A preconditioning proposal for ill-conditioned Hermitian two-level Toeplitz systems

D. Noutsos^{1,*,†}, S. Serra Capizzano² and P. Vassalos^{1,‡}

¹Department of Mathematics, University of Ioannina, GR-451 10, Ioannina, Greece ²Dipartimento di Fisica e Matematica, Università dell'Insubria-Sede di Como, via Vallegio 11, 22100 Como, Italy

SUMMARY

Large 2-level Toeplitz systems arise in many applications and thus an efficient strategy for their solution is often needed. The already known methods require the explicit knowledge of the generating function f of the considered system $T_{nm}(f)\mathbf{x} = b$, an assumption that usually is not fulfilled in real applications. In this paper, we extend to the 2-level case a technique proposed in the literature in such a way that, from the knowledge of the coefficients of $T_{nm}(f)$, we determine optimal preconditioning strategies for the solution of our systems. More precisely, we propose and analyse an algorithm for the economical computation of minimal features of f that allow us to select optimal preconditioners. Finally, we perform various numerical experiments which fully confirm the effectiveness of the proposed idea. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: two-level Toeplitz matrix; conjugate gradient; preconditioning; PCG

1. INTRODUCTION

We introduce and discuss a new algorithm for the preconditioning of the two-level Toeplitz system of the form $T_{nm}(f)\mathbf{x} = b$ where n,m are large, the symbol f is assumed to be real-valued and continuous, $(T_{nm}(f))_{(j,k)(p,q)} = t_{k-j,q-p}$ with $t_{r,s}$ being the Fourier coefficients of f, i.e. $t_{r,s} = (1/4\pi^2) \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} f(x, y) e^{-i(rx+sy)} dx dy$, $i^2 = -1$. Here the 2-index notation $(T_{nm}(f))_{(j,k)(p,q)}$ indicates that we are selecting the block (j,k) of size m with $j,k \in \{1,\ldots,n\}$ and, in that block, we are selecting the entry (p,q), $p,q \in \{1,\ldots,m\}$. Such a kind of matrices (often also called block Toeplitz with Toeplitz blocks) arise in several applications (see e.g. Reference [1]) such as Markov chains, integral equations, in the solution of certain partial differential equations (PDEs), image restoration, etc. In some contexts the generating function f is explicitly given or can be easily obtained, but in many others, like image processing,

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^{*}Correspondence to: D. Noutsos, Department of Mathematics, University of Ioannina, GR-451 10, Ioannina, Greece. †E-mail: dnoutsos@cc.uoi.gr

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Markov chains, tomography, etc. 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, their multiplicities, etc. 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 References [2, 3]). The unilevel case has been treated in Reference [4] using band Toeplitz preconditioners and in Reference [5], using circulant-like preconditioners constructed by positive reproducing kernels. Unfortunately, the use of circulant preconditioners, as well as those belonging to more general matrix algebras, cannot be extended to the 2-level setting by preserving neither the superlinear nor the optimal behaviour (see References [6-8] for negative results regarding the notion of superlinearity and References [9, 10] for negative results regarding the notion of optimality). In addition, it is well known (see e.g. Reference [11]) that the spectral properties of the Toeplitz matrices are described very precisely by the symbol. For instance, if zero belongs to the range of f then the sequence $\{T_{nm}(f)\}_{n,m}$ is asymptotically ill-conditioned: more precisely, the problem will be ill-posed in a discrete sense if fhas non-definite sign while we have invertibility but asymptotical ill-conditioning if f is nonnegative (or equivalently non-positive). In the latter we need preconditioning and an optimal technique consists in using $T_{nm}(g)$ as preconditioner where g is a polynomial and has the same zeros as f with the same orders. The system related to $T_{nm}(g)$ is banded and can be solved by multigrid methods [12]; moreover the preconditioning sequence is optimal so that only a fixed number of preconditioned conjugate gradient (PCG) iterations (independent of nand of m) has to be performed in order to reach the solution within a preassigned accuracy. In conclusion we need algorithms for determining these analytical information on the zeros of f: in Reference [4], Serra Capizzano has studied the unilevel case for generating functions only known through the matrix coefficients (i.e. the Fourier coefficients of f). He proposed two kinds of approximations of f by Fourier expansion and by Rayleigh quotient. Here, following a similar approach, we study the 2-level problem by approximating the unknown generating function f from the coefficients of the matrix. We extend the same techniques for the approximation of f into the two-dimensional setting. The main idea is to approximate fover the grid

