A First Szegő’s Limit Theorem for a class of non-Toeplitz matrices

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Abstract

We compute the limiting statistical distribution of the eigenvalues of sequences of matrices whose entries satisfy what we call a vanishing mean variation condition and are \( \mu \)-distributed for some probability measure. As an application of our results, we extend the well-known class of Kac-Murdock-Szegő generalized Toeplitz matrices to sequences of matrices whose diagonal entries are modeled by Riemann integrable functions.

Keywords: First Szegő’s Limit Theorem, Kac-Murdock-Szegő matrices, vanishing mean variation, equidistributed sequences.

MSC: 35P20, 47B35, 41A60, 15B05

1 Introduction

Kac, Murdock and Szegő [9] introduced generalized Toeplitz matrices in 1953. These are defined in the following way. Let \( a(s, t) \) be a complex valued function (called the symbol of the matrix) such that the Fourier coefficients

\[
\hat{a}_k(s) = \frac{1}{2\pi} \int_{-\pi}^{\pi} a(s, t)e^{-ikt} \, dt
\]  

are defined on \([0,1]\). For each integer \(n\), define the \(n \times n\) matrix

\[
T_n(a) = \left[ \hat{a}_{j-i} \left( \frac{i+j}{2n+2} \right)^{n-1} \right]_{i,j=0}^{n-1}
\]

The following generalizes Szegő’s First Limit Theorem.

**Theorem** (Kac, Murdock and Szegő (1953)). Suppose the following conditions hold.

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(i) The symbol \( a(s, t) \) is real valued.

(ii) The functions \( \hat{a}_k(s) \) are continuous on \([0, 1]\).

(iii) There exists a constant \( N \) such that

\[
N := \sum_{k=-\infty}^{\infty} \| \hat{a}_k \|_\infty < \infty.
\]  

(1.3)

Denote the eigenvalues of \( T_n(a) \) by \( \lambda_k(T_n(a)) \). Then \( \lambda_k(T_n(a)) \in [-N, N] \), and one has the following:

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(T_n(a))) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{0}^{1} \varphi(a(s, t)) \, ds \, dt
\]  

(1.4)

for any \( \varphi \in C([-N, N]) \).

The above theorem says, roughly, that as \( n \to \infty \), the eigenvalues of \( T_n(a) \) distribute like the values of \( a(s, t) \) sampled at regularly spaced points in the rectangle \([0, 1] \times [-\pi, \pi]\). Thus, one obtains the limiting statistical distribution (LSD) of the eigenvalues of \( T_n(a) \). In the case when the symbol does not depend on \( s \), \( a(s, t) = a(t) \), (1.4) reduces to the First Szegő’s Limit Theorem for Toeplitz matrices [7].

The Kac-Murdock-Szegő matrices are generalizations of Toeplitz matrices, in one sense, since as long as the functions \( \hat{a}_k \) are continuous, the diagonals of \( T_n(a) \) satisfy a small deviation condition. A key point we want to make with this paper is that it is the small deviation condition that allows the calculation to go through. Taking the diagonals from continuous functions, as Kac, Murdock, and Szegő do, is only one way to ensure this condition. (See §3.3 for examples of matrix sequences that are not of the Kac-Murdock-Szegő type.)

The main purpose of this paper is to generalize (1.4) to a larger class of operators. More precisely, we compute the LSD, defined as the weak-limit of the measures \( \frac{1}{n} \sum_{k=1}^{n} \delta_{\lambda_k(A_n)} \), for the eigenvalues \( \lambda_k(A_n) \) of sequences of matrices \( \{A_n\} \) for which the entries along each of their diagonals satisfy what we call a vanishing mean variation condition (see Definition 2.1) and are asymptotically distributed for some probability measure \( \mu \) on some compact subspace \( X \) in \( C^k \) or \( l^1(\mathbb{C}) \) (see Definition 2.2). In this case we have

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{X} \varphi(F(z, t)) \, d\mu(z) \, dt
\]  

(1.5)

where \( F(z, t) \) is the Fourier series defined in (2.4). For Hermitian matrices \( A_n \), the formula (1.5) holds for compactly supported continuous functions \( \varphi \) on \( \mathbb{R} \), and hence gives the LSD of the sequence \( \{A_n\} \). For arbitrary matrices, the formula holds for analytic \( \varphi \) in \( \mathbb{C} \).

In addition to the small deviation condition, another important aspect of (1.5) is the presence of the measure \( \mu \). Because of its greater generality, we use
to rederive and extend a number of results. For instance, in Theorem 3.6 below, we show that condition (ii) in the Kac-Murdock-Szeg˝ o Theorem above may be replaced by the condition that the \( \hat{a}_k \) are Riemann integrable.

Our approach is based on the standard moments method. We begin by setting up some terminology and definitions in the next section. In the third section, we start by computing the moments of sequences of matrices of fixed band size and then extend our results to the non-band case. In §3.3 we give some examples to illustrate the novelty of our approach. We conclude with a discussion of open questions.

