{k-1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & y_{k-1} & a_k \end{bmatrix} \tag{3.1}$$

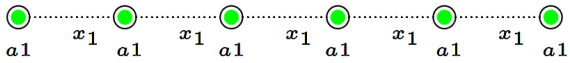

Figure 3.2: One-dimensional free-free mono-atomic lattice,($a_k = a_1, \forall k$, $x_k = x_1, \forall k$, and $y_k = x_k, \forall k$.)

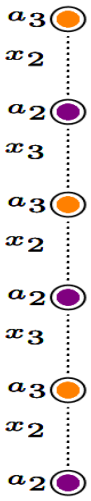

Figure 3.3: One-dimensional free-free Di-atomic lattice, ($a_k = a_2, \forall$ odd k, $a_k = a_3, \forall$ even k, $x_k = x_2, \forall$ odd k, $x_k = x_3, \forall$ even k, and $y_k = x_k, \forall k$.)

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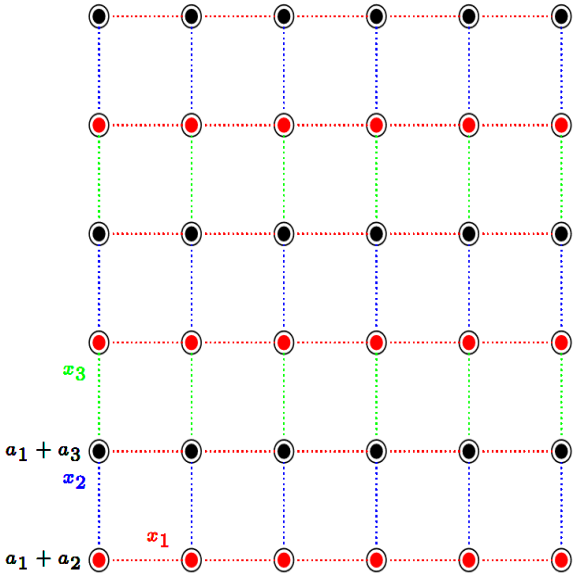

Figure 3.4: Two-dimensional lattice with free-free boundary condition (This lattice is the Kronecker sum of mono-atomic chain with free-free boundary condition in x direction(Figure 3.2) and di-atomic chain with free-free boundary condition in y direction(Figure 3.3))

3.0.2 Fixed Boundary Condition

In the case of fixed boundary conditions [17], the two ends of the atomic chain can be perturbed. So for fixed boundary conditions, the adjacency matrix is the tridiagonal k-Toeplitz matrix with perturbation in $(1,1)$ and (N,N) entries.

$$A_{fixed} = \begin{bmatrix} \tilde{a_2} & x1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ y1 & a2 & x2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & y2 & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & a_k & x_k & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_k & a_1 & x_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & y_1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & y_{k-2} & a_{k-1} & x_{k-1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & y_{k-1} & \tilde{a_3} \end{bmatrix} \tag{3.2}$$

Here $\tilde{a_2}$ and $\tilde{a_3}$ are the perturbations in the chain.

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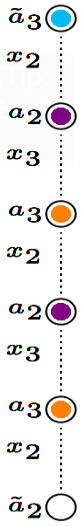

Figure 3.5: One-dimensional di-atomic lattice with fixed boundary condition,$a_k = a_2, \forall$ odd k except the boundary, $a_k = a_3, \forall$ even k except the boundary, $x_k = x_2, \forall$ odd k, $x_k = x_3, \forall$ even k, and $y_k = x_k, \forall k$. $\tilde{a_2}$ and $\tilde{a_3}$ represent the perturbation in the chain.

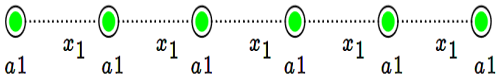

Figure 3.6: One-dimensional mono-atomic lattice with free-free boundary condition ($a_k = a_1, \forall k$, $x_k = x_1, \forall k$, and $y_k = x_k, \forall k$.)

Pictorial representation of the 2D lattice which is formed by 3.6 and 3.5 is given below.

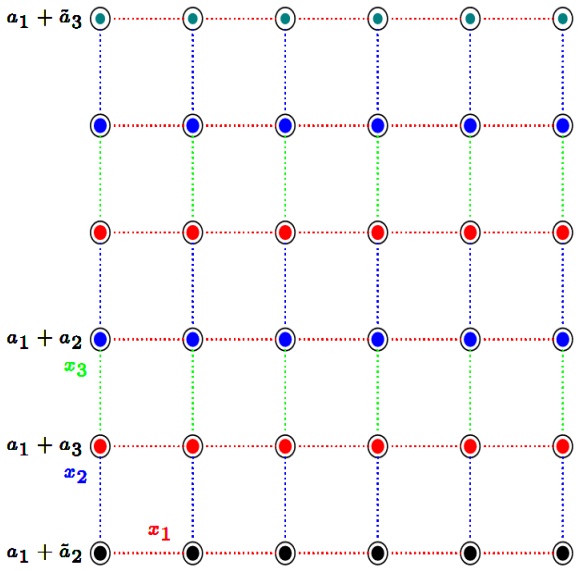

Figure 3.7: Two dimensional lattice with fixed boundary condition (This lattice is the Kronecker sum of di-atomic chain with fixed boundary condition in y direction (Figure 3.5) and mono-atomic chain with free-free boundary condition in x direction (Figure 3.6))

3.0.3 Periodic Boundary Condition

By imposing the periodic boundary condition [17] on a system, we can approximate a large system using a small part of it. Periodic boundary conditions are also called cyclic boundary conditions [18]. The adjacency matrix of a chain with only nearest neighbor interaction under periodic boundary conditions is formed by replacing $(1, N)$ and $(N, 1)$ zero entries with non-zero entries of tridiagonal k-Toeplitz matrix. Here $N \times N$ is the size of the adjacency matrix.

$$A_{periodic} = \begin{bmatrix} a1 & x1 & 0 & 0 & 0 & 0 & 0 & 0 & y_k \\ y1 & a2 & x2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & y2 & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & a_k & x_k & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_k & a_1 & x_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & y_1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & y_{k-2} & a_{k-1} & x_{k-1} \\ x_k & 0 & 0 & 0 & 0 & 0 & 0 & y_{k-1} & a_k \end{bmatrix} \tag{3.3}$$

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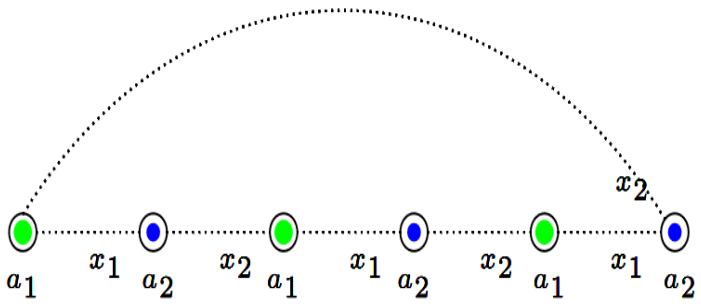

Figure 3.8: One-dimensional di-atomic lattice with periodic boundary condition ($a_k = a_1, \forall$ odd k, $a_k = a_2, \forall$ even k, $x_k = x_1, \forall$ odd k, $x_k = x_2, \forall$ even k, and $y_k = x_k, \forall k$.)

3.0.4 Lattices with Dimension ≥ 2

Adjacency matrices of the multi-dimensional lattices are the Kronecker sum of the adjacency matrices of the corresponding one-dimensional chains [19]. The adjacency matrix of a 2D lattice can be represented as,

$$L_{2D} = L_{xx} \oplus L_{yy} = L_{xx} \otimes I_y + I_x \otimes L_{yy} \tag{3.4}$$

Similarly, the adjacency matrix of a 3D lattice can be represented as

$$L_{3D} = L_{xx} \oplus L_{yy} \oplus L_{zz} = L_{xx} \otimes I_y \otimes I_z + I_x \otimes L_{yy} \otimes I_z + I_x \otimes I_y \otimes L_{zz} \tag{3.5}$$

where L_{xx}, L_{yy} and L_{zz} are adjacency matrices of individual chains. I_x, I_y and I_z are the identity matrices of x, y and z directional chains respectively.

In this manner, we can form all other higher dimensional lattices using the adjacency matrices of chains in each direction. The eigenvalues of such lattice models [20] are the pairwise sum of the individual one-dimensional chain eigenvalues.

3.0.5 Example Application: Tight-Binding Model

The applications of tridiagonal k-Toeplitz matrices under different boundary conditions include the vibrational frequency of atomic lattice [21], the chain model in quantum mechanics [22] and the periodic tight-binding model. Here we will discuss the periodic tight-binding model in detail.

The tight-binding model is a quantum mechanical model which studies the electronic properties of solids. Here, we focus on the periodic tight binding lattice with a single orbital per site and the nearest-neighbor hopping [23]. Hamiltonian of such a one-dimensional periodic tight-binding model with different boundary conditions can be represented as tridiagonal k-Toeplitz matrices and their perturbations.

The tight binding system of equations for a 1D lattice composed of N sites with a single orbital per site and nearest-neighbor hopping is given below[24].

$$E\psi = \epsilon_n \psi_n + t_{n,n-1}\psi_{n-1} + t_{n,n+1}\psi_{n+1} \tag{3.6}$$

$\forall n = 1, 2, ...N.$

In the above equation, E is the energy of the lattice, and ϵ_n is the onsite energy of lattice site n. ψ_n is the wave function of lattice site n and $t_{n,n-1}$ is the hopping term interaction between n and $n-1$ lattice sites. With free-free boundary conditions, the Hamiltonian matrix of the periodic tight binding chain with only the nearest neighbor interaction is tridiagonal k-toeplitz [25].

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$$H_{free-free} = \begin{bmatrix} \epsilon_1 & t_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ t_{12} & \epsilon_2 & t_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & t_{23} & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \epsilon_k & t_{k1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & t_{k1} & \epsilon_1 & t_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & t_{12} & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & t_{k-2,k-1} & \epsilon_{k-1} & t_{k-1,k} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & t_{k-1,k} & \epsilon_k \end{bmatrix} \tag{3.7}$$

Here $\{\epsilon_1,\epsilon_2,.....,\epsilon_k\}$ and $\{t_{12},t_{23},.....,t_{k-2,k-1},t_{k-1,k}\}$ represents onsite energies and nearest neighbor hopping terms respectively.

For fixed boundary conditions, the Hamiltonian of the tight binding one-dimensional lattice with only nearest neighbor interaction is a tridiagonal k-Toeplitz matrix with perturbation in $(1,1)$ and (N,N) entries.

$$H_{fixed} = \begin{bmatrix} a & t_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ t_{12} & \epsilon_2 & t_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & t_{23} & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \epsilon_k & t_{k1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & t_{k1} & \epsilon_1 & t_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & t_{12} & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & t_{k-2,k-1} & \epsilon_{k-1} & t_{k-1,k} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & t_{k-1,k} & b \end{bmatrix} \tag{3.8}$$

Here a and b are the onsite energies of lattice sites at the two ends of the finite lattice.

Under periodic boundary conditions, the Hamiltonian matrix for the tight binding one-dimensional lattice with only nearest neighbor interactions is a tridiagonal k-Toeplitz matrix with $(1,N)$ and $(N,1)$ non-zero entries [26].

To find the energy of the tight-binding model, we have to calculate the eigenvalues of the corresponding Hamiltonian matrix [27]. Since the Hamiltonian of a one-dimensional tight-binding model with only the nearest neighbor interaction is the tridiagonal k-Toeplitz matrix, the energy eigenvalues can be calculated using Chebyshev or Chebyshev Taylor approximations. For systems under fixed perturbation and periodic perturbation, we have to develop methods to find eigenvalues with less computational cost.

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$$H_{periodic} = \begin{bmatrix} \epsilon_1 & t_{12} & 0 & 0 & 0 & 0 & 0 & 0 & t_{k1} \\ t_{12} & \epsilon_2 & t_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & t_{23} & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & \epsilon_k & t_{k1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & t_{k1} & \epsilon_1 & t_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & t_{12} & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & t_{k-2,k-1} & \epsilon_{k-1} & t_{k-1,k} \\ t_{k1} & 0 & 0 & 0 & 0 & 0 & 0 & t_{k-1,k} & \epsilon_k \end{bmatrix} \tag{3.9}$$

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Chapter 4

Error Analysis of the Eigenvalues and Eigenvectors of Free-Free Chain

Chapter-outline

Using special cases of tridiagonal k-Toeplitz matrices where closed-form expressions for the eigenvalues are tractable, we compare the results of the semi-analytical method and the direct numerical method for matrices of finite size.

In this chapter, we will perform the error analysis of the eigenvalue calculation methods of the unperturbed tridiagonal k-toeplitz matrix, Chebyshev, and Chebyshev Taylor approximations. We will also develop an algorithm to find the eigenvectors of the k-Toeplitz tridiagonal matrices.

4.1 Error Analysis of Eigenvalues Using Special Matrices

To perform the error analysis of eigenvalues, we need to know the exact eigenvalues of the tridiagonal k-Toeplitz matrices. Eigenvalues of tridiagonal k-Toeplitz matrices show a repeated pattern when $\gamma = 0$. So it is possible to find out the exact eigenvalues of high dimensional tridiagonal k-Toeplitz matrices with $\gamma = 0$ manually. These non-symmetric matrices can have high condition numbers and they are used to illustrate the potential failure of the direct numerical methods.

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4.1.1 Chebyshev Approximation

Error analysis of Chebyshev approximated eigenvalues is done by comparing the average relative error of Chebyshev approximated eigenvalues with that of the direct numerical method eigenvalues.

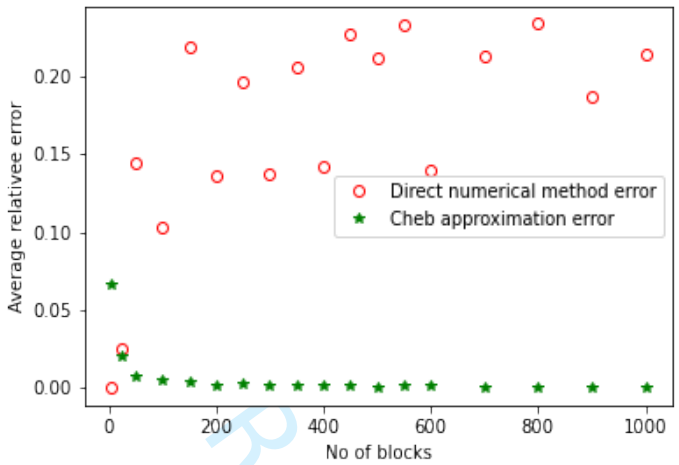

Figure 4.1: Error analysis of Chebyshev approximated vs the direct numerical method eigenvalues: diagonal=[0,0,0], upper diagonal=[0,0,-1], lower diagonal=[1,1,1]. Since the average relative error of eigenvalues of the direct numerical method is around 0.2 when the size of the matrix is greater than $100k$, the direct numerical method can't be considered a stable computing method. The eigenvalues of this matrix are $n+2$ number of zeros, $n-1$ number of $1j$, and $n-1$ number of $-1j$ where $k=3$ is the period of chain and $nk \times nk$ is the size of the matrix. $C \to \infty$, where C is the condition number of the matrix.

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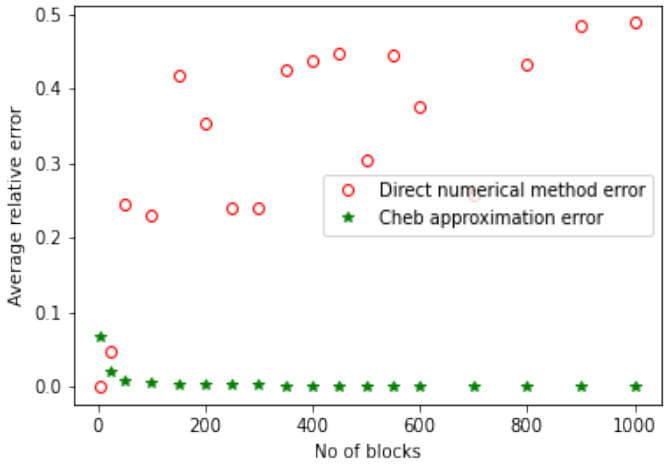

Figure 4.2: Error analysis of Chebyshev approximated vs the direct numerical method eigenvalues: diagonal=[0,0,0], upper diagonal=[0,0,1], lower diagonal=[-1,-1,-1]. Since the average relative error of eigenvalues of the direct numerical method is around 0.5 when the size of the matrix is greater than $100k$, the direct numerical method can't be considered a reliable computing method. The eigenvalues of this matrix are $n+2$ number of zeros, $n-1$ number of $1j$, and $n-1$ number of $-1j$ where $k=3$ is the period of chain and $nk \times nk$ is the size of the matrix. $C \to \infty$, where C is the condition number of the matrix.

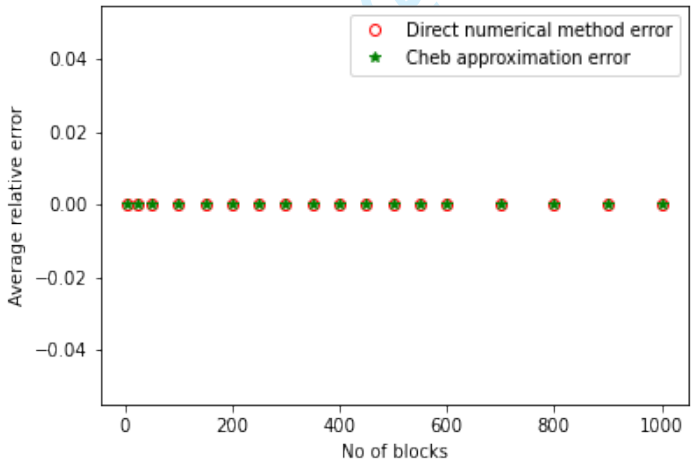

Figure 4.3: Error analysis of Chebyshev approximated vs the direct numerical method eigenvalues: diagonal=[0,0,0], upper diagonal=[0,0,1], lower diagonal=[-1,0,-1]. Since the average relative error of the direct numerical method is zero, here the direct numerical method is a reliable computation method. The eigenvalues of this matrix are $n+2$ number of zeros, $n-1$ number of $1j$, and $n-1$ number of $-1j$ where $k=3$ is the period of chain and $nk \times nk$ is the size of the matrix. $C \to \infty$, where C is the condition number of the matrix.

The eigenvalue calculation of the above-used matrices is given in the appendix section.

From the above figures, we can observe that for tridiagonal k-Toeplitz matrices, Chebyshev approximated eigenvalues are more accurate compared to the direct numerical

method eigenvalues. When the number of chains increases, the average relative error of the Chebyshev approximated eigenvalues always decrease or remains the same. We can confirm this with more examples that are included in the appendix section of this report.