$$\mathscr{S}_{nm} = \left\{ \left(-\pi + \frac{2k\pi}{n}, -\pi + \frac{2j\pi}{m} \right), \ k = 1, 2, \dots, n, \ j = 1, 2, \dots, m \right\}$$
(1)

on the square $(-\pi, \pi]^2$, then to look for the roots of f, to estimate their multiplicities, to characterize the problem (well-conditioned, ill-conditioned, ill-posed), and finally to choose the appropriate method. 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 paper is organized as follows. In Section 2 the basic theory is briefly sketched and in Section 3 the proposed approach is analysed and some numerical results are given.

2. BASIC THEORY

First we report the basic property for an approximation theory based construction of an efficient 2-level band Toeplitz preconditioner. Indeed, as the numerical examples show, Proposition 1

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is based on a strong numerical evidence and could be easily proved, as in the unilevel setting (see References [4, 13]), by making use of Theorem 3.1 and of the results of Section 2.3 in Reference [13] (for a detailed proof we refer to Reference [14]).

Proposition 1 (Noutsos et al. [14])

Let f(x, y) be a non-negative 2-variate, 2π -periodic continuous function which is equivalent to the trigonometric polynomial g(x, y) in the sense that f/g is bounded away from zero and from infinity. Suppose that (x_0, y_0) is a root of even multiplicity of g or suppose that g defines a curve of roots of even multiplicity C(x, y) = 0 in the domain $(-\pi, \pi]^2$. Let also $(\tilde{x}_0, \tilde{y}_0)$ be an approximation of (x_0, y_0) with $\varepsilon = (\varepsilon_1, \varepsilon_2)^T = (\tilde{x}_0, \tilde{y}_0)^T - (x_0, y_0)^T$ or $\tilde{C}(x, y) = 0$ be an approximation of C(x, y) = 0 with $\varepsilon(x, y) = \tilde{C}(x, y) - C(x, y)$. Then, under the restriction $\|\varepsilon\|_{\infty} \leq c \min\{1/n, 1/m\}$ or $\|\varepsilon(x, y)\|_{\infty} \leq c \min\{1/n, 1/m\}$, c being a positive constant independent of n and m, the spectrum of the preconditioned matrix $T_{nm}^{-1}(\tilde{g})T_{nm}(f)$ is contained in a strictly positive, bounded interval independent of n and m. Here $\tilde{g}(x, y)$ is the trigonometric polynomial which approximates g(x, y) and having as roots the point $(\tilde{x}_0, \tilde{y}_0)$ or the curve $\tilde{C}(x, y) = 0$ with the same multiplicity. Under these assumptions the 2-level band Toeplitz matrix $T_{nm}(\tilde{g})$ can be used as preconditioner for the 2-level Toeplitz system $T_{nm}(f)\mathbf{x} = b$ and the convergence will be optimal (i.e. with a linear rate of convergence independent of both n and m).

We remark here that the above property holds also in the case where the polynomial g has more than one point or curve or combination of points and curves of roots. We will use the following theorem concerning the approximation of a 2-variate function by Rayleigh quotient.

Theorem 1 (Noutsos et al. [14])

Let f be a 2π -periodic continuously differentiable 2-variate function with bounded second derivative. We consider $\theta_x = e^{ix}$, $\theta_y = e^{iy}$ and the associated unitary vectors $\Theta_x^{T} = 1/\sqrt{n}(1 \ \theta_x \ \theta_x^2 \ \cdots \ \theta_x^{n-1})$, $\Theta_y^{T} = 1/\sqrt{m}(1 \ \theta_y \ \theta_y^2 \ \cdots \ \theta_y^{m-1})$. Let $\Theta_{xy} = \Theta_x \otimes \Theta_y$ be the tensor product of the above vectors. Then

$$r_{nm}[f](x,y) = \frac{\Theta_{xy}^H T_{nm}(f)\Theta_{xy}}{\Theta_{xy}^H \Theta_{xy}} = f(x,y) + \mathcal{O}\left(\max\left\{\frac{1}{n}, \frac{1}{m}\right\}\right)$$
(2)

Regarding the Fourier expansion $F_{n-1,m-1}(f)$ of f of degree n-1 and m-1, we observe that the latter approximation is much faster when f is very smooth (due to its Lebesgue constant of order $\log(n) + \log(m)$), 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 will be the main theoretical tools for the construction of our banded preconditioners.