## 2 Notation and definitions

All of the results below are greatly simplified if we number the entries of matrices along their diagonals rather than the usual row-column positions. For this reason, we write the \( n \times n \) matrix \( A_n \) in the following form:

\[
A_n = [a_{k,j}] = \begin{bmatrix}
  a_{0,0} & a_{1,0} & \ldots & a_{k,0} & a_{n-1,0} \\
  a_{-1,0} & a_{0,1} & \ldots & \ldots & \ldots \\
  a_{-1,1} & \ldots & \ldots & \ldots & \ldots \\
  a_{-k,0} & \ldots & \ldots & a_{1,n-2} \\
  a_{-n+1,0} & \ldots & a_{-k,n-k} & a_{0,n-1} & a_{1,n-2} \\
  a_{-n+2,0} & \ldots & \ldots & a_{-1,n-2} & a_{0,n-1} \\
\end{bmatrix}.
\] (2.1)

In other words, \( a_{k,j} = a_{k,j}(n) \) denotes the \( j \)th term on the \( k \)th diagonal, with \( k = 0 \) corresponding to the main diagonal. A Toeplitz matrix has \( a_{k,j} = a_k \).

The entries may depend on the size \( n \) of the matrix, but we will usually suppress the dependence of \( a_{k,j} = a_{k,j}(n) \) on \( n \) where this is clear. A matrix with band size \( k_0 \) is zero outside the band \( k_0 \) from the main diagonal, i.e. \( a_{k,j} = 0 \) for \( |k| > k_0 \).

We denote the eigenvalues of \( A_n \) by \( \lambda_1(A_n), \ldots, \lambda_n(A_n) \) and its singular values by \( \sigma_1(A_n) \geq \cdots \geq \sigma_n(A_n) \). The trace norm of \( A_n \) is defined by

\[
\|A\|_{tr} = \|A\|_1 = \sum_{k=1}^{n} \sigma_k(A).
\] (2.2)

On a few occasions, we also need to consider the spectral norm defined by

\[
\|A\|_{\infty} = \sigma_1(A).
\] (2.3)

We denote by \( l^1 = l^1(\mathbb{C}) \), the space of all complex sequences \( \{z_k\}_{k \in \mathbb{Z}} \) for which \( \sum_{k \in \mathbb{Z}} |z_k| \) is finite. We also denote throughout the paper the Fourier
series with coefficients $z = \{z_k\}_{k \in \mathbb{Z}} \in l^1$ by
\[
F(z, t) := \sum_{k \in \mathbb{Z}} z_k e^{ikt} \quad (t \in [-\pi, \pi]).
\] (2.4)

Note that $F(z, \cdot) \in A(\mathbb{T})$, the Wiener algebra of summable Fourier series. When $z_k = 0$ for $|k| > k_0$, we write $z = (z_{-k_0}, \ldots, z_{k_0})$ and let
\[
P(z, t) := \sum_{|k| < k_0} z_k e^{ikt} \quad (t \in [-\pi, \pi])
\] (2.5)
be the trigonometric polynomial with coefficients $z \in \mathbb{C}^{2k_0+1}$.

2.1 Vanishing mean variation sequences

In his seminal work on the spectral theory of Jacobi matrices, Simon [15] introduced the Cesàro-Nevai class as the set of Jacobi matrices $J(\mathbf{a}, \mathbf{b})$ whose sequences $\mathbf{a} = \{a_k\}$ and $\mathbf{b} = \{b_k\}$ satisfy the condition
\[
\sum_{k=1}^n |a_k| + |b_k - 1| = o(n).
\] (2.6)

His definition was motivated by the study of Jacobi matrices that are perturbations of the free discrete Schrödinger operator $J(0, 1)$. In particular, if (2.6) holds, then $J(\mathbf{a}, \mathbf{b})$ has the same LSD as $J(0, 1)$. Following (2.6), the first author considered in [2] sequences of Jacobi matrices $\{J_n\}$ that satisfy
\[
\sum_{k=1}^n |a_{k+1}(n) - a_k(n)| + |b_{k+1}(n) - b_k(n)| = o(n).
\] (2.7)

In the definition below, we extend (2.7) to sequences of general matrices.

**Definition 2.1.** We say that a matrix sequence $\{A_n\}$ is of vanishing mean variation if the entries along the diagonals of $A_n$ satisfy the asymptotic condition
\[
\sum_{j=0}^{n-k-1} |a_{k+j+1}(n) - a_{k+j}(n)| = o(n)
\] (2.8)
for each $k$. We denote by $\mathcal{VMV}$ the set of all such matrix sequences.

In particular, the vanishing mean variation condition allows us to shift the indices of products of entries of $A_n$. This observation will play a crucial role in the proof of Theorem 3.1 below. Here are some basic examples of sequences that belong to $\mathcal{VMV}$ and that we consider later on:

1. If $T(\mathbf{a})$ is a Toeplitz operator with symbol $\mathbf{a} \in A(\mathbb{T})$, then the sequence $\{T_n(\mathbf{a})\}$ is obviously in $\mathcal{VMV}$. 


(ii) More generally, any sequence \( \{A_n\} \) with diagonals entries given by density one convergent sequences, i.e. for every \( \varepsilon > 0 \),
\[
\# \{ j \leq n : |a_{k;j}(n) - a_k| > \varepsilon \} = o(n)
\]
is easily seen to belong to \( \mathcal{VMV} \).

(iii) Results for the Kac-Murdock-Szegő matrices can be extended to sequences \( \{A_n\} \) whose diagonals are modeled by Riemann integrable functions. Indeed, let \( P_n = \{t_{0; n}, t_{1; n}, ..., t_{n; n}\} \) be a sequence of partitions of \([0, 1]\) with \( \text{mesh}(P_n) = o(1) \) and let \( a_{k;j}(n) = \hat{a}_k(t_{j;n}) \) for some Riemann integrable functions \( \hat{a}_k \) on \([0, 1]\). It is straightforward to prove that \( \{A_n\} \in \mathcal{VMV} \).

