Evaluating roots of polynomials generated by a three-term recurrence: General solutions for eigenvalue problems of chain and lattice models

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Abstract. We first show the existence and nature of convergence to a limiting set of roots for polynomials in a three-term recurrence of the form $p_{n+1}(z) = Q_k(z)p_n(z) + \gamma p_{n-1}(z)$ as $n \to \infty$, where the coefficient $Q_k(z)$ is a k^{th} degree polynomial, and z, γ are $\mathbb{C}^1$. We extend these results into relations approximating roots of such polynomials for finite n. General solutions for the evaluation are motivated by large computational efforts and errors in direct numerical methods. Later, we also apply this solution to the eigenvalue problems represented by tridiagonal matrices with a periodicity k in its entries. Generality in k and complex entries of the matrix in this solution provides an efficient numerical method for evaluation of spectra of chains and other lattice models.

Keywords. polynomial recurrence relations; limiting roots; complex roots; periodic systems; chain models; k-Toeplitz matrices.

Consider the polynomials in a three-term recurrence of the form

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

where coefficient $Q_k(z)$ is a k^{th} degree polynomial and z, γ are $\mathbb{C}^1$. This recurrence is of general interest, with widely used special cases such as the Chebyshev polynomials where $Q_1 = 2z$, $\gamma = -1$ and z is $\mathbb{R}^1$. In the first section, we establish relations for the limiting set of roots of polynomials as $n \to \infty$, and other useful approximations of these roots for finite n. Limiting roots of polynomials generated by a general three-term recurrence was recently studied by other approaches [13] where the effect of initial conditions p_o and p_1 had to be analyzed separately. Our analysis here includes initial conditions, the different rates of convergence to the limiting set, approximations for finite n and their errors. These approximations are motivated by both large errors and the large computational efforts required in direct numerical methods applied to eigenvalue problems or the corresponding

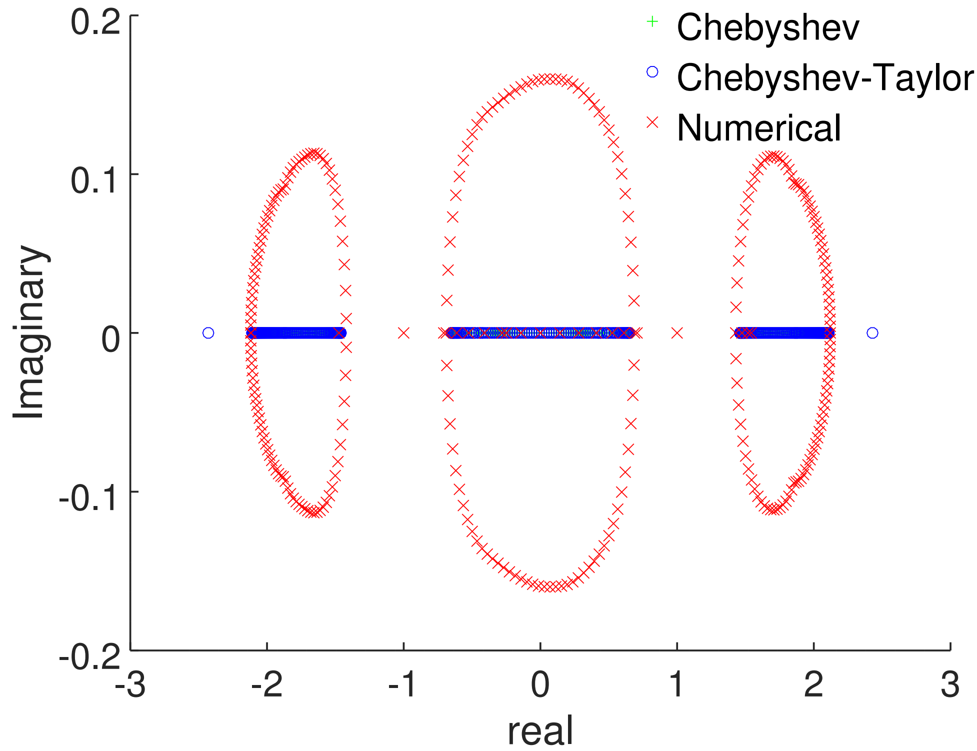


Figure 1: Example of numerical errors : A polynomial with purely real roots that is generated by the 3-term recurrence with $Q_k = z^3 - 3.5z$, $\gamma = -1$, $p_1 = z^3 - 1.5z$, $p_0 = 1$; here k=3 and for n=100 we have 300 roots. Computing effort using the proposed Chebyshev approximation is $\mathcal{O}(nk^2)$, cost of corresponding Chebyshev-Taylor approximation is $\mathcal{O}(nk^3)$, and numerical evaluation using MATLAB as eigenvalues of a matrix is $\mathcal{O}(n^2k^2)$. Scale of Y axis is enlarged to resolve the erroneous imaginary parts.

root-finding problems. Large errors due to the accumulation of digital round-offs are common when some roots are close to zero, as often is the case when modeling natural and man-made systems (see figure 1 for an example). In the second part of the paper, we show the significance of these results for eigenvalue problems that represent any chain of periodicity $k \geq 1$, and other lattice models. Note that roots of these polynomials can also represent eigenvalues of tridiagonal matrices with k-periodicity in their entries. A few examples are presented as a demonstration of the theorems.

1 Existence of a limiting set and the nature of convergence of roots

To show that roots of these polynomials have a limiting set as $n \to \infty$, it is sufficient to show that there exists a corresponding n-eigenvalue problem with a limiting distribution. In the context of this work, it is also important for nk roots of the polynomial to have a simple relation with these n eigenvalues. This would allow us to study its convergence and apply it effectively for approximations in the case of finite n. Here polynomials $p_n(z)$ are of degree nk and can be expanded as determinant of the following $n \times n$ matrix, using $p_o(z) = 1$ without loss of generality.

$$\begin{bmatrix} p_1(z) & i\sqrt{\gamma} & 0 & 0 & 0 & 0 & 0 & 0 \\ i\sqrt{\gamma} & Q_k(z) & i\sqrt{\gamma} & 0 & 0 & 0 & 0 & 0 \\ 0 & i\sqrt{\gamma} & Q_k(z) & i\sqrt{\gamma} & 0 & 0 & 0 & 0 \\ 0 & 0 & i\sqrt{\gamma} & Q_k(z) & i\sqrt{\gamma} & 0 & 0 & 0 \\ 0 & \vdots & \cdots & \ddots & \ddots & \ddots & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & i\sqrt{\gamma} & Q_k(z) & i\sqrt{\gamma} \\ 0 & 0 & 0 & 0 & 0 & 0 & i\sqrt{\gamma} & Q_k(z) \end{bmatrix}_{n\times n} \tag{2}$$

Let $\zeta = \frac{p_1(z)-Q_k(z)}{\sqrt{\gamma}}$. By factoring out $\sqrt{\gamma}$, the nk roots of $p_n(z)$ can be reformulated as the solutions of $\lambda = -\frac{Q_k(z)}{\sqrt{\gamma}}$ where λ is an eigenvalue of the $n \times n$ matrix

$$\begin{bmatrix} \zeta & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & \vdots & \cdots & \ddots & \ddots & \ddots & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}_{n\times n} \tag{3}$$

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

$$\begin{bmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & \vdots & \cdots & \ddots & \ddots & \ddots & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}_{n\times n} \tag{4}$$

Then we have

$$L_n(\zeta,\lambda) = (\zeta-\lambda)T_{n-1} + T_{n-2} \tag{5}$$

$$L_n(\zeta,\lambda) = \zeta T_{n-1} + (-\lambda)T_{n-1} + T_{n-2} \tag{6}$$

$$L_n(\zeta,\lambda) = \zeta T_{n-1} + T_n \tag{7}$$

In the above, we have used recurrence relations for the characteristic polynomials of $T_n(\lambda)$ given by

$$\begin{bmatrix} T_n \\ T_{n-1} \end{bmatrix} = \begin{bmatrix} -\lambda & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} T_{n-1} \\ T_{n-2} \end{bmatrix} = \begin{bmatrix} -\lambda & 1 \\ 1 & 0 \end{bmatrix}^n \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{8}$$

From equations (7) and (8), we also have

$$L_n(\zeta,\lambda) = \begin{bmatrix} 1 & \zeta \end{bmatrix} \begin{bmatrix} -\lambda & 1 \\ 1 & 0 \end{bmatrix}^n \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{9}$$

