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TWO-LEVEL TOEPLITZ PRECONDITIONING: APPROXIMATION RESULTS FOR MATRICES AND FUNCTIONS*

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Abstract. Large 2-level Toeplitz systems arise in a variety of applications (see, e.g., [R. H. Chan and M. Ng, *SIAM Rev.*, 38 (1996), pp. 427–482]) for which efficient numerical methods for their solution are required. Some successful numerical techniques need the explicit knowledge of the generating function f of the considered system $T_n(f)\mathrm{x} = b$, an assumption that usually is not fulfilled in real applications. In this paper we analyze and complete the procedure proposed in [D. Noutsas, S. Serra Capizzano, and P. Vassalos, *Numer. Linear Algebra Appl.*, 12 (2005), pp. 231–239] for the 2-level case. In such a way, from the knowledge of the coefficients of $T_n(f)$, we determine optimal preconditioning strategies for the solution of our systems. Finally, some numerical experiments are performed and discussed in connection with our theoretical analysis.

Key words. 2-level Toeplitz matrix, conjugate gradient, preconditioning, preconditioned conjugate gradient

AMS subject classifications. 65F10, 47B25, 64T10, 15A18

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1. Introduction.

In this paper we consider the preconditioning of 2-level Toeplitz systems of the form $T_n(f)\mathrm{x} = b$, where $n = (n_1, n_2)$ have large components, the symbol f is assumed to be defined on $\mathbf{R}$, real-valued, 2π-periodic, and continuous, $(T_n(f))_{(j,k)(p,q)} = t_{k-j,q-p}$ with $t_{r,s}$ being the Fourier coefficients of f, i.e.,

$$t_{r,s} = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} f(x,y)\exp(-\mathbf{i}(rx+sy))dxdy, \quad \mathbf{i}^2 = -1.$$

Here the 2-index notation $(T_n(f))_{(j,k)(p,q)}$, $n = (n_1, n_2)$, indicates that we are selecting the block (j,k) of size n_2 with $j,k \in \{1,\ldots,n_1\}$ and, in that block, we are selecting the entry (p,q), $p,q \in \{1,\ldots,n_2\}$.

Such matrices (often also called block Toeplitz with Toeplitz blocks) arise in several applications (see, e.g., [6, 11, 13]), such as Markov chains, integral equations, in the solution of certain partial differential equations (PDEs), and image restoration. In some contexts the generating function f is explicitly given or can be easily obtained, but in many others, like image processing, Markov chains, and tomography, the analytic expression of the symbol is not available and, as a consequence, we do not know crucial properties such as the presence of zeros, their localization, or their multiplicities. We recall that the considered information is essential to understand the spectral properties (extreme eigenvalues, ill-conditioning, ill-posedness) of the matrices and therefore to select the most suitable preconditioning methods (see [19, 12]). The 1-level case has been treated in [23] using band Toeplitz preconditioners and in

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[18] using circulant-like preconditioners constructed by positive reproducing kernels. These circulant preconditioners, as well as those belonging to more general matrix algebras, possess a natural extension in the 2-level setting. However, a quite general theory shows that it is impossible to find any of these 2-level extensions preserving either the superlinear or the optimal behavior: see [31, 25, 32] for negative results regarding the notion of superlinearity and [14, 15] for negative results regarding the notion of optimality.

We recall that the spectral properties of the Toeplitz matrices are described very precisely by the symbol (see, e.g., [3, 16]). For instance, if zero belongs to the range of f, then the sequence $\{T_n(f)\}_n$ is asymptotically ill-conditioned (for $n \to \infty$, $n = (n_1, n_2)$, i.e., for $n_1, n_2 \to \infty$): more precisely, the problem will be ill-posed in a discrete sense if f has a nondefinite sign while we have invertibility but asymptotical ill-conditioning if f is nonnegative (or equivalently nonpositive). In the latter we need preconditioning and an optimal technique consists in using $T_n(g)$ as a preconditioner where g is a nonnegative trigonometric polynomial which has the same zeros as f with the same orders. Any system related to $T_n(g)$ is banded and can be solved, under suitable assumptions, by multigrid methods [9] or cyclic reduction techniques [4, 5] in linear time; moreover, the preconditioning sequence is optimal so that only a fixed number of preconditioned conjugate gradient (PCG) iterations (independent of n_1 and of n_2) has to be performed in order to reach the solution within a preassigned accuracy. In conclusion, we need algorithms for determining analytical information on the zeros of f. In [17], by extending the proposal in [23], the 2-level case is considered for generating functions only known through the matrix coefficients (i.e., the Fourier coefficients of f): the main idea is to approximate f over the grid

$$\mathcal{S}_n = \left\{ \left(-\pi + \frac{2k\pi}{n_1} \ , \ -\pi + \frac{2j\pi}{n_2} \right), k = 1, 2, \dots, n_1 \ , \ j = 1, 2, \dots, n_2 \right\} \tag{1.1}$$

on the square $Q = (-\pi, \pi]^2$, and then we proceed by looking for the roots of f, by estimating their multiplicities, by characterizing the problem (well-conditioned, ill-conditioned, ill-posed), by choosing the appropriate method, and finally by constructing the chosen preconditioner. Since the zeros cannot be computed exactly in general, we also need to check the robustness of the preconditioning technique with regard to numerical/approximation errors in the computation of the position of the zeros. The contribution of this paper relies in giving a theoretical support to the heuristic proposal given in [17], by using and extending new tools developed in [29], and in giving a numerical procedure for approximating the polynomial factors of the symbol in the case of curves of zeros.

The paper is organized as follows. In section 2 we report basic results from the quoted literature, and in section 3 the proposed approach is theoretically analyzed and some numerical results are given.

2. Basic theory.

2.1. Results from the literature.

In the following when we write inf and sup we mean the essential infimum and the essential supremum, i.e., up to zero measure sets (with respect to the Lebesgue measure); when we write $f \sim g$ we mean that there exist positive real constants r and R such that $rg(x, y) \leq f(x, y) \leq Rg(x, y)$ for almost every (x, y) in the definition set of f and g. Moreover, when we write $a_n \sim b_n$ and $\{a_n\}$ and $\{b_n\}$ are sequences, we understand that there exist positive real constants r and R such that $rb_n \leq a_n \leq Rb_n$ for every n. (Notice that in both the instances, the case $R = +\infty$ is excluded.) A nonnegative function f has a zero at (x_0, y_0) if for every neighborhood I of (x_0, y_0) we have $\inf_{(x,y)\in I} f(x, y) = 0$. A set $\mathcal{S}$ of zeros of $f \geq 0$ is isolated if there exists a neighborhood J of $\mathcal{S}$ such that for every neighborhood $I \subset J, I \neq J$ of $\mathcal{S}$ we have $\inf_{(x,y)\in J\setminus I} f(x, y) > 0$. Furthermore, we write that a nonnegative function f has a zero of order at least $\alpha \geq 0$ at (x_0, y_0) if and only if there exist a positive constant c such that $f(x, y) \leq c\|(x, y) - (x_0, y_0)\|^\alpha$ in a suitable neighborhood of (x_0, y_0) and for some norm $\|\cdot\|$. We write that its order is $+\infty$ if it is of order at least α for every $\alpha > 0$ or in other words if

$$\lim_{(x,y)\to(x_0,y_0)} \frac{f(x, y)}{\|(x, y) - (x_0, y_0)\|^\alpha} = 0 \quad \forall\alpha > 0.$$

For our purpose, we will consider the following general definition for a zero of order $\alpha > 0$.

DEFINITION 1. *Let f be a nonnegative $L^1(Q)$ function having a zero at (x_0, y_0). We say that its order is $\alpha \in (0, \infty)$ if there exists a finite number p of curves $\mathcal{C}_i$, $i = 1, \ldots, p$, defined by $l_i(x, y) = 0$ passing through (x_0, y_0) and regular in it such that $f \sim \breve{f}$ and*

$$\breve{f}(x, y) = \sum_{i=1}^{p} |l_i(x, y)|^\alpha + g(x, y),$$

where g has a zero at (x_0, y_0) of order at least $\beta > \alpha$.

The above definition is quite general and includes many different cases, such as $f(x, y) = |x - x_0|^4 + |y - y_0|^3$ ($f = \breve{f}$, isolated zero at (x_0, y_0), $p = 1$, $\alpha = 3$, $\beta = 4$, $l_1(x, y) = y - y_0$, $g(x, y) = |x - x_0|^4$); $f(x, y) = |1 - x^2 - y^2|^2 + h(x, y)\exp(-1/(1 - x^2 - y^2))$, $h(x, y) \in L^\infty(Q)$ with positive essential range ($f = \breve{f}$, isolated curve of zeros represented by the circle centered at zero with radius 1, $p = 1$, $\alpha = 2$, $\beta = \infty$, $l_1(x, y) = 1 - x^2 - y^2$, $g(x, y) = h(x, y)\exp(-1/(1 - x^2 - y^2))$); $f(x, y) = |\sin(x^2+y^4+(x-y)^2)|+(x^2+y^2)^4$ ($\breve{f}(x, y) = x^2+y^4+(x-y)^2+(x^2+y^2)^4$, isolated zero at $(0, 0)$, $p = 2$, $\alpha = 2$, $\beta = 4$, $l_1(x, y) = x$, $l_2(x, y) = x - y$, $g(x, y) = y^4 + (x^2 + y^2)^4$).