2.2 \( \mu \)-distributed sequences

Our second definition is based on the standard notion of asymptotically distributed sequences with respect to a probability measure \( \mu \) on compact metric spaces \( X \). A sequence \( \{x_k\} \) in \( X \) is said to be asymptotically distributed wrt \( \mu \) if the measures \( \frac{1}{n} \sum_{j=0}^{n} \delta_{x_j} \) converge weakly to \( \mu \). We extend this notion to sequences of matrices in the following manner.

**Definition 2.2.** Let \( X \) be a compact subspace of \( l^1 \). The sequence of matrices \( \{A_n\} \) is said to be \( \mu \)-distributed for some Borel probability measure \( \mu \) on \( X \) if
\[
\frac{1}{n} \sum_{j=0}^{n} \delta_{a_j(n)} \text{ converge weakly to } \mu
\]
with
\[
a_j(n) = \{..., 0, a_{-j}; j, a_{-j+1}; j, ..., a_{n-j}; j, 0, ...\}.
\]

For \( \{A_n\} \) of fixed band size \( k_0 \), we write \( a_j(n) = (a_{-k_0}; j, ..., a_{k_0}; j) \) and take \( X \) to a be compact subspace in \( C^{2k_0+1} \).

All of the examples given in the previous section are \( \mu \)-distributed. Indeed, we have:

(i) The sequence \( \{T_n(a)\} \) obtained from a Toeplitz matrix \( T(a) \) with \( a \in \mathcal{A}(\mathbb{T}) \) is \( \delta_a \)-distributed on \( l^1 \) with \( a = \{a_k\} \in l^1 \).

(ii) If \( \{A_n\} \) has density one convergent diagonal sequences as in (ii) above to \( a = \{a_k\} \in l^1 \), then \( \{A_n\} \) is \( \delta_a \)-distributed.

(iii) Let \( \{A_n\} \) be as in (iii) above and let \( \alpha : [0, 1] \to l^1 \) be the map defined by
\[
\alpha(t) = \{\hat{a}_k(t)\}.
\]

If for all \( t, \alpha(t) \in X \) for some compact \( X \subset l^1 \), then \( \{A_n\} \) is \( m_\alpha \)-distributed with \( m_\alpha \) the push-forward of the Lebesgue measure \( m \) under the map \( \alpha \).
3 Main results

We now come to the main results of the paper, i.e. Szegő’s Limit Theorems for VMV sequences of matrices that are \( \mu \)-distributed. We begin by computing the moments for sequences of matrices \( \{A_n\} \in \mathcal{VMV} \) of fixed band-size, then we extend our result to sequences of arbitrary band sizes.

3.1 Sequences of band matrices

We now consider sequences \( \{A_n\} \) of fixed band-size \( k_0 \), i.e. \( a_{k,j}(n) = 0 \) for all \( |k| > k_0 \). Throughout this section, we make the assumption that the entries of \( \{A_n\} \) are uniformly bounded, i.e.

\[
\sup_n (\max_{j,k} |a_{k,j}(n)|) < \infty. \tag{3.1}
\]

The proof of the following theorem is a modification of that of Kac-Murdock-Szegő \[9, 7\], modified for the \( \mu \)-distributed case, and couched in terms of the notation of \[21\].

**Theorem 3.1.** Let \( \{A_n\} \in \mathcal{VMV} \) of fixed band size \( k_0 \) be \( \mu \)-distributed on some compact \( X \subset \mathbb{C}^{2k_0+1} \). Then for any \( r, s \in \mathbb{N} \), we have

\[
\lim_{n \to \infty} \frac{1}{n} \text{Tr} [A_n^r (A_n^*)^s] = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_X P^r(z,t)P^s(z,t) d\mu(z) dt. \tag{3.2}
\]

The proof of this theorem relies on the fact that we can shift indices modulo an \( o(n) \) term. This is the content of the following lemma. In what follows we define \( a_{k,j} = a_{k,j}(n) \) to be zero if \( j < 0, j > n - k \), or \( |k| > n \).

**Lemma 3.2.** Let \( \{A_n\} \in \mathcal{VMV} \). Then for any integers \( \nu_1, \nu_2, \ldots, \nu_p \) and \( h_1, h_2, \ldots, h_p \),

\[
\sum_{j=0}^{n} a_{h_1;\nu_1+j} a_{h_2;\nu_2+j} \cdots a_{h_p;\nu_p+j} = \sum_{j=0}^{n} a_{h_1;j} a_{h_2;j} \cdots a_{h_p;j} + o(n)
\]

**Proof.** Shift the index in the first term:

\[
\sum_{j=0}^{n} a_{h_1;\nu_1+j} a_{h_2;\nu_2+j} \cdots a_{h_p;\nu_p+j} = \sum_{j=0}^{n} a_{h_1;j} a_{h_2;j} \cdots a_{h_p;j} + \sum_{j=0}^{n} (a_{h_1;\nu_1+j} - a_{h_1;j}) a_{h_2;\nu_2+j} \cdots a_{h_p;\nu_p+j}
\]
Since the entries of $A_n$ are uniformly bounded, we can assume that they are bounded by 1. Thus the error from shifting the first term is

$$\left| \sum_{j=0}^{n} (a_{h_{1};\nu_{1}+j} - a_{h_{1};j}) a_{h_{2};\nu_{2}+j} \cdots a_{h_{p};\nu_{p}+j} \right| \leq \sum_{j=0}^{n} |a_{h_{1};\nu_{1}+j} - a_{h_{1};j}|$$

$$\leq |\nu_{1}| \sum_{j=0}^{n} |a_{h_{1};j+1} - a_{h_{1};j}|$$

$$= o(n)$$

by the triangle inequality. Shifting the indices in the remaining terms similarly will result in at most an $o(n)$ error.