For the matrix $\begin{bmatrix} -\lambda & 1 \\ 1 & 0 \end{bmatrix}$, let $t_\pm = \frac{-\lambda \pm \sqrt{\lambda^2+4}}{2}$ be the eigenvalues and hence $\lambda = \frac{1}{t_+} - t_+)$. Since $t_+ t_- = -1$, we also know $t_- = \frac{-1}{t_+}$. Let the matrix in equation (9) have a determinant D, and by using its diagonal decomposition we rewrite it as

$$L_n(\zeta,\lambda)D =$$

$$\begin{bmatrix} 1 & \zeta \end{bmatrix} \begin{bmatrix} \frac{t_+}{\sqrt{1+|t_+|^2}} & \frac{t_-}{\sqrt{1+|t_-|^2}} \\ \frac{1}{\sqrt{1+|t_+|^2}} & \frac{1}{\sqrt{1+|t_-|^2}} \end{bmatrix} \begin{bmatrix} t_+^n & 0 \\ 0 & t_-^n \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{1+|t_-|^2}} & -\frac{t_-}{\sqrt{1+|t_-|^2}} \\ \frac{-1}{\sqrt{1+|t_+|^2}} & \frac{t_+}{\sqrt{1+|t_+|^2}} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$L_n(\zeta,\lambda)D = \begin{bmatrix} \frac{t_+ + \zeta}{\sqrt{1+|t_+|^2}} & \frac{t_- + \zeta}{\sqrt{1+|t_-|^2}} \end{bmatrix} \begin{bmatrix} t_+^n & 0 \\ 0 & \frac{(-1)^n}{t_+^n} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{1+|t_-|^2}} \\ \frac{1}{\sqrt{1+|t_+|^2}} \end{bmatrix} \tag{10}$$

Since $D \neq 0$, when $L_n(\zeta,\lambda) = 0$ we have

$$\begin{bmatrix} t_+^n \frac{t_+ + \zeta}{\sqrt{1+|t_+|^2}} & \frac{(-1)^n}{t_+^n} \frac{t_- + \zeta}{\sqrt{1+|t_-|^2}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{1+|t_-|^2}} \\ \frac{1}{\sqrt{1+|t_+|^2}} \end{bmatrix} = 0 \tag{11}$$

This gives us the following relation for zeros of $L_n(\zeta,\lambda)$ that solve the required eigenvalue problem in equation (3)

$$t_+^n(t_+ + \zeta) + \frac{(-1)^n}{t_+^n}(\frac{-1}{t_+} + \zeta) = 0 \tag{12}$$

$$t_+^{2n+2} + \zeta t_+^{2n+1} + (-1)^n(\zeta t_+ - 1) = 0 \tag{13}$$

In equation (13) the absolute value of product of all zeros is one. By applying Landau's inequality [1], product of the zeros with absolute values greater than one is $< \sqrt{2+2|\zeta|^2}$. Note that ζ is bounded in the region of interest. So as n increases the absolute value of zeros approaches one, and so does the fraction of such zeros. This establishes the existence of a limiting spectrum for $L_n(\zeta, \lambda)$.

Convergence to the limiting set

The convergence of zeros of $L_n(\zeta, \lambda)$ can be obtained using Rouche's theorem. If we are able to find an R such that

$$|a_p|R^p > |a_0| + |a_1|R + \cdots + |a_{p-1}|R^{p-1} + |a_{p+1}|R^{p+1} + \cdots |a_n|R^n$$

then there are exactly p zeros of the polynomial which have magnitude less than R. Let us denote $|\zeta|$ by y. In equation (13) we are concerned with the polynomial $R^{2n+2} + yR^{2n+1} + yR + 1$. So for a value of $R = R_1$, let

$$R_1^{2n+2} > yR_1^{2n+1} + yR_1 + 1. \tag{14}$$

Now by dividing the equation above by R_1^{2n+2} we get,

$$1 > y\frac{1}{R_1^{2n+1}} + y\frac{1}{R_1} + \frac{1}{R_1^{2n+2}} \tag{15}$$

This implies if R_1 is the upper bound for magnitude of $2n+2$ zeros of $L_n(\zeta, \lambda)$, then from equation (15) $\frac{1}{R_1}$ is the lower bound for the magnitude of all its zeros. Similarly if R_2 is the upper bound for magnitude of $2n+1$ zeros, then $\frac{1}{R_2}$ is an upper bound for magnitude of one zero. We divide the analysis into $|\zeta| < 1$, $|\zeta| = 1$ and $|\zeta| > 1$, and consider these three cases separately.

1. When $|\zeta| = y < 1$, lets assume $1 + \frac{cy}{n}$ be the upper bound R, and find c.

$$R^{2n+2} > yR^{2n+1} + yR + 1 \tag{16}$$

$$(R - y)R^{2n+1} > yR + 1 \tag{17}$$

$$\left(1 + \frac{cy}{n} - y\right)\left(1 + \frac{cy}{n}\right)^{2n+1} > y\left(1 + \frac{cy}{n}\right) + 1 \tag{18}$$

Note that $(1 + \frac{cy}{n})^{2n+1} > 1 + 2cy$ and $\left(1 + \frac{cy}{n} - y\right) > 1 - y$. Also, $\left(1 + \frac{cy}{n}\right) < 2$ for some $n > cy$. Forcing the lower bound of the L.H.S to be greater than the upper bound of R.H.S, we get a lower bound on c as follows.

[1] Absolute value of the product of all zeros with an absolute value greater than one is $\leq \sqrt{\sum_{i=0}^{n} |a_i|^2}$

$$(1-y)(1+2cy) > 2y+1 \tag{19}$$
$$1+(2c-1)y-2cy^2 > 2y+1 \tag{20}$$
$$2c(1-y) > 3 \tag{21}$$
$$c > \frac{3}{2(1-y)} \tag{22}$$

This implies for some $\delta > 0$, this upper bound for magnitude of all zeros given by $R_1 = 1 + \frac{3y+\delta}{2(1-y)n}$ asymptotically approaches one. From the previous arguments $\frac{1}{R_1} > 1 - \frac{3y+\delta}{2(1-y)n}$ is a lower bound for magnitude of all zeros, and this asymptotically approaches one as well.

2. When $|\zeta| = y = 1$, we assume $1+\alpha$ is the upper bound for magnitude of $2n+2$ zeros, and derive a lower bound for α in the following manner, starting with equation (17) again.

$$(1+\alpha)^{2n+1}(1+\alpha-1) > 1+1+\alpha \tag{23}$$
$$(1+(2n+1)\alpha)\alpha > 2+\alpha \tag{24}$$
$$\alpha^2 > \frac{2}{2n+1} \tag{25}$$
$$\alpha > \sqrt{\frac{2}{2n+1}} \tag{26}$$

Thus an upper bound for magnitude of all the zeros is $1 + c\sqrt{\frac{2}{2n+1}}$ with any $c > 1$, and lower bound for the magnitudes is $1 - c\sqrt{\frac{2}{2n+1}}$, and these asymptotically approach one as well.

3. When $|\zeta| = y > 1$, consider

$$yR^{2n+1} > R^{2n+2} + yR + 1$$
$$R^{2n+1}(y-R) > 1 + yR$$

Assuming $R = 1 + \frac{cy}{n}$, we get

$$\left(1+\frac{cy}{n}\right)^{2n+1}\left(y-\left(1+\frac{cy}{n}\right)\right) > 1 + y\left(1+\frac{cy}{n}\right) \tag{27}$$

Note that $\left(1+\frac{cy}{n}\right)^{2n+1} > 1+2cy$ and also $\left(1+\frac{cy}{n}\right) < 2$ for some $n > cy$. Forcing the lower bound of the L.H.S to be greater than the upperbound of R.H.S, we get a lower bound on c as follows.

$$(1+2cy)(y-1-\frac{cy}{n}) > 1+2y \tag{28}$$

Since $(\frac{y-1}{2})$ is a sufficient lower bound for $(y-1-\frac{cy}{n})$ in the case of limiting large n

$$(1+2cy)\frac{(y-1)}{2} > 1+2y \tag{29}$$

$$2cy > \frac{3y+3}{y-1} \tag{30}$$

$$2cy > \frac{6y}{y-1} \tag{31}$$

$$c > \frac{3}{y-1} \tag{32}$$

$R_2 = 1 + \frac{3y+\delta}{(y-1)n}$ is the upperbound for magnitude of $2n+1$ zeros, and $\frac{1}{R_2} > 1 - \frac{3y+\delta}{(y-1)n}$ is an upper bound for magnitude of one zero. This implies except two zeros, all other zeros asymptotically converge to one. Consider (13) which can be rearranged to

$$t+\zeta = \frac{(-1)^{n-1}(\zeta t-1)}{t^{2n+1}} \tag{33}$$

Since $|\zeta| > 1$ we have

$$\lim_{n\to\infty}\lim_{t\to-\zeta}\frac{1}{t^{2n+1}} = 0$$

Hence $-\zeta$ is one of the limiting zeros of $L_n(\zeta,\lambda)$. A similar limit of $t_+ \to \frac{1}{\zeta}$ for large limiting n in (33) shows us that $\frac{1}{\zeta}$ is the other zero which does not converge to the unit circle. These two zeros of $L_n(\zeta,\lambda)$ also provide a condition for the limiting spectrum of a tridiagonal k-Toeplitz matrix; in addition to all the other limiting eigenvalues of $L_n(\zeta,\lambda)$ that converge to the unit circle as shown before.