4.1.2 Chebyshev-Taylor Approximation

The Chebyshev-Taylor approximation for the eigenvalues of tridiagonal k-Toeplitz matrices is not defined when $\gamma = 0$. It is not possible to obtain the exact eigenvalues of a high dimensional tridiagonal k-Toeplitz matrix with non-zero γ manually. So we don't perform a similar error analysis for Chebyshev-Taylor approximated eigenvalues.

4.2 Eigenvector Calculation for k-Toeplitz Tridiagonal Matrices

In this section, we propose a method to find the eigenvalues and eigenvectors of tridiagonal k-Toeplitz matrices. With the Chebyshev approximated eigenvalues, eigenvectors can be found using the Inverse Iteration and the Thomas algorithm. While we use Inverse Iteration, Chebyshev approximated eigenvalues are taken as the initial guess. The Thomas algorithm is used to solve the tridiagonal system as required in Inverse iteration. The code to find eigenvalues and eigenvectors of tridiagonal k-Toeplitz matrices is freely available on GitHub (Github link for my codes: Github link).

4.2.1 Thomas Algorithm

Thomas Algorithm [28] is the simplified form of Gaussian elimination and it is used to solve tridiagonal systems. A tridiagonal system of n unknowns can be written as the equation given below.

$$\begin{bmatrix} b_1 & c_1 & \dots & \dots & 0 & 0 \\ a_2 & b_2 & c_2 & \dots & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & \dots & 0 \\ 0 & \vdots & \ddots & \ddots & \dots & 0 \\ 0 & \dots & \vdots & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & 0 & \dots & \vdots & a_n & b_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ \vdots \\ d_{n-1} \\ d_n \end{bmatrix} \tag{4.1}$$

To solve systems like the above, we can use the Thomas algorithm with the computational cost of $O(n)$.

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Algorithm 7 Thomas Algorithm

for $i = 1, 2...n$ **do**
  $w \leftarrow a_i/b_{i-1}$
  $b_i \leftarrow b_i - w \times c_{i-1}$
  $d_i \leftarrow d_i - w \times d_{i-1}$
end for
followed by back substitution
for $i = n-1, n-2, ...1$ **do**
  $x_n \leftarrow d_n/b_n$
  $x_i \leftarrow \frac{d_i - c_i \times x_{i+1}}{b_i}$
end for

As the output of Inverse Iteration, we can also get eigenvalues. The limitations of the Inverse Iteration algorithm [29] in further improving the eigenvalues given by the Chebyshev approximation of the limiting set, are given below.

Limitations of Inverse Iteration in Improving the Chebyshev Approximation

- The Inverse Iteration cannot be used for matrices with complex eigenvalues.
- Modified eigenvalue due to Inverse Iteration, need not be as accurate as the original Chebyshev approximated eigenvalue, due to numerical degradation and high condition numbers of the large eigenvalue problem.

4.2.2 Error Analysis of Eigenvalues Obtained after Inverse Iteration

The following figures, do a comparative study of errors of Chebyshev approximated eigenvalues, modified Chebyshev approximated eigenvalues (eigenvalues as the result of Inverse Iteration), and built-in eigenvalues.

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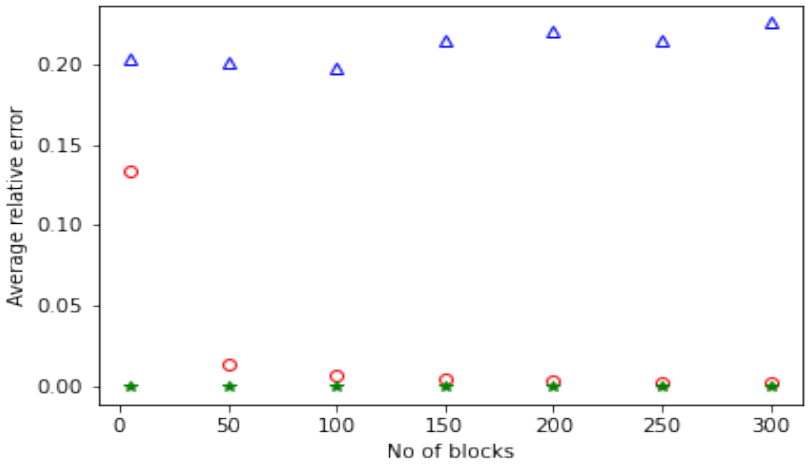

Figure 4.4: Error analysis of eigenvalues: diagonal= $[0, 0, 0]$, upper diagonal= $[0, 0, 1]$, lower diagonal= $[1, 0, 1]$. Since the average relative error of improved Chebyshev is 0.2, it is not a reliable computation method. The eigenvalues of this matrix are $n + 2$ number of zeros, $n - 1$ number of 1, and $n - 1$ number of -1 where $k = 3$ is the period of chain and $nk \times nk$ is the size of the matrix. $C \to \infty$, where C is the condition number of the matrix.

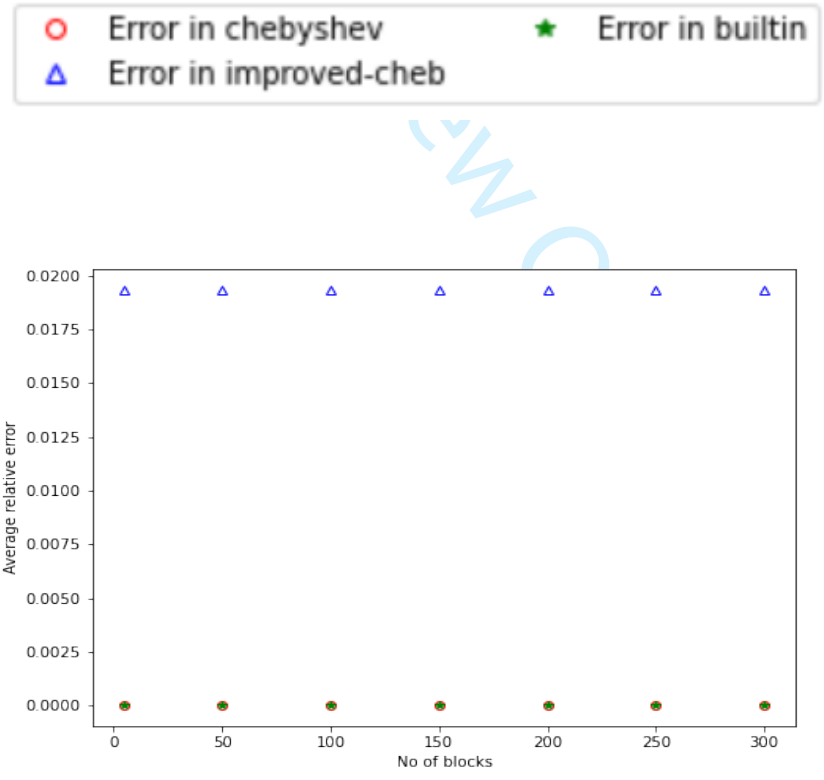

Figure 4.5: Error analysis of eigenvalues: diagonal= $[0, 0, 0]$, upper diagonal= $[0, 0, 1]$, lower diagonal $= [1, 1, 0]$. Since the average relative error of improved Chebyshev is 0.02 only, it is a stable computation method here. The eigenvalues of this matrix are $3n$ number of zeros, where $k = 3$ is the period of chain and $nk \times nk$ is the size of the matrix. $C \to \infty$, where C is the condition number of the matrix.

From the above figures, we can observe that there is no guarantee that the average relative error of the eigenvalues obtained as the result of Inverse Iteration is lesser than that of Chebyshev approximated eigenvalues. So it is better to omit the eigenvalues modified by the Inverse Iteration and keep only eigenvectors.

The computational cost of eigenvalue and eigenvector computation of this Inverse Iteration method is $O(n^2k^3)$. This method is not computationally cheaper compared to built-in methods [30]. Since it is not possible to manually find the eigenvectors of high-dimensional matrices, we can't perform the error analysis of eigenvectors separately.

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Chapter 5

Fixed Perturbation Analysis of Tridiagonal *k*-Toeplitz Matrix

Chapter-outline

The closed-form expressions for the characteristic polynomials, of a perturbed tridiagonal k-Toeplitz matrix are derived, for different boundary conditions i.e. entries of the first two rows and the last two rows may have to be perturbed representing the boundary condition on the chain. We show that a general solution for the roots of these characteristic polynomials is intractable, unlike the free-free chain in the previous chapter. Hence we suggest a few methods for identifying and updating only the perturbed eigenvalues of the free-free chain due to the boundary conditions applied. In the case of a lattice, the corresponding perturbations apply to all the chains required to construct the lattice.

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In this chapter, we study the feasibility of analytical methods for the eigenvalues of a tridiagonal k-Toeplitz matrix under fixed boundary conditions.

5.1 Fixed Boundary Condition: Perturbation Theory

The perturbed tridiagonal k-Toeplitz matrix under fixed boundary conditions is represented as $\tilde{M}_k$. Here M_k is the tridiagonal k-Toeplitz matrix without any perturbations. In order to obtain $\tilde{M}_k$, the following conditions are applied on the entries of M_k, $M_k(1,1) = a$

and $M_k(N,N) = b$, where a and b are different from a_1 and a_k.

$$\tilde{M}_k = \begin{bmatrix} a & x1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ y1 & a2 & x2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & y2 & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & a_k & x_k & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_k & a_1 & x_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & y_1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & y_{k-2} & a_{k-1} & x_{k-1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & y_{k-1} & b \end{bmatrix} \tag{5.1}$$

5.2 Recurrence Relation for the Fixed Perturbed Tridiagonal *k*-Toeplitz Matrices

We will derive the characteristic polynomial of the tridiagonal k-Toeplitz matrix under fixed boundary conditions.

5.2.1 Perturbation Only in (N, N) Entry

With perturbation in (N,N) entry, the initial condition for the characteristic polynomial becomes

$$\begin{bmatrix} p'_1(z) \\ q'_1(z) \end{bmatrix} = \begin{bmatrix} z+a_1 & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} z+a_{k-1} & -u_{k-1} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+b \\ 1 \end{bmatrix} \tag{5.2}$$

$$\begin{bmatrix} p'_n(z) \\ q'_n(z) \end{bmatrix} = \begin{bmatrix} A(z) & B(z) \\ C(z) & D(z) \end{bmatrix} \begin{bmatrix} p'_{n-1}(z) \\ q'_{n-1}(z) \end{bmatrix} \tag{5.3}$$

Here $A(z)$, $B(z)$, $C(z)$, and $D(z)$ are polynomials in z, which comes in the characteristic polynomial derivation of tridiagonal k-Toeplitz matrices without any perturbation.

Solving the above matrix, we will get

$$p'_n(z) = A(z)p'_{n-1}(z) + B(z)q'_{n-1}(z) \tag{5.4}$$

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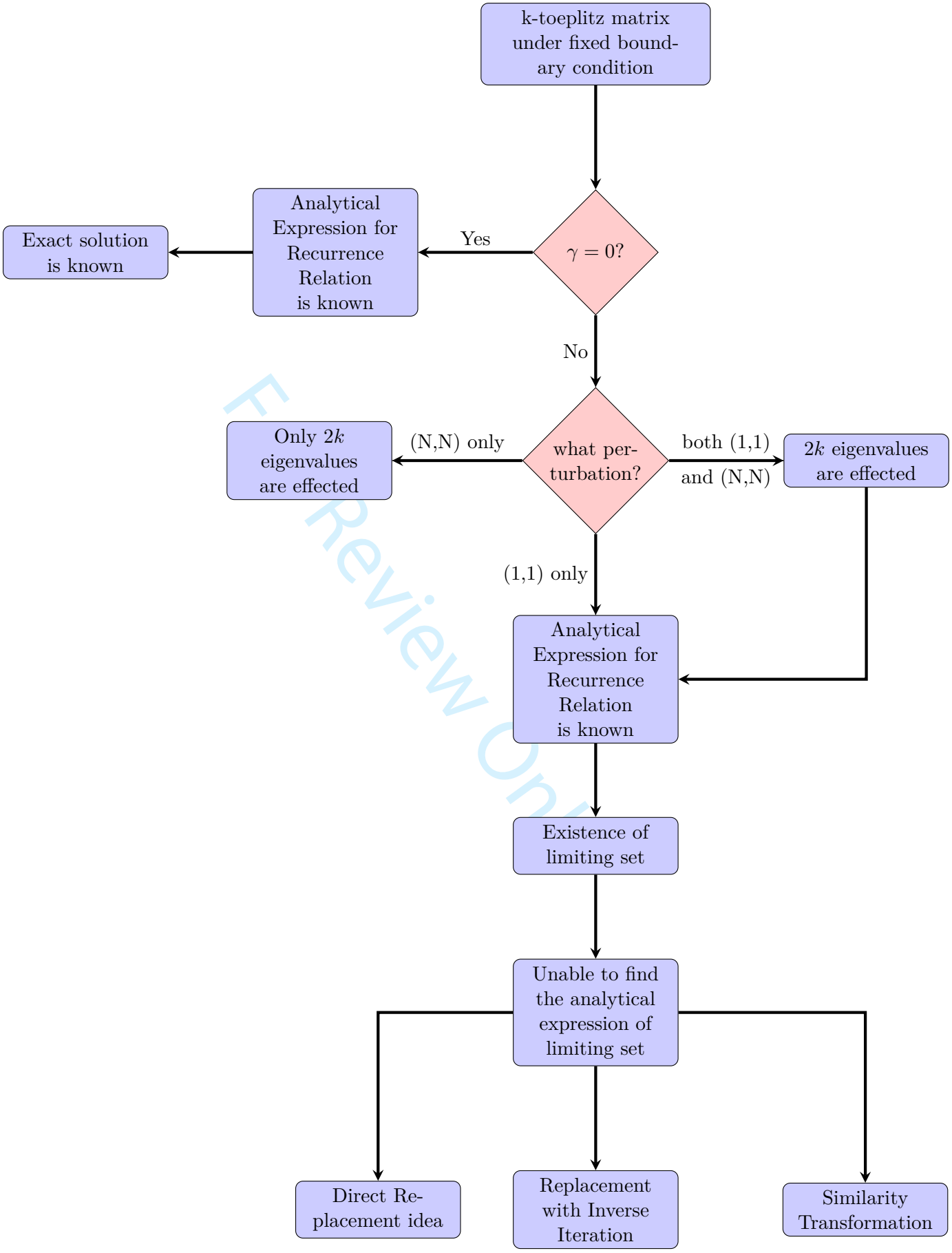

Figure 5.1: This flowchart summarizes the approaches used for computing the eigenvalues of tridiagonal k-toeplitz matrices under fixed boundary conditions.

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$$q'_n(z) = C(z)p'_{n-1}(z) + D(z)q'_{n-1}(z) \tag{5.5}$$

With (N, N) perturbation, the three-term recurrence relation of the characteristic polynomial changes to,

$$p'_{n+1}(z) = Q_k(z)p'_n(z) + \gamma p'_{n-1}(z) \tag{5.6}$$

Without any perturbation, the recurrence relation is,

$$p_{n+1}(z) = Q_k(z)p_n(z) + \gamma p_{n-1}(z) \tag{5.7}$$

So with (N, N) perturbation, the format of the recurrence relation of the characteristic polynomial remains the same, and only the initial condition for the characteristic polynomial changes. Thus continuous spectra of the limiting set are not affected by (N, N) entry perturbation. Only the initial condition of the recurrence relation changes and $2k$ eigenvalues which are not part of the continuous spectra of limiting set change by the equation given below.

$$Q_k(z) = \frac{\gamma}{p'(z)} - p'(z) \tag{5.8}$$

where $p'(z) = p'_1(z) - Q_k(z)$

The $2k$ eigenvalues are the solutions of the equation 5.8.

5.2.2 Perturbation Only in (1,1) Entry

When we add perturbation in $(1, 1)$ entry, the equation 2.5 becomes

$$\begin{bmatrix} \tilde{p}_n(z) \\ \tilde{q}_n(z) \end{bmatrix} = \begin{bmatrix} z+a & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} z+a_k & -u_k \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ q_{n-1}(z) \end{bmatrix} \tag{5.9}$$

Let,

$$\begin{bmatrix} \tilde{A}(z) & \tilde{B}(z) \\ \tilde{C}(z) & \tilde{D}(z) \end{bmatrix} = \begin{bmatrix} z+a & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} z+a_k & -u_k \\ 1 & 0 \end{bmatrix} \tag{5.10}$$

Then,

$$\begin{bmatrix} \tilde{p}_n(z) \\ \tilde{q}_n(z) \end{bmatrix} = \begin{bmatrix} \tilde{A}(z) & \tilde{B}(z) \\ \tilde{C}(z) & \tilde{D}(z) \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ q_{n-1}(z) \end{bmatrix} \tag{5.11}$$

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From the above matrix, we get

$$\tilde{p}_n(z) = \tilde{A}(z)p_{n-1}(z) + \tilde{B}(z)q_{n-1}(z) \tag{5.12}$$

$$\tilde{p}_n(z) = \tilde{A}(z)p_{n-1}(z) + \frac{\tilde{B}(z)}{B(z)}(p_n(z) - A(z)p_{n-1}(z)) \tag{5.13}$$

$$\tilde{p}_n(z) = p_n(z)\frac{\tilde{B}(z)}{B(z)} + p_{n-1}(z)(\tilde{A}(z) - R(z)A(z)) \tag{5.14}$$

where $R(z) = \frac{\tilde{B}(z)}{B(z)}$ and $S(z) = \frac{\tilde{A}(z)}{R(z)} - A(z)$.

Substitution of $R(z)$ and $S(z)$ in the 5.14 gives

$$\frac{\tilde{p}_n(z)}{R(z)} = p_n(z) + p_{n-1}(z)S(z) \tag{5.15}$$

Using Equation 2.10, we can write the above equation as

$$\frac{\tilde{p}_n(z)}{R(z)} = Q_k(z)p_{n-1}(z) + \gamma p_{n-2}(z) + p_{n-1}(z)S(z) \tag{5.16}$$

$$\frac{\tilde{p}_n(z)}{R(z)} = (Q_k(z) + S(z))p_{n-1}(z) + \gamma p_{n-2}(z) \tag{5.17}$$

Writing above equation in matrix format,

$$\begin{bmatrix} \frac{\tilde{p}_n(z)}{R(z)} \\ p_{n-1}(z) \end{bmatrix} = \begin{bmatrix} Q_k(z) + S(z) & \gamma \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ p_{n-2}(z) \end{bmatrix} \tag{5.18}$$

$$\begin{bmatrix} p_{n-1}(z) \\ p_{n-2}(z) \end{bmatrix} = \begin{bmatrix} Q_k(z) & \gamma \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_{n-2}(z) \\ p_{n-3}(z) \end{bmatrix} \tag{5.19}$$

Applying 5.19 in 5.18,

$$\begin{bmatrix} \frac{\tilde{p}_n(z)}{R(z)} \\ p_{n-1}(z) \end{bmatrix} = \begin{bmatrix} Q_k(z) + S(z) & \gamma \\ 1 & 0 \end{bmatrix} \begin{bmatrix} Q_k(z) & \gamma \\ 1 & 0 \end{bmatrix}^{n-2} \begin{bmatrix} p_1(z) \\ 1 \end{bmatrix} \tag{5.20}$$

From the above equation, it can be shown that $\frac{\tilde{p}_n(z)}{R(z)}$ can be written as a determinant of the matrix given below.