With this lemma we can proceed to the proof of Theorem 3.1.

**Proof of Theorem 3.1** As in [9], we write $A_n$ as the sum of diagonals:

$$A_n = \sum_{|k| \leq k_0} D_k,$$  \hspace{1cm} (3.3)

where $D_k$ denotes the $k$th diagonal matrix of $A_n$, i.e.

$$D_k = \begin{bmatrix}
    a_{k;0} & \cdots & \cdots & a_{k;n-k} \\
    a_{k;1} & & & \\
    \vdots & & & \\
    a_{k;n-k} & & & \\
\end{bmatrix}$$

Thus, $A_n^r(A_n^s)^*$ is the sum

$$\sum \prod_{j=1}^{r} D_{h_j} \prod_{l=1}^{s} D_{-k_l},$$

where the sum is taken over all possible combinations. The main diagonal entries of each product in the last sum will be nonzero only if

$$|h| - |k| = \sum h_j - \sum k_j = 0.$$

Using the Kac, Murdock and Szegő [11] approach, we can calculate the entries on the main diagonal of the product $\prod_{j=1}^{r} D_{h_j} \prod_{l=1}^{s} D_{-k_l}$. For $|h| = |k|$, the $i$th term on the diagonal of the product is

$$\left( \prod_{j=1}^{r} D_{h_j} \prod_{l=1}^{s} D_{-k_l} \right)_{0;0} = \prod_{j=1}^{r} a_{h_j;\nu_{j}+i} \prod_{l=1}^{s} a_{-k_l;\nu_{p+l}+i} \hspace{1cm} (3.4)$$
where
\[ \nu_j = \begin{cases} h_1 + \cdots + h_{j-1} + h_j^- & \text{if } 1 \leq j \leq p \\ h_p - k_1 - \cdots - k_j^- & \text{if } p < j \leq q. \end{cases} \]
and \( h_j^- = \min\{h_j, 0\} \). Therefore, we obtain
\[
\text{Tr} [A_n^r(A_n^s)^*] = \sum_{j=0}^{n} \sum_{|h| = |k|} \prod_{l=1}^{r} a_{h_i;j} \prod_{m=1}^{s} z_{k_m} + o(n) \tag{3.5}
\]
Since \( \{A_n\} \) is banded, the sum \( \sum_{|h| = |k|} \) above is finite. Thus we can use Lemma 3.2 to shift the indices modulo an \( o(n) \) term:
\[
\text{Tr} [A_n^r(A_n^s)^*] = \sum_{j=0}^{n} \sum_{|h| = |k|} \prod_{l=1}^{r} a_{h_i;j} \prod_{m=1}^{s} \bar{z}_{k_m} + o(n). \tag{3.6}
\]
Finally, it follows from the \( \mu \)-distribution of \( \{A_n\} \) that
\[
\frac{1}{n} \text{Tr} [A_n^r(A_n^s)^*] = \int_X \sum_{|h| = |k|} \prod_{l=1}^{r} z_{h_i} \prod_{m=1}^{s} \bar{z}_{k_m} \ d\mu(z) + o(1)
\]
\[
= \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_X \prod_{m=1}^{s} \bar{z}_{k_m} \ d\mu(z) e^{i(|k| - |h|)} \ d\mu(z) \ dt + o(1)
\]
\[
= \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_X P^r(z, t) \bar{P}^s(z, t) \ d\mu(z) \ dt + o(1)
\]
as desired.

For sequences of normal band matrices, one can use the Stone-Weierstrass Theorem and the functional calculus for normal operators together with our previous trace formula to obtain their LSD. More precisely, we have the following result.

**Corollary 3.3.** Let \( \{A_n\} \) be a sequence of normal matrices of fixed band size \( k_0 \). If \( \{A_n\} \in \mathcal{VMV} \) is \( \mu \)-distributed on some compact \( X \subset \mathbb{C}^{2k_0+1} \), then we have
\[
\lim_{n \to \infty} \frac{1}{n} \text{Tr}[\varphi(A_n)] = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_X \varphi(P(z, t)) \ d\mu(z) \ dt. \tag{3.7}
\]
for any \( \varphi \in C_c(\mathbb{C}) \), the space of compactly supported continuous functions on \( \mathbb{C} \).

### 3.2 Sequences of non-band size matrices

We now extend our previous results to sequences of matrices of arbitrary band size. We start with a basic lemma that gives a general condition for when two sequences have the same LSD.
Lemma 3.4. Let \( \{A_n\} \) and \( \{B_n\} \) be two sequences of matrices that satisfy \( \|A_n\|_\infty = O(1) = \|B_n\|_\infty \). If \( \|A_n - B_n\|_{tr} = o(n) \), then we have
\[
\left| \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) - \sum_{k=1}^{n} \varphi(\lambda_k(B_n)) \right| = o(n)
\]
for any analytic function \( \varphi \) on \( D_M \), i.e. \( \varphi \in C^\omega(D_M) \). If the sequences are Hermitian, then we can choose \( \varphi \in C(D_M) \).