From the above three cases we have the limiting zeros of $L_n(\zeta,\lambda)$ as unit circle $t_+ = e^{i\theta}$. Given $\lambda = \frac{1}{t_+} - t_+$, we get the condition $\frac{Q_k(z)}{\sqrt{\gamma}} = -\lambda = 2i\sin\theta$ for the limiting set, which corresponds to continuous curves. But in case of $|\zeta| > 1$, we have two zeros of $L_n(\zeta,\lambda)$ that do not converge to the unit circle. These two zeros provide the same additional eigenvalue problem $-\frac{Q_k(z)}{\sqrt{\gamma}} = \zeta - \frac{1}{\zeta} = \frac{p(z)}{\sqrt{\gamma}} - \frac{\sqrt{\gamma}}{p(z)}$. Here $p(z)$ is a polynomial of degree utmost k given by $p_1(z) - Q_k(z)$. This solution represents up to a maximum of $2k$ points that may lie outside the continuous curves.

Theorem 1. *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 $\mathbb{C}^1$, 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 $p(z) = p_1(z) - Q_k(z)$.*

The proof is from the previous analysis.

We denote the set $C = \{z : Q_k(z) = 2i\sqrt{\gamma}\sin\theta\}$ and the set $P = \{z : Q_k(z) = \frac{\gamma}{p(z)} - p(z)\}$, so that $C \cup P$ contains the limiting set. The set C is continuous and can be viewed as the curve $Q_k(z) = L$ in three dimension ($\mathbb{R}^3$), with real and imaginary part of z being X, Y axis and L being the Z axis (see section 2.3 for graphic examples).

corollary 1. *For the continuous set C, we have following three cases when γ is real.*

- *When γ is purely real and positive, then $Q_k(z) = 2\sqrt{|\gamma|}i\sin\theta$; and line L is a purely imaginary interval $\{-2\sqrt{|\gamma|}i, 2\sqrt{|\gamma|}i\}$.*
- *When $\gamma = 0$, the spectrum reduces to $2k$ distinct points independent of dimension N.*
- *When γ is purely real and negative, then $Q_k = -2\sqrt{|\gamma|}\sin\theta$ and L is a purely real interval $\{-2\sqrt{|\gamma|}, 2\sqrt{|\gamma|}\}$.*

corollary 2. *The limiting roots of the polynomials in a three-term recurrence of the form $p_{n+1}(z) = Q_k(z)p_n(z) + \gamma p_{n-1}(z)$ with z, γ in $\mathbb{C}^1$, are dense on the continuous set C.*

For the rigorous proof of this statement we refer the reader to another work [13] which makes use of Ismail's q-Discriminants along with theorems from other works [11]. There can be several notions of a limiting set [9].
Here, using equation (7) i.e. $L_n(\zeta, \lambda) = \zeta T_{n-1} + T_n$, we provide a reasonable argument for the above. Let $\lambda_i^{(n)}$ for $i = 1, 2, \ldots$ be the roots of T_n and $\lambda_i^{(n-1)}$ be the roots of T_{n-1}. We know $T_{n-1}(\lambda_i^{(n)}) = \cos(\frac{n-1}{n}[\frac{\pi}{2}(2i+1)]) \to 0$ as $n \to \infty$. Thus for all i we have from equation (7), as $n \to \infty$

$$L(\zeta, \lambda_i^{(n)}) = \zeta T_{n-1}(\lambda_i^{(n)}) \to 0 \tag{34}$$

Note that the roots of T_n are dense on its support in its limiting case, and so the zeros of L have to be dense as well.

1.1 Finite-n approximations

Equation (34) justifies approximating 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 second kind, we call this a Chebyshev approximation. The nk roots are the solution of z in the following equation, where λ_i with $i = 1, 2 \ldots n$ are the roots of T_n.

$$Q_k(z) = -\sqrt{\gamma}\lambda_i \tag{35}$$

With the limiting behavior of zeros in equation (34), one can also further expand equation (7) by a Taylor series approximation which is denoted as Chebyshev-Taylor approximation in this work. Let λ_i and λ_j be the roots of T_n and T_{n-1} respectively that are closest to each other.

Then the zero of $L_n(\zeta, \lambda)$ can be approximated using a first order Taylor approximation as the following. Given $T_n(\lambda_i) = T_{n-1}(\lambda_j) = 0$,

$$L_n(\zeta, \lambda) = T_n + \zeta T_{n-1} \tag{36}$$

$$0 \approx (\lambda - \lambda_i)T_n'(\lambda_i) + \zeta(\lambda - \lambda_j)T_{n-1}'(\lambda_j) \tag{37}$$

$$\lambda \approx \frac{\lambda_i T_n'(\lambda_i) + \zeta\lambda_j T_{n-1}'(\lambda_j)}{T_n'(\lambda_i) + \zeta T_{n-1}'(\lambda_j)} \tag{38}$$

So the roots of p_n are approximated by solving for z' in the equation

$$Q_k(z') = -\sqrt{\gamma}\lambda \approx -\sqrt{\gamma}\frac{\lambda_i T_n'(\lambda_i) + \zeta\lambda_j T_{n-1}'(\lambda_j)}{T_n'(\lambda_i) + \zeta T_{n-1}'(\lambda_j)} \tag{39}$$

For each Chebyshev-Taylor approximation of eigenvalue, we use roots of T_n and T_{n-1}. We compute the k solutions of z using equation (35) and a λ_i. We improve this Chebyshev approximation of a root by evaluating $\zeta(z)$, followed by solving equation (39) for z'. We finally identify the solution closest to z among the k solutions of z', as the improved approximation. This approach, in principle, can be further extended into an iterative procedure or an higher-order approximation if required. Further, knowing $\zeta(z)$ and n, we can use the previous analysis of convergence to bound the error in the Chebyshev approximation. Note that ζ values away from 1 indicates a faster rate of convergence as $\frac{1}{n}$ to the limiting case. When $|\zeta(z)| \sim 1$, the error in λ_i used in equation (35) is $\leq \sqrt{\frac{2}{2n+1}}$. In other cases, the error in λ_i is upper-bound by

$$|\lambda - \lambda_i| < \Delta \tag{40}$$

where

$$\Delta = \begin{cases} \frac{3|\zeta|}{2(1-|\zeta|)n} & |\zeta| < 1 \\ \\ \frac{3|\zeta|}{(|\zeta|-1)n} & |\zeta| > 1 \end{cases} \tag{41}$$

This allows a numerical estimate of maximum error in each evaluated eigenvalue z (or z') for a given Q_k without much computational effort. Note that such bounds on the error in each eigenvalue evaluated, is not possible in the case of a direct numerical method.

