# Eigenvalues of banded symmetric Toeplitz matrices are known almost in close form?

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**Abstract**

It is well-known that the eigenvalues of (real) symmetric banded Toeplitz matrices of size $n$ are approximately given by an equispaced sampling of the symbol $f(\theta)$, up to an error which grows at most as $h = (n+1)^{-1}$, where the symbol is a real-valued cosine polynomial. Under the condition that $f$ is monotone, we show that there is hierarchy of symbols so that

$$\lambda_j^{(h)} - f\left(\theta_j^{(h)}\right) = \sum_k c_k\left(\theta_j^{(h)}\right) h^k, \qquad \theta_j^{(h)} = j\pi h, j = 1, \ldots, n,$$

with $c_k(\theta)$ higher order symbols. In the general case, a more complicate expression holds but still we find a structural hierarchy of symbols. The latter asymptotic expansions constitute a starting point for computing the eigenvalues of large symmetric banded Toeplitz matrices by using classical extrapolation methods. Selected numerics are shown in 1D and a similar study is briefly discussed in the multilevel setting ($d$D, $d \geq 2$) with blocks included, so opening the door to a fast computation of the spectrum of matrices approximating partial differential operators.

*Keywords:* Toeplitz matrix, generating function and spectral symbol, GLT matrix sequence, approximation of differential operators

## 1. Introduction

Let $A_n$ be a Toeplitz matrix of order $n$

$$A_n = \begin{bmatrix} a_0 & \cdots & a_m & & & \\ \vdots & \ddots & & \ddots & & \\ & & \ddots & & \ddots & \\ a_m & & & \ddots & & \\ & \ddots & & & \ddots & a_m \\ & & \ddots & & & \vdots \\ & & & a_m & \cdots & a_0 \end{bmatrix} \tag{1}$$

where the coefficients $a_k$, $k = 0, \ldots, m$, are supposed real.

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Let $g \in L^1(-\pi,\pi)$ and let $T_n(g)$ be the Toeplitz matrix generated by $g$ i.e. $(T_n(g))_{s,t} = \gamma_{s-t}$, $s,t = 1,\ldots,n$, with $g$ indicated as generating function of $\{T_n(g)\}$ and with $\gamma_k$ being the $k$-th Fourier coefficient of $g$ that is

$$\gamma_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} g(\theta)\, \exp(-\mathbf{i}k\theta)\, d\theta, \quad \mathbf{i}^2 = -1. \tag{2}$$

If $g$ is real-valued then several spectral properties (localization, extremal behavior, collective distribution) are known (see [5, 11] and references therein) and $g$ is also the spectral symbol of $\{T_n(g)\}$ in the Weyl sense [5, 10, 15, 16]. According to the notation above, our setting is very special since by direct computation the generating function of the Toeplitz matrix in (1) is the real-valued function $f(\theta)$, defined as $a_0 + 2\sum_{k=1}^{m} a_k \cos(k\theta)$, that is $A_n = T_n(f)$.

In this special setting also quantitative estimates are avaliable. In fact, using an embedding argument in the Tau algebra (that is the set of matrices diagonalized by a sine transform [2]), we are lead to the conclusion that the $j$-th eigenvalue $\lambda_j^{(h)}$ of a matrix $A_n$ as in (1) can be approximated by the value $f\left(\theta_j^{(h)}\right)$ with an error bounded by $K_f h$, where $K_f$ is a constant depending on $f$, but independent of $h$ and $j$ (see [2, 3, 12] and references therein).

In this note, the key idea is that the error is much more regular and if fact an asymptotic expansion is numerically observed (and partly proved in [4]), so that the computation of $\lambda_{j_h}^{(h)}$ for large dimension $n$ can be obtained by the computation of few terms $\lambda_{j_H}^{(H)}$ for much smaller sizes $N$ and $\theta_{j_h}^{(h)} = \theta_{j_H}^{(H)} = \bar{\theta}$, with the use of extrapolation-type algorithms [6], variations of those used for the computation of composed trapezoidal integration of a smooth function.