Proof. By linearity of the trace and Mergelyan’s Theorem, it suffices to consider \( \varphi(z) = z^m \) for \( m \in \mathbb{N} \). Writing \( A_n^m = ((A_n - B_n) + B_n)^m \) and using the elementary properties of the trace, we have
\[
\text{Tr}[A_n^m] - \text{Tr}[B_n^m] = \text{Tr}[(A_n - B_n) C_n]
\]
for some matrix \( C_n \) that is a finite sum of products of \( A_n - B_n \) and \( B_n \). By the sub-multiplicative property of the spectral norm, we easily deduce that \( \|C_n\|_\infty = O(1) \). Finally, we apply Von Neumann’s trace inequality (see [8], Theorem 7.4.10, p. 433) to obtain
\[
|\text{Tr}[(A_n - B_n) C_n]| \leq \sum_{k=1}^{n} \sigma_k(A_n - B_n) \sigma_k(C_n) = O(\|A_n - B_n\|_{tr}) = o(n)
\]
as desired. \( \square \)

The basic idea underlying the proof of the results below is to approximate the LSD of the original matrix sequence by the LSD of another sequence of band-matrices with fixed band size. Consequently, we make the assumption similar to that of Kac, Murdock and Szegö [1, 3] that \( \{A_n\} \) satisfies the condition
\[
\mathcal{M} := \sup_n \left[ \sum_{|k| \leq n} \max_{0 \leq j \leq n-k} |a_{k,j}(n)| \right] < \infty. \tag{3.8}
\]

From Gershgorin’s Circle Theorem [8], the spectrum of \( A_n \) lies inside the closed disk \( D_M = \{z : |z| \leq \mathcal{M}\} \). Moreover, by Qi’s extension of Gergorin’s Theorem [13], the singular values of \( A_n \) are also contained \([0, \mathcal{M}]\).

Theorem 3.5. Let \( \{A_n\} \in \mathcal{V} \mathcal{M} \mathcal{V} \) be a \( \mu \)-distributed on some compact \( X \subset l^1 \). Then, we have
\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_X \varphi(F(z, t)) \, d\mu(z) \, dt
\]
for any \( \varphi \in C^\omega(D_M) \). In addition, if the \( A_n \)'s are assumed to be Hermitian, then we can take \( \varphi \in C([-\mathcal{M}, \mathcal{M}]) \).
Proof. For any $\varepsilon > 0$, condition (3.8) implies there exists $k_0 \in \mathbb{N}$ such that

$$\sum_{|k| > k_0} \max_{1 \leq j \leq n-k} |a_{k,j}| < \varepsilon. \quad (3.9)$$

Let $\{B_n\}$ be the sequence of band-matrices of size $k_0$ obtained from $A_n$, i.e. $B_n = [b_{k;j}]$ with

$$b_{k;j} = \begin{cases} a_{k;j} & \text{if } |k| \leq k_0 \\ 0 & \text{otherwise} \end{cases}$$

In particular, by Qi’s result we deduce $\|A_n - B_n\|_\text{tr} = \mathcal{O}(n\varepsilon)$. Thus, by Lemma [3.4] it suffices to prove the result for $\{B_n\}$. But this follows from our trace formula in Theorem 3.1. Indeed, if $\pi_{k_0} : l^1 \to C^{2k_0+1}$ denotes the standard projection defined by

$$\pi_{k_0}(z) = (z_{-k_0}, \ldots, z_{k_0})$$

then the sequence $\{B_n\}$ is $(\pi_{k_0})_\ast(\mu)$-distributed on the compact set $\pi_{k_0}(X) \subset C^{2k_0+1}$. Hence, we have

$$\frac{1}{n} \text{Tr}[B_n^m] = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_X F^m(\pi_{k_0}(z), t) d\mu(z) dt + o(1). \quad (3.10)$$

Moreover, by the compactness of $X$, we can choose $k_0$ large enough so that

$$|F(z, t) - F(\pi_{k_0}(z), t)| < \varepsilon$$

uniformly in $z$ and $t$. Consequently, it follows

$$\frac{1}{n} \text{Tr}[A_n^m] = \frac{1}{n} \text{Tr}[B_n^m] + \mathcal{O}(\varepsilon)$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_X F^m(z, t) d\mu(z) dt + \mathcal{O}(\varepsilon) + o(1).$$

The conclusion is then an immediate consequence of the linearity of the trace and Mergelyan’s Theorem. \qed

As a first consequence of the above result, we extend the class of Kac-Murdock-Szegő sequences of matrices to sequences whose diagonals are modeled by Riemann integrable functions.

