Asymptotics of the eigenvectors of large Toeplitz-Hessenberg matrices generated by symbols with a power singularity

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### Toeplitz matrices

Denote by $\mathbb{T}$ the unit circle in the complex plane: $\mathbb{T} = \{z \in \mathbb{C}: |z| = 1\}$. Given $a \in L^1(\mathbb{T})$ denote by $a_k$ the Fourier coefficients of $a$:

$$a_k = \frac{1}{2\pi} \int_0^{2\pi} a(e^{i\theta})e^{-ik\theta} \, d\theta.$$  

The **Toeplitz matrices** generated by $a \in L^1(\mathbb{T})$ are

$$T_n(a) = [a_{j-k}]_{j,k=1}^n.$$  

For example,

$$T_4(a) = \begin{bmatrix}
a_0 & a_{-1} & a_{-2} & a_{-3} \\
a_1 & a_0 & a_{-1} & a_{-2} \\
a_2 & a_1 & a_0 & a_{-1} \\
a_3 & a_2 & a_1 & a_0
\end{bmatrix}.$$  

The function $a$ is referred to as the **generating function** or the **generating symbol** of the matrix sequence $\{T_n(a)\}_{n=1}^\infty$. 
Hessenberg-Toeplitz matrices

Note if \( h \in \text{Hardy class } H^\infty(\mathbb{T}) \), then \( T_n(h) \) are lower-triangular:

\[
T_4(h) = \begin{bmatrix}
    h_0 & 0 & 0 & 0 \\
    h_1 & h_0 & 0 & 0 \\
    h_2 & h_1 & h_0 & 0 \\
    h_3 & h_2 & h_1 & h_0
\end{bmatrix}.
\]

Here we consider another case which is not so trivial:

\[
a(t) = \frac{h(t)}{t}
\]

where \( h \in H^\infty(\mathbb{T}) \).

In this case \( T_n(a) \) are Hessenberg matrices:

\[
T_4(h) = \begin{bmatrix}
    h_1 & h_0 & 0 & 0 \\
    h_2 & h_1 & h_0 & 0 \\
    h_3 & h_2 & h_1 & h_0 \\
    h_4 & h_3 & h_2 & h_1
\end{bmatrix}.
\]
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- Toeplitz matrices
- Challenge from statistical mechanics
- Asymptotics of the eigenvalues
- Eigenvectors and cofactors

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- Numerical experiments
Result of Dai, Geary, and Kadanoff

In 2009 a group of investigators in statistical mechanics published some numerical results about the eigenvalues and eigenvectors of a class of Toeplitz matrices:


They considered a special family of the so-called Fisher-Hartwig symbols:

\[ a(t) = \left( 2 - t - \frac{1}{t} \right)^{\alpha/2} (-t)^{\beta} \]

with

\[ 0 < \frac{\alpha}{2} < -\beta < 1. \]
Result of Dai, Geary, and Kadanoff

Using numerical experiments they found (but not proved, in the strict mathematical sense) the following asymptotic formulas for the eigenvalues and eigenvectors:

**Conjecture (Dai, Geary, and Kadanoff)**

As \( n \to \infty \),

\[
\lambda_{j,n} \approx a \left( n^{\frac{\alpha+1}{n}} \omega_n^j \right),
\]

\[
\nu_{s(j,n)} \approx \frac{1}{\left( n^{\frac{\alpha+1}{n}} \omega_n^j \right)^s}.
\]

Here

\[
\omega_n := \exp \left( -\frac{2\pi i}{n} \right).
\]
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Determinants of Hessenberg-Toeplitz matrices

M. Bogoya, A. Böttcher, S. Grudsky,
Asymptotics of individual eigenvalues of large Hessenberg Toeplitz matrices, 2010.

My colleagues considered the symbols of the form

$$a(t) = \frac{h(t)}{t} \quad \text{with} \quad h(t) = (1 - t)^\alpha f(t).$$

fulfilling the following conditions:

- $f$ is analytic and does not vanish in a neighborhood $W$ of $\mathbb{D}$.
- $\alpha > 0$, $\alpha \notin \mathbb{Z}$ (so, the function $a$ has a singularity of the power type).
- The range of $a$ denoted by $\mathcal{R}(a)$ is a Jordan curve in $\mathbb{C}$, and $a'(t) \neq 0$ for every $t \in \mathbb{T} \setminus \{1\}$.