The paper is organized as follows. In Section 2 we present few numerical tests, the related asymptotic expansion, and the associated algorithmic proposal, in the case of monotone symbols as those appearing in the certain approximations of differential operators in 1D and 2D. In Section 3 we discuss the general case and few open questions related to the (block) multilevel case, to the case of nonmonotone symbols, and to the rich setting of numerically approximated differential operators.

## 2. The asymptotic expansion and the algorithmic proposal in the monotone setting

In order to show the results in a clean way and in order to describe clearly the strong applicative potential, we start from the easiest case, that is a specific class of monotone trigonometric polynomials. In particular, we take

$$f_q(\theta) = (2 - 2\cos(\theta))^q, \qquad q = 1, 2, \ldots \tag{3}$$

and its 2D counterpart $f_q(\theta_1,\theta_2) = f_q(\theta_1) + f_q(\theta_2)$. We notice that $A_n^{(q)} = T_n(f_q(\theta))$ is the approximation of the operator $(-1)^q \frac{d^{2q}}{dx^{2q}} u$ over the interval $(0,1)$ by using equispaced Finite Differences (see [1]) with stepsize $h = (n+1)^{-1}$ and homogeneous boundary conditions $u^{(j)}(0) = u^{(j)}(1) = 0$, $j = 0,\ldots,q-1$ while $A_{\mathbf{n}}^{(q)} = T_{\mathbf{n}}(f_q(\theta_1,\theta_2))$, $\mathbf{n} = (n_1,n_2)$, is its 2D counterpart with $n_1$ gridpoints in the $x_1$ direction and $n_2$ gridpoints in the $x_2$ direction.

Denoted by $\{\lambda_j^{(h)}\}_{j=1}^n$ the set of all the eigenvalues of the matrix $A_n^{(q)}$, we can generate reasonable approximations $\{\tilde{\lambda}_j^{(h)}\}_{j=1}^n$ by evaluating the symbol $f(\theta)$ over $(0,\pi)$, $n$ times equidistantly, with stepsize $\pi h = \pi/(n+1)$,

$$\tilde{\lambda}_j^{(h)} = f(\theta_j^{(h)}) = f\left(\frac{\pi j}{n+1}\right) = f\left(j\pi h\right), \quad j = 1,\ldots,n. \tag{4}$$

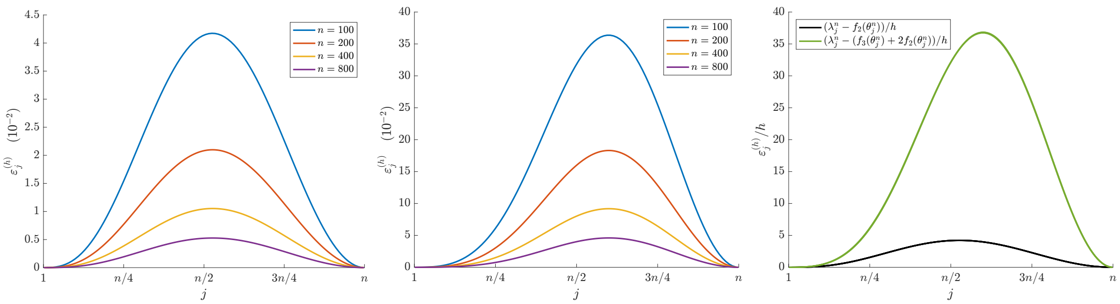


Figure 1: Errors for eigenvalue approximation of matrices with symbol $f_2(\theta)$ (left pane) and $f_3(\theta) + 2f_2(\theta)$ (middle pane) using equidistant sampling, $\theta_j^n = j\pi/(n+1)$ for $n = 100, 200, 400, 800$. Left: The error distribution for the different $n$ for $f_2(\theta)$. Middle: The error distribution for the different $n$ for $f_3(\theta) + 2f_2(\theta)$. Right: The errors for the different $n$, for both $f_2(\theta)$ (black) and $f_3(\theta)+2f_2(\theta)$ (green), scaled with $h = (n+1)^{-1}$. The scaled errors superpose forming faithful approximations of the respective $c_1(\theta)$.