LEMMA 1 (see [21, 16]). *Let f be a nonnegative $L^1(Q)$ function having zeros expressible as a finite collection of curves and isolated points and having maximal order $\alpha < \infty$ (according to Definition 1). Then $T_n(f)$, $n = (n_1, n_2)$, is positive definite and its minimal eigenvalue $\lambda_{\min}(T_n(f))$ is such that $\lambda_{\min}(T_n(f)) \sim \nu^{-\alpha}$ with $n_1 \sim n_2 \sim \nu$. The same conclusion is true if $f = f_n$ depends on n, as long as the notion of order of zeros (which may depend on n) is well defined and independent of n according to Definition 1.*

For a generic n-by-n matrix X with complex entries we define

$$\|X\|_p = \begin{cases} \left(\frac{\sum_{j=1}^{n} \sigma_j^p}{n}\right)^{1/p} & \text{if } p \in [1, \infty), \\ \sigma_1 & \text{if } p = \infty \end{cases}$$

with $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ denoting the singular values of X. Furthermore, indicating by $m\{\cdot\}$ the Lebesgue measure (on Q in the present case), for $f \in L^p(Q)$ and $p \in [1, \infty)$, we define $\|f\|_p = \left[\frac{1}{m\{Q\}} \int_Q |f(x)|^p\, dx\right]^{1/p}$ and $\|f\|_\infty = \sup_{x\in Q} |f(x)|$ for $f \in L^\infty(Q)$, $p = \infty$, and sup denoting the essential supremum, i.e., up to zero measure sets.

LEMMA 2 (see [30, 26]). *Let f be an $L^p(Q)$ function. Then $\|T_n(f)\|_p \leq \|f\|_p$ and $\lim_{n\to\infty} \|T_n(f)\|_p = \|f\|_p$ $\forall p \in [1, \infty]$.*

Finally, for θ Lebesgue measurable over $D \subset \mathbf{R}^k$, with k positive integer and $0 < m\{D\} < \infty$, the expression "$\{A_n\}$ is distributed as the measurable function θ" with A_n of size $N(n)$ is equivalent to writing that for any $F \in \mathcal{C}_0$ (continuous with bounded support) it holds

$$\lim_{n\to\infty} \frac{1}{N(n)} \sum_{j=1}^{N(n)} F\left(\lambda_j\left(A_n\right)\right) = \frac{1}{m\{D\}} \int_D F\left(\theta(x)\right)\, dx,$$

where $\{\lambda_j\left(A_n\right) : \ j = 1, \ldots, N(n)\}$ denotes the complete set of the eigenvalues of A_n and where n could be either a positive integer or a positive multi-index. Often the considered distribution results for the eigenvalues hold for Hermitian sequences, but there exist many noteworthy exceptions in the complex field (concerning non-Hermitian sequences): the case of Toeplitz sequences generated by complex-valued symbols whose range has nonempty interior and for which the complement of the range is a connected set in the complex field (see [33]), the case of quasi-Hermitian discretizations of finite difference differential operators (see [10]), and the case of the preconditioned sequences considered in Lemma 3. In our context we have $D = Q$, $k = 2$, and the matrices A_n are either Hermitian Toeplitz or preconditioned matrices (see Lemma 3) which can be turned into Hermitian ones by similarity transformations.

Now we recall a basic result which is the foundation of the band Toeplitz preconditioning.

Lemma 3 (see [8, 27]). *Let f and g be two essentially nonnegative functions (not identically zero) belonging to $L^1(Q)$ and such that f/g is not constant. Then*

$$\inf f/g < \lambda(T_n^{-1}(g)T_n(f)) < \sup f/g$$

and moreover $\{T_n^{-1}(g)T_n(f)\}$ is distributed as f/g.

We explain the band Toeplitz preconditioning approach with an example. Consider the function $f(x, y) = x^2 + y^2$ which has a unique zero of order two at $z_0 = (0, 0)$. The matrix $T_n(f)$ is full but can be optimally preconditioned by the simple band Toeplitz matrix

$$T_n(g) = \begin{bmatrix} B & -I & & & \\ -I & \ddots & \ddots & & \\ & \ddots & & \ddots & \\ & & \ddots & \ddots & -I \\ & & & -I & B \end{bmatrix}_{n_1 \times n_1}, \quad B = \begin{bmatrix} 4 & -1 & & & \\ -1 & \ddots & \ddots & & \\ & \ddots & & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 4 \end{bmatrix}_{n_2 \times n_2}$$

with I denoting the $n_2 \times n_2$ identity matrix and with $g(x, y) = 4 - 2\cos(x) - 2\cos(y) = 4\sin^2(x/2) + 4\sin^2(y/2)$. By Lemma 3 we deduce that the eigenvalues of the preconditioned matrix $T_n^{-1}(g)T_n(f)$ are

1. contained in the interval $(1, \pi^2/4)$, $1 = \min f/g$, $\pi^2/4 = \max f/g$, and
2. globally distributed as the function f/g.

Therefore, irrespectively of the 2-index $n = (n_1, n_2)$ and of the size $N(n) = n_1 n_2$ of the considered linear system, the number of PCG iterations for which we need to find the solution within a fixed accuracy $\epsilon > 0$ can be bounded by a universal constant independent of n (which can be estimated as a function of ϵ [1]). Moreover, for the solution of a system with matrix $T_n(g)$, we can use solvers based on fast sine transforms (see, e.g., [34]) costing $\mathcal{O}(N(n) \log N(n))$ arithmetic operations (flops), multigrid methods [9], or just classical Poisson solvers (based on the cyclic reduction idea; see, e.g., [4, 5]) with cost of $\mathcal{O}(N(n))$ flops. In conclusion the associated PCG method is optimal (in the sense of Axelsson and Neytcheva [2]) since

1. the cost of each iteration is $\mathcal{O}(N(n)\log N(n))$ flops, $N(n) = n_1 n_2$, that is of the same order as the cost of a matrix vector product, and
2. the number of iterations does not depend on n.

We observe that the main point for deriving such a result does not rely on the regularity of the function f. Actually, if $f(x,y) = x^2 + y^2$ is replaced by $f(x,y) = (x^2+y^2)h(x,y)$, where $h(x,y)$ is any function in $L^\infty(Q)$ with positive essential range, then the same $T_n(g)$ is still an optimal preconditioner.

Therefore, the crucial points are the number of the zeros or curves of zeros of f, which should be finite, and their order, which should be even (for the case where the order of the zeros is not even, to our knowledge, the best idea is the use of multigrid strategies [9, 28]).

However, in many practical situations we possess the coefficients $\{t_{r,s}\}$, in some cases we know the positive definiteness of the matrix $T_n(f)$ or even the fact that $T_n(f)$ is asymptotically ill-conditioned, but very often we do not have an explicit expression for f. In that cases we have to recover the minimal information for devising an optimal preconditioning technique, i.e., the position and the order of the zeros of f.

In [23] an economic strategy was devised for the numerical evaluation of the order and the position of the zeros in the 1-dimensional case. The technique has been heuristically extended to two dimensions in [17]: in [29] the theoretical explanation of the goodness of the procedure for the 1-dimensional case was given. Here we complete the picture by giving theoretical results in the 2-dimensional setting and giving a numerical procedure for approximating the polynomial factors of the symbol in the case of curves of zeros. In actuality, under the assumption that the zeros are even, we can determine exactly the order of the zeros but the position of these zeros is affected by an error for which we can provide a rough a priori bound.

In conclusion, we would like to study the spectral behavior of

$$T_n^{-1}(\tilde{g})T_n(f),$$

where $f \sim g$, g is a trigonometric polynomial of fixed degrees and the zeros of $\tilde{g}$ are an approximation of those of g. A simple example is given by the situation

$$\begin{aligned} g(x,y) &= \prod_{j=0}^{k}(4 - 2\cos(x-x_j) - 2\cos(y-y_j))^{\alpha_j}, \\ \tilde{g}(x,y) &= \prod_{j=0}^{k}(4 - 2\cos(x-\tilde{x}_j) - 2\cos(y-\tilde{y}_j))^{\alpha_j} \end{aligned}$$

and $(\tilde{x}_j, \tilde{y}_j)$ is an approximation of (x_j, y_j) $\forall j = 0,\dots,k$, even if the most challenging case is the one where the zeros form a curve: in this respect there is the problem of approximating such a curve by using the zeros of a trigonometric polynomial; since the symbol f is known only through the set of its Fourier coefficients, a direct fast solution (requiring only FFTs) can be obtained by considering the zeros of approximations of f such as the Fourier polynomial of degree n or its Cesaro sum of the same degree.

In the following subsection we furnish some mathematical tools with which to answer this question and in the subsequent subsection we analyze the spectral features of (approximate) preconditioned matrix sequences.