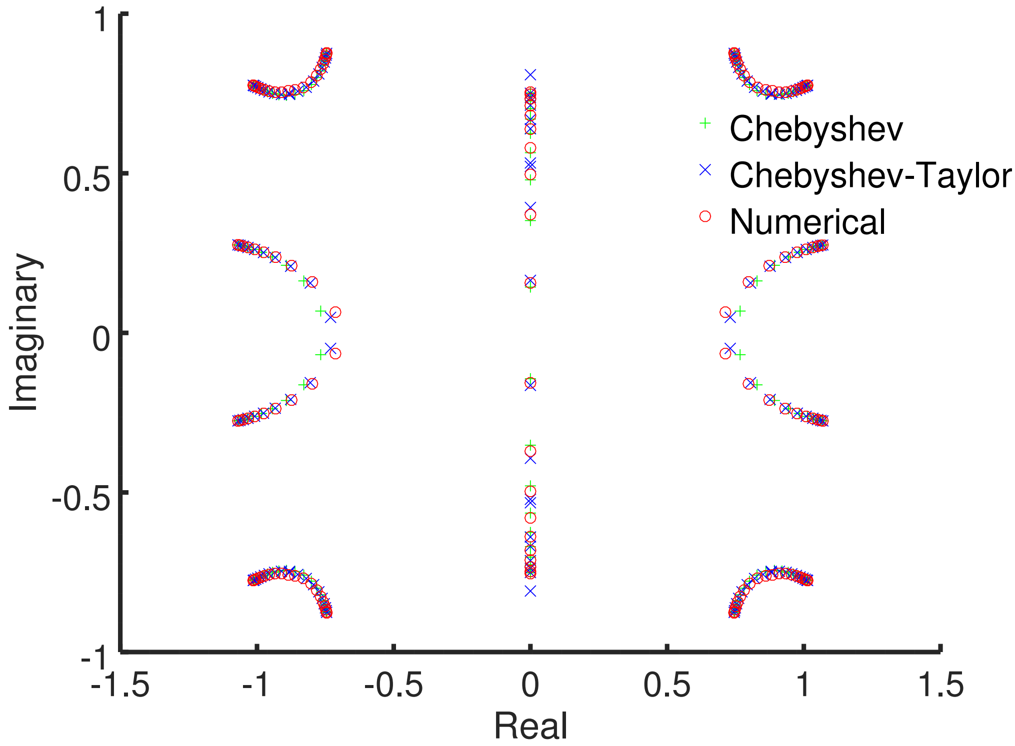


Figure 2: Approximation of roots in case of finite n, for the 3-term recurrence described in section 2.2 as S_7. Here k=7, n=20 results in 140 roots. Computing effort using a Chebyshev approximation on limiting roots is $\mathcal{O}(nk^2)$, cost of corresponding Chebyshev-Taylor approximation is $\mathcal{O}(nk^3)$, and numerical evaluations is $\mathcal{O}(n^2k^2)$.

2 Evaluating spectra of chain and lattice models

The analyzed three-term recurrence is also satisfied by characteristic polynomials of tridiagonal matrices with k-periodic entries on the three diagonals, and of corresponding dimensions nk. Here initial condition p_1 for the recurrence is restricted and not independent of the polynomial Q_k. If k is the natural number representing periodicity of entries, such matrices can be called tridiagonal k-Toeplitz matrices. Roots of these characteristic polynomials represent the behavior of man-made and natural systems which contain a large number of units arranged periodically. Periodicity in natural and man-made systems have been of great interest and resulted in corresponding theories of Bloch, Hill, Floquet, Lyapunov and others. For example, Bloch's theory of sinusoidal waves in a simple periodic potential (k=1, $n \to \infty$) has been widely applied; here real-valued spectra representing basis waves of the system results from a periodic phase-condition applied on the set of all possible waves. In this work, with variables in $\mathbb{C}$ and imaginary entries that need not result in a Hermitian, we allow for both dissipative and generative properties in the chain and thus conditions on both phase and amplitude define the limiting complex roots.

Many problems in physics, economics, biology and engineering are modelled using chains and lattices. In a chain each repeated unit can in-turn be composite, and thus contain interconnected elements or elements of multiple types resulting in a periodicity $k > 1$. There are classical chain models like Ising model, the structural model for graphene [6] and worm like chains in microbiology [12]. Such chain models can be reduced to a system of equations represented by a tridiagonal matrix [10], [1], [8] with periodic entries. The tridiagonal matrix of interest is Hermitian with real spectra in cases like some spring-mass systems, electrical ladder networks and Markov chains. It can be non-Hermitian in the case of other chain models in economics and physical systems that break certain reflection symmetries, behave non-locally, or do not entail conservation of energy [16], [2]. Limiting cases of tridiagonal 2-Toeplitz and 3-Toeplitz matrices with real entries were studied [5], and so were tridiagonal k-Toepltiz matrices similar to a real symmetric matrix [1], all of which produce the above three-term polynomial recurrence for z, γ in $\mathbb{R}^1$.

In most cases, a physical lattice in more than one dimension is well approximated using such chain models when complemented by laws such as conservation of momentum. A chain with periodicity $k > 1$ is especially useful in modeling a lattice of higher dimensions, which then is decomposed into a small set of such chains based on the symmetry properties of the lattice, or using mean-field representations. In the context of this work, one can solve for roots of polynomials generated by a family of co-efficient polynomials Q_k in the case of a lattice. Alternately, we know the existence of a limiting set of roots even for a recurrence with more than three terms [3], and thus the proposed approach can be extended to a general lattice. In case of tridiagonal k-Toeplitz matrices, we also show in the appendix that the continuous part of the limiting set of roots can alternately be derived using Widom's conditional theorems for existence of limiting spectra of block-Toeplitz operators [14], [15] and its recent extensions [4]. Whereas, the analysis in previous sections also included nature of convergence and the up-to $2k$ critical roots that depend on initial conditions of the recurrence, which may not converge to this continuous set; evaluation of these critical roots are significant in chain and lattice models.

In the next section 2.1, characteristic polynomials of tridiagonal k-Toeplitz matrices are shown to satisfy the recurrence of interest. This is followed by a section on some chain models and special k-Toeplitz matrices S_k, which serves as an example for important such recurrence relations with variables in $\mathbb{C}$. Finally, a few numerical examples are used in section 2.3 to demonstrate the utility of theorems and the generalized spectral relations of chains for variables in $\mathbb{C}$. We begin with characteristic polynomials of tridiagonal k-Toeplitz matrices; here tridiagonal elements in the first k rows repeat after k rows. They are of the form

$$M_k = \begin{bmatrix} a_1 & x_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ y_1 & a_2 & x_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & y_2 & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \ddots & a_k & x_k & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & y_k & a_1 & x_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & y_1 & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & y_{k-1} & a_k & x_k \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & y_k & a_1 \end{bmatrix}$$

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.

2.1 Three term recurrence of polynomials from a general tridiagonal k-Toeplitz matrix

Our objective in this section is to get a three-term recurrence relation of characteristic polynomial of 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 $(n-2)k \times (n-2)k$. We do this by expanding the determinant.

Characteristic equation of matrix M_k is given by the polynomial $\det(M_k - \lambda I) = 0$ and let $-\lambda = z$.

$$M_k - \lambda I = \begin{bmatrix} z + a_1 & x_1 & 0 & 0 & 0 \\ y_1 & z + a_2 & x_2 & 0 & 0 \\ 0 & y_2 & z + a_3 & x_3 & 0 \\ 0 & 0 & y_3 & \ddots & \ddots \\ 0 & 0 & 0 & \ddots & \ddots \end{bmatrix}$$

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

$$p_n \quad = (z + a_1)q_n - u_1 r_n. \tag{42}$$

In the matrix form, we have

$$\begin{bmatrix} p_n(z) \\ q_n(z) \end{bmatrix} = \begin{bmatrix} z + a_1 & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} q_n(z) \\ r_n(z) \end{bmatrix} \tag{43}$$

This gives us

$$\begin{bmatrix} p_n(z) \\ q_n(z) \end{bmatrix} = \begin{bmatrix} z + a_1 & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z + a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} z + a_k & -u_k \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ q_{n-1}(z) \end{bmatrix} \tag{44}$$

With the initial condition,

$$\begin{bmatrix} p_1(z) \\ q_1(z) \end{bmatrix} = \begin{bmatrix} z + a_1 & -u_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z + a_2 & -u_2 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} z + a_{k-1} & -u_{k-1} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} z + a_k \\ 1 \end{bmatrix} \tag{45}$$

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 $U(i) = \begin{bmatrix} z + a_i & -u_i \\ 1 & 0 \end{bmatrix}$. Also let $U_k = \Pi_{i=1}^{k} U(i)$. Entries of U_k are polynomials in z, and for generality let us denote them as $U_k = \begin{bmatrix} A(z) & B(z) \\ C(z) & D(z) \end{bmatrix}$ where $A(z), B(z), C(z)$ and $D(z)$ are some polynomials of degree utmost k. Therefore

$$\begin{bmatrix} p_n(z) \\ q_n(z) \end{bmatrix} = \begin{bmatrix} A(z) & B(z) \\ C(z) & D(z) \end{bmatrix} \begin{bmatrix} p_{n-1}(z) \\ q_{n-1}(z) \end{bmatrix} \tag{46}$$

Lemma 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.*

$$p_{n+1}(z) = Q_k(z)p_n(z) + \gamma p_{n-1}(z) \tag{47}$$

Here $Q_k(z)$ is a polynomial of degree k, and γ is in $\mathbb{C}^1$.