**Theorem 3.6.** Let $\{A_n\}$ be a sequence of matrices such that there exists a sequence of partitions $\{P_n\}$ of $[0, 1]$ with $P_n = \{t_{j;n}\}_{j=0}^n$ and $\text{mesh}(P_n) = o(1)$ such that

$$a_{k;j}(n) = \hat{a}_k(t_{j;n}),$$

where $\hat{a}_k$ are Riemann integrable functions on $[0, 1]$ satisfying

$$\mathcal{N} := \sum_{k=0}^{\infty} \|\hat{a}_k\|_\infty < \infty. \quad (3.11)$$
For any \( \varphi \in \mathcal{C}^\omega(D_N) \), we have

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{0}^{1} \varphi(a(s, t)) \, ds \, dt \quad (3.12)
\]

where \( a(s, t) = \sum_{k \in \mathbb{Z}} \hat{a}_k(s) e^{ikt} \). If the \( A_n \) are Hermitian, then one can take \( \varphi \in \mathcal{C}([-N, N]) \).

Proof. From the integrability of \( \hat{a}_k \), we have \( \{A_n\} \in \mathcal{VMV} \). Let \( \alpha : [0, 1] \to l^1 \) be the map given by (2.10). Under condition (3.11), it is not hard to verify that the closure of the set \( \alpha([0, 1]) \) is compact in \( l^1 \). By example (iii) of Section 2.2, the sequence

\[
\hat{a}_j(n) = \{..., 0, \hat{a}_{-j}(t_{j;n}), \hat{a}_{-j+1}(t_{j;n}), \ldots, \hat{a}_{n-j}(t_{j;n}), 0, ...\} \quad (3.13)
\]

is asymptotically equidistributed for the push-forward measure \( m_\alpha \). Consequently, Theorem 3.5 implies that

\[
\lim_{n \to \infty} \frac{1}{n} \text{Tr}[A_n^m] = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{0}^{1} F^m(z, t) \, dm_\alpha(z) \, dt = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{0}^{1} a^m(s, t) \, ds \, dt
\]

as desired. \( \square \)

The results of the above theorem also hold if the entries of \( A_n \) are asymptotically modeled by Riemann integrable functions.

**Corollary 3.7.** Let \( \{A_n\} \) be a sequence of matrices that satisfies (3.8) and let \( \{\hat{A}_n\} \) be a sequence as in Theorem 3.6. If we assume

\[
|a_{k,j} - \hat{a}_k(t_{j;n})| = o(1), \quad (3.14)
\]

then we have

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{0}^{1} \varphi(a(s, t)) \, ds \, dt \quad (3.15)
\]

for any \( \varphi \in \mathcal{C}^\omega(D_{M'}) \) with \( M' = \max\{M, N\} \). In the Hermitian case, \( \mathcal{C}^\omega(D_{M'}) \) is replaced by \( \mathcal{C}([-M', M']) \).

**Proof.** Arguing as in the proof of Theorem 3.5, we can use Lemma 3.4 together with conditions (3.8) and (3.11) to reduce the problem to the case when \( \{A_n\} \) and \( \{\hat{A}_n\} \) are sequences of band matrices of fixed band size \( k_0 \). Under the
assumption \[3.14\] and Qi’s Theorem, one has \(\|A_n - \hat{A}_n\|_{tr} = o(n)\), so another application of Lemma \[3.3\] yields
\[
\frac{1}{n} \text{Tr}[\varphi(A_n)] = \frac{1}{n} \text{Tr}[\varphi(\hat{A}_n)] + o(1) \quad (3.16)
\]
Moreover, by Corollary \[3.6\] we also have
\[
\frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(\hat{A}_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \varphi(a(s,t)) \, ds \, dt + o(1). \quad (3.17)
\]
The conclusion is then an immediate consequence of last two estimates. □

We conclude this section with two applications of the above results. First, we use Theorem \[3.5\] to give a new proof of Szegő’s First Limit Theorem. We state Szegő’s Theorem in its most general form, i.e. for real-valued symbols \(a \in L^1(\mathbb{T})\) as considered by Tyrtyshnikov and Zamarashkin \[18\].

**Corollary 3.8.** (First Szegő’s Limit Theorem) Let \(T(a)\) be a Toeplitz matrix with real valued symbol \(a \in L^1(\mathbb{T})\). Then, we have
\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \varphi(a(t)) \, dt \quad (3.18)
\]
for any \(\varphi \in C_c(\mathbb{R})\), the space of compactly supported functions on \(\mathbb{R}\).

**Proof.** First, note that \(T_n(a)\) is Hermitian since \(a\) is real valued. For \(a > 0\), so \(T_n(a)\) is positive semi-definite, we have
\[
\|T_n(a)\|_{tr} = \sum_{k=1}^{n} \lambda_k(T_n(a)) = na_0 = \frac{n}{2\pi} \int_{-\pi}^{\pi} a(t) \, dt = \frac{n}{2\pi} \|a\|_1.
\]
By writing \(a = a^+ - a^-\) with \(a^+(t) = \max\{a(t), 0\}\) and \(a^-(t) = -\min\{a(t), 0\}\), it follows that \(\|T_n(a)\|_{tr} \leq \pi^{-1} n \|a\|_1\) for any \(a \in L^1(\mathbb{T})\). By the density of \(C^1(\mathbb{R})\) in \(C_c(\mathbb{R})\) for the sup norm, we only need to consider \(\varphi \in C^1_c(\mathbb{R})\). By the Mean-Value Theorem and the p-Wielandt-Hoffman inequality \[8\] with \(p = 1\), we have
\[
\sum_{k=1}^{n} |\varphi(\lambda_k(T_n(a))) - \varphi(\lambda_k(T_n(b)))| \leq \|\varphi\|_\infty \|T_n(a) - T_n(b)\|_{tr}
\]
\[= \|\varphi\|_\infty \|T_n(a - b)\|_{tr}\]
\[
\leq \frac{n}{\pi} \|\varphi'\|_\infty \|a - b\|_1
\]
for \(a, b \in L^1(\mathbb{T})\). Hence, it suffices to consider \(a\) in a dense subset of \(L^1(\mathbb{T})\), e.g. \(\mathcal{A}(\mathbb{T})\).