2.2. Theoretical results. We read the first part of Lemma 3 in the following way: if f and g are two essentially nonnegative functions (not identically zero) such that f/g is not constant and $f \sim g$, then

$$\kappa_p\left(T_n^{-1/2}(g)T_n(f)T_n^{-1/2}(g)\right) < C := (\sup f/g)(\inf f/g)^{-1} < \infty$$

for any $p \in [1,\infty]$ and with $\kappa_p(X) = \|X\|_p\|X^{-1}\|_p$ being the condition number of an invertible matrix X with respect to the (scaled) Schatten norm $\|\cdot\|_p$, $p \in [1,\infty]$. In the following we suppose to have a perturbed g, let us say g_n, such that g_n is not equivalent to f but it is close in norm to g. We try to see what happens to the condition numbers of the perturbed symmetrized preconditioned matrix

$$T_n^{-1/2}(g_n)T_n(f)T_n^{-1/2}(g_n).$$

THEOREM 1. *Let $f \sim g$ and let $f_n \sim g_n$ such that the constants of equivalence are independent of $n = (n_1, n_2)$ and suppose that $f, f_n, g, g_n \in L^p(Q)$, $p \in [1,\infty]$. Suppose that f has zeros expressible as a finite collection of curves and isolated points and having maximal order $\alpha < \infty$ (according to Definition 1); suppose also that f_n has zeros expressible as a finite collection of curves and isolated points and having maximal order $\beta < \infty$ (according to Definition 1). Then there exist proper constants C_1, C_2, q_1, q_2 independent of n such that*

$$\kappa_p\left(T_n^{-1/2}(g_n)T_n(f)T_n^{-1/2}(g_n)\right) \le \left[C_1 + q_1\nu^\alpha\|g_n - g\|_p\right]\left[C_2 + q_2\nu^\beta\|f_n - f\|_p\right]$$

with $n_1 \sim n_2 \sim \nu$.

Proof. From the equivalence relationships $f_n \sim g_n$ and $f \sim g$, we infer that there exists constants C_1 and C_2, independent of n, such that

$$\sup g/f \le C_1, \quad \sup f_n/g_n \le C_2. \tag{2.1}$$

Moreover, from the nonnegativity of f and g_n and from the assumption on the maximal order of their zeros, by applying Lemma 1, we deduce that $\lambda_{\min}(T_n(f)) \sim \nu^{-\alpha}$ and that $\lambda_{\min}(T_n(g_n)) \sim \nu^{-\beta}$. Therefore, there exist absolute constants q_1 and q_2 independent of n for which we have

$$\|T_n^{-1}(f)\|_\infty \le q_1\nu^\alpha, \quad \|T_n^{-1}(g_n)\|_\infty \le q_2\nu^\beta. \tag{2.2}$$

Then, by the plain definition of the condition number, we have

$$\kappa_p\left(T_n^{-1/2}(g_n)T_n(f)T_n^{-1/2}(g_n)\right) = X_nY_n,$$

where

$$X_n = \|T_n^{-1/2}(g_n)T_n(f)T_n^{-1/2}(g_n)\|_p, \quad Y_n = \|T_n^{1/2}(g_n)T_n^{-1}(f)T_n^{1/2}(g_n)\|_p.$$

Moreover, since $\sigma_j(XY) \le \|X\|_\infty\sigma_j(Y)$, by definition of $\|\cdot\|_p$ norm, it follows that

$$\|XY\|_p \le \|X\|_\infty\|Y\|_p, \tag{2.3}$$

which corresponds to the submultiplicative property if $p = \infty$. Since $f_n \sim g_n$ with equivalence constants independent of n, by Lemma 3 we deduce that the spectrum of $T_n^{-1/2}(g_n)T_n(f_n)T_n^{-1/2}(g_n)$ is uniformly bounded away from zero and infinity (refer to the constant C_2 in (2.1)). By invoking Lemma 2, we know that $\|T_n(f-f_n)\|_p \le \|f_n - f\|_p$ and by (2.2) we know that $\|T_n^{-1}(g_n)\|_\infty \le q_2\nu^\beta$. Therefore, by invoking the triangle inequality and (2.3) applied twice, we have

$$\begin{aligned} X_n &\le \|T_n^{-1/2}(g_n)T_n(f_n)T_n^{-1/2}(g_n)\|_p + \|T_n^{-1/2}(g_n)T_n(f-f_n)T_n^{-1/2}(g_n)\|_p \\ &\le C_2 + q_2\nu^\beta\|f_n - f\|_p. \end{aligned}$$

Moreover, since $T_n^{1/2}(g_n)T_n^{-1}(f)T_n^{1/2}(g_n)$ is positive definite, its spectral norm Y_n coincides with its maximal eigenvalue and since $T_n^{1/2}(g_n)T_n^{-1}(f)T_n^{1/2}(g_n)$ is similar to $T_n(g_n)T_n^{-1}(f)$ and the latter is similar to $T_n^{-1/2}(f)T_n(g_n)T_n^{-1/2}(f)$ which is positive definite, it follows that

$$\begin{aligned} Y_n &= \|T_n^{-1/2}(f)T_n(g_n)T_n^{-1/2}(f)\|_p \\ &\le \|T_n^{-1/2}(f)T_n(g)T_n^{-1/2}(f)\|_p + \|T_n^{-1/2}(f)T_n(g_n-g)T_n^{-1/2}(f)\|_p \\ &\le C_1 + q_1\nu^\alpha\|g_n - g\|_p, \end{aligned}$$

where in last inequality we have made recourse to Lemma 3 with the constant C_1 in (2.1), to Lemma 2, and to relations (2.2) and (2.3).

Finally we conclude that

$$\kappa_p\left(T_n^{-1/2}(g_n)T_n(f)T_n^{-1/2}(g_n)\right) \le [C_1 + q_1\nu^\alpha\|g_n - g\|_p]\left[C_2 + q_2\nu^\beta\|f_n - f\|_p\right]$$

and the proof is over. $\square$

2.3. The robustness of the inexact band Toeplitz preconditioning. First we show that the error that we make in the evaluation of the zeros must be infinitesimal: if this is not the case, then the associated "inexact" band Toeplitz preconditioning is no longer optimal.

For the sake of simplicity, let us take a nonnegative essentially bounded function f with a unique zero of order 2α (α positive integer) at (x_0, y_0) and suppose that $g(x,y) = (2-2\cos(x-x_0))^\alpha + (2-2\cos(y-y_0))^\alpha$ and $\tilde g(x,y) = (2-2\cos(x-\tilde x_0))^\alpha + (2-2\cos(y-\tilde y_0))^\alpha$ with $(\tilde x_0, \tilde y_0) = (x_0, y_0) + (\delta_1, \delta_2)$. Here δ_1, δ_2 are fixed quantities independent of $n = (n_1, n_2)$ with $\|(\delta_1, \delta_2)\|_\infty \ne 0$. The following facts hold:

1. $\lim_{n\to\infty} \lambda_{\min}(T_n(f)) = 0$, $\lambda_{\max}(T_n(f)) \le \|f\|_\infty < \infty$;
2. $\lim_{n\to\infty} \lambda_{\min}(T_n^{-1}(\tilde g)T_n(f)) = 0$, $\lim_{n\to\infty} \lambda_{\max}(T_n^{-1}(\tilde g)T_n(f)) = \infty$,

where the claim in 1 is a consequence of Lemma 1 and the claim in 2 follows from the second part of Lemma 3. In actuality, by Lemma 3, the sequence $\{T_n^{-1}(\tilde g)T_n(f)\}$ is distributed as $h = f/\tilde g$ where h has a zero at (x_0, y_0) which is responsible for the relation $\lim_{n\to\infty} \lambda_{\min}(T_n^{-1}(\tilde g)T_n(f)) = 0$ and has a pole at $(\tilde x_0, \tilde y_0) = (x_0, y_0) + (\delta_1, \delta_2)$ which is responsible for the relation $\lim_{n\to\infty} \lambda_{\max}(T_n^{-1}(\tilde g)T_n(f)) = \infty$. In conclusion, it is self-evident that the associated PCG algorithm cannot be optimal and therefore we have to determine the root (x_0, y_0) within an error infinitesimal as n goes to infinity.

2.3.1. Isolated zeros. We proceed as follows. In full generality, let us suppose that f has $k+1$ zeros of even order $2\alpha_0, 2\alpha_1, \ldots, 2\alpha_k$ at $(x_0, y_0), (x_1, y_1), \ldots, (x_k, y_k)$ and let us take

$$g_n(x,y) = \prod_{j=0}^{k} \left[(2-2\cos(x-x_{j,n}))^{\alpha_j} + (2-2\cos(y-y_{j,n}))^{\alpha_j}\right]$$

with $\|(x_j, y_j) - (x_{j,n}, y_{j,n})\|_\infty \le \epsilon_\nu$, $n = (n_1, n_2)$, $n_1 \sim n_2 \sim \nu$. We wish to determine ϵ_ν such that

$$\kappa_\infty \left(T_n^{-1/2}(g_n) T_n(f) T_n^{-1/2}(g_n) \right) \le K, \tag{2.4}$$

where K is a universal constant independent of $n = (n_1, n_2)$.