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$$\begin{bmatrix} p_1(z) & i\sqrt{\gamma} & 0 & 0 & \dots & 0 \\ i\sqrt{\gamma} & Q_k(z) & i\sqrt{\gamma} & 0\dots & 0 & \\ 0 & i\sqrt{\gamma} & Q_k(z) & i\sqrt{\gamma} & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0\dots & \dots & \dots & \dots & i\sqrt{\gamma} & Q_k(z)+S(z) \end{bmatrix}_{n\times n} \tag{5.21}$$

Let $p_1(z) = Q_k(z) + p(z)$. Then zeros of $\frac{\tilde{p}_n(z)}{R(z)}$ can be written as $\lambda = -\frac{Q_k(z)}{\sqrt{\gamma}}$. λ is the eigenvalue of W matrix and it is given below.

$$W = \begin{bmatrix} \frac{p(z)}{\sqrt{\gamma}} & -1 & 0 & 0 & \dots & 0 \\ 1 & 0 & -1 & 0 & \dots & 0 \\ 0 & 1 & 0 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & \dots & 0 & \frac{S(z)}{\sqrt{\gamma}} \end{bmatrix}_{n\times n} \tag{5.22}$$

$L_n(\zeta, \lambda)$ is the characteristic polynomial for the above matrix and $T_n(\lambda)$ is the characteristic polynomial for the skew-symmetric matrix given below.

$$\begin{bmatrix} 0 & -1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & -1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & -1 & 0 & \dots & 0 \\ 0 & \dots & \ddots & \vdots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{bmatrix}_{n\times n} \tag{5.23}$$

Let $\zeta_1 = \frac{p(z)}{\sqrt{\gamma}}$ and $\zeta_2 = \frac{S(z)}{\sqrt{\gamma}}$

Then by first expanding determinant along $(1,1)$ entry and further by (N,N) entry, we have

$$\begin{aligned} L_n(\zeta,\lambda) &= (\zeta_1-\lambda)((\zeta_2-\lambda)T_{n-2}+T_{n-3}) + (\zeta_2-\lambda)T_{n-3} + T_{n-4} \\ &= (\zeta_1-\lambda)(\zeta_2-\lambda)T_{n-2} + (\zeta_1+\zeta_2-2\lambda)T_{n-3} + T_{n-4} \\ &= -\lambda T_{n-1} - \lambda(\zeta_1+\zeta_2)T_{n-3} + T_{n-2} + \zeta_1\zeta_2 T_{n-2} \end{aligned} \tag{5.24}$$

Using $T_n = -\lambda T_{n-1} + T_{n-2}$ and $T_{n-1} = -\lambda T_{n-2} + T_{n-3}$, the above equation can be reduced to,

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$$L_n(\zeta,\lambda) = T_n + (\zeta_1+\zeta_2)T_{n-1} + \zeta_1\zeta_2 T_{n-2} \tag{5.25}$$

Writing in matrix form, we will get

$$L_n(\zeta,\lambda) = \begin{bmatrix} 1 & \zeta_1+\zeta_2 & \zeta_1\zeta_2 \end{bmatrix} \begin{bmatrix} T_n \\ T_{n-1} \\ T_{n-2} \end{bmatrix} \tag{5.26}$$

Next step is to find the solution of $L_n(\zeta,\lambda) = 0$.

5.2.3 Reducing into the Family of Polynomials

We outline two methods for further reductions.

Method 1

Using $T_n = -\lambda T_{n-1} + T_{n-2}$ and $T_{n-1} = -\lambda T_{n-2} + T_{n-3}$, we can write the below matrix equation.

$$\begin{bmatrix} T_n \\ T_{n-1} \\ T_{n-2} \end{bmatrix} = \begin{bmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} T_{n-1} \\ T_{n-2} \\ T_{n-3} \end{bmatrix} \tag{5.27}$$

Eigenvalues of the matrix, $\begin{bmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & 0 \end{bmatrix}$ are $t_0 = -\lambda$, $t_+ = \frac{-\lambda+\sqrt{\lambda^2+4}}{2}$ and $t_- = \frac{-\lambda-\sqrt{\lambda^2+4}}{2}$

.

The corresponding eigenvectors are $\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$, $\begin{bmatrix} \frac{|t_+|^2}{\sqrt{1+|t_+|^2+|t_+|^4}} \\ \frac{|t_+|}{\sqrt{1+|t_+|^2+|t_+|^4}} \\ \frac{1}{\sqrt{1+|t_+|^2+|t_+|^4}} \end{bmatrix}$, and $\begin{bmatrix} \frac{|t_-|^2}{\sqrt{1+|t_-|^2+|t_-|^4}} \\ \frac{|t_-|}{\sqrt{1+|t_-|^2+|t_-|^4}} \\ \frac{1}{\sqrt{1+|t_-|^2+|t_-|^4}} \end{bmatrix}$

Equation 5.26 can be written as

$$L_n(\zeta,\lambda) = \begin{bmatrix} 1 & \zeta_1+\zeta_2 & \zeta_1\zeta_2 \end{bmatrix} \begin{bmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & 0 \end{bmatrix}^{n-2} \begin{bmatrix} t_0 \\ 1 \\ 0 \end{bmatrix} \tag{5.28}$$

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where

$$\begin{bmatrix} T_n \\ T_{n-1} \\ T_{n-2} \end{bmatrix} = \begin{bmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & 0 \end{bmatrix}^{n-2} \begin{bmatrix} t_0 \\ 1 \\ 0 \end{bmatrix} \tag{5.29}$$

Using matrix decomposition, we get

$$\begin{bmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 0 & 1 & 0 \end{bmatrix} = Q \wedge Q^{-1} \tag{5.30}$$

where

$$Q = \begin{bmatrix} 1 & \frac{|t_+|^2}{\sqrt{1+|t_+|^2+|t_+|^4}} & \frac{|t_-|^2}{\sqrt{1+|t_-|^2+|t_-|^4}} \\ 0 & \frac{|t_+|}{\sqrt{1+|t_+|^2+|t_+|^4}} & \frac{|t_-|}{\sqrt{1+|t_-|^2+|t_-|^4}} \\ 0 & \frac{1}{\sqrt{1+|t_+|^2+|t_+|^4}} & \frac{1}{\sqrt{1+|t_-|^2+|t_-|^4}} \end{bmatrix} \tag{5.31}$$

$$\wedge = \begin{bmatrix} t_0 & 0 & 0 \\ 0 & t_+ & 0 \\ 0 & 0 & t_- \end{bmatrix} \tag{5.32}$$

and

$$Q^{-1} = \begin{bmatrix} \frac{t_+ - t_-}{\sqrt{1+|t_+|^2+|t_+|^4}\sqrt{1+|t_-|^2+|t_-|^4}} & \frac{|t_-|^2-|t_+|^2}{\sqrt{1+|t_+|^2+|t_+|^4}\sqrt{1+|t_-|^2+|t_-|^4}} & \frac{{t_+}^2 t_- - {t_-}^2 t_+}{\sqrt{1+|t_+|^2+|t_+|^4}\sqrt{1+|t_-|^2+|t_-|^4}} \\ 0 & \frac{1}{\sqrt{1+|t_-|^2+|t_-|^4}} & \frac{-t_-}{\sqrt{1+|t_-|^2+|t_-|^4}} \\ 0 & \frac{-1}{\sqrt{1+|t_+|^2+|t_+|^4}} & \frac{t_+}{\sqrt{1+|t_+|^2+|t_+|^4}} \end{bmatrix} \tag{5.33}$$

Here Q is the eigenvector matrix and $\wedge$ is the eigenvalue matrix.

Using the equations 5.28, 5.29, 5.30, 5.31 and 5.32 , $L_n(\zeta, \lambda) = 0$ can be written as

$$\begin{aligned}(t_+ - \frac{1}{t_+})^{n-2}[(t_+ + \frac{1}{t_+})(t_+ - \frac{1}{t_+}) + \frac{1}{t_+^2} - t_+^2] + (t_+)^{n-2}[t_+^2 + (\zeta_1+\zeta_2)t_+ + \zeta_1\zeta_2] \\ - \frac{(-1)^{n-2}}{t_+^{n-2}}[\frac{1}{t_+^2} + (\zeta_1+\zeta_2)\frac{-1}{t_+} + \zeta_1\zeta_2] = 0\end{aligned} \tag{5.34}$$

$$t_+^{2n} + (\zeta_1+\zeta_2)t_+^{2n-1} + (\zeta_1\zeta_2)t_+^{2n-2} - (-1)^n[1 - t_+(\zeta_1+\zeta_2) + (\zeta_1\zeta_2)t_+^2] = 0 \tag{5.35}$$

Method 2

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$$\begin{bmatrix} T_n \\ T_{n-1} \end{bmatrix} = \begin{bmatrix} -\lambda & 1 \\ 1 & 0 \end{bmatrix}^{n-1} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{5.36}$$

By applying matrix decomposition, we can write

$$\begin{bmatrix} -\lambda & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} \frac{t_+}{\sqrt{1+|t_+|^2}} & \frac{t_-}{\sqrt{1+|t_-|^2}} \\ \frac{1}{\sqrt{1+|t_+|^2}} & \frac{1}{\sqrt{1+|t_-|^2}} \end{bmatrix} \begin{bmatrix} t_+ & 0 \\ 0 & t_- \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{1+|t_-|^2}} & \frac{-t_-}{\sqrt{1+|t_-|^2}} \\ \frac{-1}{\sqrt{1+|t_+|^2}} & \frac{t_+}{\sqrt{1+|t_+|^2}} \end{bmatrix} \tag{5.37}$$

Then,

$$T_n = \frac{1}{\sqrt{1+|t_-|^2}\sqrt{1+|t_+|^2}}[t_+^n - t_-^n] \tag{5.38}$$

$$T_{n-1} = \frac{1}{\sqrt{1+|t_-|^2}\sqrt{1+|t_+|^2}}[t_+^{n-1} - t_-^{n-1}] \tag{5.39}$$

For $L_n(\zeta, \lambda) = 0$,

$$[t_+^n - t_-^n] + (\zeta_1 + \zeta_2)[t_+^{n-1} - t_-^{n-1}] + (\zeta_1\zeta_2)[t_+^{n-2} - t_-^{n-2}] = 0 \tag{5.40}$$

Using $t_- = \frac{-1}{t_+}$,

$$[t_+^n - \frac{(-1)^n}{t_+^n}] + (\zeta_1 + \zeta_2)[t_+^{n-1} - \frac{(-1)^{n-1}}{t_+^{n-1}}] + (\zeta_1\zeta_2)[t_+^{n-2} - \frac{(-1)^{n-2}}{t_+^{n-2}}] = 0 \tag{5.41}$$

$$[t_+^{2n} - (-1)^n] + (\zeta_1 + \zeta_2)[t_+^{2n-1} - (-1)^n t_+] + (\zeta_1\zeta_2)[t_+^{2n-2} - (-1)^{n-1}t_+^2] = 0 \tag{5.42}$$

On further reduction,

$$t_+^{2n} + (\zeta_1 + \zeta_2)t_+^{2n-1} + (\zeta_1\zeta_2)t_+^{2n-2} - (-1)^n[1 - t_+(\zeta_1 + \zeta_2) + (\zeta_1\zeta_2)t_+^2] = 0 \tag{5.43}$$

By method 1 and method 2, we get the identical polynomial relation for t_+. Since there are two ζ terms in the equation 5.43, we cannot find the limiting set by applying Rouche's theorem [31] and other similar approaches.

5.2.4 Perturbation in Both (1, 1) and (N, N) Entries

When there is (N, N) entry perturbation to the tridiagonal k-Toeplitz matrix, the recurrence relation becomes,

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$$p'_{n+1}(z) = Q_k(z)p'_n(z) + \gamma p'_{n-1}(z) \tag{5.44}$$

When only (N, N) perturbation is present, only the initial condition of recurrence relation changes, and because of that the $2k$ eigenvalues are not part of the continuous spectra of the limiting set change.

When both $(1, 1)$ and (N, N) perturbations are present,

$$\begin{bmatrix} \tilde{p'}_n(z) \\ \tilde{q'}_n(z) \end{bmatrix} = \begin{bmatrix} z+a & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} z+a_k & -u_k \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p'_{n-1}(z) \\ q'_{n-1}(z) \end{bmatrix} \tag{5.45}$$

$$\begin{bmatrix} \tilde{p'}_n(z) \\ \tilde{q'}_n(z) \end{bmatrix} = \begin{bmatrix} \tilde{A(z)} & \tilde{B(z)} \\ \tilde{C(z)} & \tilde{D(z)} \end{bmatrix} \begin{bmatrix} p'_{n-1}(z) \\ q'_{n-1}(z) \end{bmatrix} \tag{5.46}$$

Here $\tilde{A}(z)$, $\tilde{B}(z)$, $\tilde{C}(z)$ and $\tilde{D}(z)$ are polynomials in z.

$$\tilde{p'}_n(z) = \tilde{A}(z)p'_{n-1}(z) + \tilde{B}(z)q'_{n-1}(z) \tag{5.47}$$

Thus,

$$\tilde{p'}_n(z) = p'_n(z)\frac{\tilde{B}(z)}{B(z)} + p'_{n-1}(z)(\tilde{A}(z) - R(z)A(z)) \tag{5.48}$$

where $R(z) = \frac{\tilde{B}(z)}{B(z)}$ and $S(z) = \frac{\tilde{A}(z)}{R(z)} - A(z)$.

$$\frac{\tilde{p'}_n(z)}{R(z)} = p'_n(z) + p'_{n-1}(z)S(z) \tag{5.49}$$

Applying Equation 5.44 in 5.49,

$$\frac{\tilde{p'}_n(z)}{R(z)} = (Q_k(z) + S(z))p'_{n-1}(z) + \gamma p'_{n-2}(z) \tag{5.50}$$

Writing in matrix format,

$$\begin{bmatrix} \frac{\tilde{p'}_n(z)}{R(z)} \\ p'_{n-1}(z) \end{bmatrix} = \begin{bmatrix} Q_k(z) + S(z) & \gamma \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p'_{n-1}(z) \\ p'_{n-2}(z) \end{bmatrix} \tag{5.51}$$

$$\begin{bmatrix} p'_{n-1}(z) \\ p'_{n-2}(z) \end{bmatrix} = \begin{bmatrix} Q_k(z) & \gamma \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p'_{n-2}(z) \\ p'_{n-3}(z) \end{bmatrix} \tag{5.52}$$

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combining 5.52 and 5.53,

$$\begin{bmatrix} \frac{\tilde{p'}_n(z)}{R(z)} \\ {p'}_{n-1}(z) \end{bmatrix} = \begin{bmatrix} Q_k(z)+S(z) & \gamma \\ 1 & 0 \end{bmatrix} \begin{bmatrix} Q_k(z) & \gamma \\ 1 & 0 \end{bmatrix}^{n-2} \begin{bmatrix} {p'}_1(z) \\ 1 \end{bmatrix} \tag{5.53}$$

From the above equation, it can be shown that $\frac{\tilde{p'}_n(z)}{R(z)}$ can be written as a determinant of the matrix given below.

$$\begin{bmatrix} {p'}_1(z) & i\sqrt{\gamma} & 0 & 0 & \dots & 0 \\ i\sqrt{\gamma} & Q_k(z) & i\sqrt{\gamma} & 0\dots & 0 & \\ 0 & i\sqrt{\gamma} & Q_k(z) & i\sqrt{\gamma} & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0\dots & \dots & \dots & \dots & i\sqrt{\gamma} & Q_k(z)+S(z) \end{bmatrix}_{n\times n} \tag{5.54}$$

Let, ${p'}_1(z) = Q_k(z) + p'(z)$.

Then zeros of $\frac{\tilde{p'}_n(z)}{R(z)}$ can be written as $\lambda' = -\frac{Q_k(z)}{\sqrt{\gamma}}$, where λ' is the eigenvalue of W'.

$$W' = \begin{bmatrix} \frac{p'(z)}{\sqrt{\gamma}} & -1 & 0 & 0 & \dots & 0 \\ 1 & 0 & -1 & 0 & \dots & 0 \\ 0 & 1 & 0 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & \dots & 0 & \frac{S(z)}{\sqrt{\gamma}} \end{bmatrix}_{n\times n} \tag{5.55}$$

$L'_n(\zeta', \lambda')$ is the characteristic polynomial for the above matrix and $T_n(\lambda)$ is the characteristic polynomial for the below skew-symmetric matrix.

$$\begin{bmatrix} 0 & -1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & -1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & -1 & 0 & \dots & 0 \\ 0 & \dots & \ddots & \vdots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 \end{bmatrix}_{n\times n} \tag{5.56}$$

Let $\zeta'_1 = \frac{p'(z)}{\sqrt{\gamma}}$ and $\zeta_2 = \frac{S(z)}{\sqrt{\gamma}}$.

Then by first expanding determinant along $(1,1)$ entry and further by (N,N) entry, we have

$$L'_n(\zeta', \lambda') = T_n + (\zeta'_1 + \zeta_2)T_{n-1} + (\zeta'_1\zeta_2)T_{n-2} \tag{5.57}$$

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$$L'_n(\zeta', \lambda') = \begin{bmatrix} 1 & \zeta'_1 + \zeta_2 & \zeta'_1\zeta_2 \end{bmatrix} \begin{bmatrix} T_n \\ T_{n-1} \\ T_{n-2} \end{bmatrix} \tag{5.58}$$

Now we have to find the solution of $L'_n(\zeta', \lambda') = 0$.

Using the same approach we used in section 3.2.3, $L'_n(\zeta', \lambda') = 0$ can be written as

$$\begin{aligned}(t_+ - \frac{1}{t_+})^{n-2}[(t_+ + \frac{1}{t_+})(t_+ - \frac{1}{t_+}) + \frac{1}{t_+^2} - t_+^2] + (t_+)^{n-2}[t_+^2 + (\zeta'_1 + \zeta_2)t_+ + \zeta'_1\zeta_2] \\ -\frac{(-1)^{n-2}}{t_+^{n-2}}[\frac{1}{t_+^2} + (\zeta'_1 + \zeta_2)\frac{-1}{t_+} + \zeta'_1\zeta_2] = 0\end{aligned} \tag{5.59}$$

$$t_+^{2n} + (\zeta'_1 + \zeta_2)t_+^{2n-1} + (\zeta'_1\zeta_2)t_+^{2n-2} - (-1)^n[1 - t_+(\zeta'_1 + \zeta_2) + (\zeta'_1\zeta_2)t_+^2] = 0 \tag{5.60}$$

As we discussed in section 5.2.3, since there are two ζ terms in equation 5.60, we cannot find the limiting set by applying Rouche's theorem or equivalent approaches.