3. THE PROPOSED METHOD—NUMERICAL EXAMPLES

In this section, we propose and describe the procedure in which, starting from the sole knowledge of the entries of $T_{nm}(f)$, we approximate the generating function f and consequently we determine the appropriate preconditioner. We present also various numerical experiments

3	n = m	out	$\varepsilon n = \varepsilon m$	λ_{\min}	$\lambda_{ m max}$	3	out	$\varepsilon n = \varepsilon m$	λ_{\min}	λ_{\max}
	4	0	0.2 < 1	1.3834	16.4384		0	0.04 < 1	1.6741	15.7964
0.05	8	0	0.4 < 1	1.2598	18.8287	0.01	0	0.08 < 1	1.2130	17.8996
	16	0	0.8 < 1	1.1134	20.2060		0	0.16 < 1	1.0321	19.2999
	32	9	1.6 > 1	1.0690	27.4340		0	0.32 < 1	1.0181	19.9149
	64	61	3.2>1	0.5231	60.1832		0	0.64 < 1	1.0077	20.5311

Table I. Number of outliers for $T_{nm}^{-1}(\tilde{g})T_{nm}(f)$, range (f/g) = [1, 20.73921].

to test the effectiveness of the proposed method. The testing functions have been chosen in such a way to cover a wide class of generating functions. First, we consider a numerical example which underlies the main idea described in Proposition 1: 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 f/g.

Numerical example 1: We consider the Toeplitz matrix $T_{nm}(f)$ 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 $T_{nm}(f)x = b$ by a PCG iteration we use as preconditioner the 2-level band Toeplitz matrix $T_{nm}(\tilde{g})$ instead of $T_{nm}(g)$, where $\tilde{g}(x, y) = (2\cos(x - \varepsilon) - \sin(x + 2y + \varepsilon))^2$ is an approximation of g(x, y). In Table I we show the strict relation existing between the approximation error and the number of outlying eigenvalues. It is observed that, only when $n\varepsilon = m\varepsilon$ exceeds 1, there exist eigenvalues of the preconditioned matrix that lie outside the range of f/g. We give the outline of our procedure in the following 4 steps and then we describe each of them:

- 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.

Indeed we have to admit that there are still a lot of details to be taken into account in order to produce a real algorithm; in this sense Steps 1–4 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 two-level Toeplitz systems.

Step 1: First of all, from the coefficients of the matrix $T_{nm}(f)$, we approximate the function f over the grid $\mathscr{G}_{nm} \subset (-\pi, \pi]^2$ defined in (1). By taking into account of Theorem 1 and of the subsequent remark, we restrict our attention to two possible approximations of the function f, namely by Fourier expansion or by Rayleigh quotient (2). There are advantages and disadvantages of the above approximations. The approximation by Rayleigh quotient leads to a smoother shape (less oscillations) of the function with respect to (w.r.t.) the Fourier approximation. Moreover, whenever $T_{nm}(f)$ is positive definite, the Rayleigh quotient approximation is uniformly positive while the Fourier approximation could lead to negative values in some points (especially if $T_{nm}(f)$ is ill-conditioned and positive definite as in the case of a non-negative symbol). On the other hand, the Fourier approximation is much faster when f is smooth. The computational cost for both the approximation methods is $\mathcal{O}(nm(\log n + \log m))$ since both the quantities can be evaluated through a constant number of fast Fourier

transforms (FFTs). In practice, we use the Fourier approximation for all points of the grid and then we check by Rayleigh quotient only the points in which the first approximation gave absolutely small negative values. If the algorithm estimates that the function changes sign, then we assume that the problem is ill-posed in a discrete sense (the matrix $T_{nm}(f)$ is non-definite and potentially singular). In the last case, it could be necessary to use some kind of regularization and the above procedure stops here. Otherwise we proceed to Step 2.

Step 2: First of all we must search for the local minima. Since the approximated function f does not change sign, we assume that f is a non-negative function. The possible roots would be points from the set of the local minima. The searching is done along the directions of x and y comparing the approximated values of the successive points. If the approximated value in a local minimum is of order $\mathcal{O}(\max\{1/n, 1/m\})$, then it is possible that f has a root in that point. To check it, we must also take the grid \mathscr{G}_{2n2m} and compute only the value of the corresponding (new grid) point.