By reading Theorem 1 with $p = \infty$ in our specific case, we obtain that

$$\begin{aligned} \kappa_\infty \left(T_n^{-1/2}(g_n) T_n(f) T_n^{-1/2}(g_n) \right) \le & \left[C_1 + q_1 \nu^{2\alpha_{\max}} \|g_n - g\|_\infty \right] \\ & \left[C_2 + q_2 \nu^{2\alpha_{\max}} \|f_n - f\|_\infty \right] \end{aligned} \tag{2.5}$$

with $n_1 \sim n_2 \sim \nu$. In the above equation the functions g and f_n have to be chosen in order to minimize $\|g_n - g\|_\infty$ and $\|f_n - f\|_\infty$ but with the constraint that $g \sim f$ and $f_n \sim g_n$. In such a way we hope to obtain a bound like the one in (2.4). An obvious proposal is represented by

$$\begin{aligned} g(x, y) &= g_n(x + (x_{j,n} - x_j), y + (y_{j,n} - y_j)), \\ f_n(x, y) &= f(x + (x_j - x_{j,n}), y + (y_j - y_{j,n})). \end{aligned} \tag{2.6}$$

It is evident that

$$g(x, y) = \prod_{j=0}^{k} [(2 - 2\cos(x - x_j))^{\alpha_j} + (2 - 2\cos(y - y_j))^{\alpha_j}],$$

$g \sim f$, and $f_n \sim g_n$; moreover a simple manipulation shows that

$$\|g - g_n\|_\infty \le \|\nabla g\|_\infty \epsilon_\nu \quad \text{and} \quad \|f - f_n\|_\infty \le L\epsilon_\nu^\gamma$$

if f is Hölder continuous with parameter $\gamma \in (0, 1]$ and constant $L > 0$. (In the regular case, e.g., if f is continuously differentiable, then f is Lipschitz continuous and therefore $L = \|\nabla f\|_\infty$ and $\gamma = 1$.) Here when we write $\|\nabla g\|_\infty$ and $\|\nabla f\|_\infty$, we mean the 1-norm of the vector composed by the infinity norms of the two components.

However, we can obtain a better estimate by choosing

$$g(x, y) = \begin{cases} g_n(x, y) & \text{if } \mathcal{A} \text{ holds true,} \\ g_n(x + (x_{j,n} - x_j), y + (y_{j,n} - y_j)) & \text{if } \mathcal{B} \text{ holds true,} \end{cases} \tag{2.7}$$

$$f_n(x, y) = \begin{cases} f(x) & \text{if } \mathcal{A} \text{ holds true,} \\ f(x + (x_j - x_{j,n}), y + (y_j - y_{j,n})) & \text{if } \mathcal{B} \text{ holds true} \end{cases}$$

with $\delta = 2\epsilon_\nu$, condition $\mathcal{A}$ being $\|(x, y) - (x_{j,n}, y_{j,n})\|_\infty > \delta \; \forall j = 0, \ldots, k$ and condition $\mathcal{B}$ being $\exists j \in \{0, \ldots, k\}$ such that $\|(x, y) - (x_{j,n}, y_{j,n})\|_\infty \le \delta$. In this way, due to the definition of order of zero, we have $\|g_n - g\|_\infty \le z_1 \epsilon_\nu^{2\alpha_{\min}}$ and $\|f_n - f\|_\infty \le z_2 \epsilon_\nu^{2\alpha_{\min}}$ for suitable absolute constants z_1 and z_2: beside the better approximation estimate, a surprising further advantage, when compared with the proposal in (2.6), is that we do not have to require any regularity to the function f. Furthermore, to apply the crucial relation (2.5) we have to verify that $f \sim g$ and $f_n \sim g_n$. This result is contained in the following theorem.

THEOREM 2. *Let us suppose that f has $k + 1$ zeros of even order $2\alpha_0, 2\alpha_1, \ldots, 2\alpha_k$ at $(x_0, y_0), (x_1, y_1), \ldots, (x_k, y_k)$ and let us take*

$$g_n(x, y) = \prod_{j=0}^{k} [(2 - 2\cos(x - x_{j,n}))^{\alpha_j} + (2 - 2\cos(y - y_{j,n}))^{\alpha_j}]$$

with $\|(x_j, y_j) - (x_{j,n}, y_{j,n})\|_\infty \le \epsilon_\nu$, $n = (n_1, n_2)$, $n_1 \sim n_2 \sim \nu$. *Let* f_n *and* g *be defined as in* (2.7). *Then* $f \sim g$ *and* $f_n \sim g_n$.

Proof. The proof of $f \sim g$ is equivalent to writing that $\frac{f}{g}$ and $\frac{g}{f}$ are uniformly bounded. Setting

$$g^*(x,y) = \prod_{j=0}^{k} \left[(2 - 2\cos(x - x_j))^{\alpha_j} + (2 - 2\cos(y - y_j))^{\alpha_j}\right],$$

by the assumptions on f, we have $\max\{\sup \frac{f(x,y)}{g^*(x,y)}, \sup \frac{g^*(x,y)}{f(x,y)}\} = C^* < \infty$. Therefore

$$\begin{aligned}
\sup \frac{f(x,y)}{g(x,y)} &= \max\left\{ \sup_{(x,y):\ \mathcal{A}\text{ holds}} \frac{f(x,y)}{g(x,y)}, \sup_{(x,y):\ \mathcal{B}\text{ holds}} \frac{f(x,y)}{g(x,y)} \right\} \\
&= \max\left\{ \sup_{(x,y):\ \mathcal{A}\text{ holds}} \frac{f(x,y)}{g(x,y)}, \sup_{(x,y):\ \mathcal{B}\text{ holds}} \frac{f(x,y)}{g^*(x,y)} \right\} \\
&\le \max\left\{ \sup_{(x,y):\ \mathcal{A}\text{ holds}} \frac{f(x,y)}{g(x,y)},\ \sup \frac{f(x,y)}{g^*(x,y)} \right\} \\
&\le \max\left\{ \sup_{(x,y):\ \|(x,y)-(x_{j,n},y_{j,n})\|_\infty > 2\epsilon_\nu} \frac{f(x,y)}{g(x,y)},\ C^* \right\}.
\end{aligned}$$

Now, by exploiting the asymptotical behavior of f and g in a neighborhood of the roots, we obtain

$$\sup \frac{f(x,y)}{g(x,y)} \le \sup_{(x,y):\ \|(x,y)-(x_{j,n},y_{j,n})\|_\infty > 2\epsilon_\nu} \hat{C} \frac{\|(x,y) - (x_j, y_j)\|_\infty^{2\alpha_{\max}}}{\|(x,y) - (x_{j,n}, y_{j,n})\|_\infty^{2\alpha_{\max}}} + C^*$$

with $\hat{C}$ absolute constant independent of n. Hence by triangle inequality we deduce

$$\begin{aligned}
\sup \frac{f(x,y)}{g(x,y)} &\le \sup_{(x,y):\ \|(x,y)-(x_{j,n},y_{j,n})\|_\infty > 2\epsilon_\nu} \hat{C} \left[1 + \frac{\|(x_{j,n}, y_{j,n}) - (x_j, y_j)\|_\infty}{\|(x,y) - (x_{j,n}, y_{j,n})\|_\infty}\right]^{2\alpha_{\max}} + C^* \\
&\le \hat{C}(1.5)^{2\alpha_{\max}} + C^*,
\end{aligned}$$

where in the last inequality we have made recourse to the relations $\|(x_j, y_j) - (x_{j,n}, y_{j,n})\|_\infty \le \epsilon_\nu$ and $\|(x,y) - (x_{j,n}, y_{j,n})\|_\infty > 2\epsilon_\nu$.

A uniform bound (independent of n) is found along the same reasoning lines also for $\sup \frac{g(x,y)}{f(x,y)}$, $\sup \frac{f_n(x,y)}{g_n(x,y)}$ and $\sup \frac{g_n(x,y)}{f_n(x,y)}$ and therefore the theorem is proven. ☐

Finally, taking into account (2.5), the optimality is maintained i.e. (2.4) is satisfied if $\epsilon_\nu^{2\alpha_{\min}} \nu^{2\alpha_{\max}} = \mathcal{O}(1)$ which is equivalent to the relation $\epsilon_\nu = \mathcal{O}(\nu^{-\frac{\alpha_{\max}}{\alpha_{\min}}})$.

2.3.2. Curves of zeros. In the case of curves of zeros we suppose that f has $k+1$ regular curves of zeros of even order $2\alpha_0, 2\alpha_1, \ldots, 2\alpha_k$ at $(x_0(t), y_0(t)), (x_1(t), y_1(t)), \ldots, (x_k(t), y_k(t))$, $t \in [0,1]$, where $(x_j(t), y_j(t))$, $j = 0, \ldots, k$, is the solution of the implicit equation $l_j(x,y) = 0$. Let us take

$$g_n(x,y) = \prod_{j=0}^{k} (2 - 2\cos(l_{j,n}(x,y)))^{\alpha_j}$$

with $(x_{j,n}(t), y_{j,n}(t))$, $j = 0, \ldots, k$, being solution of the (approximate) implicit equation $l_{j,n}(x, y) = 0$, $\|(x_j(t), y_j(t)) - (x_{j,n}(t), y_{j,n}(t))\|_\infty \le \epsilon_\nu$, $n = (n_1, n_2)$, $n_1 \sim n_2 \sim \nu$. As in the case of isolated zeros the goal is to determine ϵ_ν such that

$$\kappa_\infty \left(T_n^{-1/2}(g_n) T_n(f) T_n^{-1/2}(g_n) \right) \le K, \tag{2.8}$$

where K is a universal constant independent of $n = (n_1, n_2)$. We consider Theorem 1 with $p = \infty$ in the latter context and then we have (2.5) with $n_1 \sim n_2 \sim \nu$ and where the functions g and f_n have to be chosen in order to minimize $\|g_n - g\|_\infty$ and $\|f_n - f\|_\infty$ but with the constraint that $g \sim f$ and $f_n \sim g_n$. In such a way, as in the case of the isolated zeros, we wish to obtain a bound as in (2.8). We consider the proposal described by