5.2.5 Special Case: $\gamma = 0$

Let's see a special case where $\gamma = 0$. Then the equation 5.50 becomes,

$$\tilde{p'}_n(z) = R(z)[Q_k(z) + S(z)]p'_{n-1}(z) \tag{5.61}$$

and the equation 5.6 changes to,

$$p'_n(z) = Q_k(z)p'_{n-1}(z) \tag{5.62}$$

From the above equations, we get

$$\tilde{p'}_n(z) = R(z)[Q_k(z) + S(z)][Q_k(z)]^{n-1} \tag{5.63}$$

This leads to

$$\tilde{p'}_n(z) = Q_k(z)\tilde{p'}_{n-1}(z) \tag{5.64}$$

So when $\gamma = 0$, instead of a three-term recurrence relation, we can obtain a two-term recurrence relation. The above recurrence relation indicates that the eigenvalues of tridiagonal k-Toeplitz matrices with $\gamma = 0$ are getting repeated. Here we propose an

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algorithm to find the eigenvalues of the tridiagonal k-Toeplitz matrix whose $\gamma = 0$, under fixed perturbation.

Let n be the number of blocks of the perturbed tridiagonal k-Toeplitz matrix whose eigenvalue we have to find.

Algorithm 8 Algorithm to find eigenvalues of $\gamma = 0$ tridiagonal k-Toeplitz matrix under fixed perturbation

Require: Two null arrays Q and pert.

Find the eigenvalues of the unperturbed tridiagonal k-Toeplitz matrix using the python built-in function with number of blocks = 1 and store it in the Q array.

Calculate the eigenvalues of the perturbed tridiagonal k-Toeplitz matrix using builtin function with number of blocks = 2 and store it in pert array.

Append the pert array $(n-2)$ times by adding all elements in Q.

The pert array gives the eigenvalues of the tridiagonal k -Toeplitz matrix whose $\gamma = 0$ under fixed perturbation. The computational cost of this method is $O(k^2)$.

5.2.6 Off-Diagonal Perturbation

Under the fixed-fixed boundary conditions, there can be perturbation in $(1,2)$, $(2,1)$, $(N-1,N)$, and $(N,N-1)$ entries of the matrix. In the presence of fixed boundary conditions, we will obtain the characteristic polynomial of the tridiagonal k-Toeplitz matrix considering the perturbations in the off-diagonal entries.

Perturbation in (N, N), (N-1, N) and (N, N-1) Entries

With perturbation in (N,N), $(N-1,N)$ and $(N,N-1)$ entries, the tridiagonal k-Toeplitz matrix changes to

$$\tilde{M_k}' = \begin{bmatrix} a_1 & x_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ y_1 & a2 & x2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & y2 & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & a_k & x_k & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_k & a_1 & x_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & y_1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & y_{k-2} & a_{k-1} & x \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & y & b \end{bmatrix} \tag{5.65}$$

The initial condition for the characteristic polynomial of the above matrix can be

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written as,

$$\begin{bmatrix} p''_1(z) \\ q''_1(z) \end{bmatrix} = \begin{bmatrix} z+a_1 & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} z+a_{k-1} & -\tilde{u}_{k-1} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+b \\ 1 \end{bmatrix} \tag{5.66}$$

where $\tilde{u}_{k-1} = xy$.

$$\begin{bmatrix} p''_n(z) \\ q''_n(z) \end{bmatrix} = \begin{bmatrix} A(z) & B(z) \\ C(z) & D(z) \end{bmatrix} \begin{bmatrix} p''_{n-1}(z) \\ q''_{n-1}(z) \end{bmatrix} \tag{5.67}$$

Here $A(z)$, $B(z)$, $C(z)$, and $D(z)$ are polynomials in z, which comes in the characteristic polynomial derivation of tridiagonal k-Toeplitz matrices without any perturbation.

From the above matrix, we can get

$$p''_n(z) = A(z)p''_{n-1}(z) + B(z)q''_{n-1}(z) \tag{5.68}$$

The format of this three-term recurrence relation for the characteristic polynomial remains the same as that of the tridiagonal k-Toeplitz matrix without any perturbation. So the limiting set is unchanged under this perturbation and only $2k$ eigenvalues are getting changed.

Perturbation in $(1,1)$, $(1,2)$ and $(2,1)$ Entries

When we add perturbation in $(1,1)$, $(1,2)$ and $(2,1)$ entries, the tridiagonal k-Toeplitz matrix becomes,

$$\tilde{M_k}'' = \begin{bmatrix} a & \tilde{x} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \tilde{y} & a2 & x2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & y2 & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & a_k & x_k & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_k & a_1 & x_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & y_1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & y_{k-2} & a_{k-1} & x_{k-1} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & y_{k-1} & a_k \end{bmatrix} \tag{5.69}$$

The characteristic polynomial equation for the above matrix can be written as,

$$\begin{bmatrix} \tilde{\tilde{p}}_n(z) \\ \tilde{\tilde{q}}_n(z) \end{bmatrix} = \begin{bmatrix} z+a & -\tilde{u}_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} z+a_k & -u_k \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ q_{n-1}(z) \end{bmatrix} \tag{5.70}$$

where $\tilde{u}_1 = \tilde{x}\tilde{y}$.

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Let,

$$\begin{bmatrix} \tilde{\tilde{A}}(z) & \tilde{\tilde{B}}(z) \\ \tilde{\tilde{C}}(z) & \tilde{\tilde{D}}(z) \end{bmatrix} = \begin{bmatrix} z+a & -\tilde{u}_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z+a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \dots \begin{bmatrix} z+a_k & -u_k \\ 1 & 0 \end{bmatrix} \tag{5.71}$$

Then,

$$\begin{bmatrix} \tilde{\tilde{p}}_n(z) \\ \tilde{\tilde{q}}_n(z) \end{bmatrix} = \begin{bmatrix} \tilde{\tilde{A}}(z) & \tilde{\tilde{B}}(z) \\ \tilde{\tilde{C}}(z) & \tilde{\tilde{D}}(z) \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ q_{n-1}(z) \end{bmatrix} \tag{5.72}$$

From the above matrix, we get

$$\tilde{\tilde{p}}_n(z) = \tilde{\tilde{A}}(z)p_{n-1}(z) + \tilde{\tilde{B}}(z)q_{n-1}(z) \tag{5.73}$$

$$\tilde{\tilde{p}}_n(z) = \tilde{\tilde{A}}(z)p_{n-1}(z) + \frac{\tilde{\tilde{B}}(z)}{B(z)}(p_n(z) - A(z)p_{n-1}(z)) \tag{5.74}$$

$$\tilde{\tilde{p}}_n(z) = p_n(z)\frac{\tilde{\tilde{B}}(z)}{B(z)} + p_{n-1}(z)(\tilde{\tilde{A}}(z) - \tilde{R}(z)A(z)) \tag{5.75}$$

where $\tilde{R}(z) = \frac{\tilde{\tilde{B}}(z)}{B(z)}$ and $\tilde{S}(z) = \frac{\tilde{\tilde{A}}(z)}{\tilde{R}(z)} - A(z)$.

Substitution of $\tilde{R}(z)$ and $\tilde{S}(z)$ in equation 5.75 gives

$$\frac{\tilde{\tilde{p}}_n(z)}{\tilde{R}(z)} = p_n(z) + p_{n-1}(z)\tilde{S}(z) \tag{5.76}$$

The characteristic polynomial of tridiagonal k-Toeplitz matrix under perturbation in (1, 1), (1, 2), and (2, 1) entries also follows a three-term recurrence relation. We can show that there exists a limiting set for the eigenvalues of tridiagonal k-Toeplitz matrices under perturbation in (1, 1), (1, 2), and (2, 1) entries for finite large n [32].

5.3 Methods to Approximate the Limiting Set for Fixed Perturbation

Since we couldn't find the limiting set for the eigenvalues of the tridiagonal k -Toeplitz matrix under fixed boundary conditions, we have to develop methods to approximate the limiting set.

To begin with, we show below that a straightforward one-rank perturbation of the tridiagonal k -Toeplitz matrix is not useful in imposing the fixed boundary condition on

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the chain. One rank perturbation [33] on a $n \times n$ square matrix A can be written as $A + uv^T$.

$$uv^T = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_n \end{bmatrix} \begin{bmatrix} v_1 & v_2 & \dots & \dots & v_n \end{bmatrix} \tag{5.77}$$

$$uv^T = \begin{bmatrix} u_1v_1 & u_1v_2 & \dots & u_1v_{n-1} & u_1v_n \\ u_2v_1 & u_2v_2 & \dots & u_2v_{n-1} & u_2v_n \\ \vdots & \vdots & \dots \vdots & \vdots & \vdots \\ \vdots & \vdots & \dots \vdots & \vdots & \vdots \\ \vdots & \vdots & \dots \vdots & \vdots & \vdots \\ u_nv_1 & u_nv_2 & \dots & u_nv_{n-1} & u_nv_n \end{bmatrix} \tag{5.78}$$

Here u is one of the eigenvectors of A and v can be a random vector with the same size of u.

***Theorem**: Let u and v be two n-dimensional column vectors such that u is an eigenvector of A associated with the eigenvalue λ_1. Then, the eigenvalues of $A + uv^T$ are $(\lambda_1 + v^Tu, \lambda_2, ...\lambda_n)$.*

If the fixed perturbation can be written as a one-rank perturbation, we can easily find the eigenvalues of a tridiagonal k-Toeplitz matrix under fixed perturbation using the above theorem. For fixed perturbation, we need perturbation only in $(1, 1)$ and (N, N) entries of the tridiagonal k-Toeplitz matrix. Then, all the entries of uv^T have to be zero except $(1, 1)$ and (N, N) entries. That is, $u_1v_1 \neq 0$, $u_nv_n \neq 0$ and $u_jv_j = 0, \forall j \neq 0$ and n. To get perturbation only in $(1, 1)$ and (N, N) entries, we have to apply conditions on the entries of both u and v. Since u is the eigenvector of matrix A, it is not possible to put conditions on the entries of u. So we can't use one rank perturbation method to find the eigenvalues of the tridiagonal k-Toeplitz matrix under fixed perturbation.

5.3.1 Similarity Transformation

Two matrices A and B are similar if there exists an invertible matrix X such that $A = X^{-1}BX$ [34].

***Theorem**: Suppose A and B are similar matrices. Then A and B have the same characteristic polynomial and hence the same eigenvalues.*

Similarity transformation [35] provides a way to connect two symmetric tridiagonal k-Toeplitz matrices, whose $x_1 = 0$ and $x_{k-1} = 0$ and their $(1, 1)$ and (N, N) entries are

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interchanged. Here we are going to use the idea that eigenvalues won't change when we apply similarity transformation to matrices.

Consider a symmetric tridiagonal k-Toeplitz matrix , M_{k1} whose $k = 3$ and the number of block$(n) = 1$. Let, Y_{k1} be the matrix generated by applying (N, N) entry perturbation $= \epsilon$ in M_{k1}.

$$M_{k1} = \begin{bmatrix} a_1 & x_1 & 0 \\ x_1 & a_2 & x_2 \\ 0 & x_2 & a_3 \end{bmatrix} \text{ and } Y_{k1} = \begin{bmatrix} a_1 & x_1 & 0 \\ x_1 & a_2 & x_2 \\ 0 & x_2 & a_3 + \epsilon \end{bmatrix}.$$

$$P_{13}Y_{k1}P_{13} = \begin{bmatrix} a_3 + \epsilon & x_2 & 0 \\ x_2 & a_2 & x_1 \\ 0 & x_1 & a_1 \end{bmatrix} \tag{5.79}$$

Here P_{13} is the permutation matrix which is formed by the permutation of 1 and 3 columns of I_3 matrix. Since $P_{13}^{-1} = P_{13}$, Y_{k1} and $P_{13}Y_{k1}P_{13}$ are similar matrices. We can see that if $x_1 = 0$ and $x_2 = 0$, $P_{13}Y_{k1}P_{13}$ can be written as M_{k1} matrix with $(1, 1)$ entry perturbation $= a_3 + \epsilon - a_1$ and (N, N) entry perturbation $= a_1 - a_3$.

$$P_{13} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \text{ and } P_{16} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

P_{16} is the permutation matrix which is formed by the permutation of 1 and 6 columns of I_6 matrix.

When $n = 2$ and $k = 3$,

$$M_{k2} = \begin{bmatrix} a_1 & x_1 & 0 & 0 & 0 & 0 \\ x_1 & a_2 & x_2 & 0 & 0 & 0 \\ 0 & x_2 & a_3 & x_3 & 0 & 0 \\ 0 & 0 & x_3 & a_1 & x_1 & 0 \\ 0 & 0 & 0 & x_1 & a_2 & x_2 \\ 0 & 0 & 0 & 0 & x_2 & a_3 \end{bmatrix} \text{ and } Y_{k2} = \begin{bmatrix} a_1 & x_1 & 0 & 0 & 0 & 0 \\ x_1 & a_2 & x_2 & 0 & 0 & 0 \\ 0 & x_2 & a_3 & x_3 & 0 & 0 \\ 0 & 0 & x_3 & a_1 & x_1 & 0 \\ 0 & 0 & 0 & x_1 & a_2 & x_2 \\ 0 & 0 & 0 & 0 & x_2 & a_3 + \epsilon \end{bmatrix}$$

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$$P_{16}Y_{k2}P_{16} = \begin{bmatrix} a_3+\epsilon & 0 & 0 & 0 & x_2 & 0 \\ 0 & a_2 & x_2 & 0 & 0 & x_1 \\ 0 & x_2 & a_3 & x_3 & 0 & 0 \\ 0 & 0 & x_3 & a_1 & x_1 & 0 \\ x_2 & 0 & 0 & x_1 & a_2 & 0 \\ 0 & x_1 & 0 & 0 & 0 & a_1 \end{bmatrix} \tag{5.80}$$

Here M_{k2} be a symmetric tridiagonal k-Toeplitz matrix with $k = 3$ and the number of blocks$(n) = 2$. Y_{k2} is a matrix formed by applying ϵ perturbation in (N, N) entry of M_{k2}. $P_{16}Y_{k2}P_{16}$ is a similarity transformation of Y_{k2}. If $x_1 = 0$ and $x_2 = 0$, $P_{16}Y_{k2}P_{16}$ can be written as M_{k2} matrix with $(1, 1)$ entry perturbation $= a_3 + \epsilon - a_1$ and (N, N) entry perturbation $= a_1 - a_3$.

Let us generalize the above-discussed idea. P_{1N} is the permutation matrix which is formed by the permutation of 1 and N columns of I_N matrix and M_k is a symmetric tridiagonal k-Toeplitz matrix with $x_1 = 0$ and $x_{k-1} = 0$. Y_k matrix is formed by applying (N, N) entry perturbation $= \epsilon$ on M_k. When Y_k is left and right multiplied by P_{1N} permutation matrix result in $P_{1N}Y_kP_{1N}$ matrix. $P_{1N}Y_kP_{1N}$ matrix has perturbation in both (1,1) and (N, N) entries with (1,1) entry perturbation $= a_k + \epsilon - a_1$ and (N, N) entry perturbation $= a_1 - a_k$. Here Y_k has only (N, N) entry perturbation, so eigenvalues of Y_k can be found using the Chebyshev approximation of M_k matrix and the equation 5.8. Since $P_{1N}Y_kP_{1N}$ is the similarity transform of Y_k, they have same eigenvalues.

5.3.2 Direct Replacement Method for Perturbed Eigenvalues

We have derived three-term recurrence relation for the tridiagonal-toeplitz matrix under the fixed perturbation. The polynomials with a three-term recurrence have a limiting set [32], and to find only the difference between the two limiting sets of eigenvalues i.e. with and without perturbation, we can use direct replacement method.

The direct replacement is a method to approximate the limiting set of the tridiagonal k-Toeplitz matrix after $(1, 1)$ entry perturbation. This method is based on the replacement of eigenvalues which has maximum change during the $(1, 1)$ entry perturbation.

Here we consider a tridiagonal k-Toeplitz matrix with period $= k$, number of blocks $= n$, and size of the matrix $= nk \times nk$.

Graphs of error analysis of direct replacement eigenvalues are given in the next chapter.

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Algorithm 9 Direct Replacement Algorithm

Require: Null arrays called C, R, and TR.

Calculate the Chebyshev approximated eigenvalues for the unperturbed tridiagonal k-Toeplitz matrix for the no of blocks (n) we want, and store it as C.

Compare Chebyshev approximated eigenvalues of the unperturbed tridiagonal k-Toeplitz matrix at $n = 2$ with builtin eigenvalues of the (1,1) entry perturbed tridiagonal k-Toeplitz matrix at $n = 2$.

Then find the two Chebyshev approximated eigenvalues, which are getting maximum change during perturbation in (1,1) entry when $n = 2$, and store it in a null array called R.

Find those two built-in eigenvalues of the (1,1) entry perturbed tridiagonal k-Toeplitz matrix at $n = 2$, which are getting the maximum change after perturbation and store it in the TR array.

Replace the two eigenvalues from the C array which are close to R array elements with the TR elements.

5.3.3 Replacement for Perturbed Eigenvalues with Inverse Iteration

Replacement using Inverse Iteration is a modified version of the Direct Replacement algorithm. Here we use the Inverse Iteration algorithm to replace the eigenvalues which have the maximum change due to $(1, 1)$ entry perturbation. The algorithm for this method is given below.

We consider tridiagonal k-Toeplitz matrix with period $= k$, number of blocks $= n$ and size of the matrix $= nk \times nk$.

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Algorithm 10 Replacement using Inverse Iteration

Require: Null arrays called C, R, I, and TR.

Calculate the Chebyshev approximated eigenvalues for the unperturbed tridiagonal k-Toeplitz matrix for the no of blocks(n) we want, and store it as C.

Compare Chebyshev approximated eigenvalues of the unperturbed tridiagonal k-Toeplitz matrix at $n = 2$, with builtin eigenvalues of the $(1, 1)$ entry perturbed tridiagonal k-Toeplitz matrix at $n = 2$.

Then find the two Chebyshev approximated eigenvalues, which are getting maximum change during perturbation in (1,1) entry when $n = 2$, and store it in a null array called R.

Find those two built-in eigenvalues of the (1,1) entry perturbed tridiagonal k-Toeplitz matrix at $n = 2$, which are getting the maximum change after perturbation and store it in the TR array.

Perform the Inverse Iteration algorithm taking TR eigenvalues as input and store the output eigenvalues in the I array.

Replace the two eigenvalues from the C array which are close to R array elements with the I elements.

Error analysis of the eigenvalues generated by replacement using the Inverse Iteration algorithm is given in the next chapter.

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Chapter 6

Example Results for Fixed and Periodic Boundary Conditions

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Chapter-outline

Here, the approaches suggested in the previous chapter to identify the perturbed Chebyshev eigenvalues, and correct them using direct numerical methods, is demonstrated.

6.1 Fixed Perturbation

During only (N, N) entry perturbation in the tridiagonal k-Toeplitz matrix, $2k$ eigenvalues that are not part of the continuous limiting set are getting affected and the continuous part of the limiting set remains the same.