For such \(a\), it is readily seen that condition \[3.8\] holds with \(\mathcal{M} = \|a\|_1\). Moreover, the sequence \(\{T_n(a)\}\) is \(\mu\)-distributed in \(X = \{a\}\) with \(\mu = \delta_a\), and \(\mathbf{a} = \{a_k\}\) the sequence made by the Fourier coefficients of \(a\). The conclusion is then an immediate consequence of Theorem \[3.5\] The last part is a consequence that \(T_n(a)\) is Hermitian if \(a\) is real-valued. □
As a second application, we present a natural extension of the well-known $M(a,b)$-class of Jacobi matrices introduced by Nevai \[12\]. Recall, a Jacobi matrix $J(a,b) \in M(a,b)$ if it has convergent diagonals, i.e.

$$\lim_{k \to \infty} a_k = a \quad \text{and} \quad \lim_{k \to \infty} b_k = b > 0.$$ 

The LSD of such matrices is well-known to be the arcsine distribution over the interval $[a-2b,a+2b]$. In the next result, we extend Nevai’s class to sequences of matrices $\{A_n\}$ whose diagonals are given by density one convergent sequences.

**Corollary 3.9.** Let $\{A_n\}$ satisfy, for each $\epsilon > 0$,

$$\# \{ j : \|a_j(n) - a\|_\infty > \epsilon \} = o(n)$$

for some $a = \{a_k\}_{k \in \mathbb{Z}} \in l^1$, and $a_j(n)$ given by (2.14). For any $\varphi \in C^\infty(D_N)$, we have

$$\lim_{n \to \infty} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \varphi(a(t)) \, dt \quad \text{for any } \varphi \in C([-N,N]).$$

with $a(t) = \sum_{k \in \mathbb{Z}} a_k e^{ikt}$. If the $A_n$’s are Hermitian, then the statement holds for any $\varphi \in C([-N,N])$.

**Proof.** This is a simple application of Theorem 3.5. Indeed, $\{A_n\} \in \mathcal{VMV}$ since the diagonals are given by density one convergent sequences and $\{A_n\}$ is $\delta_a$-distributed. \qed

### 3.3 Illustrative examples

Here we elaborate two examples of how our results apply to matrix sequences that are not of the Kac-Murdock-Szegő type or other generalizations that have been previously considered. We only consider sequences of finite finite band size as our results can easily be extended to arbitrary sequences of matrices if one imposes conditions (3.8) or (3.11).

Let $\{r_n\}$ be a sequence of positive numbers such that $r_n = o(n)$ and $r_n \to \infty$. Also, let $\{c_n\}$ be a sequence that is $\nu$-distributed for some probability measure $\nu$ on $[0,1]$, i.e.

$$\frac{1}{n} \sum_{k=1}^{n} \delta_{c_k} \to \nu.$$ 

We break up the diagonals into $\lfloor n/r_n \rfloor$ bins, where in each bin the entries tend toward constants. To be precise, let $\{a(n)\}$ be a sequence for which $a_{k \lfloor r_n \rfloor + j} \to c_k$ as $j \to \infty$ with $k = 0, \ldots, \lfloor n/r_n \rfloor$ and $j = 0, \ldots, \lfloor r_n \rfloor$. For instance, construct the sequence $\{a(n)\}$ in the following way. In the first $\lfloor r_n \rfloor$ entries of $a(n)$ place the constant $c_1$; in the next $\lfloor r_n \rfloor$ entries place $c_2$, and so on up to $a_{\lfloor r_n \rfloor}$, so that

$$a(n) = \{c_1, c_1, \ldots, c_1, c_2, c_2, \ldots, c_2, \ldots, c_{\lfloor r_n \rfloor}, c_{\lfloor r_n \rfloor}, c_{\lfloor r_n \rfloor}, \ldots, c_{\lfloor r_n \rfloor}\}$$

$\lfloor r_n \rfloor$ times $\lfloor r_n \rfloor$ times $n-\lfloor n/r_n \rfloor \lfloor r_n \rfloor$ times
Now, consider Riemann integrable functions \( \hat{\alpha}_{-k_0}, \ldots, \hat{\alpha}_{k_0} \) on \([0, 1]\) and construct the sequence of matrices \( \{A_n\} \) by putting \( \hat{\alpha}_k(a(n)) \) on its \( k \)th diagonal. Then \( \{A_n\} \in \mathcal{VMV} \) and is \( \mu \)-distributed with \( \mu \) the push-forward of \( \nu \) under the map \( \alpha(s) = (\hat{\alpha}_{-k_0}(s), \ldots, \hat{\alpha}_{k_0}(s)) \) for \( s \in [0, 1] \). Hence, we deduce

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{0}^{1} \varphi(a(s,t)) \, d\nu(s) \, dt \quad (3.20)
\]

for every \( \varphi \in C_c(D_M) \).