$$g(x, y) = \begin{cases} g_n(x, y) & \text{if } \mathcal{A} \text{ holds true}, \\ g_n(x + (x_{j,n} - x_j), y + (y_{j,n} - y_j)) & \text{if } \mathcal{B} \text{ holds true}, \end{cases} \tag{2.9}$$
$$f_n(x, y) = \begin{cases} f(x) & \text{if } \mathcal{A} \text{ holds true}, \\ f(x + (x_j - x_{j,n}), y + (y_j - y_{j,n})) & \text{if } \mathcal{B} \text{ holds true} \end{cases}$$

with $\delta = 2\epsilon_\nu$, condition $\mathcal{A}$ being $\|(x, y) - (x_{j,n}(t), y_{j,n}(t))\|_\infty > \delta \ \forall j = 0, \ldots, k$ and condition $\mathcal{B}$ being $\exists j \in \{0, \ldots, k\}$, $\exists \bar{t} \in [0, 1]$ such that $\|(x, y) - (x_{j,n}(\bar{t}), y_{j,n}(\bar{t}))\|_\infty \le \delta$. In this way, due to the definition of order of zero, we have $\|g_n - g\|_\infty \le z_1 \epsilon_\nu^{2\alpha_{\min}}$ and $\|f_n - f\|_\infty \le z_2 \epsilon_\nu^{2\alpha_{\min}}$ for suitable absolute constants z_1 and z_2: we stress that no regularity of the function f is explicitly required. Furthermore, to apply the crucial relation (2.5) we have to verify that $f \sim g$ and $f_n \sim g_n$. This result is contained in the following theorem.

THEOREM 3. *Let us suppose that f has $k+1$ regular curves of zeros of even order $2\alpha_0, 2\alpha_1, \ldots, 2\alpha_k$ at $(x_0(t), y_0(t)), (x_1(t), y_1(t)), \ldots, (x_k(t), y_k(t))$, $t \in [0, 1]$, where $(x_j(t), y_j(t))$, $j = 0, \ldots, k$, is the solution of the implicit equation $l_j(x, y) = 0$. Let us take*

$$g_n(x, y) = \prod_{j=0}^{k} (2 - 2\cos(l_{j,n}(x, y)))^{\alpha_j}$$

with $(x_{j,n}(t), y_{j,n}(t))$, $j = 0, \ldots, k$, being solution of the (approximate) implicit equation $l_{j,n}(x, y) = 0$, $\|(x_j(t), y_j(t)) - (x_{j,n}(t), y_{j,n}(t))\|_\infty \le \epsilon_\nu$, $n = (n_1, n_2)$, $n_1 \sim n_2 \sim \nu$. Let f_n and g be defined as in (2.9). *Then $f \sim g$ and $f_n \sim g_n$ (with essentially the same constants as in Theorem* 2).

Proof. The proof is similar to that of Theorem 2. □

In view of (2.5), the optimality of the related PCG method is maintained, i.e., (2.4) is satisfied if $\epsilon_\nu^{2\alpha_{\min}} \nu^{2\alpha_{\max}} = \mathcal{O}(1)$ which is equivalent to the relation $\epsilon_\nu = \mathcal{O}(\nu^{-\frac{\alpha_{\max}}{\alpha_{\min}}})$. We remark that a trivial combination of Theorems 2 and 3 implies that the same conclusions hold in the case of combinations of isolated zeros and (regular) curves of zeros. Finally we have to emphasize a practical (and serious) difficulty which arises when curves of zeros are present: indeed, in that case, given the approximate curves of zeros, the proposed function $g_n(x, y)$ is not necessarily a trigonometric polynomial. Therefore the corresponding matrix $T_n(g_n)$ is dense as $T_n(f)$ and a possible but tricky solution is to approximate g_n by a polynomial of fixed degree: in some cases this idea can be followed but we believe that the answer in the general case is in the negative since, when we force ϵ_ν to be small enough, the degree of the polynomial g_n cannot be controlled in general by an absolute constant independent of $n = (n_1, n_2)$, $n_1 \sim n_2 \sim \nu$.

2.4. Comments on the use of the results. In the case where the zero is unique or in the case where all the zeros have the same order, it is sufficient to choose $\epsilon_n = \nu^{-1}$: this is a very reasonable requirement from a practical point of view. When the ratio $\frac{\alpha_{\max}}{\alpha_{\min}}$ is high (case of unbalanced zeros), the required precision on the computation of the zeros becomes very high. We can meet the requirement with an effort of $\mathcal{O}(N(n)\log(N(n)))$ flops by evaluating f as the nth Fourier sum, $n = (n_1, n_2)$. However, we must emphasize that we are guaranteed to be successful only if f is regular enough: we recall that the sup norm error of the Fourier sum is, up to a $\log \nu$ factor, $n_1 \sim n_2 \sim \nu$, of the same order of the best approximation error and the latter is $o(\nu^{-K})$ if f is K times continuously differentiable. Therefore in the case of just continuous functions and in the case where we desire that the approximation of f maintain the sign of function, then we can use the Rayleigh quotient approach considered in detail in Theorem 4.

THEOREM 4. *Let f be a 2π-periodic continuously differentiable 2-variate function with bounded second derivative. We consider $\theta_x = \exp(\mathbf{i}x), \theta_y = \exp(\mathbf{i}y)$ and the associated unitary vectors*

$$\Theta_x^T = \frac{1}{\sqrt{n_1}}(1\ \theta_x\ \theta_x^2\ \cdots\ \theta_x^{n_1-1}) \quad \text{and} \quad \Theta_y^T = \frac{1}{\sqrt{n_2}}(1\ \theta_y\ \theta_y^2\ \cdots\ \theta_y^{n_2-1}).$$

Let $\Theta_{xy} = \Theta_x \otimes \Theta_y$ be the tensor product of the above vectors. Then, for $n = (n_1, n_2)$, we have

$$r_n[f](x,y) := \frac{\Theta_{xy}^H T_n(f)\Theta_{xy}}{\Theta_{xy}^H \Theta_{xy}} = f(x,y) + \mathcal{O}\left(\max\left\{\frac{1}{n_1}, \frac{1}{n_2}\right\}\right). \tag{2.10}$$

In the more general case where $f \in L^1(Q)$, if $f \geq 0$ almost everywhere, then

$$r_n[f](x,y) \geq 0 \qquad \forall\ (x,y) \in Q$$

and $r_n[f]$ is uniformly strictly positive if, in addition, the essential supremum of f is positive.

Proof. Since $\Theta_{xy}^H \Theta_{xy} = 1$ by definition of Θ_{xy}, it follows that $r_n[f](x,y) = \Theta_{xy}^H T_n(f)\Theta_{xy}$. Moreover the map $r_n[\cdot]$, as an operator from $L^1(Q)$ into the space of the trigonometric bivariate polynomials, is linear and positive: indeed the linearity is evident since $T_n(\alpha g_1 + \beta g_2) = \alpha T_n(g_1) + \beta T_n(g_2)$ by the linearity of the Fourier coefficients; moreover if f is real valued, then $T_n(f)$ is Hermitian (see, e.g., [19]) and if f is nonnegative, then $T_n(f)$ is nonnegative definite (see, e.g., [19]). As a consequence, since Θ_{xy} has unit length, we infer that $r_n[f](x,y)$ is real valued if f is and is nonnegative if f is. Finally (see again [19]), if f is nonnegative and not identically zero (essential supremum of f strictly positive), then $T_n(f)$ is positive definite and $r_n[f](x,y)$ is a strictly positive function. (In the terminology of [24] the latter property means that the operator is linear and strongly positive.)

Now we prove relation (2.10). In what follows it is important to note that (x,y) is generic but fixed and (s,t) is the pair of dummy variables internal to the operator r_n. For instance, $r_n[f(s,t)](x,y)$ is the operator r_n applied to the function f and then evaluated at the point (x,y), while $r_n[f(x,y)](x,y) = f(x,y) \cdot r_n[1](x,y) = f(x,y)$ since $f(x,y)$ is a fixed constant and r_n is linear. Having this point in mind, we proceed with the proof.