Proof. From equation (46) we have,

$$p_n(z) = A(z)p_{n-1}(z) + B(z)q_{n-1}(z) \tag{48}$$
$$q_n(z) = C(z)p_{n-1}(z) + D(z)q_{n-1}(z) \tag{49}$$

Rearranging equation (48)

$$B(z)q_{n-1}(z) = p_n(z) - A(z)p_{n-1}(z) \tag{50}$$

Replacing n by $n+1$,

$$B(z)q_n(z) = p_{n+1}(z) - A(z)p_n(z) \tag{51}$$

Multiplying (49) by $B(z)$

$$B(z)q_n(z) = B(z)C(z)p_{n-1}(z) + B(z)D(z)q_{n-1}(z) \tag{52}$$

Substituting equation (51) in (52), we obtain a three term recurrence relation

$$p_{n+1}(z) - A(z)p_n(z) = B(z)C(z)p_{n-1}(z) + D(z)(p_n(z) - A(z)p_{n-1}(z))$$

$$p_{n+1}(z) = (A(z) + D(z))p_n(z) + (B(z)C(z) - A(z)D(z))p_{n-1}(z) \tag{53}$$
$$p_{n+1}(z) = \text{trace}(U_k)p_n(z) - det(U_k)p_{n-1}(z) \tag{54}$$

This proves the theorem with $Q_k(z) = \text{trace}(U_k)$ and $\gamma = -det(U_k)$.

∎

corollary 3. *Using Lemma-1 and determinants of the factors U we have*

$$\gamma = -\Pi_{i=1}^{k} u_i$$

and

$$Q_k = A(z) + D(z)$$

corollary 4. *From the above and Lemma-1, we have three term recurrence in the matrix form,*

$$\begin{bmatrix} p_{n+1}(z) \\ p_n(z) \end{bmatrix} = \begin{bmatrix} Q_k(z) & \gamma \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_n(z) \\ p_{n-1}(z) \end{bmatrix} \tag{55}$$

Let $\Gamma = \begin{bmatrix} Q_k(z) & \gamma \\ 1 & 0 \end{bmatrix}$. The eigenvalues of Γ are

$$r_{\pm}(z) = \frac{Q_k(z) \pm \sqrt{(Q_k(z))^2 + 4\gamma}}{2} \tag{56}$$

With the corresponding eigenvectors

$$\begin{bmatrix} 1 & 1 \\ \frac{1}{r_+(z)} & \frac{1}{r_-(z)} \end{bmatrix}$$

By relationship of the determinant to eigenvalues, we have $r_+(z) \times r_-(z) = -\gamma$ for all z.

corollary 5. *Suppose two tridiagonal k-Toeplitz matrices M_k with entries x_j, a_j, y_j and M'_k with entries x'_j, a'_j, y'_j have the relation $a_j = a'_j$ and $x_j y_j = x'_j y'_j$ $\forall j$ then this is a sufficient condition for both of them to have an identical limiting spectrum. In case of $k = 2$, this is the necessary and sufficient condition.*

Proof. From equation (54), it is sufficient to have the same product $u_j = x_j y_j$ to have the same $Q_k(z)$ and γ. Theorem-1 establishes the same limiting spectra for all such matrices. In case of $k = 2, \gamma = u_1 u_2$ and $trace(U) = u_1 + u_2$. This necessary condition implies that given $Q_k(z)$ and γ, u_1, u_2 are uniquely determined in this case. ∎

2.2 A chain with complex spectra : S_k

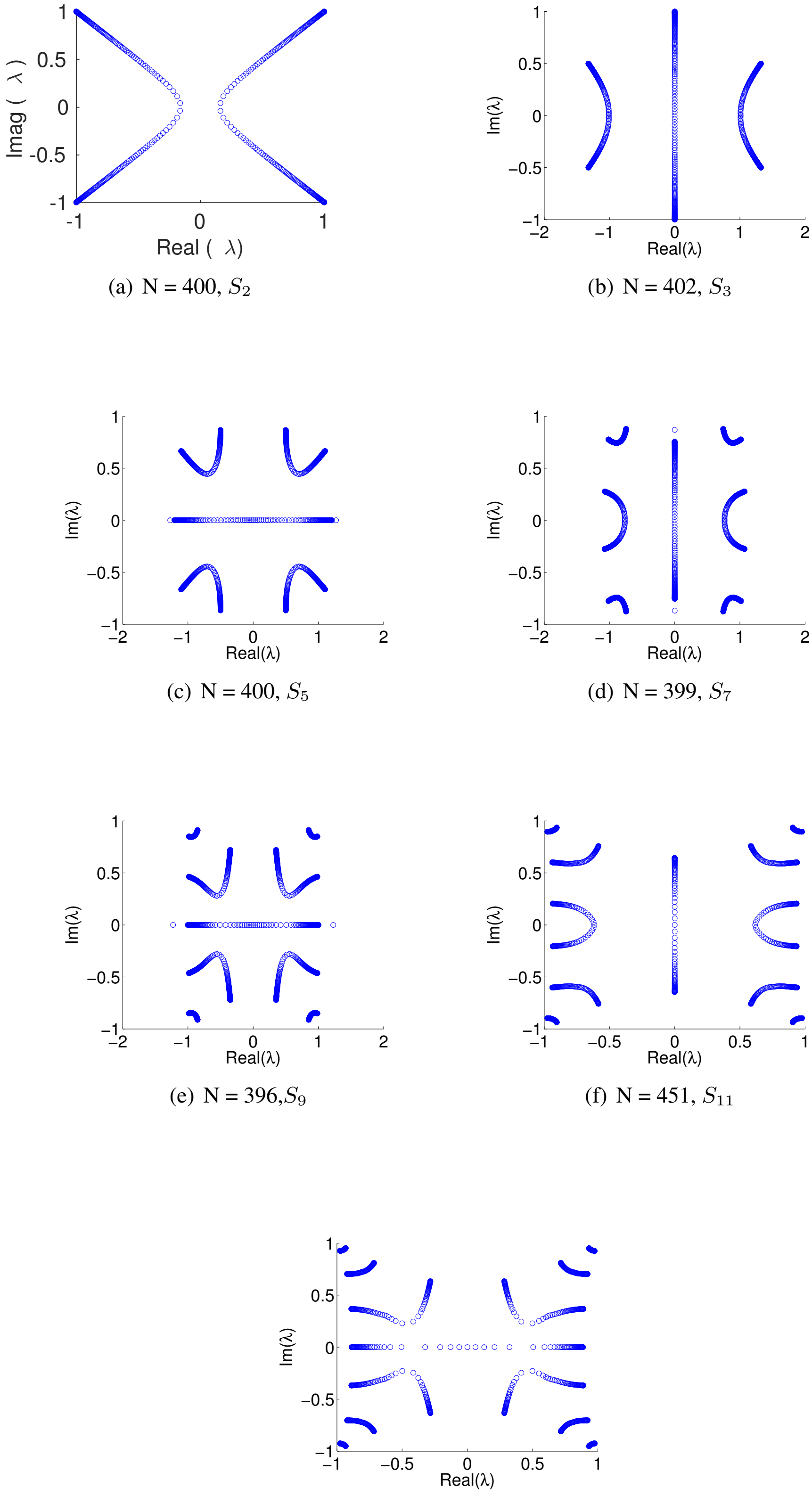
In this section, we apply our results to characteristic polynomials of tridiagonal k-Toeplitz matrices S_k that represent a chain where Hermitian blocks (representing non-dissipative units) are joined by non-Hermitian blocks (representing a source-sink pair). Such chains exhibit unique modes that span dissipative, transitive and generative properties. We define tridiagonal k-Toeplitz matrices S_k, where $a_j = a$ and $x_j y_j = (-1)^{1+(j \mod k)}$. Here k is any odd number or 2. If k is any even number other than 2, spectra of S_k is identical to that of S_2 of corresponding dimensions.