We define the vector of errors as $\varepsilon^{(h)} = \{\varepsilon_j^{(h)}\}_{j=1}^n = \lambda^{(h)} - \tilde{\lambda}^{(h)}$, where the $j$-th component is

$$\varepsilon_j^{(h)} = \lambda_j^{(h)} - \tilde{\lambda}_j^{(h)}, \qquad j = 1, \ldots, n. \tag{5}$$

For $q = 1$, that is for the matrix $A_n^{(1)}$, we know that the error is exactly zero [2] and ths is true also in 2D, while again using the results in [2], we know that the error is bounded by $Kh$ for $q > 1$ with $K = K_{f_q}$, depending on $q$ but not on $h$ that is

$$\lambda_j^{(h)} = f_q(\theta_j^{(h)}) + O(h). \tag{6}$$

However, if we plot $\varepsilon^{(h)}$ for $h = h^{(1)} > h^{(2)} > h^{(3)} > \cdots$ then we discover that the errors, as expected, decrease as $h$ decreases (see left pane of Figure 1), but there is more information since the plot of the error looks like the sampling of a (scaled) smooth function and in fact the plots of

$$\frac{\varepsilon^{(h^{(r)})}}{h^{(r)}}, \qquad r = 1, 2, 3, \ldots \tag{7}$$

superpose perfectly (see black curve on right pane of Figure 1): the latter is compatible with the existence of a new function $c_1(\cdot)$ such that $\lambda_j^{(h)} = f_q(\theta_j^{(h)}) + c_1(\theta_j^{(h)})h + O(h^2)$ (see [4] for very refined results), and in fact what is displayed in the right pane of Figure 1) is a faithful approximation of the function $c_1(\cdot)$ for $f(\cdot) = f_2(\cdot)$. The same is displayed in the middle pane of Figure 1 for $A_n = A_n^{(3)} + 2A_n^{(2)} = T_n(f_3(\theta) + 2f_2(\theta))$, and its scaled error on the green curve of the right pane of Figure 1.

By continuing in this direction we have numerically seen that higher order terms appear so suggesting that, at least for monotone symbols as $f = f_q$, we have

$$\lambda_j^{(h)} = f\left(\theta_j^{(h)}\right) + \sum_k c_k\left(\theta_j^{(h)}\right) h^k, \tag{8}$$

with $j = j_h$ depending on $h$ in a way that will be clear in the following, where we explain how to use algorithmically the asymptotic expansion, by using clarifying examples.

*2.1. The algorithmic proposal*

Consider $f = f_q$ with $q > 1$ and let us assume that $\lambda_j^{(h)}$ has to be computed for a certain $j$ and for a large $n$, with high precision. The use of the quantity $f_q(\theta_j^{(h)})$ is not sufficient because the error is of order $h$. Assume $n+1 = 10^4$ and $j = 10^3$: we consider $n^{(1)}+1 = 100$ and $n^{(2)}+1 = 200$ with $j^{(1)} = 10$ and $j^{(2)} = 20$ so that

$$\theta_j^{(h)} = \theta_{j^{(1)}}^{(h^{(1)})} = \theta_{j^{(2)}}^{(h^{(2)})} = \bar{\theta} = \pi/10. \tag{9}$$

We compute $\lambda_{j^{(1)}}^{(h^{(1)})}$ and $\lambda_{j^{(1)}}^{(h^{(1)})}$ directly using a standard eigensolver: this can be done efficiently due to the moderate size of the involved matrices i.e. $n^{(r)} \leq 200$, $r = 1, 2$.