Due to (N, N) entry perturbation, only the initial condition changes and $2k$ eigenvalues, those are not part of the continuous spectra of limiting set changes by the equation given below.

$$Q_k(z) = \frac{\gamma}{p'(z)} - p'(z) \tag{6.1}$$

where $p'(z) = p'_1(z) - Q_k(z)$

The $2k$ eigenvalues are the solutions of the equation 6.1.

If there is a perturbation in both $(1, 1)$ and (N, N) entries, we can treat $(1, 1)$ and (N, N) entry perturbations independent of each other. Due to (N, N) entry perturbation, $2k$ eigenvalues that are not part of the continuous limiting set are getting affected, and

because of $(1, 1)$ entry perturbation, the continuous part of the limiting set is getting affected.

6.1.1 Fixed Boundary Condition for $\gamma = 0$ Matrices

In Chapter 5, we have developed an algorithm to find the exact eigenvalues of the tridiagonal k-Toeplitz matrix with $\gamma = 0$ under fixed perturbation. For $\gamma = 0$, for tridiagonal k-Toeplitz matrices, the characteristic polynomial can be written as the product of at most k factors, thus the matrix has at most k different eigenvalues. $\gamma = 0$ chains can be one-directional or they can have nearest neighbors without any interaction. The following figures give the average relative error in the built-in eigenvalues for the tridiagonal k-Toeplitz matrices with $\gamma = 0$ under fixed perturbation. With our algorithm, the exact eigenvalues can be found for any n without any error for $\gamma = 0$, tridiagonal k-Toeplitz matrices.

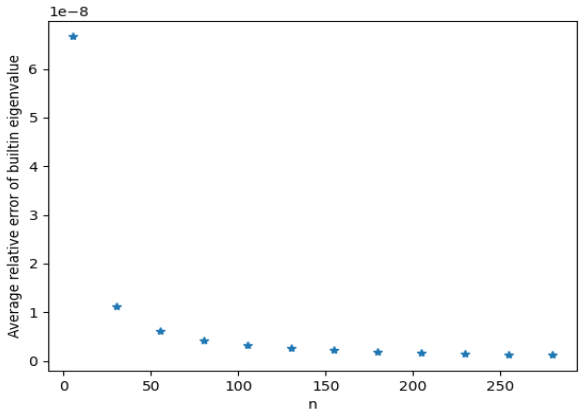

Figure 6.1: Error analysis of eigenvalues: diagonal= $[0, 0, 0]$, upper diagonal= $[1, -1, 1]$, lower diagonal= $[1, 0, -1]$, perturbation in $(1, 1)$ entry= 100, perturbation in (N, N) entry $= -2$. $C = 382.6$, where C is the condition number of the matrix when $n = 200$. Using our algorithm, we can find the eigenvalues without any error.

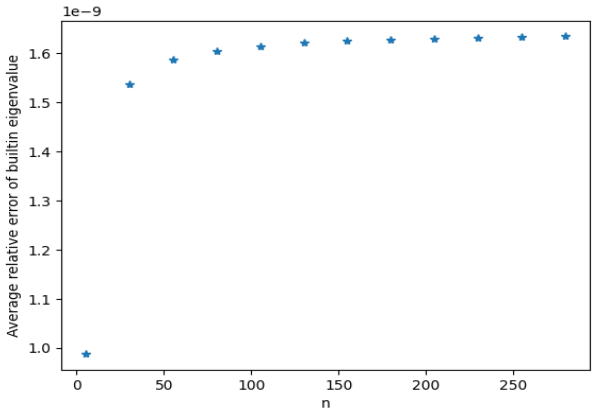

Figure 6.2: Error analysis of eigenvalues: diagonal= $[1, 2, 1]$, upper diagonal= $[0, 1, 1]$ = lower diagonal, perturbation in (1, 1) entry= 100, perturbation in (N, N) entry $= -2$. $C = 11.344$, where C is the condition number of the matrix when $n = 200$. Using our algorithm, we can find the eigenvalues without any error.

6.1.2 Similarity Transformation

Using similarity transformation, we can connect the eigenvalues of only (N, N) entry perturbed symmetric tridiagonal k-Toeplitz matrix whose $x_1 = 0$ and $x_{k-1} = 0$ and symmetric tridiagonal k-Toeplitz matrix with perturbation in both $(1, 1)$ and (N, N) entries. Since symmetric tridiagonal k-Toeplitz matrix whose $x_1 = 0$ and $x_{k-1} = 0$ with $(1, 1)$ entry perturbation $= a_1 - a_k + \epsilon$ and (N, N) entry perturbation $= a_k - a_1$ is similar to symmetric tridiagonal k-Toeplitz matrix whose $x_1 = 0$ and $x_{k-1} = 0$ with (N, N) entry perturbation $= \epsilon$, they have same eigenvalues. When there is only (N, N) entry perturbation ((N, N) entry perturbation $= \epsilon$) in the symmetric tridiagonal k-Toeplitz matrix (M_k), the $2k$ eigenvalues which are not part of the continuous limiting set are getting changed. With this idea we can find the eigenvalues of symmetric tridiagonal k-Toeplitz matrix with both $(1, 1)$ and (N, N) entry perturbations ($(1, 1)$ entry perturbation $= a_1 - a_k + \epsilon$ and (N, N) entry perturbation $= a_k - a_1$).

6.1.3 Direct Replacement Method for Perturbed Eigenvalues

The given below graphs show how the average relative error of eigenvalues of tridiagonal k-Toeplitz matrices under (1, 1) entry perturbation calculated using the direct replacement algorithm changes when the number of blocks (n) increases.

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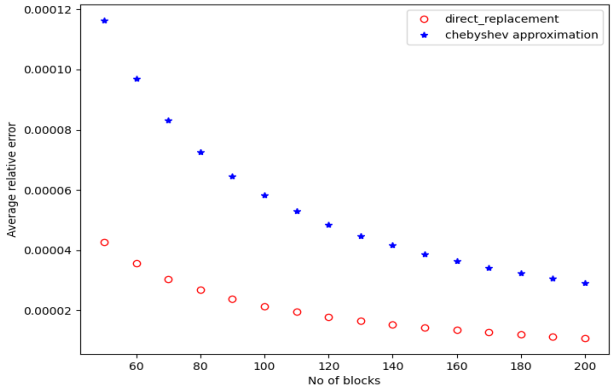

Figure 6.3: Direct Replacement: diagonal= $[10, 12, 3]$, upper diagonal= $[1, 41, 5]$, lower diagonal=upper diagonal, $k = 3$ is the period of chain, perturbation in (1, 1) entry = 0.1. Here average relative error of the direct replacement method is lesser than that of the Chebyshev approximated eigenvalues, so the direct replacement method works better than the Chebyshev approximation method. Condition number of the matrix = 5.024.

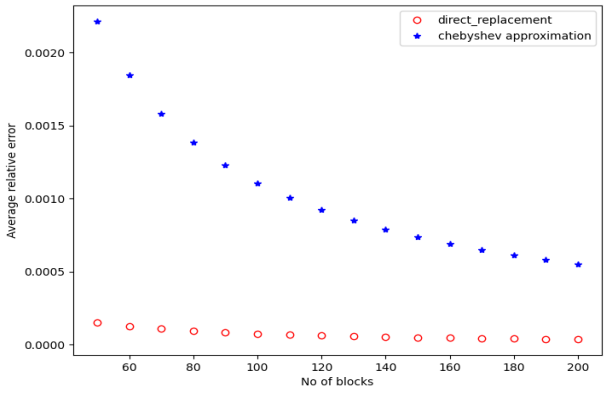

Figure 6.4: Direct Replacement: diagonal= $[10, 12, 3]$, upper diagonal= $[1, 41, 5]$, lower diagonal=upper diagonal, $k = 3$ is the period of chain, perturbation in (1, 1) entry = 5. Here average relative error of the direct replacement method is lesser than that of the Chebyshev approximated eigenvalues, so the direct replacement method works better than the Chebyshev approximation method. Condition number of the matrix = 5.024.

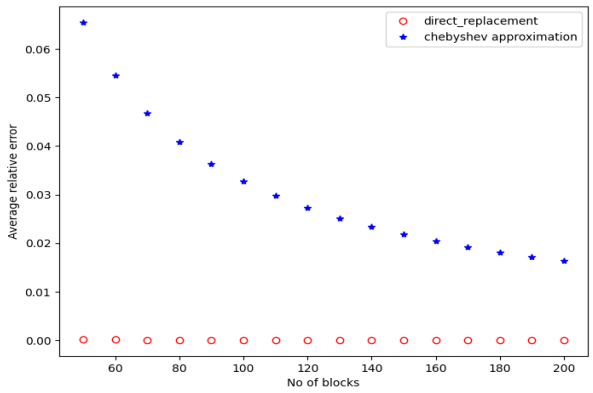

Figure 6.5: Direct Replacement: diagonal= $[10, 12, 3]$, upper diagonal= $[1, 41, 5]$, lower diagonal=upper diagonal, $k = 3$ is the period of chain, perturbation in (1, 1) entry $= -10$. Here average relative error of the direct replacement method is lesser than that of the Chebyshev approximated eigenvalues, so the direct replacement method is not better than the Chebyshev approximation method. Condition number of the matrix $= 5.024$.

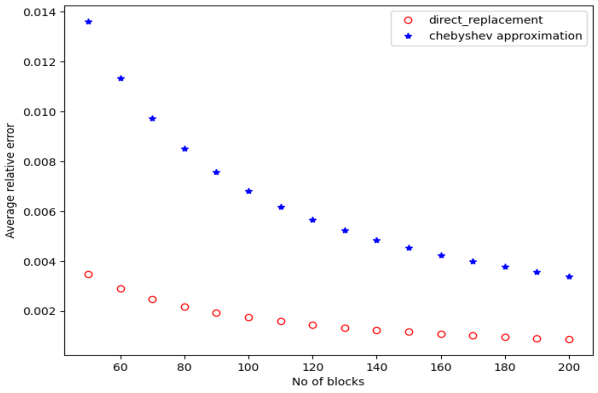

Figure 6.6: Direct Replacement: diagonal= $[1, 2, 3]$, upper diagonal= $[1, 4, -2]$, lower diagonal=upper diagonal, $k = 3$ is the period of chain, perturbation in (1, 1) entry $= 50$. Here average relative error of the direct replacement method is almost zero, so the direct replacement method works better than the Chebyshev approximation method. The condition number of the matrix when $n = 50$ is 17.7936, the condition number of the matrix when $n = 100$ is 17.8525, the condition number of the matrix when $n = 150$ is 17.8645, and the condition number of the matrix when $n = 200$ is 17.8688.

The direct replacement method works better in most cases, but we can't give any guarantee that the direct replacement idea will work for every case of $(1, 1)$ entry perturbation.

6.1.4 Replacement for Perturbed Eigenvalues with Inverse Iteration

Replacement using Inverse Iteration is a modification to the direct replacement method and given below graphs represent the error diagram of eigenvalues that are generated by replacement with Inverse Iteration.

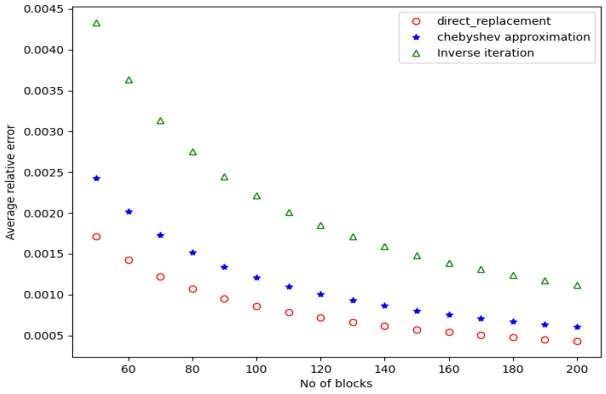

Figure 6.7: Replacement using Inverse Iteration: diagonal= $[1, 2, 3]$, lower diagonal= $[1, 4, -2]$, upper diagonal=lower diagonal, $k = 3$ is the period of chain, perturbation in (1, 1) entry $= 0.001$. Eigenvalues modified using Inverse Iteration are more erroneous than both the direct replacement method and the Chebyshev approximation method. Thus modification of eigenvalues using Inverse Iteration fails here. The condition number of the matrix when $n = 50$ is 17.7936, the condition number of the matrix when $n = 100$ is 17.8525, the condition number of the matrix when $n = 150$ is 17.8645, and the condition number of the matrix when $n = 200$ is 17.8688. Here n is the number of blocks of the matrix.

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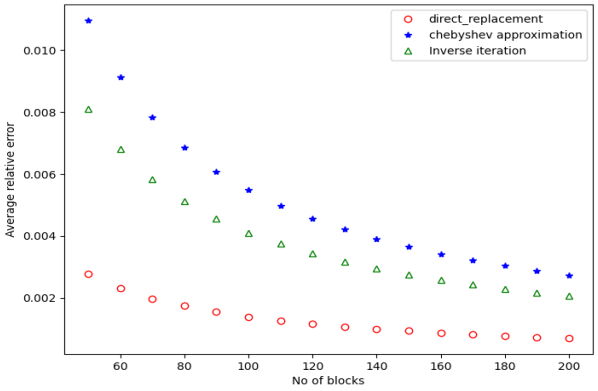

Figure 6.8: Replacement using Inverse Iteration: diagonal= $[1, 2, 3]$, lower diagonal = $[1, 4, -2]$, upper diagonal=lower diagonal, $k = 3$ is the period of chain, perturbation in (1, 1) entry = -5. Eigenvalues modified using Inverse Iteration are more erroneous than the direct replacement method. Thus modification of eigenvalues using Inverse Iteration fails here. The condition number of the matrix when $n = 50$ is 17.7936, the condition number of the matrix when $n = 100$ is 17.8525, the condition number of the matrix when $n = 150$ is 17.8645, and the condition number of the matrix when $n = 200$ is 17.8688. Here n is the number of blocks of the matrix.

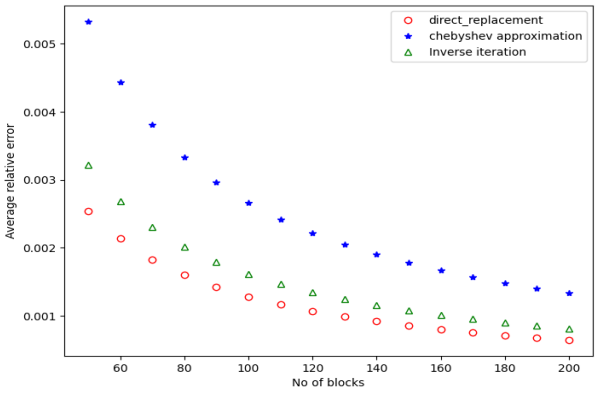

Figure 6.9: Replacement using Inverse Iteration: diagonal= $[1, 2, 3]$, lower diagonal= $[1, 4, -2]$, upper diagonal=lower diagonal, $k = 3$ is the period of chain, perturbation in (1, 1) entry = 2. Eigenvalues modified using Inverse Iteration are more erroneous than the direct replacement method. Thus modification of eigenvalues using Inverse Iteration fails here. The condition number of the matrix when $n = 50$ is 17.7936, the condition number of the matrix when $n = 100$ is 17.8525, the condition number of the matrix when $n = 150$ is 17.8645, and the condition number of the matrix when $n = 200$ is 17.8688. Here n is the number of blocks of the matrix.

From the above graphs, we can conclude that replacement for perturbed eigenvalues using Inverse Iteration need not be better than the direct replacement method.

6.2 Periodic Perturbation Analysis

In this section, we compare the eigenvalues of open and closed k-periodic chains.

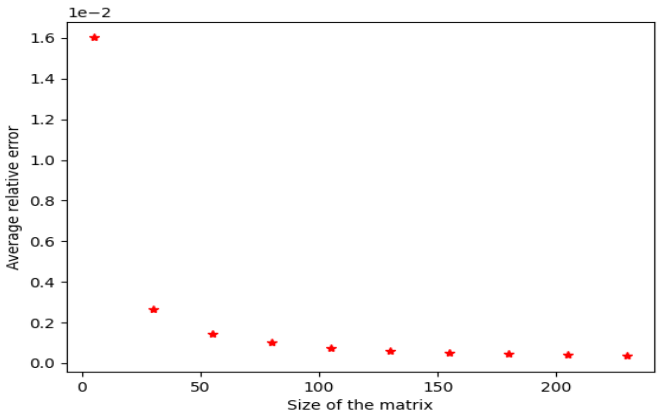

Figure 6.10: Error analysis of eigenvalues under periodic perturbation: diagonal= $[-500, 1000, 80, -100, 50]$, upper diagonal= $[20, 19, 50, 40, -50]$, lower diagonal=upper diagonal.

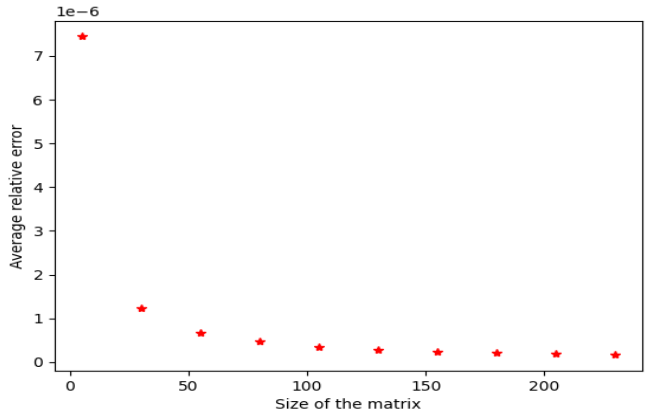

Figure 6.11: Error analysis of eigenvalues under periodic perturbation: diagonal = $[-500, 1000, 80, -100, 50]$, upper diagonal= $[20, 19, 50, 40, -1]$, lower diagonal=upper diagonal.

In the above figures, the error is the difference between eigenvalues with and without periodic perturbation. We can reach the following conclusions through the analysis of the figures and n is the number of blocks of the matrix.

- At large n, eigenvalues of tridiagonal k-Toeplitz matrices with periodic perturbation converge to the eigenvalues of tridiagonal k-Toeplitz matrices with free-free boundary condition.
- For large n, we can approximate the Chebyshev approximated eigenvalues for the tridiagonal k-Toeplitz matrix with periodic boundary conditions.

- For large n, we can find the eigenvalues of the tridiagonal k-Toeplitz matrix under periodic boundary conditions with the computational cost of $O(nk^2)$.