Examples:

$$S_2 = \begin{bmatrix} a & i & 0 & 0 & 0 & 0 \\ -i & a & -1 & 0 & 0 & 0 \\ 0 & 1 & a & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \ddots & a & -1 \\ 0 & 0 & 0 & 0 & 1 & a \end{bmatrix}$$

$$S_3 = \begin{bmatrix} a & 1 & 0 & 0 & 0 & 0 \\ 1 & a & \frac{i}{4} & 0 & 0 & 0 \\ 0 & 4i & a & 1 & 0 & 0 \\ 0 & 0 & 1 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & \ddots & a & 1 \\ 0 & 0 & 0 & 0 & 1 & a \end{bmatrix}$$

For S_k with $N \gg k$, where N be the dimension of matrix, eigenvalues are plotted in figure 3. The corresponding values of k are $2, 3, 5, 7, 9, 11$ and 13. We discuss cases with $a = 0$ without loss of generality as any other constant just induces a shift in the spectra by the value a. The following observations on spectra of S_k will be later derived using theorem-1 stated in the first part of this paper.



(a) N = 400, S_2

(b) N = 402, S_3

(c) N = 400, S_5

(d) N = 399, S_7

(e) N = 396,S_9

(f) N = 451, S_{11}

(g) N = 533, S_{13}

Figure 3: Eigenvalues plotted real vs imaginary part. N indicates the dimension of matrix S_k.

2.2.1 Observations and claims on S_k

1. All $S_k \in \mathbb{C}^{n\times n}$ for a fixed k have same limiting spectrum.
2. Spectrum of S_k (plotted real versus imaginary part of eigenvalues of large dimension S_k) for $N \gg k$ converges to k distinct curves.
3. Let k be of the form $2m-1$ where $m>1$ is a natural number. One of the k curves traced by eigenvalues is along the imaginary axis if m is even, and the eigenvalues trace a line on the real axis if m is odd.

Here dimension N of the matrix S_k is taken exactly as an integer multiple of k. If it is not a multiple of k then $r = N \mod k$ number of eigenvalues may lie outside the k curves traced in complex plane. Note that a general requirement of symmetry in eigenvalues exists for matrices with alternating zero and non-zero sub-diagonals; this is shown in the appendix.

2.2.2 Limiting spectra of S_k

In this section we use the procedure described in section 2.1 to explicitly derive Q_k and γ in the three-term recurrence relations of characteristic polynomials of matrices S_k. This allows us to prove the properties of limiting spectra of matrices S_k claimed in section 2.2.1 by simply applying the theorems in section 1. As mentioned before, spectrum of S_k for an even number k reduces to that of S_2 and hence is not discussed further. Let the odd natural number $k = 2m-1$ where $m > 1$. Let $s_1 = \frac{2m-6}{4}$ when m is odd and $s_2 = \frac{2m-4}{4}$ when m is even.

Theorem 2. *Characteristic polynomial of any S_k of dimension nk satisfies the three-term recurrence relation given by*

$$p_n(z) = Q_k(z)p_{n-1}(z) + (-1)^{\frac{k+1}{2}} p_{n-2}(z) \tag{57}$$

where

$$Q_k(z) = \sum_{t=0}^{s_1} \left(\binom{m-t-1}{t} z^{2m-4t-1} - \binom{m-t-2}{t} z^{2m-4t-3} \right) + z \tag{58}$$

when m is odd, and

$$Q_k(z) = \sum_{t=0}^{s_2} \left(\binom{m-t-1}{t} z^{2m-4t-1} - \binom{m-t-2}{t} z^{2m-4t-3} \right) \tag{59}$$

when m is even.

The proof of the above theorem is provided in the appendix.

Note that we have $\gamma = 1$ when m is even and $\gamma = -1$ when m is odd. When we apply theorem-1 and corollary-1 using the above derived values of γ and $Q_k(z)$, all observations about the limiting spectra of S_k in section 2.2.1 are proved to be true in generality.

2.3 Numerical examples

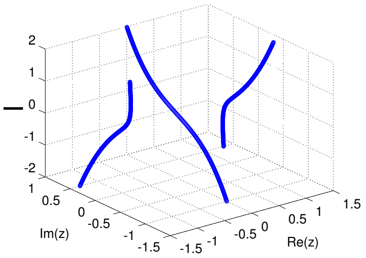
In this section we present a few example solutions of eigenvalues, both in the case of a matrix S_k and other general tridiagonal k-Toeplitz matrices M_k. The polynomial $Q_k(z) = L$ has k distinct roots for any point in L. These nk roots can be well approximated using n Chebyshev roots on line L which become dense in the limiting case (section 1.1). As pointed before, such evaluations cost $\mathcal{O}(nk^2)$ arithmetic operations while numerical evaluations cost $\mathcal{O}(n^2k^2)$. In many applications where n is large, tracing these curves as the support for eigenvalues using fewer points on L may be sufficient. As the points on L vary smoothly, these roots can be viewed as k curves in three dimensional space (X, Y axis representing real and imaginary parts of z, and Z axis corresponding to L). Therefore limiting eigenvalues are supported by the curve $Q_k(z) = L$ in $\mathbb{C} - L$ space.

2.3.1 S_k

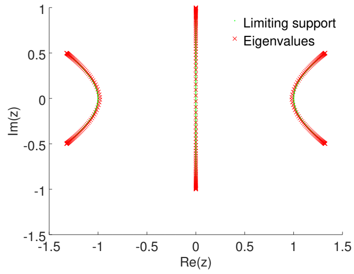
1. For a graphic example of S_3, we have $Q_3(z) : z^3 - z = L$ with $L \in [-2i, 2i]$. For S_5, we have $Q_5(z) : z^5 - z^3 + z = L$, with $L \in [-2, 2]$. For S_7 we have $Q_7(z) : z^7 - z^5 + 2z^3 - z = L$ with $L \in [-2i, 2i]$. These curves, their projections and eigenvalues for a large N can be seen in figure 4.

2. Note that when k is of the form $4m + 1$, spectrum contains real axis as one of the curve and k of the form $4m + 3$ spectrum contains imaginary axis as one of the curves (Theorem 2).

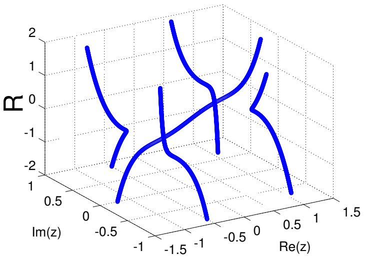
3. Convergence of the absolute value of eigenvalues of 2×2 recurrence matrix i.e. $|r_{\pm}|$ defined in section 2.1, indicates the convergence to the limiting spectrum for tridiagonal k-Toeplitz matrices (as shown in appendix using Widom's theorems). In figure 5, the maximum, minimum and average of absolute r are plotted for S_3 with $N \in \{3, 6, 9, \cdots 300\}$.



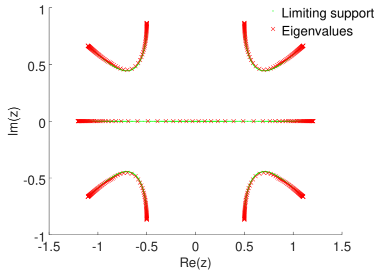
(a) $Q_3 = L$ as C-I space for S_3



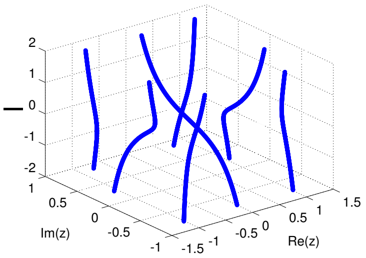
(b) N = 300, $Q_3(z) = L$ represented in figure 4a projected on the complex plane as the support for limiting spectra



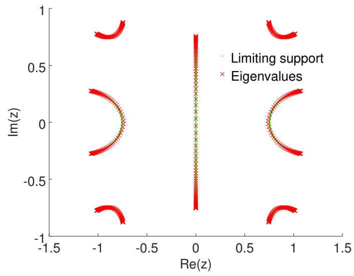
(c) $Q_5 = L$ as C-R space for S_5



(d) N = 500, $Q_5(z) = L$ represented in figure 4c projected on the complex plane as the support for limiting spectra



(e) $Q_7 = L$ as C-I space for S_7



(f) N = 700, $Q_7(z) = L$ represented in figure 4e projected on the complex plane as the support for limiting spectra

Figure 4: Traces of $Q_k = L$ when L is a purely real or imaginary interval for the Chebyshev approximation, and corresponding spectrum of matrices S_k.