From the regularity assumptions we know that

$$f(s,t) = f(x,y) + [\nabla f]^T(x,y) \begin{pmatrix} \sin(s-x) \\ \sin(t-y) \end{pmatrix} + C(s,t,x,y),$$

where $|C(s,t,x,y)| \le K\left[\sin^2((s-x)/2)+\sin^2((t-y)/2)\right]$ with K pure constant only depending on the infinity norms of ∇f and H_f and with H_f denoting the Hessian of f. (For this kind of Taylor-style theorem in the periodic setting see [7] and references therein.) Now we perform the main step for proving the desired result which makes use (1) of the linearity and positivity of the operator, (2) of the above Taylor style representation, (3) of the simple identities (related to the Korovkin test; see subsection 4.1.1 in [22]) $r_n[1](x,y) \equiv 1$, $r_n[\sin(s)](x,y) \equiv \sin(x) + \mathcal{O}(\frac{1}{n_1})$, $r_n[\sin(t)](x,y) \equiv \sin(y) + \mathcal{O}(\frac{1}{n_2})$, $r_n[\cos(s)](x,y) \equiv \cos(x) + \mathcal{O}(\frac{1}{n_1})$, $r_n[\cos(t)](x,y) \equiv \cos(y) + \mathcal{O}(\frac{1}{n_2})$, and (4) of the boundedness of the second derivative H_f: indeed calling $E_{n,f}(x,y) = |r_n[f(s,t)](x,y) - f(x,y)|$ the approximation error, we have

$$\begin{aligned}
E_{n,f}(x,y) \quad &=_{(3)} \quad |r_n[f(s,t)](x,y) - r_n[f(x,y)](x,y)| \\
&=_{\text{linearity}} |r_n[f(s,t) - f(x,y)](x,y)| \\
&=_{(2)} \left| r_n \left[[\nabla f]^T(x,y) \begin{pmatrix} \sin(s-x) \\ \sin(t-y) \end{pmatrix} + C(s,t,x,y) \right](x,y) \right| \\
&=_{\text{linearity}} \left| \frac{\partial f}{\partial x}(x,y) r_n[\sin(s-x)](x,y) + \frac{\partial f}{\partial y}(x,y) r_n[\sin(t-y)](x,y) \right. \\
&\qquad \left. + r_n\left[C(s,t,x,y)\right](x,y) \right| \\
&\le_{\text{positivity}} \left| \frac{\partial f}{\partial x}(x,y) \right| |r_n[\sin(s-x)](x,y)| + \left| \frac{\partial f}{\partial y}(x,y) \right| |r_n[\sin(t-y)](x,y)| \\
&\qquad + r_n\left[|C(s,t,x,y)|\right](x,y) \\
&\le_{\text{regularity}} \|\nabla f\|_\infty \left[|r_n[\sin(s-x)](x,y)| + |r_n[\sin(t-y)](x,y)| \right] \\
&\qquad + K r_n\left[\sin^2((s-x)/2) + \sin^2((t-y)/2))\right](x,y).
\end{aligned}$$

Finally the claimed thesis is equivalent to proving that

$$\begin{aligned}
&|r_n[\sin(s-x)](x,y)| + |r_n[\sin(t-y)](x,y)| \\
&\quad + r_n\left[\sin^2((s-x)/2) + \sin^2((t-y)/2))\right](x,y) = \mathcal{O}\left(\max\left\{\frac{1}{n_1}, \frac{1}{n_2}\right\}\right)
\end{aligned}$$

and, taking into account the identities $\sin^2((s-x)/2) = (1-\cos(s-x))/2$, $\sin^2((t-y)/2)) = (1-\cos(t-y))/2$, the latter is proven if we prove that

$$|r_n[\sin(s-x)](x,y)| = \mathcal{O}\left(\max\left\{\frac{1}{n_1}, \frac{1}{n_2}\right\}\right), \tag{2.11}$$

$$|r_n[\sin(t-y)](x,y)| = \mathcal{O}\left(\max\left\{\frac{1}{n_1}, \frac{1}{n_2}\right\}\right), \tag{2.12}$$

$$r_n[1-\cos(s-x)](x,y) = \mathcal{O}\left(\max\left\{\frac{1}{n_1}, \frac{1}{n_2}\right\}\right), \tag{2.13}$$

$$r_n[1-\cos(t-y)](x,y) = \mathcal{O}\left(\max\left\{\frac{1}{n_1}, \frac{1}{n_2}\right\}\right). \tag{2.14}$$

By the explicit computation in the banded case (taking into account that $r_n[f]$ is the Césaro sum of f [23, 22]), it is easy to verify that relationships (2.11)–(2.14) hold.

Here, for the sake of completeness, we just give a detailed look at the last one:

$$\begin{aligned} r_n[1-\cos(t-y)](x,y) &=_{\text{trigonometric identity}} r_n[1-\cos(t)\cos(y)-\sin(t)\sin(y)](x,y) \\ &=_{\text{linearity}} \quad r_n[1](x,y)-\cos(y)r_n[\cos(t)](x,y) \\ &\qquad -\sin(y)r_n[\sin(t)](x,y) \\ &=_{(3)} \quad 1-\cos(y)\left[\cos(y)+\mathcal{O}\left(\frac{1}{n_2}\right)\right] \\ &\qquad -\sin(y)\left[\sin(y)+\mathcal{O}\left(\frac{1}{n_2}\right)\right]=\mathcal{O}\left(\frac{1}{n_2}\right). \quad \square \end{aligned}$$

Regarding the Fourier expansion $F_{n_1-1,n_2-1}(f)$ of f of degree n_1-1 and n_2-1, we observe that the latter approximation is much faster when f is very smooth (due to its Lebesgue constant of order $\log(n_1)+\log(n_2)$), but may fail to converge when f is only continuous. On the other hand, thanks to the Korovkin theory, the Rayleigh quotient approximation always converges when f is continuous and preserves the sign of f, but its order of approximation is not sensitive to the regularity of f. We point out that these two types of approximation have been the main theoretical tools for the construction of our banded preconditioners (see [17]).

3. Numerical examples and related discussions. As a preliminary step, we consider two numerical examples which give evidence of the main ideas described in Theorem 2 and Theorem 3 (whose result was essentially conjectured in Proposition 1 of [17]): a good approximation of the "exact" trigonometric polynomial $g(x,y)$ leads to a controlled number of spectral outliers laying outside the main clustering mass described by the range of $\frac{f}{g}$.

Numerical example 1. We consider the Toeplitz matrix $T_n(f)$ produced by the generating function $f(x,y)=(1+x^2+y^2)(2\cos(x)-\sin(x+2y))^2$. It is obvious that the trigonometric polynomial $g(x,y)=(2\cos(x)-\sin(x+2y))^2$ has an infinite number of roots which form a curve of roots. For the solution of the system $T_n(f)\mathrm{x}=b$ by a PCG iteration we use as preconditioner the 2-level band Toeplitz matrix $T_n(\tilde{g})$ instead of $T_n(g)$, where $\tilde{g}(x,y)=(2\cos(x-\epsilon)-\sin(x+2y+\epsilon))^2$ is an approximation of $g(x,y)$. In Table 3.1 we show the strict relation existing between the approximation error and the number of outlying eigenvalues. It is observed that, only when $n_1\epsilon=n_2\epsilon$ exceeds 1, there exist eigenvalues of the preconditioned matrix that lie outside the range of $\frac{f}{g}$.

Numerical example 2. We consider the Toeplitz matrix $T_n(f)$ generated by $f(x,y)=(3+\cos(x))(4-2\cos(x)-2\cos(y))(2-2\cos(x-\pi))^2$. It is obvious that it has a zero of order 2 at $(0,0)$ and a line of zeros at $x=\pi$ of order 4. We make a theoretical check on the use of the preconditioner $T_n(\tilde{g})$, where $\tilde{g}(x,y)=((4-2\cos(x+\epsilon)-2\cos(y+\epsilon))(2-2\cos(x-\pi-\epsilon))^2$ is an approximation of $g(x,y)$ with $g(x,y)=(4-2\cos(x)-2\cos(y))(2-2\cos(x-\pi))^2$. In Table 3.2 we report the tight relationship between the approximation error and the number of outlying

TABLE 3.1
Number of outliers for $T_n^{-1}(\tilde{g})T_n(f)$, range$\left(\frac{f}{g}\right)=[1\ ,\ 20.73921]$.

ϵ	$n_1=n_2$	out	$\epsilon n_1=\epsilon n_2$	$\lambda_{\min}$	$\lambda_{\max}$	ϵ	out	$\epsilon n_1=\epsilon n_2$	$\lambda_{\min}$	$\lambda_{\max}$
	8	0	$.4<1$	1.26	18.83		0	$.08<1$	1.21	17.9
.05	16	0	$.8<1$	1.11	20.2	.01	0	$.16<1$	1.03	19.3
	32	9	$1.6>1$	1.07	27.43		0	$.32<1$	1.02	19.91
	64	61	$3.2>1$	0.52	60.18		0	$.64<1$	1.01	20.5

Table 3.2
Number of outliers for $T_n^{-1}(\tilde{g})T_n(f)$, *range*$\left(\frac{f}{g}\right) = [2\ ,\ 4]$.

ϵ	$n_1 = n_2$	out	$\epsilon n_1^2 = \epsilon n_2^2$	$\lambda_{\min}$	$\lambda_{\max}$	ϵ	out	$\epsilon n_1^2 = \epsilon n_2^2$	$\lambda_{\min}$	$\lambda_{\max}$
	8	13	$3.2 > 1$	1.9	4.42		0	$.06 < 1$	2.28	3.96
	16	52	$12.8 > 1$	1.42	5.15		0	$.25 < 1$	2.1	3.99
.05	32	225	$51.2 > 1$	0.95	5.5	.001	8	$1.02 > 1$	2.01	4.03
	64	931	$204.8 > 1$	0.64	8.87		177	$4.09 > 1$	1.95	4.01

eigenvalues. It can be noted that, only if $n_1^2\epsilon = n_2^2\epsilon$ exceeds 1, then there exist eigenvalues of the preconditioned matrix that lie outside the range of $\frac{f}{g}$: we stress that this case falls into the one of nonbalanced zeros for which we should expect $\epsilon_\nu \sim \nu^{-2}$, $\nu = n_1 = n_2$ since $\frac{\alpha_{\max}}{\alpha_{\min}} = 2$. Therefore the suggestion from this example is that the bounds found in Theorems 2 and 3 cannot be improved in general. (Possibly, a local analysis of the Toeplitz operators could help refine the analysis in the case of special sets of symbols with nonbalanced zeros.)