Now we make use of formula (8) in this specific case by obtaining

$$\lambda_{j^{(r)}}^{(h^{(r)})} = f_q\left(\bar{\theta}\right) + c_1\left(\bar{\theta}\right)\, h^{(r)} + c_2\left(\bar{\theta}\right)\, (h^{(r)})^2 + \cdots, \qquad r = 1, 2. \tag{10}$$

By a direct computation we find

$$\phi \equiv \frac{4\lambda_{j^{(2)}}^{(h^{(2)})} - \lambda_{j^{(1)}}^{(h^{(1)})} - 3f_q(\bar{\theta})}{2h^{(2)}} = c_1(\bar{\theta}) - 2c_3(\bar{\theta})(h^{(2)})^2 + O\left((h^{(2)})^3\right), \tag{11}$$

where all the quantities in the left-hand side are known or can be computed explicitly, with a negligible arithmetic cost. Using the quantity $\phi$ we have

$$\lambda_j^{(h)} = f_q\left(\bar{\theta}\right) + \phi h + s_h, \qquad s_h = O\left(h^2 + h(h^{(2)})^2\right) \tag{12}$$

and therefore, since $h = 10^{-4}$, $h^{(2)} = 5 \cdot 10^{-3}$, the error $s_h$ is proportional to $10^{-8}$ which is already machine precision (see Table 1). On the other hand, by using the same idea, we can approximate also the quantity $c_2(\theta)$ and indeed

$$\psi \equiv -\frac{2\lambda_{j^{(2)}}^{(h^{(2)})} - \lambda_{j^{(1)}}^{(h^{(1)})} - f_q(\bar{\theta})}{2(h^{(2)})^2} = c_2(\bar{\theta}) + 3c_3(\bar{\theta})h^{(2)} + O\left((h^{(2)})^2\right). \tag{13}$$

Therefore, if we find $\tilde{\phi}$ approximating $c_1(\bar{\theta})$ with a precision of $10^{-6}$, then, using the computable quantity $f_q\left(\bar{\theta}\right) + \tilde{\phi}h + \psi h^2$, we obtain an approximation of $\lambda_j^{(h)}$ with a precision $10^{-10}$ (see Table 1).

For the computation of $\tilde{\phi}$ we have to find a linear combination that eliminates the quadratic and the cubic term of the expansion in formula (10) and hence we need the computation of $\lambda_{j^{(3)}}^{(h^{(3)})}$ for a further $j^{(3)} = 15$ and $n^{(3)}+1 = 150$. In particular, taking into account $h^{(j)} = r_j h^{(2)}$, $r_1 = 2$, $r_2 = 1$, $r_3 = 4/3$, we find

$$\lambda_{j^{(i)}}^{(h^{(i)})} = f_q\left(\bar{\theta}\right) + r_i c_1(\bar{\theta})\, h^{(2)} + r_i^2 c_2(\bar{\theta})\, (h^{(2)})^2 + r_i^3 c_3(\bar{\theta})\, (h^{(2)})^3 + O\left((h^{(2)})^4\right), \quad i = 1, 2, 3. \tag{14}$$

If we take a real nonzero vector $(y_1, y_2, y_3)$ orthogonal to the vectors $(r_1^2, r_2^2, r_3^2)$ and $(r_1^3, r_2^3, r_3^3)$, then the linear combination of the three equations above with coefficients $y_1, y_2, y_3$ leads to the computation of $\tilde{\phi}$ approximating $c_1(\bar{\theta})$ with the desired precision. In reality

$$\tilde{\phi} = \frac{\sum_{l=1}^3 y_l \lambda_{j^{(l)}}^{(h^{(l)})} - f(\bar{\theta}) \sum_{l=1}^3 y_l}{h^{(2)} \sum_{l=1}^3 y_l r_l} = c_1\left(\bar{\theta}\right) + \left(\sum_{l=1}^3 y_l r_l^4\right)(h^{(2)})^3 + O\left((h^{(2)})^4\right). \tag{15}$$