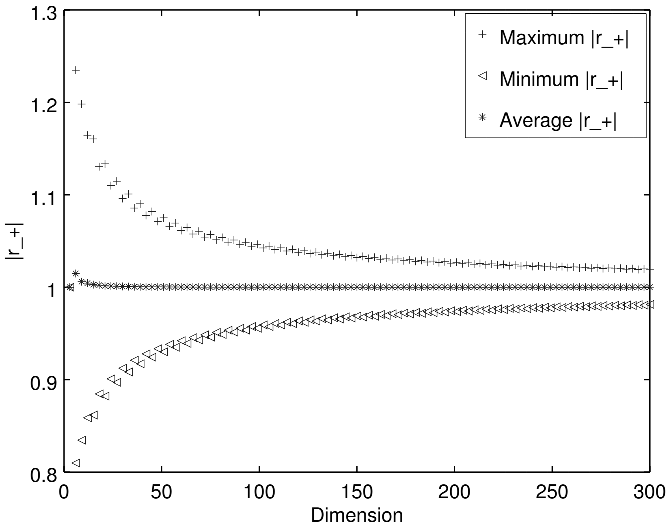


Figure 5: $|r\pm|$ for S_3 vs N.

2.3.2 M_k

In M_k, when $a_j = a$ we can limit our discussion to matrices of the form

$$M'_k = \begin{bmatrix} 0 & x_1 & 0 & 0 & 0 & 0 \\ y_1 & 0 & x_2 & 0 & 0 & 0 \\ 0 & y_2 & 0 & \ddots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & x_j & 0 \\ 0 & 0 & 0 & y_j & 0 & \ddots \\ 0 & 0 & 0 & 0 & \ddots & \ddots \end{bmatrix}.$$

Here $M_k = M'_k + aI$ and spectrum of the matrix M_k is shifted from that of M'_k by a value a. In this section we consider examples of M'_5. When we apply Lemma-1 we get expressions for Q_5 and γ for these examples.

Let $u_j = x_j y_j$; then

$$Q_5 = z^5 - \left(\sum_{i=0}^{4} u_i\right) z^3 + \left(\sum_{i=0}^{2}\sum_{j=i+2}^{4} u_i u_j\right) z \tag{60}$$

$$\gamma = -u_0 u_1 u_2 u_3 u_4 \tag{61}$$

As an example, x_j and y_j were taken from uniform disc of radius 1 in the complex plane and theorem-1 was applied to generate limiting supports for the eigenvalue distribution. Matrices of dimension 500 are shown in Figures 6 and 7.

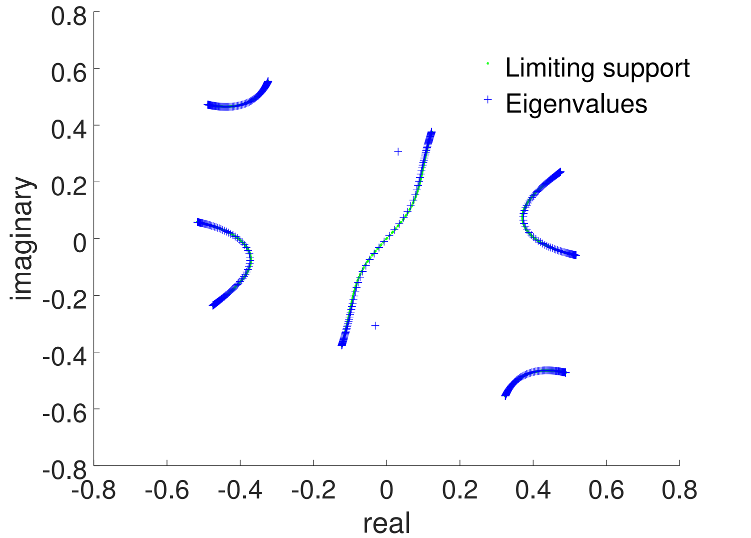


Figure 6: Example spectrum of M_5' of dimension 500 and corresponding continuous limiting support for $Q_5 - L = 0$.

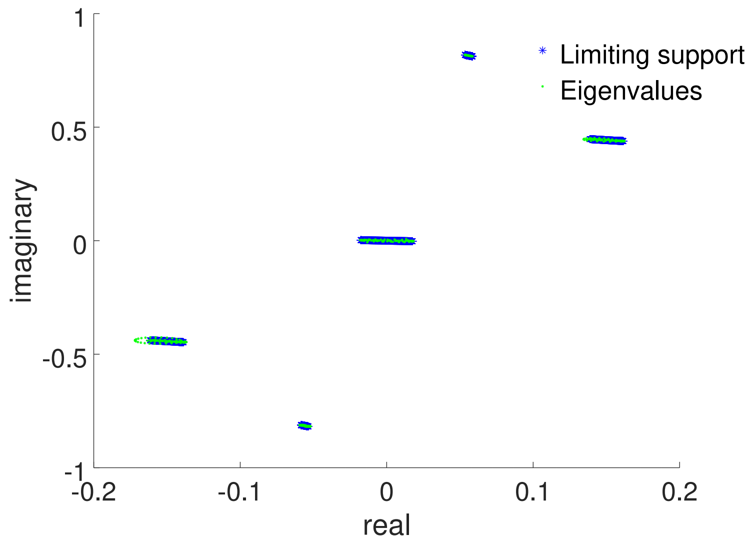


Figure 7: Example spectrum of M_5' of dimension 500 and corresponding continuous limiting support for $Q_5 - L = 0$.

In figure 6,

$$
\begin{aligned}
x =&[0.14786 - 0.14549i, 0.49296 - 0.14926i, -0.49709 + 0.31233i, \\
&- 0.66051 - 0.63714i, -0.47679 + 0.10519i] \\
y =&[-0.46743 - 0.33319i, 0.23728 + 0.09273i, -0.63907 - 0.29653i, \\
&0.52739 - 0.24468i, -0.32003 + 0.10717i]
\end{aligned}
$$

In figure 7,

$$
\begin{aligned}
x =&[0.54284 + 0.13073i, -0.38154 - 0.59148i, -0.26609 - 0.04314i, \\
&- 0.41213 + 0.59500i, 0.10894 + 0.11749i] \\
y =&[-0.33995 + 0.23836i, -0.11798 + 0.00038i, 0.44581 + 0.19947i, \\
&0.59770 + 0.51966i, 0.00649 - 0.00344i]
\end{aligned}
$$

3 Summary

We analyzed the behavior of roots of polynomials with a three-term recurrence relation of the form $p_{n+1}(z) = Q_k(z)p_n(z) + \gamma p_{n-1}(z)$, where the coefficient $Q_k(z)$ is any k^{th} degree polynomial, and z, γ are $\mathbb{C}^1$. In addition to establishing existence and convergence to a limiting set of roots for generality of variables in $\mathbb{C}$ and any k, useful approximations for roots in case of finite n were derived. A slower convergence to the limiting set of roots by an order of $1/\sqrt{n}$ was shown to be possible for some cases, compared to the expected order of $1/n$. Relations for the up-to $2k$ critical roots which depend on the initial conditions and lie outside the continuous limiting set, were also derived. These results were applied to eigenvalue problems of tridiagonal k-Toeplitz matrices which are significant for chain and lattice models. Numerical examples were used as a demonstration of theorems later. These closed-form solutions and approximations can substitute direct numerical solution of these eigenvalue problems which involve significantly larger computational effort and are error prone.

Appendix

Proof of theorem 2 :

Let the odd natural number $k = 2m - 1$. Let $s_1 = \frac{2m-6}{4}$ when m is odd and $s_2 = \frac{2m-4}{4}$ when m is even.

Theorem 2: Characteristic polynomial of any S_k of dimension nk satisfies the three-term recurrence relation given by

$$p_n(z) = Q_k(z)p_{n-1}(z) + (-1)^{\frac{k+1}{2}} p_{n-2}(z) \tag{62}$$

where

$$Q_k(z) = \sum_{t=0}^{s_1} \left(\binom{m-t-1}{t} z^{2m-4t-1} - \binom{m-t-2}{t} z^{2m-4t-3} \right) + z \tag{63}$$

when m is odd, and

$$Q_k(z) = \sum_{t=0}^{s_2} \left(\binom{m-t-1}{t} z^{2m-4t-1} - \binom{m-t-2}{t} z^{2m-4t-3} \right) \tag{64}$$

when m is even.

Proof. For the matrices S_k we have $U(i) = \begin{bmatrix} z & (-1)^i \\ 1 & 0 \end{bmatrix}$ for $1 \leq i \leq k$. Also $U_k = \prod_{i=1}^{k} \begin{bmatrix} z & (-1)^i \\ 1 & 0 \end{bmatrix}$. For S_k and S_{k+2} we have, $U_{k+2} = \begin{bmatrix} z^2 - 1 & z \\ z & 1 \end{bmatrix} U_k$. Therefore we obtain, $\det(U_{k+2}) = -\det(U_k)$ and trace$(U_{k+4}) = z^2$trace$(U_{k+2}) +$ trace(U_k).