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Chapter 7

Appendix

7.0.1 Adjacency Matrices for the Lattices in Chapter 2

(a) Figure 3.4

$$L_{xx} = \begin{bmatrix} a_1 & x_1 & 0 \\ x_1 & a_1 & x_1 \\ 0 & x_1 & a_1 \end{bmatrix} \text{ and } L_{yy} = \begin{bmatrix} a_2 & x_2 & 0 & 0 & 0 & 0 \\ x_2 & a_3 & x_3 & 0 & 0 & 0 \\ 0 & x_3 & a_2 & x_2 & 0 & 0 \\ 0 & 0 & x_2 & a_3 & x_3 & 0 \\ 0 & 0 & 0 & x_3 & a_2 & x_2 \\ 0 & 0 & 0 & 0 & x_2 & a_3 \end{bmatrix}$$

Here L_{xx} and L_{yy} represent adjacency matrices of the chains in figure 3.2 and figure 7.7 respectively. Adjacency matrix for the 2D lattice formed by L_{xx} and L_{yy} is given by,

$$A_{2D-free-free} = L_{xx} \oplus L_{yy} = L_{xx} \otimes I_2 + I_1 \otimes L_{yy}$$

$$L_{xx} \otimes I_2 = \begin{bmatrix} a_1 & 0 & x_1 & 0 & 0 & 0 \\ 0 & a_1 & 0 & x_1 & 0 & 0 \\ x_1 & 0 & a_1 & 0 & x_1 & 0 \\ 0 & x_1 & 0 & a_1 & 0 & x_1 \\ 0 & 0 & x_1 & 0 & a_1 & 0 \\ 0 & 0 & 0 & x_1 & 0 & a_1 \end{bmatrix} \text{ and } I_1 \otimes L_{yy} = L_{yy}$$

So,

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$$A_{2D-free-free} = \begin{bmatrix} a_1+a_2 & x_2 & x_1 & 0 & 0 & 0 \\ x_2 & a_1+a_3 & x_3 & x_1 & 0 & 0 \\ x_1 & x_3 & a_1+a_2 & x_2 & x_1 & 0 \\ 0 & x_1 & x_2 & a_1+a_3 & x_3 & x_1 \\ 0 & 0 & x_1 & x_3 & a_1+a_2 & x_2 \\ 0 & 0 & 0 & x_1 & x_2 & a_1+a_3 \end{bmatrix}$$

(b) Figure 3.7

The adjacency matrices of the chains in figures 3.6 and 3.5 can be represented as L_{xx} and L_{yy}.

$$L_{xx} = \begin{bmatrix} a_1 & x_1 & 0 \\ x_1 & a_1 & x_1 \\ 0 & x_1 & a_1 \end{bmatrix} \text{ and } L_{yy} = \begin{bmatrix} \tilde{a}_2 & x_2 & 0 & 0 & 0 & 0 \\ x_2 & a_3 & x_3 & 0 & 0 & 0 \\ 0 & x_3 & a_2 & x_2 & 0 & 0 \\ 0 & 0 & x_2 & a_3 & x_3 & 0 \\ 0 & 0 & 0 & x_3 & a_2 & x_2 \\ 0 & 0 & 0 & 0 & x_2 & \tilde{a}_3 \end{bmatrix}$$

Adjacency matrix for the 2D lattice formed by L_{xx} and L_{yy} is given below.

$A_{2D-fixed} = L_{xx} \oplus L_{yy} = L_{xx} \otimes I_2 + I_1 \otimes L_{yy}$

$$L_{xx} \otimes I_2 = \begin{bmatrix} a_1 & 0 & x_1 & 0 & 0 & 0 \\ 0 & a_1 & 0 & x_1 & 0 & 0 \\ x_1 & 0 & a_1 & 0 & x_1 & 0 \\ 0 & x_1 & 0 & a_1 & 0 & x_1 \\ 0 & 0 & x_1 & 0 & a_1 & 0 \\ 0 & 0 & 0 & x_1 & 0 & a_1 \end{bmatrix} \text{ and } I_1 \otimes L_{yy} = L_{yy}$$

$$A_{2D-fixed} = \begin{bmatrix} a_1+\tilde{a}_2 & x_2 & x_1 & 0 & 0 & 0 \\ x_2 & a_1+a_3 & x_3 & x_1 & 0 & 0 \\ x_1 & x_3 & a_1+a_2 & x_2 & x_1 & 0 \\ 0 & x_1 & x_2 & a_1+a_3 & x_3 & x_1 \\ 0 & 0 & x_1 & x_3 & a_1+a_2 & x_2 \\ 0 & 0 & 0 & x_1 & x_2 & a_1+\tilde{a}_3 \end{bmatrix}$$

7.0.2 Figures and Adjacency Matrix for the Tight Binding Lattices

(a) When both x and y directional chains are diatomic and under the free-free boundary condition.

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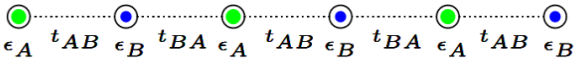

Figure 7.1: One-dimensional free-free di-atomic lattice, ($\epsilon_k = \epsilon_A, \forall$ odd k, $\epsilon_k = \epsilon_B, \forall$ even k, $t_k = t_{AB}, \forall$ odd k, $t_k = t_{BA}, \forall$ even k)

Figure 7.2: One-dimensional free-free di-atomic lattice, ($\epsilon_k = \epsilon_C, \forall$ odd k, $\epsilon_k = \epsilon_D, \forall$ even k, $t_k = t_{CD}, \forall$ odd k, $t_k = t_{DC}, \forall$ even k)

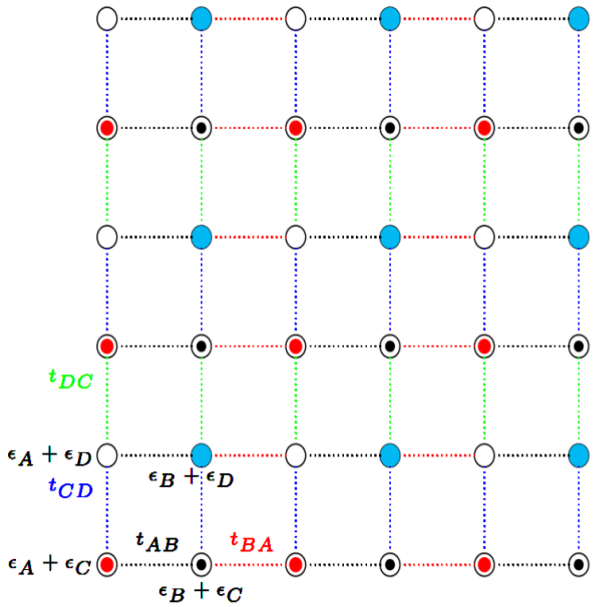

Figure 7.3: Two-dimensional lattice with free-free boundary condition (This lattice is the Kronecker sum of diatomic chain with free-free boundary condition in the x direction(Figure 7.1) and diatomic chain with free-free boundary condition in the y direction(Figure 7.2))

Let's see how to find the adjacency matrix for the above 2D lattice.

$$\text{Let, } L_{xx} = \begin{bmatrix} \epsilon_A & t_{AB} & 0 & 0 \\ t_{AB} & \epsilon_B & t_{BA} & 0 \\ 0 & t_{BA} & \epsilon_A & t_{AB} \\ 0 & 0 & t_{AB} & \epsilon_B \end{bmatrix} \text{ and } L_{yy} = \begin{bmatrix} \epsilon_C & t_{CD} & 0 & 0 \\ t_{CD} & \epsilon_D & t_{DC} & 0 \\ 0 & t_{DC} & \epsilon_C & t_{CD} \\ 0 & 0 & t_{CD} & \epsilon_D \end{bmatrix}$$

Adjacency matrix for the 2D lattice formed by L_{xx} and L_{yy} is given by,

$$A_{2D-free-free} = L_{xx} \oplus L_{yy} = L_{xx} \otimes I_2 + I_2 \otimes L_{yy}$$

$$L_{xx} \otimes I_2 = \begin{bmatrix} \epsilon_A & 0 & t_{AB} & 0 & 0 & 0 & 0 & 0 \\ 0 & \epsilon_A & 0 & t_{AB} & 0 & 0 & 0 & 0 \\ t_{AB} & 0 & \epsilon_B & 0 & t_{BA} & 0 & 0 & 0 \\ 0 & t_{AB} & 0 & \epsilon_B & 0 & t_{BA} & 0 & 0 \\ 0 & 0 & t_{BA} & 0 & \epsilon_A & 0 & t_{AB} & 0 \\ 0 & 0 & 0 & t_{BA} & 0 & \epsilon_A & 0 & t_{AB} \\ 0 & 0 & 0 & 0 & t_{AB} & 0 & \epsilon_B & t_{CD} \\ 0 & 0 & 0 & 0 & 0 & t_{AB} & 0 & \epsilon_B \end{bmatrix}$$

$$I_2 \otimes L_{yy} = \begin{bmatrix} \epsilon_C & t_{CD} & 0 & 0 & 0 & 0 & 0 & 0 \\ t_{CD} & \epsilon_D & t_{DC} & 0 & 0 & 0 & 0 & 0 \\ 0 & t_{DC} & \epsilon_C & t_{CD} & 0 & 0 & 0 & 0 \\ 0 & 0 & t_{CD} & \epsilon_D & t_{DC} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \epsilon_C & t_{CD} & 0 & 0 \\ 0 & 0 & 0 & 0 & t_{CD} & \epsilon_D & t_{DC} & 0 \\ 0 & 0 & 0 & 0 & 0 & t_{DC} & \epsilon_C & t_{CD} \\ 0 & 0 & 0 & 0 & 0 & 0 & t_{CD} & \epsilon_D \end{bmatrix}$$

$$A_{2D-free-free} = \begin{bmatrix} \epsilon_A + \epsilon_C & t_{CD} & t_{AB} & 0 & 0 & 0 & 0 & 0 \\ t_{CD} & \epsilon_A + \epsilon_D & t_{DC} & t_{AB} & 0 & 0 & 0 & 0 \\ t_{AB} & t_{DC} & \epsilon_B + \epsilon_C & t_{CD} & t_{BA} & 0 & 0 & 0 \\ 0 & t_{AB} & t_{CD} & \epsilon_B + \epsilon_D & t_{DC} & t_{BA} & 0 & 0 \\ 0 & 0 & t_{BA} & 0 & \epsilon_A + \epsilon_C & t_{CD} & t_{AB} & 0 \\ 0 & 0 & 0 & t_{BA} & t_{CD} & \epsilon_A + \epsilon_D & t_{DC} & t_{AB} \\ 0 & 0 & 0 & 0 & t_{AB} & t_{DC} & \epsilon_B + \epsilon_C & t_{CD} \\ 0 & 0 & 0 & 0 & 0 & t_{AB} & t_{CD} & \epsilon_B + \epsilon_D \end{bmatrix}$$

(b) When the x chain is triatomic with free-free boundary condition and the y chain is diatomic with free-free boundary condition.

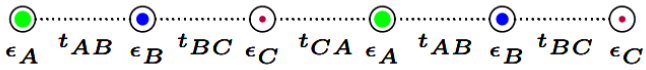

Figure 7.4: One-dimensional free-free di-atomic lattice, ($\epsilon_k = \epsilon_A$, for $k = 1, 4, 7..$, $\epsilon_k = \epsilon_B$, for $k = 2, 5, 8..$ and, $\epsilon_k = \epsilon_C$ for $k = 3, 6, 9..$, $t_k = t_{AB}$, for $k = 1, 4, 7..$, $t_k = t_{BC}$, for $k = 2, 5, 8..$ and $t_k = t_{CA}$ for $k = 3, 6, 9..$)

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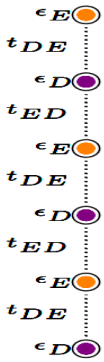

Figure 7.5: One-dimensional free-free di-atomic lattice, ($\epsilon_k = \epsilon_D, \forall$ odd k, $\epsilon_k = \epsilon_E, \forall$ even k, $t_k = t_{DE}, \forall$ odd k, $t_k = t_{ED}, \forall$ even k)

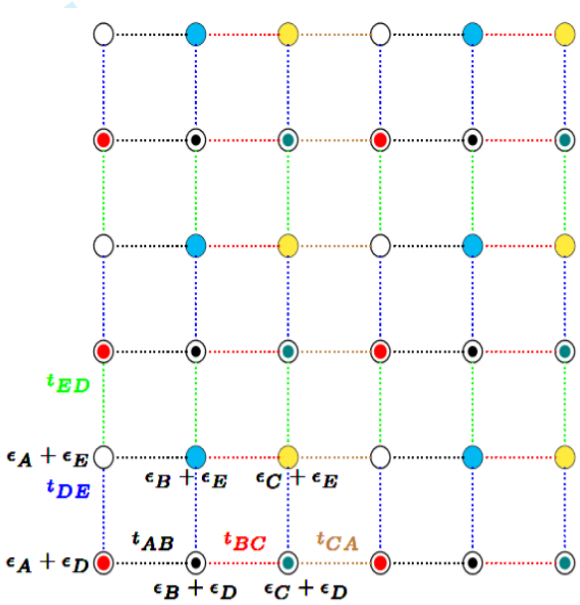

Figure 7.6: Two-dimensional lattice with free-free boundary condition (This lattice is the Kronecker sum of tri-atomic chain with free-free boundary condition in the x direction(Figure 7.4) and di-atomic chain with free-free boundary condition in the y direction(Figure 7.5))

Let's see how to find the adjacency matrix for the above 2D lattice.

$$\text{Let, } L_{xx} = \begin{bmatrix} \epsilon_A & t_{AB} & 0 & 0 & 0 & 0 \\ t_{AB} & \epsilon_B & t_{BC} & 0 & 0 & 0 \\ 0 & t_{BC} & \epsilon_C & t_{CA} & 0 & 0 \\ 0 & 0 & t_{CA} & \epsilon_A & t_{AB} & 0 \\ 0 & 0 & 0 & t_{AB} & \epsilon_B & t_{BC} \\ 0 & 0 & 0 & 0 & t_{BC} & \epsilon_C \end{bmatrix} \text{ and } L_{yy} = \begin{bmatrix} \epsilon_D & t_{DE} & 0 & 0 \\ t_{DE} & \epsilon_E & t_{ED} & 0 \\ 0 & t_{ED} & \epsilon_D & t_{DE} \\ 0 & 0 & t_{DE} & \epsilon_E \end{bmatrix}$$

Adjacency matrix for the 2D lattice formed by L_{xx} and L_{yy} is given by,

$$A_{2D-free-free} = L_{xx} \oplus L_{yy} = L_{xx} \otimes I_2 + I_3 \otimes L_{yy}$$

$L_{xx} \otimes I_2$ and $I_3 \otimes L_{yy}$ are 12×12 dimensional matrices. But we are considering only the first 6 rows and the first 6 columns of these matrices.

$$L_{xx} \otimes I_2 = \begin{bmatrix} \epsilon_A & 0 & t_{AB} & 0 & 0 & 0 \\ 0 & \epsilon_A & 0 & t_{AB} & 0 & 0 \\ t_{AB} & 0 & \epsilon_B & 0 & t_{BC} & 0 \\ 0 & t_{AB} & 0 & \epsilon_B & 0 & t_{BC} \\ 0 & 0 & t_{BC} & 0 & \epsilon_C & 0 \\ 0 & 0 & 0 & t_{BC} & 0 & \epsilon_C \end{bmatrix}$$

$$I_3 \otimes L_{yy} = \begin{bmatrix} \epsilon_D & t_{DE} & 0 & 0 & 0 & 0 \\ t_{DE} & \epsilon_E & t_{ED} & 0 & 0 & 0 \\ 0 & t_{ED} & \epsilon_D & t_{DE} & 0 & 0 \\ 0 & 0 & t_{DE} & \epsilon_E & 0 & t_{BC} \\ 0 & 0 & 0 & 0 & \epsilon_D & t_{DE} \\ 0 & 0 & 0 & 0 & t_{DE} & \epsilon_E \end{bmatrix}$$

$$A_{2D-free-free} = \begin{bmatrix} \epsilon_A + \epsilon_D & t_{DE} & t_{AB} & 0 & 0 & 0 \\ t_{DE} & \epsilon_A + \epsilon_E & t_{ED} & t_{AB} & 0 & 0 \\ t_{AB} & t_{ED} & \epsilon_B + \epsilon_D & t_{DE} & t_{BC} & 0 \\ 0 & t_{AB} & t_{DE} & \epsilon_B + \epsilon_E & 0 & t_{BC} \\ 0 & 0 & t_{BC} & 0 & \epsilon_C + \epsilon_D & t_{DE} \\ 0 & 0 & 0 & t_{BC} & t_{DE} & \epsilon_C + \epsilon_E \end{bmatrix} \tag{7.1}$$

(c) When the x directional chain is di-atomic with free-free boundary condition and the y directional chain is di-atomic with fixed-fixed boundary condition.