These conditions imply that $h \in H^\infty(\mathbb{D})$, $h_0 \neq 0$, and $\text{wind}_\lambda(a) = -1$ for each $\lambda \in \mathcal{D}(a) := \text{interior region of } \mathcal{R}(a)$. 
Range of $a = \frac{(1-t)^{3/4}}{t}$ and the eigenvalues of $T_n(a)$
Range of $a = \frac{(1-t)^{3/4}}{t}$ and the eigenvalues of $T_n(a)$
Asymptotics of the determinants

Let $W_0$ be a neighborhood of 0 in $\mathbb{C}$. For each $\lambda \in \mathcal{D}(a) \cap a(W) \setminus W_0$ there exists a unique $t_\lambda$ with $|t_\lambda| > 1$ such that

$$a(t_\lambda) = \lambda.$$ 

Theorem (Bogoya, Böttcher, Grudsky)

For each $\lambda \in \mathcal{D}(a) \cap a(W) \setminus W_0$,

$$\det(T_n(a - \lambda)) = (-h_0)^{n+1} \left( \frac{1}{t_\lambda^{n+2} a'(t_\lambda)} - \frac{1}{c_\alpha \lambda^2 n^{\alpha+1}} + \mathcal{O}(n^{-\alpha-\alpha_0-1}) \right).$$

The upper bound of the residue term is uniform in $\lambda \in a(W) \setminus W_0$.

Here

$$\alpha_0 := \min\{\alpha, 1\}, \quad c_\alpha := \frac{\pi}{f(1)\Gamma(\alpha + 1)\sin(\alpha\pi)}.$$
Asymptotics of the eigenvalues

In the first approximation, \( \lambda_{j,n} \approx a(\omega_n^j) \).

To stay away from the singular point 0 consider \( \lambda_{j,n} \) with \( j \in \mathcal{J}_n \),

\[
\mathcal{J}_n := \{ j \in \{1, \ldots, n\} : a(\omega_n^j) \notin W_0 \}.
\]

Theorem (Bogoya, Böttcher, Grudsky)

For \( n \) large enough and \( j \in \mathcal{J}_n \),

\[
\lambda_{j,n} = a(\omega_n^j) + \omega_n^j a'(\omega_n^j) \left( (\alpha + 1) \frac{\log(n)}{n} + \log(D_1(\omega_n^j)) \frac{1}{n} + R_1(j, n) \right)
\]

where

\[
D_1(u) := \frac{c_\alpha a^2(u)}{u^2 a'(u)}, \quad R_1(j, n) = O \left( \frac{1}{n^{\alpha_0+1}} \right) + O \left( \frac{\log^2(n)}{n^2} \right).
\]
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General relation between eigenvectors and cofactors

Given a matrix $A \in \mathbb{C}^{n \times n}$ denote by adj$(A)$ the classical adjoint of $A$, i.e. the transposed matrix of the cofactors of $A$.

Observation (well known)

Let $\lambda$ be an eigenvalue of a matrix $A$. Then each non-zero column $\nu$ of adj$(A - \lambda I)$ is an eigenvector associated with $\lambda$:

$$A\nu = \lambda \nu.$$

Proof.

By the main property of the classical adjoint matrix,

$$(A - \lambda I) \text{adj}(A - \lambda I) = \det(A - \lambda I)I = 0.$$ 

So, for each column $\nu$ of adj$(A - \lambda I)$ we have

$$(A - \lambda I)\nu = 0.$$
Minors of the first row of a Hessenberg-Toeplitz matrix

To calculate the first column of \( \text{adj}(T_n(a)) \) consider the minors of the first row of \( T_n(a) \). For example:

\[
\text{Minor}_1^5(T_6(a)) =\begin{vmatrix}
h_1 & h_0 & 0 & 0 & 0 & 0 & 0 \\
h_2 & h_1 & h_0 & 0 & 0 & 0 & 0 \\
h_3 & h_2 & h_1 & h_0 & 0 & 0 & 0 \\
h_4 & h_3 & h_2 & h_1 & h_0 & 0 & 0 \\
h_5 & h_4 & h_3 & h_2 & h_1 & h_0 & 0 \\
h_6 & h_5 & h_4 & h_3 & h_2 & h_1 & h_0
\end{vmatrix}
\]