Which can also be written as

$$\gamma_{k+2} = -\gamma_k \tag{65}$$

$$Q_{k+4} = z^2 Q_{k+2} + Q_k \tag{66}$$

Corresponding initial U_k matrices with $k = 1$ and $k = 3$ are

$$U_1 = \begin{bmatrix} z & -1 \\ 1 & 0 \end{bmatrix}$$

$$U_3 = \begin{bmatrix} z^3 & 1 - z^2 \\ 1 + z^2 & -z \end{bmatrix}$$

We use these initial conditions to solve equation (65) and equation (66). Thus

$$\det(U_k) = (-1)^{\frac{k-1}{2}} \tag{67}$$

For equation (66), initial conditions are

$$\text{trace}(U_1) = z$$

$$\text{trace}(U_3) = z^3 - z$$

With these two initial conditions and recurrence relation (66) we obtain coefficients c_i of Q_k where

$$Q_k = \text{trace}(U_k) = c_k z^k + c_{k-1} z^{k-1} + \cdots + c_0$$

z^{13}	z^{11}	z^9	z^7	z^5	z^3	z	Value of k	m
0	0	0	0	0	0	1	1	1
0	0	0	0	0	1	-1	3	2
0	0	0	0	1	-1	1	5	3
0	0	0	1	-1	2	-1	7	4
0	0	1	-1	3	-2	1	9	5
0	1	-1	4	-3	3	-1	11	6
1	-1	5	-4	6	-3	1	13	7

Table 1: Coefficients of $Q_k(z)$

Table 1 shows c_i values corresponding to first few k. Let $f(m,n)$ be an element at m^{th} row n^{th} column in table 1. Where m and n start from top right corner. Here $f(m,n) = c_{2n+1}$ corresponding to $Q_{2m-1}(z)$. From equation (66) we have

$$f(m,n) = f(m-1,n-1) + f(m-2,n) \tag{68}$$

with appropriate initial conditions.

The table 1 can be seen as two pascal triangles one with initial condition 1 and another with initial condition -1. $f(m, m-2t)$ is the entry in the row $m-t$ and the column $t+1$ of the pascal triangle and that will be $\binom{m-t-1}{t}$. Similarly $f(m, m-2t-1)$ is given by entries in row $m-t-1$ and column $t+1$ of another pascal triangle and this is $-\binom{m-t-2}{t}$. Using the above, we construct the polynomial as

$$Q_{2m-1}(z) = \sum_{t=0}^{s} \left(\binom{m-t-1}{t} z^{2m-4t-1} - \binom{m-t-2}{t} z^{2m-4t-3} \right) + z \tag{69}$$

when m is odd, and

$$Q_{2m-1}(z) = \sum_{t=0}^{s} \left(\binom{m-t-1}{t} z^{2m-4t-1} - \binom{m-t-2}{t} z^{2m-4t-3} \right) \tag{70}$$

when m is even. ∎

The limiting set C and Widom's conditional theorems on block-Toeplitz operators

In the special case of characteristic polynomials of tridiagonal matrices and the recurrence relation of interest here, the continuous limiting set C can be as well derived from theorems for existence of the limiting spectrum for block-Toeplitz matrices. These were shown to exist under certain conditions by H. Widom [14] and [15]. Extension of this theory to the equilibrium problem for an arbitrary algebraic curve was presented in a recent article [4], and in this brief note, we maintain the notations used there. Here we treat the tridiagonal k-Toeplitz matrix as a block-Toeplitz matrix. The $symbol$ for the matrix was defined as

$$A(z) = A_0 + A_1 z^{-1} + A_{-1} z \tag{71}$$

Here,

$$A(z) = \begin{bmatrix} a_1 & x_1 & 0 & 0 & zy_k \\ y_1 & a_2 & x_2 & 0 & 0 \\ 0 & y_2 & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & a_{k-1} & x_{k-1} \\ \frac{x_k}{z} & 0 & 0 & y_k - 1 & a_k \end{bmatrix}$$

The spectrum is determined by an algebraic curve $zf(z,\lambda) = z\det(A(z)-\lambda I)$ and in this case it is a quadratic polynomial. The limiting spectrum of the tridiagonal block-Toeplitz matrix is given by all z where both roots of the quadratic polynomial have same magnitude [14]. This is valid under certain assumptions (named H1,H2, H3) as shown by Delvaux [4]. Let the quadratic polynomial $zf(z,\lambda)$ be of the form $a(\lambda)z^2 + b(\lambda)z + c(\lambda)$. Below we show that b and Q_k are identical, also showing that the relevant theorems of Widom and Delvaux can be reduced to derive the continuous set C in the limiting spectra of tridiagonal k-Toeplitz matrices. The coefficients have to be evaluated by finding the determinant. To do this, consider a permutation matrix

$$J = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & \iddots & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$J^2 = I$ and $\det(J^2) = \det(J)^2 = 1$ and $\det(A(z)) = \det(JA(z)J)$. By applying the expansion for determinant of such matrices (provided in [7]) to $\det(JA(z)J)$ we get

$$zf(z,\lambda) = \Pi_{i=1}^{k} x_i + z^2 \Pi_{i=1}^{k} y_i + zb(\lambda)$$

With,

$$b(\lambda) =$$

$$\text{trace}\left(\begin{bmatrix} a_1 - \lambda & -x_1 y_1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a_2 - \lambda & -x_2 y_2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a_3 - \lambda & -x_3 y_3 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} a_k - \lambda & -x_k y_k \\ 1 & 0 \end{bmatrix}\right)$$

Let $r_\pm = \frac{-b(\lambda) \pm \sqrt{b(\lambda)^2 - 4a(\lambda)c(\lambda)}}{2a(\lambda)}$ be the roots of quadratic equation $zf(z,\lambda) = 0$. In the case of limiting large n it was shown by those authors that the quadratic polynomial has two roots of equal magnitude. So this gives a corresponding condition $|r_+| = |r_-| = \sqrt{\frac{|c(\lambda)|}{|a(\lambda)|}}$. So the coefficient $b(\lambda)$ is related to the determinant as

$$\sqrt{|a(\lambda)c(\lambda)|} = \frac{1}{2}| - b(\lambda) \pm \sqrt{b(\lambda)^2 - 4a(\lambda)c(\lambda)}| \tag{72}$$

With a change of notation from λ to z, by rewriting $b(\lambda) = Q_k(z)$ and $a(\lambda)c(\lambda) = -\gamma$ we get,

$$\sqrt{|\gamma|}e^{i\theta} = \frac{-Q_k(z) \pm \sqrt{Q_k(z)^2 + 4\gamma}}{2} \tag{73}$$

This also defines the continuous set C for the special case of these matrices, and implies the same condition on $Q_k(z)$ in theorem-1.

Symmetry in spectrum of odd diagonal matrices

Let the diagonals of a square matrix be indexed such that the main diagonal is zeroth diagonal, and diagonals above and below it are numbered sequentially using positive and negative integers respectively. Then, odd-diagonal matrices refer to matrices with non-zero entries only on the odd-numbered diagonals. In this section we show that a significant reflection symmetry exists in the spectra of all odd diagonal matrices with constant entries on the main diagonal, including k-Toeplitz matrices of this kind.

Proposition 1. *Suppose two square matrices $A, B \in \mathbb{C}^{n\times n}$ commute up to a constant $k \in \mathbb{C}$, i.e. $AB = kBA$ and B is non-singular, then if λ is eigenvalue of A with eigenvector x, then $k\lambda$ is also an eigenvalue with a corresponding eigenvector Bx.*

Proof. From the statement of the theorem,

$$Ax = \lambda x \tag{74}$$
$$AB^{-1}Bx = \lambda B^{-1}Bx \tag{75}$$
$$BAB^{-1}Bx = \lambda Bx \tag{76}$$
$$\frac{1}{k}ABB^{-1}Bx = \lambda Bx \tag{77}$$
$$ABx = k\lambda Bx \tag{78}$$

∎

corollary 6. *For a square matrix A with zeros on the even indexed diagonals, and a square matrix B with $(1, -1, 1, -1\cdots)$ as entries in the diagonal and all other entries as zeros, the above theorem applies with $k = -1$. Therefore eigenvalues of S_k and M_k occur in $a \pm \lambda$ pairs, when the main diagonal consists of constant entries $'a'$.*

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