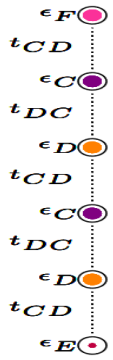

Figure 7.7: One-dimensional fixed-fixed di-atomic lattice, ($\epsilon_k = \epsilon_C, \forall$ odd k except the boundaries, $\epsilon_k = \epsilon_D, \forall$ even k except the boundaries , $t_k = t_{CD}, \forall$ odd k, $t_k = t_{DC}, \forall$ even k)

For Review Only

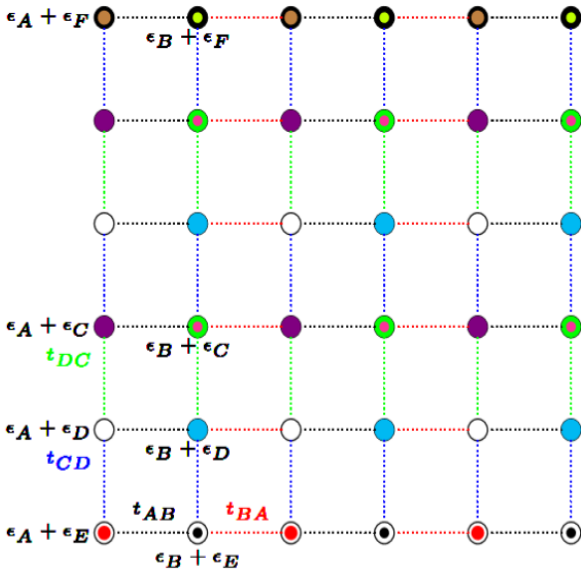

Figure 7.8: Two-dimensional lattice with free-free boundary condition (This lattice is the Kronecker sum of di-atomic chain with free-free boundary condition in the x direction(Figure 7.4) and di-atomic chain with fixed boundary condition in the y direction(Figure 7.7))

Let's see how to find the adjacency matrix for the above 2D lattice.

$$\text{Let, } L_{xx} = \begin{bmatrix} \epsilon_A & t_{AB} & 0 & 0 & 0 & 0 \\ t_{AB} & \epsilon_B & t_{BA} & 0 & 0 & 0 \\ 0 & t_{BA} & \epsilon_A & t_{AB} & 0 & 0 \\ 0 & 0 & t_{AB} & \epsilon_B & t_{BA} & 0 \\ 0 & 0 & 0 & t_{BA} & \epsilon_A & t_{AB} \\ 0 & 0 & 0 & 0 & t_{AB} & \epsilon_B \end{bmatrix} \text{ and } L_{yy} = \begin{bmatrix} \epsilon_E & t_{CD} & 0 & 0 & 0 & 0 \\ t_{CD} & \epsilon_D & t_{DC} & 0 & 0 & 0 \\ 0 & t_{DC} & \epsilon_C & t_{CD} & 0 & 0 \\ 0 & 0 & t_{CD} & \epsilon_D & t_{DC} & 0 \\ 0 & 0 & 0 & t_{DC} & \epsilon_C & t_{CD} \\ 0 & 0 & 0 & 0 & t_{CD} & \epsilon_F \end{bmatrix}$$

Adjacency matrix for the 2D lattice formed by L_{xx} and L_{yy} is given below.

$$A_{2D-fixed} = L_{xx} \oplus L_{yy} = L_{xx} \otimes I_2 + I_2 \otimes L_{yy}$$

$L_{xx} \otimes I_2$ and $I_2 \otimes L_{yy}$ are 12×12 dimensional matrices. But we are considering only the first 6 rows and the first 6 columns of these matrices.

$$L_{xx} \otimes I_2 = \begin{bmatrix} \epsilon_A & 0 & t_{AB} & 0 & 0 & 0 \\ 0 & \epsilon_A & 0 & t_{AB} & 0 & 0 \\ t_{AB} & 0 & \epsilon_B & 0 & t_{BA} & 0 \\ 0 & t_{AB} & 0 & \epsilon_B & 0 & t_{BA} \\ 0 & 0 & t_{BA} & 0 & \epsilon_A & 0 \\ 0 & 0 & 0 & t_{BA} & 0 & \epsilon_A \end{bmatrix}$$

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$$I_2 \otimes L_{yy} = \begin{bmatrix} \epsilon_E & t_{CD} & 0 & 0 & 0 & 0 \\ t_{CD} & \epsilon_D & t_{DC} & 0 & 0 & 0 \\ 0 & t_{DC} & \epsilon_C & t_{CD} & 0 & 0 \\ 0 & 0 & t_{CD} & \epsilon_D & t_{DC} & 0 \\ 0 & 0 & 0 & t_{DC} & \epsilon_C & t_{CD} \\ 0 & 0 & 0 & 0 & t_{CD} & \epsilon_F \end{bmatrix}$$

$$A_{2D-fixed} = \begin{bmatrix} \epsilon_A + \epsilon_E & t_{CD} & t_{AB} & 0 & 0 & 0 \\ t_{CD} & \epsilon_A + \epsilon_D & t_{DC} & t_{AB} & 0 & 0 \\ t_{AB} & t_{DC} & \epsilon_B + \epsilon_C & t_{CD} & t_{BA} & 0 \\ 0 & t_{AB} & t_{CD} & \epsilon_B + \epsilon_D & 0t_{DC} & t_{BA} \\ 0 & 0 & t_{BA} & t_{DC} & \epsilon_A + \epsilon_C & t_{CD} \\ 0 & 0 & 0 & t_{BA} & t_{CD} & \epsilon_A + \epsilon_F \end{bmatrix} \tag{7.2}$$

7.0.3 Eigenvalue Derivation of the Matrices used for Error Analysis

The derivation of the characteristic polynomial is done by the method of induction.

(a) upper diagonal chain=[0,0,-1], lower diagonal chain=[1,1,1], diagonal chain=[0,0,0], period of the chain $(k) = 3$ and chain length $= nk$.

When $n = 1$

$$M_1 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{7.3}$$

The characteristic polynomial is

$$P1 = (-\lambda)^3 \tag{7.4}$$

$$\lambda = 0, 0, 0 \tag{7.5}$$

When $n = 2$,

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$$M_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{7.6}$$

The characteristic polynomial is

$$P2 = \lambda^4[1 + \lambda^2] = (-\lambda)^{2+2}(\lambda^2 + 1)^{2-1} \tag{7.7}$$

$$\lambda = 0, 0, 0, 0, i, -i \tag{7.8}$$

When $n = 3$,

$$M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{7.9}$$

Characteristic polynomial is

$$P3 = \lambda^2[-\lambda(P2) + \lambda^2(P1) - \lambda^3] = (-\lambda)^{3+2}(\lambda^2 + 1)^{3-1} \tag{7.10}$$

$$\lambda = 0, 0, 0, 0, 0, i, i, -i, -i \tag{7.11}$$

Similarly for any n, the characteristic polynomial is

$$Pn = \lambda^2[-\lambda(P_{n-1}) + \lambda^2(P_{n-2}) - \lambda^3] = (-\lambda)^{n+2}(\lambda^2 + 1)^{n-1} \tag{7.12}$$

So, for any n, λ's are n+2 number of zeros and n-1 number of i and -i.

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(b) upper diagonal chain=[0,0,1], lower diagonal chain=[-1,-1,-1], diagonal chain=[0,0,0], period of the chain $(k) = 3$ and chain length $= nk$.

When $n = 1$

$$M_1 = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix} \tag{7.13}$$

The characteristic polynomial is

$$P1 = -\lambda[-\lambda]^2 \tag{7.14}$$

$$\lambda = 0, 0, 0 \tag{7.15}$$

When $n = 2$,

$$M_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix} \tag{7.16}$$

The characteristic polynomial is

$$P2 = (-\lambda)(-\lambda)[-\lambda P1 + \frac{P1}{-\lambda}] = -[\lambda]^2[\lambda + \frac{1}{\lambda}]P1 = -\lambda[\lambda^2 + 1]P1 \tag{7.17}$$

$$\lambda = 0, 0, 0, 0, i, -i \tag{7.18}$$

When $n = 3$,

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$$M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix} \tag{7.19}$$

The characteristic polynomial is

$$P3 = (-\lambda)(-\lambda)[-\lambda P2 + \frac{P2}{-\lambda}] = -[\lambda]^2[\lambda + \frac{1}{\lambda}]P2 = -\lambda[\lambda^2 + 1]P2 = -\lambda^5[\lambda^2 + 1]^2 \tag{7.20}$$

$$\lambda = 0, 0, 0, 0, 0, i, i, -i, -i \tag{7.21}$$

Similarly for any n, characteristic polynomial is

$$P_n = -\lambda[\lambda^2 + 1]P_{n-1} = [-1]^n\lambda^{n+2}[\lambda^2 + 1]^{n-1} \tag{7.22}$$

So, for any n, λ's are n+2 number of zeros,n -1 number of i and -i.

(c) upper diagonal chain=[0,0,1], lower diagonal chain=[-1,0,-1], diagonal chain=[0,0,0], period of the chain $(k) = 3$ and chain length $= nk$.

When $n = 1$

$$M_1 = \begin{bmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{7.23}$$

The characteristic polynomial is

$$P1 = -\lambda[-\lambda]^2 \tag{7.24}$$

$$\lambda = 0, 0, 0 \tag{7.25}$$

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When $n = 2$,

$$M_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{7.26}$$

The characteristic polynomial is

$$P2 = (-\lambda)(-\lambda)[-\lambda P1 + \frac{P1}{-\lambda}] = -\lambda^2[\lambda + \frac{1}{\lambda}]P1 = -\lambda[\lambda^2 + 1]P1 = \lambda^4[\lambda^2 + 1] \tag{7.27}$$

$$\lambda = 0, 0, 0, 0, i, -i \tag{7.28}$$

When $n = 3$,

$$M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{7.29}$$

The characteristic polynomial is

$$P3 = (-\lambda)(-\lambda)[-\lambda P2 + \frac{P2}{-\lambda}] = -\lambda^2[\lambda + \frac{1}{\lambda}]P2 = -\lambda[\lambda^2 + 1]P2 = -\lambda^5[\lambda^2 + 1]^2 \tag{7.30}$$

$$\lambda = 0, 0, 0, 0, 0, i, i, -i, -i \tag{7.31}$$

Similarly for any n, the characteristic polynomial is

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$$P_n = -\lambda[\lambda^2 + 1]P_{n-1} = [-1]^n\lambda^{n+2}[\lambda^2 + 1]^{n-1} \tag{7.32}$$

So, for any n, λ's are n+2 number of zeros, $n-1$ number of i and -i.

(d) upper diagonal chain=[0,0,1], lower diagonal chain=[1,0,1], diagonal chain=[0,0,0], period of the chain $(k) = 3$ and chain length $= nk$.

When $n = 1$

$$M_1 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{7.33}$$

The characteristic polynomial is

$$P1 = -\lambda[-\lambda]^2 \tag{7.34}$$

$$\lambda = 0, 0, 0 \tag{7.35}$$

When $n = 2$,

$$M_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{7.36}$$

The characteristic polynomial is

$$P2 = (-\lambda[-\lambda P1 + \frac{P1}{\lambda}] = \lambda^2[-\lambda + \frac{1}{\lambda}]P1 = \lambda[-\lambda^2 + 1]P1 = -\lambda^4[-\lambda^2 + 1] = \lambda^4[\lambda^2 - 1] \tag{7.37}$$

$$\lambda = 0, 0, 0, 0, 1, -1 \tag{7.38}$$

When $n = 3$,

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$$M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{7.39}$$

The characteristic polynomial is

$$P3 = (-\lambda)(-\lambda)[-\lambda P2 + \frac{P2}{\lambda}] = [\lambda]^2[-\lambda + \frac{1}{\lambda}]P2 = \lambda[-\lambda^2 + 1]P2 = -\lambda^5[\lambda^2 - 1]^2 \tag{7.40}$$

$$\lambda = 0, 0, 0, 0, 0, 1, 1, -1, -1 \tag{7.41}$$

Similarly for any n, characteristic polynomial is

$$P_n = \lambda[-\lambda^2 + 1]P_{n-1} = [-1]^n\lambda^{n+2}[\lambda^2 - 1]^{n-1} \tag{7.42}$$

So, for any n, λ's are n+2 number of zeros,$n-1$ number of 1 and -1.

(e) upper diagonal chain=[0,0,1], lower diagonal chain=[1,1,0], diagonal chain=[0,0,0], period of the chain $(k) = 3$ and chain length $= nk$.

When $n = 1$

$$M_1 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{7.43}$$

Characteristic polynomial is

$$P1 = -\lambda[-\lambda]^2 \tag{7.44}$$

$$\lambda = 0, 0, 0 \tag{7.45}$$

When $n = 2$,

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$$M_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{7.46}$$

Characteristic polynomial is

$$P2 = (-\lambda)(-\lambda)[-\lambda P1] = \lambda^2[-\lambda]P1 = -\lambda^3 P1 = \lambda^6 \tag{7.47}$$

$$\lambda = 0, 0, 0, 0, 0, 0 \tag{7.48}$$

When $n = 3$,

$$M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{7.49}$$

The characteristic polynomial is

$$P3 = (-\lambda)(-\lambda)[-\lambda P2] = -\lambda^3 P2 = -\lambda^9 \tag{7.50}$$

$$\lambda = 0, 0, 0, 0, 0, 0, 0, 0, 0 \tag{7.51}$$

Similarly for any n, the characteristic polynomial is

$$P_n = -\lambda^3 P_{n-1} = [-1]^n[\lambda]^{3n} \tag{7.52}$$

So, for any n, λ's are 3n number of zeros.

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7.0.4 Error Analysis on more Examples

(1) upper diagonal chain=[0,0,1], lower diagonal chain=[1,1,1], diagonal chain=[0,0,0], period of the chain $(k) = 3$ and chain length $= nk$.

When $n = 1$

$$M_1 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{7.53}$$

The characteristic polynomial is

$$P1 = -\lambda(\lambda^2) = (-\lambda)^{1+2}(\lambda^2 - 1)^{1-1} \tag{7.54}$$

$$\lambda = 0, 0, 0 \tag{7.55}$$

When $n = 2$,

$$M_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{7.56}$$

The characteristic polynomial is

$$P2 = \lambda^4(\lambda^2 - 1) = (-\lambda)^{2+2}(\lambda^2 - 1)^{2-1} \tag{7.57}$$

$$\lambda = 0, 0, 0, 0, 1, -1 \tag{7.58}$$

When $n = 3$,

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$$M_3 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{7.59}$$

The characteristic polynomial is

$$P3 = (-\lambda)^2[-\lambda[\lambda^4(\lambda^2 - 1)] + \lambda[-\lambda(-\lambda^3) - \lambda^2]] \tag{7.60}$$

The above equation can be written as

$$P3 = \lambda^2[-\lambda(P2) + \lambda[-\lambda(P1) - \lambda^2]] = \lambda^2[-\lambda(P2) - \lambda^2(P1) - \lambda^3] = (-\lambda)^{3+2}(\lambda^2 - 1)^{3-1} \tag{7.61}$$

$$\lambda = 0, 0, 0, 0, 1, -1 \tag{7.62}$$

Similarly for any n, characteristic polynomial is

$$P_n = \lambda^2[-\lambda(P_{n-1}) - \lambda^2(P_{n-2}) - \lambda^3] = (-\lambda)^{n+2}(\lambda^2 - 1)^{n-1} \tag{7.63}$$

So, for any n, λ's are $(n + 2)$ number of zeros and $(n - 1)$ number of of 1 and -1.

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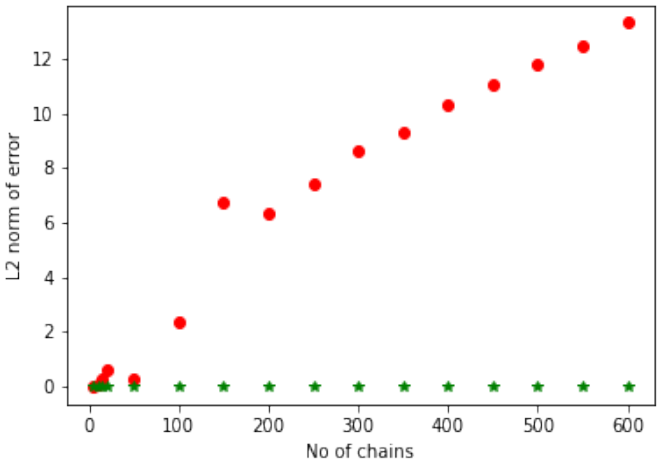

Figure 7.9: Eigenvalue error analysis-d=[0,0,0],u=[0,0,1],l=[1,1,1]

(2) upper diagonal chain= $[i, 0, 0]$, lower diagonal chain= $[i, 1, 1]$, diagonal chain = $[0, 0, 0]$, period of the chain $(k) = 3$ and chain length $= nk$.

When $n = 1$

$$M_1 = \begin{bmatrix} 0 & i & 0 \\ i & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{7.64}$$

The characteristic polynomial is

$$P1 = -[\lambda^3 + \lambda] \tag{7.65}$$

$$\lambda = 0, i, -i \tag{7.66}$$

When $n = 2$,

$$M_2 = \begin{bmatrix} 0 & i & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & i & 0 \\ 0 & 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{7.67}$$

The characteristic polynomial is

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$$P2 = -\lambda[\lambda^2(P1) + P1] = -[\lambda^3 + \lambda]P1 = [-\lambda^3 - \lambda]^2 \tag{7.68}$$

$$\lambda = 0, 0, i, i, -i, -i \tag{7.69}$$

When $n = 3$,

$$M_3 = \begin{bmatrix} 0 & i & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & i & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{7.70}$$

The characteristic polynomial is

$$P3 = -\lambda[\lambda^2 P2 + P2] = [-\lambda^3 - \lambda]P2 = [-\lambda^3 - \lambda]^3 \tag{7.71}$$

$$\lambda = 0, 0, 0, i, i, i, -i, -i, -i \tag{7.72}$$

Similarly for any n, characteristic polynomial is

$$P_n = [-\lambda^3 - \lambda]P_{n-1} = [-\lambda^3 - \lambda]^n \tag{7.73}$$

So, for any n, λ's are n number of zeros, i and -i.

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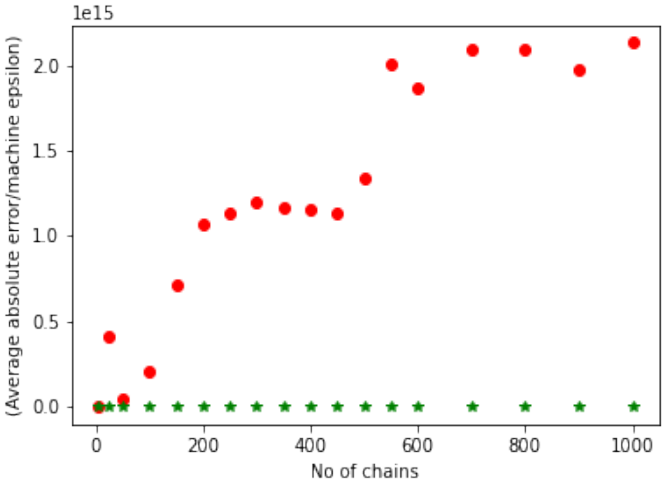

Figure 7.10: Eigenvalue error analysis-d=[0,0,0],u=[i,0,0],l=[i,1,1]

7.0.5 Other Possible Approaches to Identify Eigenvalues after (1, 1) Entry Perturbation

S Analysis

$S(z)$ and $R(z)$ are two polynomials in z which appear in the characteristic polynomial recurrence relation of the tridiagonal k-Toeplitz matrix after $(1, 1)$ entry perturbation. S Analysis is an attempt to analyze how $S(z)$ and $R(z)$ polynomial values are related to the eigenvalues of tridiagonal k-Toeplitz matrices after $(1, 1)$ entry perturbation.

The first step of this method was to analyze the relation between $|R - 1|/|S + 1|$ values and eigenvalues of the tridiagonal k-Toeplitz matrix after $(1, 1)$ entry perturbation. Since the polynomial $S(z)$ is a function of $R(z)$, it is better to study how S values and eigenvalues of the tridiagonal k-Toeplitz matrix after the $(1, 1)$ entry perturbation are related. The next step was to find if there is any relationship between the $2k$ points which are not part of the continuous limiting set and their S values. In $ds - dl$ graphs, the X axis is $|ds|^2+|dl|^2$ where dl is the difference in neighboring builtin eigenvalues under fixed perturbation and ds is the difference in corresponding S values. Then I checked whether those eigenvalues which have the maximum change after the perturbation in the $(1, 1)$ entry, are corresponding to the S values which are not in the continuous curve.

S Analysis Figures

This is an attempt to check how builtin eigenvalues of tridiagonal k-Toeplitz matrix is related to their S values.