(deleted cells are marked by gray)

\[
=\begin{vmatrix}
h_0 & 0 & 0 & 0 & 0 & 0 & 0 \\
h_1 & h_0 & 0 & 0 & 0 & 0 & 0 \\
h_2 & h_1 & h_0 & 0 & 0 & 0 & 0 \\
h_3 & h_2 & h_1 & h_0 & 0 & 0 & 0 \\
h_4 & h_3 & h_2 & h_1 & h_0 & 0 & 0 \\
h_5 & h_4 & h_3 & h_2 & h_1 & h_0 & 0 \\
h_6 & h_5 & h_4 & h_3 & h_2 & h_1 & h_0
\end{vmatrix}
\]

= \text{Minor}_{1,2}^{5,7}(T_7(h)).
Eigenvectors via Fourier coefficients

For $T_n(a - \lambda)$ the the previous trick gives:

$$\text{Minor}_1^s(T_n(a - \lambda)) = \text{Minor}_{1,2}^{s,n+1}(T_{n+1}(h\lambda)).$$

By Jacobi’s theorem a minor of a matrix $A$ can be expressed through the complementary minor of the inverse matrix $A^{-1}$.

In our case $T_{n+1}(h\lambda)$ is a lower-triangular Toeplitz matrix, and its inverse matrix can be found easily:

$$T_{n+1}^{-1}(h\lambda) = T_{n+1}(b\lambda) \quad \text{where} \quad b\lambda(t) = \frac{1}{h\lambda(t)} = \frac{1}{h(t) - \lambda t}.$$
Eigenvectors via Fourier coefficients

Denoting the Fourier coefficients of $b_{\lambda_j,n}$ by $b^{(j,n)}_s$ we finally obtain:

$$\text{Cofactor}_1^s(T_n(a - \lambda_{j,n})) = (-1)^{n+1} b^{(j,n)}_{n-1} b^{(j,n)}_{s-1}.$$  

does not depend on $s$

Proposition

If $b^{(j,n)}_{n-1} \neq 0$, then the following vector $v_{j,n}$ is an eigenvector of $T_n(a)$ associated with $\lambda_{j,n}$:

$$v_{j,n} = \left[ b^{(j,n)}_s \right]_{s=0}^{n-1}.$$

Here $b^{(j,n)}_s$ is the Fourier coefficient of $b_{\lambda_{j,n}}$:

$$b^{(j,n)}_s = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-ki\theta}}{h(t) - \lambda_{j,n}t} \, d\theta.$$
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Asymptotic formula for the eigenvectors

Proposition

For $n$ large enough and $j \in \mathcal{J}_n$,

$$b_s(j, n) = -\frac{D_2(\omega_j^n) \omega_n^{-js}}{D_1(\omega_j^n) n^{\alpha+1}} \left(1 + R_1(j, n, s)\right) s/n \left(1 + R_2(j, n, s)\right).$$

Here $R_1 = O\left(\frac{s}{n^{\alpha_0+1}}\right) + O\left(\frac{\log(n)}{n}\right)$, $R_2 = O\left(\frac{1}{s^{\alpha_0}}\right) + O\left(\frac{\log(n)}{n}\right)$, uniformly with respect to $n$ and $j \in \mathcal{J}_n$, and the expressions

$$D_1(u) = \frac{c_\alpha a^2(u)}{u^2 a'(u)}, \quad D_2(u) = \frac{1}{u^2 a'(u)}$$

are bounded and bounded away from zero when $u = \omega_j^n$ with $j \in \mathcal{J}_n$. 
Asymptotic behavior of the norms

Note that the eigenvectors given in the form

\[ v_{j,n} = \left[ b_s^{(j,n)} \right]_{s=0}^{n-1} \]

are not normalized. Here is a result about their norms:

**Proposition**

As \( n \to \infty \) and \( j \in J_n \),

\[ \|v_{j,n}\| \sim C(a, n, j) \sqrt{\frac{n}{\log(n)}}, \]

where \( C(a, n, j) \) is bounded and bounded away from zero.