| $f_q(\theta)$ | $\left(\lambda_j^{(h)} - f_q(\bar{\theta})\right) \cdot 10^4$ | $\left(\lambda_j^{(h)} - (f_q(\bar{\theta}) + \phi h)\right) \cdot 10^4$ | $\left(\lambda_j^{(h)} - (f_q(\bar{\theta}) + \tilde{\phi} h + \psi h^2)\right) \cdot 10^4$ |
|---|---|---|---|
| $f_1(\theta)$ | 0.000000000000000 | 0.000000000000000 | 0.000000000000000 |
| $f_2(\theta)$ | 0.155088139629153 | 0.000129376093397 | -0.000000894066106 |
| $f_3(\theta)$ | 0.045491164669903 | 0.000429174397452 | -0.000015082429122 |
| $f_4(\theta)$ | 0.008914500804868 | 0.000444641055132 | -0.000037091018868 |

Table 1: Errors for $f_q(\bar{\theta}), q = 1, 2, 3, 4$, and errors when approximating $c_1(\bar{\theta})$ by $\phi$ and $\tilde{\phi}$, and $c_2(\bar{\theta})$ by $\psi$.

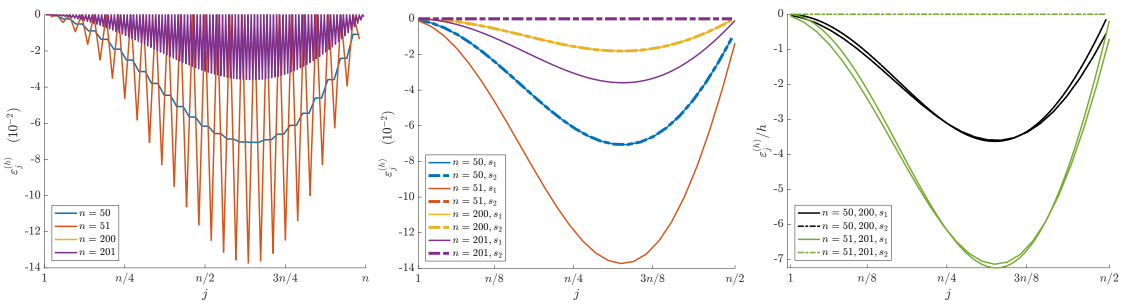


Figure 2: Left: Errors for $g_2(\theta) = 2 - 2\cos(2\theta)$, for $n = 50, 51, 200, 201$. Middle: Errors sorted into two subgrids, $s_2, s_2$, for each $n$. Right: The errors for the sorted subgrids of the different $n$, scaled with $h = (n+1)^{-1}$. The scaled errors superpose forming a faithful approximation of $c_1(\theta)$ for each subgrid $\pi(2j-1)h \in (0, \pi)$ and $\pi 2jh \in (0, \pi)$. For $g_\alpha(\theta) = 2 - 2\cos(\alpha\theta)$ with $\alpha > 2$ there is the emergence of $\alpha$ different functions $c_1(\theta)$ each on a subgrid $s_t$, $t = 1, \ldots, \alpha$, with points of the form $\pi(\alpha j - t)h \in (0, \pi)$.

## 3. Further variations, open problems, and conclusions

The numerics displayed in the previous section clearly indicate the potential of the idea and suggest several open problems and further issues to investigate.

- Since further numerical tests show that the same type of expansion holds for bivariate and multivariate functions of the form $f_q(\theta_1, \ldots, \theta_d) = \sum_{l=1}^{d} f_q(\theta_l)$ a future goal will be the formal proof of formula (8), for any dimensionality $d \geq 1$, starting from the deep analysis in [4].

- Given a positive integer $\alpha \geq 2$ and the nonmonotone function $g_\alpha(\theta) = 2 - 2\cos(\alpha\theta)$, numerical tests show that $\alpha$ different formulas like that in (8) hold on $\alpha$ disjoint subgrids of the original one (see Figure 2 for $\alpha = 2$ and the related caption): this induces the conjecture that the number of the different expansions is related to the number of sign changes of the derivative of the generating function in the basic interval $(0, \pi)$.