As a particular example, in the discrete Schrödinger case (i.e., \( \hat{\alpha}_1(s) = \hat{\alpha}_{-1}(s) = 1, \hat{\alpha}_k(s) = 0 \) for \( |k| > 1 \), and \( f(s) := \hat{\alpha}_0(s) \)), \( (3.20) \) reduces to

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{0}^{1} \varphi(f(x) + 2\cos t) \, d\nu(x) \, dt
\]

One can make a simple change of variables in order to compute the asymptotic spectral density \( \rho \) under some monotonicity assumptions. For instance, if we assume that \( f \) is increasing on \([0, 1]\) and \( f(1) - f(0) < 4 \), then we can write \( (3.20) \) as

\[
\lim_{n \to \infty} \frac{1}{n} \text{Tr}[\varphi(A_n)] = \int_{f(0)-2}^{f(1)+2} \varphi(x) \, \rho(x) \, dx
\]

for any \( \varphi \in C_c(\mathbb{R}) \) where

\[
\rho(x) = \begin{cases}
\int_{0}^{f^{-1}(x+2)} \frac{d\nu(s)}{\sqrt{4 - (x - f(s))^2}} & x \in (f(0) - 2, f(1) - 2) \\
\int_{0}^{1} \frac{d\nu(s)}{\sqrt{4 - (x - f(s))^2}} & x \in (f(1) - 2, f(0) + 2) \\
\int_{f^{-1}(x-2)}^{1} \frac{d\nu(s)}{\sqrt{4 - (x - f(s))^2}} & x \in (f(0) + 2, f(1) + 2)
\end{cases}
\]

In our second example, we model each of the \( \lfloor r_n \rfloor \) bins on the diagonals by Riemann integrable functions. Consider sequences of partitions \( \{P_n\} \) with \( P_n = \{t_{0;n}, \ldots, t_{r_n;n}\} \) of \([0, 1]\) with \( \text{mesh}(P_n) = o(1) \) and Riemann integrable functions \( \hat{\alpha}_{k;j} \) for \( |k| \leq k_0 \) and \( j \in \mathbb{N} \). We construct the sequence of matrices \( \{A_n\} \) for which the \( k \)th diagonal of \( A_n \) is given by

\[
\hat{\alpha}_{k;1}(t_{0;n}), \ldots, \hat{\alpha}_{k;1}(t_{r_n;n}), \hat{\alpha}_{k;2}(t_{0;n}), \ldots, \hat{\alpha}_{k;2}(t_{r_n;n}), \text{ etc.}
\]

The sequence \( \{A_n\} \) is obviously in \( \mathcal{VMV} \). Let \( \alpha_j \) be the maps on \([0, 1]\) defined by

\[
\alpha_j(s) = (\hat{\alpha}_{-k_0;j}(s), \ldots, \hat{\alpha}_{k_0;j}(s)) \quad (j \in \mathbb{N}).
\]
Under the assumption that the push-forward measures $n^{-1} \sum_{1 \leq i \leq n} m_{\alpha}$ converge weakly to a measure $\mu$ on some compact set $X \subset C^{2k_{0}+1}$, the sequence $\{A_n\}$ is $\mu$-distributed and hence Theorem 3.1 implies

$$\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \varphi(\lambda_k(A_n)) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \int_{X} \varphi(P(\mathbf{z}, t)) \, d\mu(\mathbf{z}) \, dt \quad (3.21)$$

for any $\varphi \in C^\omega(D_M)$.

4 Discussion

In this paper we have restricted our attention to the scalar case. Obvious extensions of results on sequences of multi-level Toeplitz matrices or block Toeplitz matrices as considered in [17, 4] will be explored in future works. Here we mention a few other directions for future research.

It would be interesting to investigate the possible connections between our results and the discretization of differential operators. For instance, Jacobi matrices have been successfully used to study the discrete Schrödinger equation (see [5]). This approach has also been used by the first author to compute the LSD of the quantum asymmetric top [1]. Tilli [17] used a similar approach in the study of Sturm-Liouville operators. We note that our results should allow one to derive results about the spectra of differential operators whose coefficients are discontinuous.

Another possible direction to extend our work would be random Toeplitz matrices. Recently, Bryc et al. [3] showed that the LSD of random Toeplitz matrices exists, but were unable to provide a closed form for it. Kargin [10] slightly improved their results by looking at different asymptotic regimes, but he was still unable to explicitly compute the LSD for every regime. We believe that our methods can be used to compute the LSD of those matrices.

All the results presented in this paper are concerned with the First Szegő’s Limit Theorem. Evidently, it would be of great interest to extend our results to the Strong Szegő’s Limit Theorem [10], which gives an explicit expression for the error term in the first theorem. In particular, the strong theorem allows one to calculate the asymptotics of the determinant (as opposed to just the $n$th roots of the determinant).

Mejlbo and Schmidt [11] derived a Strong Szegő’s Theorem for generalized Toeplitz matrices of the Kac-Murdock-Szegő type under fairly restrictive conditions. Later, Shao and Erhardt [14, 6] found a (different) expression for the error under more general conditions. Both Mejlbo and Schmidt, and Shao and Erhardt require the functions $\hat{a}_k$ modeling the diagonals to be Hölder continuous with exponent $\alpha \geq 3/2$. Our results for the trace only require Riemann integrability, so it may be possible to extend their results to a broader class of operators.
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