So, the norm of \( v_{j,n} \) tends to infinity, and after the normalizing the errors of our asymptotic formula are very small (except for the first coordinates).
How to compute the first coordinates

Our formula does not work for the first components of the eigenvectors. But $b_{\lambda_j,n}$ is the reciprocal function to $h_{\lambda_j,n}$:

$$b_{\lambda_j,n}(t)h_{\lambda_j,n}(t) = 1 \quad \text{where} \quad h_{\lambda_j,n}(t) = h(t) - \lambda_j,n t,$$

and its Fourier coefficients $b_s := b_{s, (j,n)}$ can be computed easily from the following triangular system of linear equations:

\[
\begin{align*}
 b_0 h_0 & = 1, \\
 b_1 h_0 + b_0 (h_1 - \lambda_j,n) & = 0, \\
 b_2 h_0 + b_1 (h_1 - \lambda_j,n) + b_0 h_2 & = 0, \\
 b_3 h_0 + b_2 (h_1 - \lambda_j,n) + b_1 h_2 + b_0 h_3 & = 0, \\
 & \vdots \\
\end{align*}
\]

The calculation of the first $m$ coefficients takes time $O(m^2)$. Therefore we choose $m = \lfloor \sqrt{n} \rfloor$ and obtain a linear complexity problem.
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Asymptotic formula for the last coordinates \((s = n - 1)\)

**Proposition**

\[
 b^{(n,j)}_{n-1} = \frac{2i \omega_n^{j/2} \sin \frac{\pi j}{n}}{c_\alpha a^2(\omega_n^j)} \cdot \frac{1}{n^{\alpha+1}} + O\left(\frac{\log(n)}{n^{\alpha+\alpha_0+1}}\right).
\]

We always suppose that \(j \in \mathcal{J}_n\) where

\[
 \mathcal{J}_n = \{j \in \{1, \ldots, n\} : a(\omega_n^j) \notin W_0\}.
\]

If \(j \in \mathcal{J}_n\), then the quotient \(j/n\) is separated both from 0 and 1.

**Corollary**

*If* \(n\) *is large enough and* \(j \in \mathcal{J}_n\), *then* \(b^{(n,j)}_{n-1} \neq 0\), *and the vector*

\[
 \left[ b_s^{(j,n)} \right]_{s=0}^{n-1}
\]

*is an eigenvector of* \(T_n(a)\) *associated with* \(\lambda_{j,n}\).
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Maximum errors of the coordinates of the eigenvectors

The following table shows the maximum error obtained with one-term and two-term asymptotic formulas. Only the components with $s > \lfloor \sqrt{n} \rfloor$ are taken into account.

In all the tests $a(t) = t^{-1}(1 - t)^{3/4}$, $j = n/4$.

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<th>$n = 256$</th>
<th>$n = 512$</th>
<th>$n = 1024$</th>
<th>$n = 2048$</th>
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</thead>
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<tr>
<td>one term</td>
<td>$1.5 \cdot 10^{-1}$</td>
<td>$1.3 \cdot 10^{-1}$</td>
<td>$1.1 \cdot 10^{-1}$</td>
<td>$8.8 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>two term</td>
<td>$1.1 \cdot 10^{-3}$</td>
<td>$5.3 \cdot 10^{-4}$</td>
<td>$2.2 \cdot 10^{-4}$</td>
<td>$9.3 \cdot 10^{-5}$</td>
</tr>
</tbody>
</table>
Testing the asymptotic formula for the last coordinates

We computed the last coordinates $b^{(j,n)}_{n-1}$ in two ways:

- using exact algorithms;
- with our asymptotic formula:

$$b^{(n,j)}_{n-1} \approx \frac{2i \omega^{j/2} \sin \frac{\pi j}{n}}{c_\alpha a^2(\omega^j_n)} \cdot \frac{1}{n^{\alpha+1}}.$$  

In all the tests $a(t) = t^{-1}(1 - t)^{3/4}$, $j = n/4$.

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</thead>
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<tr>
<td>abs(exact value)</td>
<td>$1.16 \cdot 10^{-5}$</td>
<td>$3.32 \cdot 10^{-6}$</td>
<td>$9.65 \cdot 10^{-7}$</td>
</tr>
<tr>
<td>abs(asymptpt value)</td>
<td>$1.06 \cdot 10^{-5}$</td>
<td>$3.16 \cdot 10^{-6}$</td>
<td>$9.38 \cdot 10^{-7}$</td>
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<tr>
<td>relative error</td>
<td>8.5%</td>
<td>4.9%</td>
<td>2.8%</td>
</tr>
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