- The case where the generating function is $s \times s$ Hermitian matrix-valued, so that the coefficient $\gamma_j$ in (2) are blocks of fixed dimension $s \times s$, is also of interest, given its occurrence [8, 9] in the approximation of constant coefficient partial differential equations (PDEs) by Finite Elements [7].

- Finally we mention that in the case of approximated PDEs with variable coefficients, a spectral symbol can be computed thanks to the theory of Generalized Locally Toeplitz (GLT) sequences [14]: also in this context it would be interesting to investigate the occurrence of asymptotic expansions like (8) and its computational use for the fast and accurate computation of eigenvalues of the involved large matrices.

**Acknowledgements**

Funded by the Graduate School in Mathematics and Computing (FMB), and Uppsala University.

[1] O. Axelsson, *Finite Difference Methods.* Encyclopedia of Computational Mechanics. 1/2 2004.

[2] D. Bini and M. Capovani, "Spectral and computational properties of band symmetric Toeplitz matrices", *Linear Algebra Appl.*, **52/53** (1983), pp. 99–126.

[3] J. Bogoya, A. Böttcher, and E. Maximenko,"From convergence in distribution to uniform convergence", *Bol. Soc. Mat. Mex.*, **3-22** (2016), pp. 695–710.

[4] A. Böttcher, S. Grudsky, and E. Maximenko,"Inside the eigenvalues of certain Hermitian Toeplitz band matrices", *J. Comput. Appl. Math.*, **233-9** (2010), pp. 2245–2264.

[5] A. Böttcher and B. Silbermann, *Introduction to Large Truncated Toeplitz Matrices.* Springer-Verlag, New York 1999.

[6] C. Brezinski and M. Redivo Zaglia, *Extrapolation methods. Theory and practice.* Studies in Computational Mathematics, 2. North-Holland Publishing Co., Amsterdam 1991.

[7] P. Ciarlet, *The Finite Element Method for Elliptic Problems.* North Holland, Amsterdam, 1978.

[8] A. Dorostkar, M. Neytcheva, and S. Serra-Capizzano, "Spectral analysis of coupled PDEs and of their Schur complements via the notion of Generalized Locally Toeplitz sequences", *Comput. Meth. Appl. Mech. Eng.*, **309** (2016), pp. 74–105.

[9] C. Garoni, S. Serra-Capizzano, and D. Sesana, "Spectral analysis and spectral symbol of $d$-variate $\mathbf{Q}_p$ Lagrangian FEM stiffness matrices", *SIAM J. Matrix Anal. Appl.*, **36-3** (2015), pp. 1100–1128.

[10] U. Grenander and G. Szegö, *Toeplitz Forms and Their Applications.* Second Edition, Chelsea, New York, 1984.

[11] S. Serra-Capizzano, "On the extreme eigenvalues of Hermitian (block) Toeplitz matrices", *Linear Algebra Appl.*, **270** (1998), pp. 109–129.

[12] S. Serra-Capizzano, "On the extreme spectral properties of Toeplitz matrices generated by L1 functions with several minima/maxima", *BIT*, **36-1** (1996), pp.135–142.

[13] S. Serra-Capizzano, "Asymptotic results on the spectra of block Toeplitz preconditioned matrices", *SIAM J. Matrix Anal. Appl.,* **20-1** (1998), pp. 31–44.

[14] S. Serra-Capizzano, "GLT sequences as a Generalized Fourier Analysis and applications", *Linear Algebra Appl.,* **419-1** (2006), pp. 180–233.

[15] P. Tilli, "A note on the spectral distribution of Toeplitz matrices", *Linear Multil. Algebra,* **45-2/3** (1998), pp.147–159.

[16] E. Tyrtyshnikov, "A unifying approach to some old and new theorems on distribution and clustering", *Linear Algebra Appl.*, **232** (1996), pp. 1–43.