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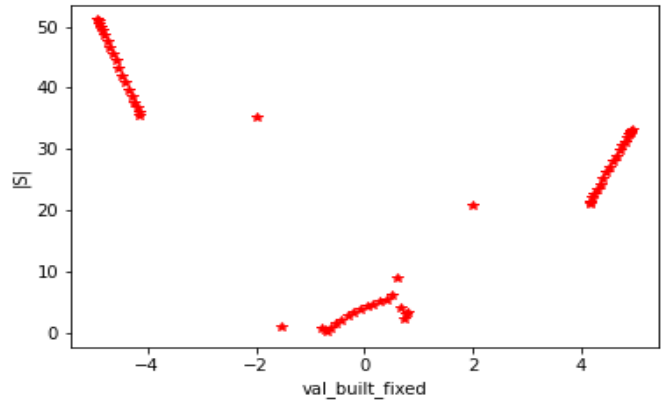

Figure 7.11: S-diagram: $d = [0, 0, 0], l = u, u = [1, 2, 4]$, $n = 20$, perturbation in (1, 1) entry $= -1$

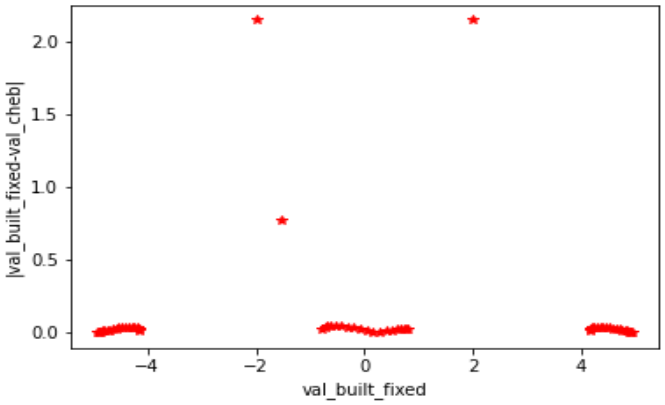

Figure 7.12: $difference$: $d = [0, 0, 0], l = u, u = [1, 2, 4]$, $n = 20$, perturbation in (1, 1) entry $= -1$

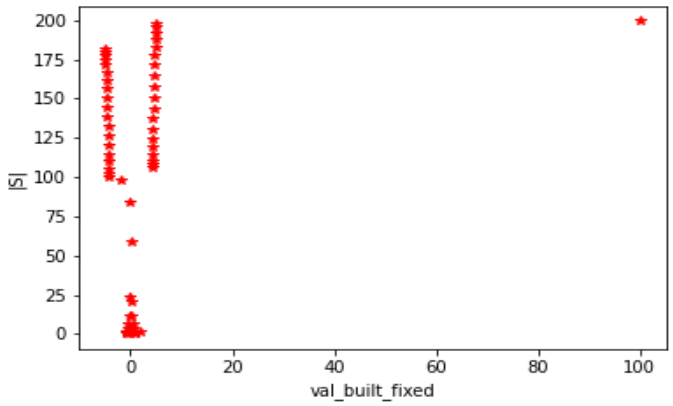

Figure 7.13: S-diagram: $d = [0, 0, 0], l = u, u = [1, 2, 4]$, $n = 20$, perturbation in (1, 1) entry $= 100$

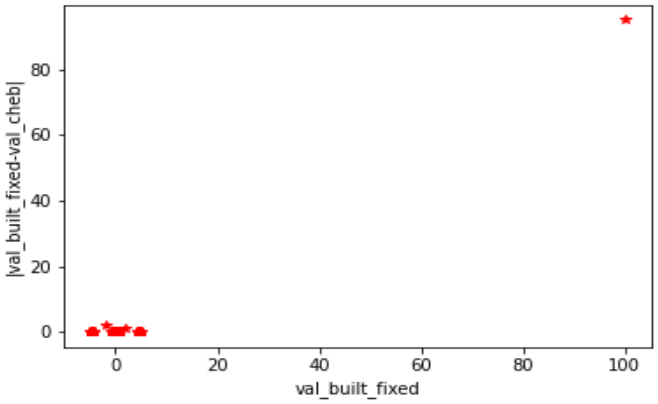

Figure 7.14: difference: $d = [0, 0, 0], l = u, u = [1, 2, 4]$, $n = 20$, perturbation in (1, 1) entry = 100

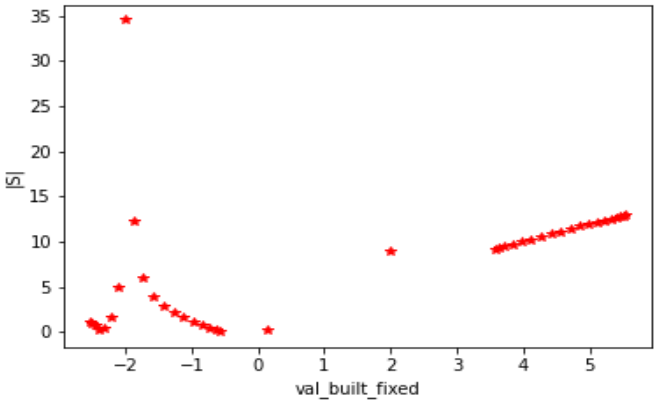

Figure 7.15: S-diagram: $d = [1, 2], l = u, u = [1, -3]$, $n = 20$, perturbation in (1, 1) entry $= -1$

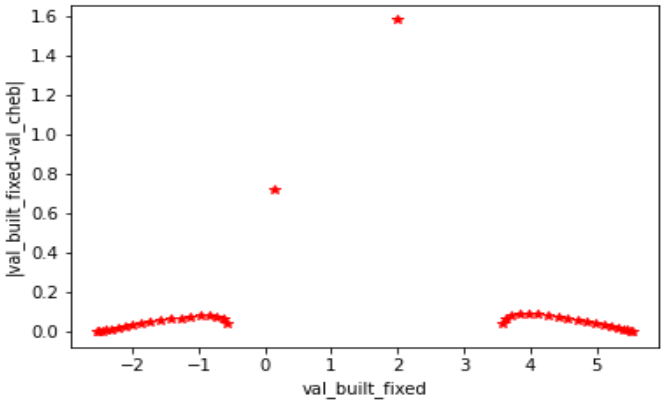

Figure 7.16: difference: $d = [1, 2], l = u, u = [1, -3]$, $n = 20$, perturbation in (1, 1) entry $= -1$

From the above graphs, we can interpret that the magnitude of the difference between builtin eigenvalues after perturbation in $(1, 1)$ entry and Chebyshev approximated eigen-

values is maximum when $|S|$ is not in the continuous curve. The same properties of $|S|$ vs eigenvalues after perturbation in $(1,1)$ entry are shown by $|ds|^2 + |dl|^2$ vs eigenvalues after perturbation in $(1,1)$ entry graph.

R-S Analysis

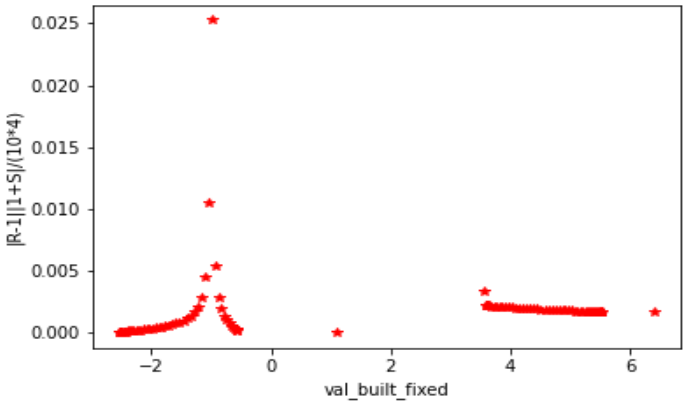

Figure 7.17: RS diagram : $d = [1,2], l = u, u = [1,-3] pert = [3,-1], n = 20$

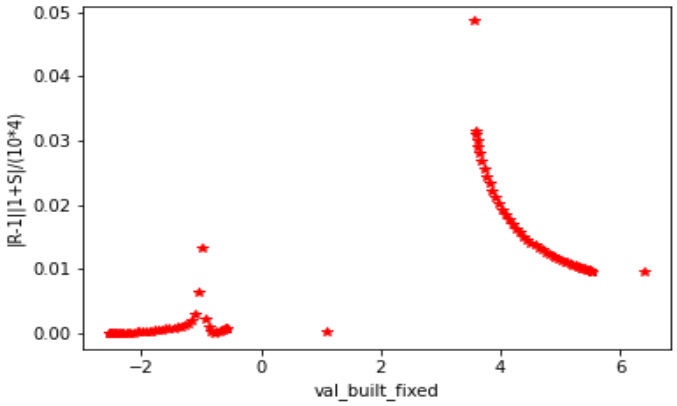

Figure 7.18: RS diagram: $d = [1,2], l = u, u = [1,-3] pert = [5,-1], n = 20$

Github link for my codes: link to github account

ds-dl Analysis

Analysis of the given below graphs lead to the following conclusion, when $|ds|^2+|dl|^2$ is not in the continuous curve, the difference between Chebyshev approximated eigenvalues and builtin eigenvalues after $(1,1)$ entry perturbation is maximum.

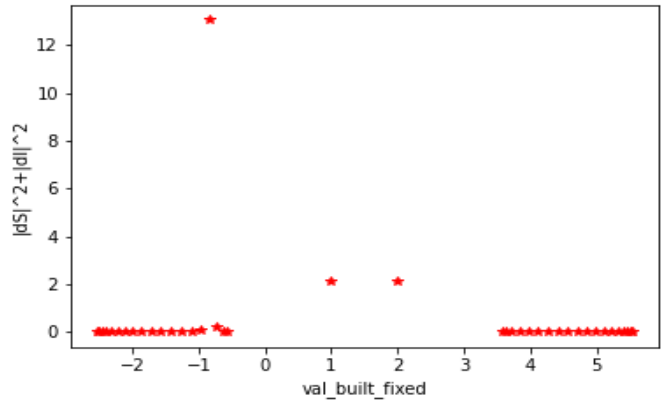

Figure 7.19: ds-dl: $d = [1, 2], l = u, u = [1, -3]$, perturbation in (1, 1) entry $= 0.1$, $n = 20$

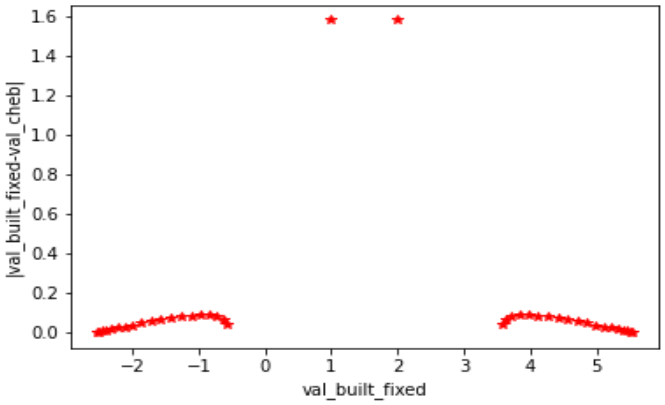

Figure 7.20: $difference$: $d = [1, 2], l = u, u = [1, -3]$, perturbation in (1, 1) entry $= 0.1$, $n = 20$

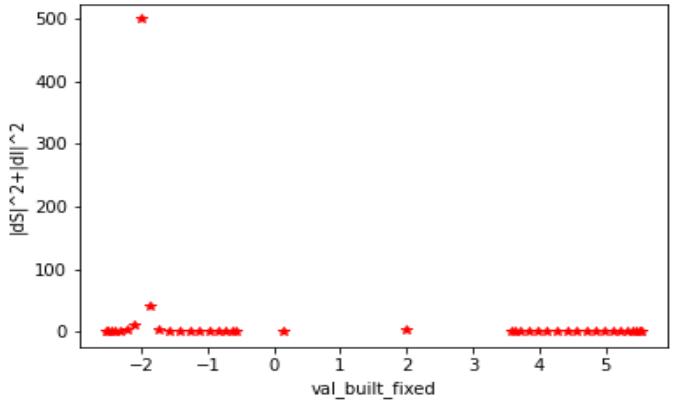

Figure 7.21: ds-dl: $d = [1, 2], l = u, u = [1, -3]$, perturbation in (1, 1) entry $= -1$, $n = 20$

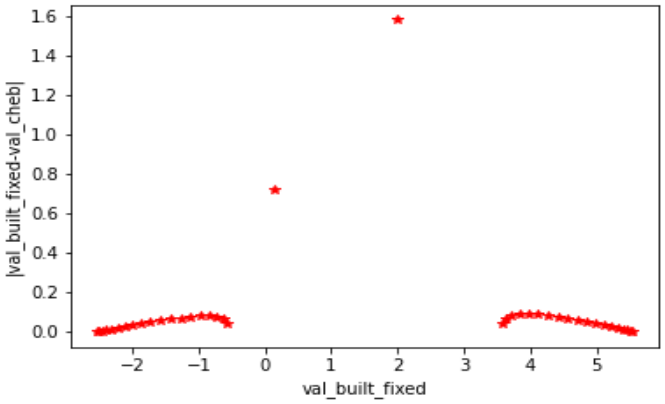

Figure 7.22: $difference$: $d = [1, 2], l = u, u = [1, -3]$, perturbation in (1, 1) entry $= -1$, $n = 20$

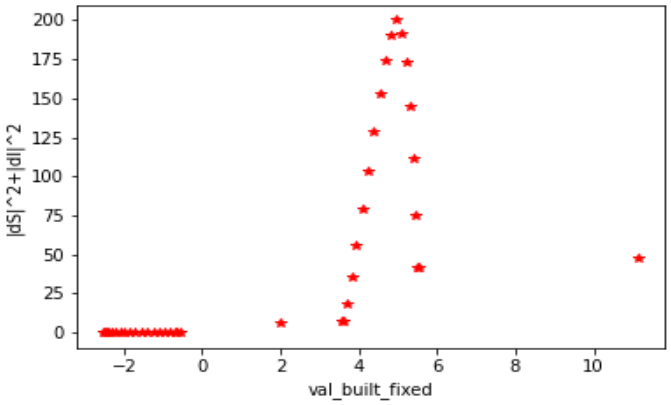

Figure 7.23: ds-dl: $d = [1, 2], l = u, u = [1, -3]$, perturbation in (1, 1) entry= 10, $n = 20$

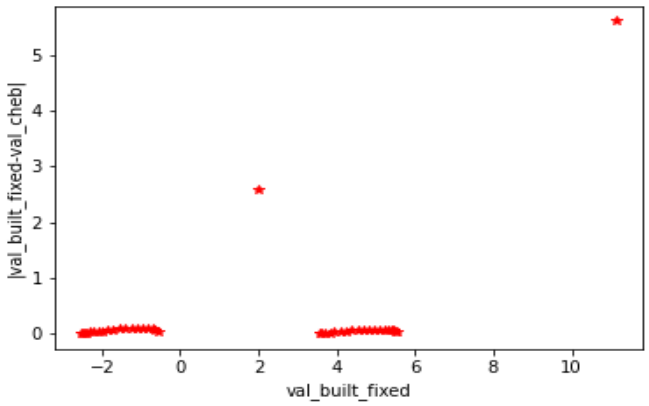

Figure 7.24: $difference$: $d = [1, 2], l = u, u = [1, -3]$, perturbation in (1, 1) entry= 10, $n = 20$

2k-S Diagram

The following graphs show how $2k$ points that are not part of the limiting set are getting affected by $(1, 1)$ entry perturbation. In the $2k - S$ diagram, S values of the $2k$ points are plotted against the $2k$ points.

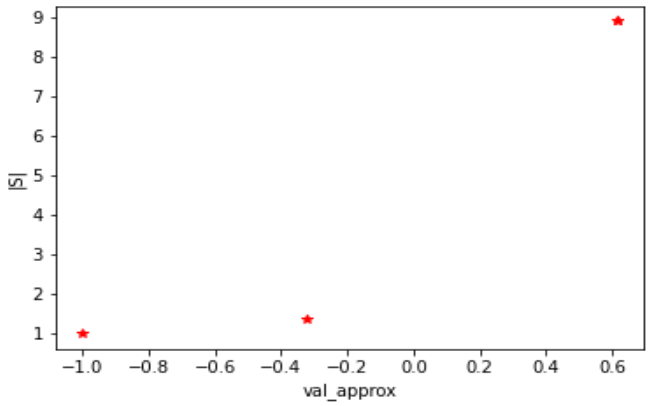

Figure 7.25: 2k-S-diagram: $d = [1, 2], l = u, [1, -3]$, $n = 20$, perturbation in (1, 1) entry = 10

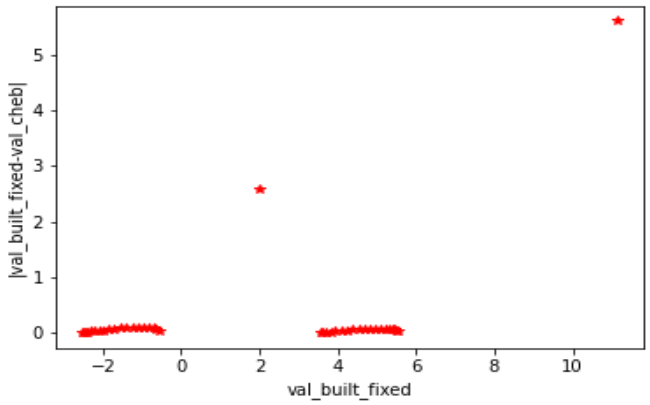

Figure 7.26: $difference$: $d = [1, 2], l = u, u = [1, -3]$, $n = 20$, perturbation in (1, 1) entry = 10

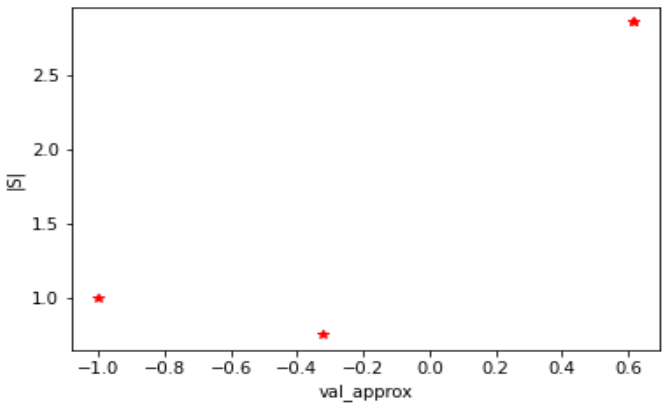

Figure 7.27: 2k-S-diagram: $d = [1, 2], l = u, [1, -3]$, $n = 20$, perturbation in (1, 1) entry = -1

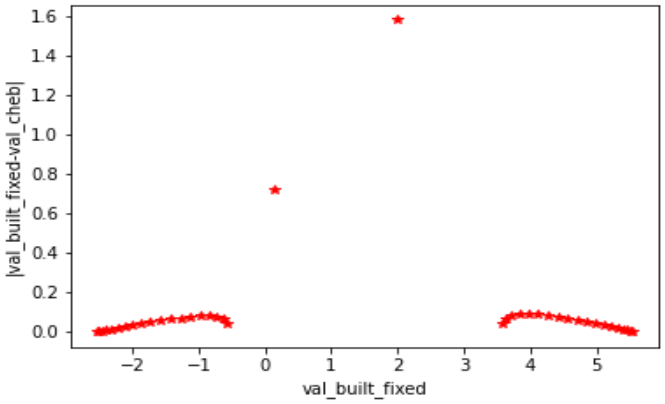

Figure 7.28: $difference : d = [1, 2], l = u, u = [1, -3]$, $n = 20$, perturbation in (1, 1) entry $= 1$

We checked whether the $2k$ points that are not part of the continuous limiting set, have the maximum change during perturbation, and we found that is not the case.

For Review Only