In the rest of the section we follow a procedure proposed in [17] which, starting from the knowledge of the entries of $T_n(f)$, is able to determine an approximation of the generating function f (with its zeros and related orders) and consequently gives all the necessary information for determining the appropriate preconditioner. We first present and complete a sketch of this procedure and then we discuss various numerical experiments to test the effectiveness of the proposed method.

The outline of the procedure in [17] (which was based on a general scheme proposed and analyzed in [23, 29], respectively) is given in the following steps:

- Step 1: Approximate the function f from the coefficients of the matrix.
- Step 2: Search for the possible roots of f.
- Step 3: Estimate the multiplicities of each root.
- Step 4: Categorize the roots and choose the appropriate preconditioner.

We observe that these steps can be regarded as a collection of ideas that eventually have the potential to lead to a real black-box procedure for the analysis, the detection and the effective preconditioning of ill-conditioned 2-level Toeplitz systems. Here we go in this direction by describing in detail a part of Step 4 concerning the case of curves of zeros, i.e., how to construct a polynomial factor having approximately the same zeros of f (curves of zeros and isolated zeros). We stress that this subroutine (i.e., Algorithm 1 reported on the next page) is essential for the effectiveness of the whole procedure and has been ignored so far in the relevant literature. Indeed, looking at Theorem 3, we see that the approximation of the curves of the zeros is not sufficient for determining the symbol of the precondition since what we really need is the approximation $l_{j,n}(x, y)$ of every implicit function $l_j(x, y)$, $j = 0, \ldots, k$, which (implicitly) defines the right curve of zeros $(x_j(t), y_j(t))$, $t \in [0, 1]$, $j = 0, \ldots, k$.

However, as emphasized in the remarks following Theorem 3, the approximate factor $2 - 2\cos(l_{j,n}(x, y))$ and even the theoretical one $2 - 2\cos(l_j(x, y))$ in general are not trigonometric polynomials. Therefore, that nontrigonometric symbol $2 - 2\cos(l_{j,n}(x, y))$ or $2 - 2\cos(l_j(x, y))$ would correspond to a useless preconditioner owing to the denseness of preconditioner itself (which would make the method not optimal according to Axelsson and Neytcheva [2], since the cost of every iteration would be much higher than the cost of a matrix-vector product). As a consequence, in Algorithm 1, we follow a computational approach described in the following pseudocode (written in a pseudo high-level language) for the direct computation of the (approximate) polynomial factor (if any) containing all the zeros of f. To estimate the polynomial factor we use least-square approximation (LSA). Since we want to have good approximation on the selected roots, we choose the information of all the points of the set

$$\mathcal{G}_n = \left\{ (x_j^{(n_1)}, y_j^{(n_2)}) \in \mathcal{S}_n, \text{ computed roots of } f \text{ on } \mathcal{S}_n,\ j = 1, \ldots, \tilde{\theta}_n \right\},$$

$\mathcal{S}_n$ being a $n_1 \times n_2$ uniform gridding on $Q = (-\pi, \pi]^2$ (see (1.1)). It is well known from the above theory that the computed values of f on these points, by Rayleigh quotient, are $\mathcal{O}(\max\{\frac{1}{n_1}, \frac{1}{n_2}\})$ instead of 0. So, these values contain a significant error. We could correct those by putting 0 but then the LSA procedure would give us a polynomial which takes negative values. To avoid this, we give positive values for f of order $\mathcal{O}(\max\{\frac{1}{n_1}, \frac{1}{n_2}\})$ (the same values for all points are acceptable). In addition, it is not sufficient to apply LSA only on the points of $\mathcal{G}_n$. It is necessary to choose some points which give enough information for the reconstruction of the shape of f. For this we choose a coarse grid $\mathcal{S}_{\hat{n}}$, $\hat{n} = (\hat{n}_1, \hat{n}_2)$, where $\hat{n}_1 << n_1$ and $\hat{n}_2 << n_2$ ($\hat{n}_1 \approx \sqrt{n_1}$, $\hat{n}_2 \approx \sqrt{n_2}$ are enough), and create all the points of $\mathcal{S}_{\hat{n}}$ which are added to the points of $\mathcal{G}_n$ for the LSA method. Let θ_n be the number of the selected points ($\theta_n = |\mathcal{G}_n| + |\mathcal{S}_{\hat{n}}|$) and $\hat{f}$ be the θ_n−dimensional vector of the approximated values of f, as these are described before. Let also $q = (q_1, q_2)$, $q_1, q_2 \geq 0$, $q_1 + q_2 \geq 1$ be the pair of orders of the trigonometric polynomial that we have to approximate in each direction. Then, we have to solve the LSA problem $\min_{\mathbf{t}} \|\hat{f} - V_q\mathbf{t}\|_2^2$, where V_q is the rectangular Vandermonde matrix defined by

$$((V_q)_{j,k})_{j=1,\ldots,\theta_n, k=1,\ldots,(2q_1+1)(2q_2+1)}$$

with $(V_q)_{j,k} = \psi_k(x_j^{(n_1)}, y_j^{(n_2)})$ and $\psi_k(x,y) = \exp(\mathbf{i}\alpha x + \mathbf{i}\beta y)$. Here the relation between the index $k \in \{1, \ldots, (2q_1+1)(2q_2+1)\}$ and the 2-index $(\alpha, \beta) \in \{-q_1, \ldots, q_1\} \times \{-q_2, \ldots, q_2\}$ is defined through the bijection $k := k(\alpha, \beta, q) = (\alpha + q_1)(2q_2 + 1) + \beta + q_2 + 1$, $q = (q_1, q_2)$. To apply LSA it is necessary to have $\theta_n \geq (2q_1 + 1)(2q_2 + 1)$; otherwise we choose additional points on the fine grid, near the estimated roots, in order to have more information about the roots, until the above inequality is satisfied.

Algorithm 1. Approximating factor.

```
b :=false;
for q_1 = 1 : q_1^max do
    for q_2 = 1 : q_2^max do
        Minimize ||f̂ − V_q t||_2^2;
        construct the polynomial p_t(x, y) = Σ_k t_k ψ_k(x, y);
        if max_{(x,y)∈G_n} |p_t(x, y)| < ε_ν then
            b :=true;
        end if
    end for
end for
if b =true then
    write: "The approximating factor is optimal";
else
    write: "The approximating factor does not insure optimality";
end if
factor: p_t(x, y);
```

Here given $q_1^{\max} > 0$, $q_2^{\max} > 0$, the procedure will compute a mask $\mathbf{t} = \mathbf{t}(q)$ of Fourier coefficients with $q = (q_1, q_2)$, $0 \le q_1 \le q_1^{\max}$, $0 \le q_2 \le q_2^{\max}$, $q_1 + q_2 \ge 1$.

Numerical example 3. In order to test our procedure we solve

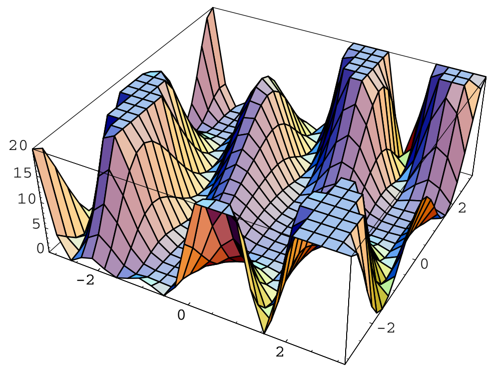
$$T_n(f)\mathrm{x} = b,$$

where the generating function is $f(x,y) = (x^2+y^2+1/4)(\cos(x+y)+\sin(2x))^2$ and has five curves of roots in the domain $Q = (-\pi,\pi]^2$ as is shown clearly in Figure 3.1(a). The knowledge of the generating function has been used only for the computation of the coefficients of $T_n(f)$. In what follows we calculate the grid $\mathcal{G}_n$ and we estimate the possible roots of f as well as their multiplicities. According to the reasoning in the previous sections, we set ϵ_ν as $.06, .03, .015, 7.5 * 10^{-3}, 3.75 * 10^{-3}$ for $\nu = n_1 = n_2 = 16, 32, 64, 128, 256$, respectively. For $\nu = 8$ we do not have enough information (points) to set up a reasonable good LSA scheme. We mention here that the cost of LSA is dominated by that of PCG since the number of columns of the overdetermined problem depends on the partial degrees q_1, q_2 of the desired trigonometric polynomial rather the dimensions n_1, n_2 of the original problem. The maximum permitted order of the approximated trigonometric polynomial is restricted by the dimension of the problem. More specifically, knowing that the cost of the solution of a band block Toeplitz system of size ν^2 $(n_1 = n_2 = \nu)$ and total bandwidth l can be done in $O(\nu^2 l^2)$ arithmetic operations, the total degree, which roughly speaking coincides with the total bandwidth, cannot exceed $\mathcal{O}(\log \nu)$. The stopping criterion of our algorithm is $p_t(x_i, y_i) < \epsilon_\nu$, where (x_i, y_i) are the estimated roots and $\epsilon_\nu = \mathcal{O}(\frac{1}{\nu})$ or the degree of the approximated polynomial is larger than $c \log \nu$ with suitable c. In practice, and for various examples, the second condition happens more often. This occurrence may lead to some eigenvalues which lay outside the range of $\frac{f}{g}$, where g is the trigonometric polynomial of minimal order which just raises the roots of f. On the other hand, by using LSA not only in the points that have been estimated as roots, we obtain a global approximation of the unknown function f and therefore we can gain a better clustering of the preconditioned system than that achieved by g. This observation is confirmed in Table 3.3, where we denote by I the unpreconditioned CG method, by $\hat{P}$ the PCG method derived from our procedure, and by P the optimal PCG method. Although the algorithm stopped because the second criterion was satisfied, the required iterations by the optimal preconditioner and the ones needed by our proposal are almost the same, and for some dimensions the global behavior is even better. We mention that the comparison with the optimal preconditioner has only theoretical meaning since, in the practical situation, we do not know the generating function and, as a consequence, the generating function of the exact preconditioner is not available. For the PCG method we used as an initial guess the null vector, as b the vector of all ones, and $\frac{\|r_k\|_2}{\|r_0\|_2} \le 10^{-5}$ as a stopping criterion, where r_k is the residual vector after k iterations.

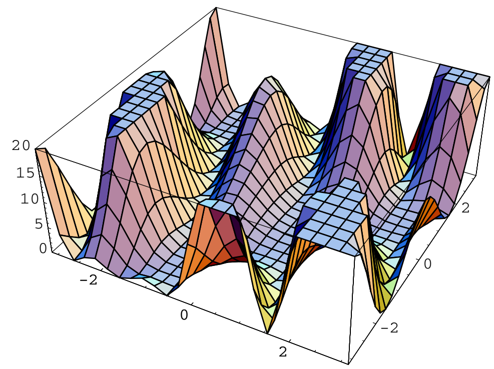
Table 3.3

Iterations of the PCG method for $f(x,y) = (x^2+y^2+1/4)(\cos(x+y)+\sin(2x))^2$.

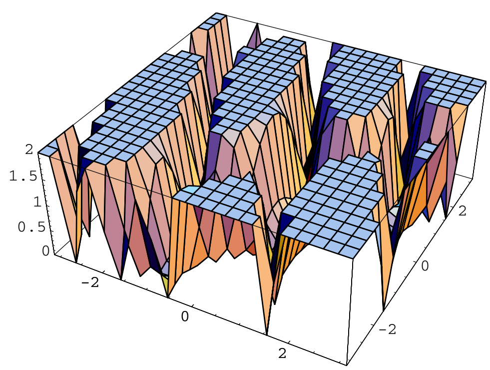
$\nu = n_1 = n_1$	I	$\hat{P}$	P
8	48	-	25
16	146	22	37
32	396	41	44
64	978	52	50
128	*	56	54
256	*	59	57



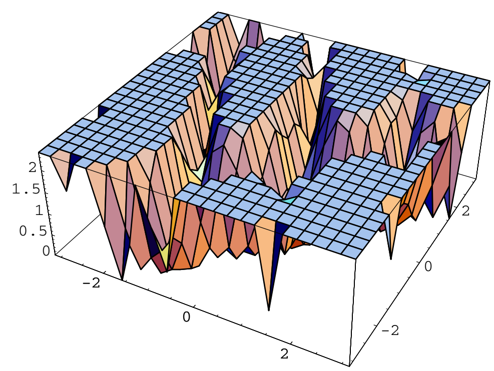
(a) The generating function in (0,20)



(b) The approximated trigonometric polynomial in (0,20)



(c) The generating function in (0,2)



(d) The approximated trigonometric polynomial in (0,2))

FIG. 3.1. *The function f and its approximated trigonometric polynomial in* $[0, 2]$ *and* $[0, 20]$.

In Figure 3.1 we give two snapshots of the graphs of the unknown generating function f and the trigonometric polynomial $\hat{p}$ that we have estimated using our algorithm when $\nu = 32$ and the order of $p_{\mathbf{t}}$ is $(5, 5)$. More precisely, in Figures 3.1(a) and 3.1(b) we observe the global approximation features of our scheme, while in 3.1(c) and 3.1(d) we concentrate our attention on comparing the exact generating function f and the approximate polynomial $p_{\mathbf{t}}$ in the domains where they attain small values: we recall that is the good approximation in such domains, which is crucial for a good performance of the associated preconditioner. In both cases, it is clear that a very good approximation has been achieved by the procedure.

Remark 1. For functions like $x^2 + (y-1)^4$ that need different treatment in each variable, our four-step algorithm can estimate very accurately the root $(0, 1)$ as well as the multiplicities 2 in the x direction and 4 in the y direction (see Example 3 in [17]).

Remark 2. Furthermore, it is worth commenting on the case where f has zeros of not even orders (not integer as well): in that case even the exact band Toeplitz

TABLE 3.4
Maximum, minimum eigenvalues and iterations of the four possible preconditioned schemes.

$n_1 = n_2$	$\lambda_{\max}(P_{2,4}^{-1}T)$	$\lambda_{\min}(P_{2,4}^{-1}T)$	$Iter_{2,4}$	$\lambda_{\max}(P_{2,6}^{-1}T)$	$\lambda_{\min}(P_{2,6}^{-1}T)$	$Iter_{2,6}$
8	13.9	.72	15	6.23	.8	10
16	15.9	.34	28	6.88	.38	17
32	17.4	.16	56	7.26	.18	33
$n_1 = n_2$	$\lambda_{\max}(P_{4,4}^{-1}T)$	$\lambda_{\min}(P_{4,4}^{-1}T)$	$Iter_{4,4}$	$\lambda_{\max}(P_{4,6}^{-1}T)$	$\lambda_{\min}(P_{4,6}^{-1}T)$	$Iter_{4,6}$
8	14	.98	15	3.63	.99	8
16	15.9	.8	24	4.04	.97	11
32	17.8	.5	39	4.76	.96	15

preconditioning (error free with respect to the position of the zeros) is no longer optimal. However, in the 1-dimensional setting, it has been proved that in the worst case (refer to [20]) the number of PCG iterations can grow at most as $\nu^{1/2}$, ν being the size of the 1-level Toeplitz matrix, which can be reasonably good for very ill-conditioned positive definite Toeplitz systems. It is remarked here that the proof of the 1-level case can be extended in the 2-level case. The obtained result is that in the worst case the number of PCG iterations can grow at most as $\nu^{1/2}$, $\nu \sim n_1 \sim n_2$. To show this we consider $f(x,y) = |x|^3 + |y|^5$ which has the isolated zero $(0,0)$ with multiplicities $(3,5)$. By applying our four-step algorithm we will get an isolated zero $(x_0,y_0) \approx (0,0)$ with the associated multiplicities $(k_1,k_2) \approx (3,5)$. If we approximate k_1 and k_2 by the closest even integers we could get four possible choices: $(2,4)$, $(2,6)$, $(4,4)$, or $(4,6)$. We describe in detail the first possibility $(2,4)$. The associated trigonometric polynomial is $2 - 2\cos(x) + (2 - 2\cos(y))^2$ and the condition number of the preconditioned matrix can be estimated by studying the limit of $\frac{|x|^3+|y|^5}{2-2\cos(x)+(2-2\cos(y))^2}$ as $(x,y) \to (0,0)$. In this case a simple analysis in polar coordinates implies that $\kappa(T_n^{-1}(g)T_n(f)) = \mathcal{O}(\nu)$. By using the tools introduced in this paper, we get $\kappa(T_n^{-1}(\tilde{g})T_n(f)) = \mathcal{O}(\nu)$, where $\tilde{g} = 2-2\cos(x+\epsilon_1)+(2-2\cos(y+\epsilon_2))^2$, $\epsilon_1 \sim \epsilon_2 \sim \frac{1}{\nu}$. Hence the number of PCG iterations grows as $\nu^{1/2}$. This is shown in Table 3.4, where we consider the above four choices. We can observe in this table that the choice $(4,6)$ is better than the one of $(4,4)$; then $(2,6)$ follows and the worst choice is $(2,4)$. An explanation of the aforementioned phenomenon is contained in the classical PCG convergence theory due to Axelsson and Lindskög [1]. In the overestimated choices, the eigenvalues of the preconditioned matrix are far away from zero but some of them grow to infinity since $\frac{f}{g}$ is far away from zero but unbounded while in the underestimated ones, they are uniformly bounded but some of them tend to zero since $\frac{f}{g}$ is bounded but has a zero at $(0,0)$. Now, from [1], it is well known that small eigenvalues disturb the PCG convergence more than big eigenvalues and, as a consequence, it is a general recommendation to overestimate the multiplicities of the roots rather than underestimate them when the involved numbers are not even integers.

Remark 3. As a conclusion, we remark here that the above theory could be extended in the d-dimensional case where $d \geq 3$. The difference is that we may have isolated roots, curves of roots, surfaces of roots, or hypersurfaces of roots. It is possible to state and prove spectral properties for the d-dimensional case analogous to the ones given in this paper for the 2-dimensional case. The difficulty is on the practical side. It is more complicated to construct an efficient algorithm which would recognize the roots, their nature (isolated, curves, surfaces, or hypersurfaces), and their multiplicities. On the other hand, concerning the applications, d-level ($d \geq 3$) Toeplitz systems arise from several discretization schemes for elliptic d-dimensional PDEs. In that case, the symbol f is known (or at least the position and the order of the zeros is known) and therefore the exact trigonometric polynomial which deletes the roots can be determined analytically.

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