Step 3: For the estimation of the multiplicities of the roots we work in grids with small values of n and m (much smaller than the dimensions of the system in such a way that the computation cost of one PCG iteration dominates). Our approach is based on the following reasoning: let (x_0, y_0) be the zero of f with multiplicity $2k_1$ w.r.t. x and $2k_2$ w.r.t. y. For the sake of simplicity and without loss of generality, we assume that $(x_0, y_0) = (0, 0)$ and f(x, y) positive elsewhere. Then the function f can be written as

$$f(x, y) = h(x, y)((2 - 2\cos(x))^{k_1} + (2 - 2\cos(y))^{k_2})$$
(3)

where h(x, y) is a continuously differentiable and strictly positive function. Therefore f is equivalent to the function $(2 - 2\cos(x))^{k_1} + (2 - 2\cos(y))^{k_2}$. Since the smallest eigenvalue of $T_{nm}(f)$ collapses to zero as n and m tends to infinity with a convergence speed depending on the order of its unique zero (see Reference [11]), it follows that it can be written in the form

$$\lambda_{nm} = \frac{c_1}{n^{2k_1}} + \frac{c_2}{m^{2k_2}} + o\left(\frac{1}{n^{2k_1}} + \frac{1}{m^{2k_2}}\right) \tag{4}$$

where c_1 and c_2 are positive constants. We suppose now that *m* has been chosen so large (w.r.t. *n*) that the dominating term is $1/n^{2k_1}$. Now we take the ratio

$$s_{nm} = \frac{\lambda_{n/4,m} - \lambda_{n/2,m}}{\lambda_{n/2,m} - \lambda_{nm}} = \frac{c_1 \left(\frac{1}{(\frac{n}{4})^{2k_1}} - \frac{1}{(\frac{n}{2})^{2k_1}}\right) + o\left(\frac{1}{n^{2k_1}}\right)}{c_1 \left(\frac{1}{(\frac{n}{2})^{2k_1}} - \frac{1}{n^{2k_1}}\right) + o\left(\frac{1}{n^{2k_1}}\right)} = 2^{2k_1} + o(1)$$
(5)

Therefore, the ratio s_{nm} is an approximation of 2^{2k_1} and consequently $\log_2(s_{nm})$ can be considered a good guess for the multiplicity $2k_1$ of the considered root (w.r.t. x). The previous analysis has been done by considering the exact values of the eigenvalues which are unknown. To follow our procedure, we have to approximate these eigenvalues. From the previous step we have in hand the approximation of the root $(\tilde{x}_0, \tilde{y}_0)$ and the value $f(\tilde{x}_0, \tilde{y}_0)$ which is an approximation of λ_{nm} . The related approximation error is of order $\mathcal{O}(\max\{1/n, 1/m\})$ which is not convenient for the estimation of the multiplicity. To improve the approximation, we use the inverse power method. Recalling Theorem 4.1 of Reference [4], we observe that it can be easily extended in the 2-level setting. In other words, the vector $\Theta_{\tilde{x}_0,\tilde{y}_0}$, defined in

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Grid	(\tilde{x}, \tilde{y})	$\widetilde{\lambda}_{n,m}$	$\log_2(\tilde{s}_{nm})$	(\tilde{x}, \tilde{y})	$\widetilde{\lambda}_{n,m}$	$\log_2(\tilde{s}_{nm})$
(8,32)	(0.349,0.286)	0.777		(1.047,1.999)	0.735	
(16,32)	(0.185,0.286)	0.227		(0.924,1.999)	0.227	
(32,32)	(0.095,0.095)	0.092	2.03	(1.047,1.999)	0.093	1.92
(32,8)	(0.095,0.349)	0.622		(1.047,1.745)	0.645	
(32,16)	(0.095, 0.185)	0.215		(1.047,2.033)	0.219	
(32,32)	(0.095,0.095)	0.092	1.73	(1.047,1.999)	0.093	1.76

Table II. Positions and multiplicities of the zeros: $f(x, y) = (x^2 + y^2)((x - 1)^2 + (y - 2)^2)$.

Table III. Iterations of PCG method: $f(x, y) = (x^2 + y^2)((x - 1)^2 + (y - 2)^2)$.

(n,m)	(16,16)	(16,32)	(32,16)	(16,64)	(64,16)	(32,32)	(32,64)	(64,32)
Inm	166	237	216	308	311	325	467	479
$T_{nm}(\tilde{g})$	34	50	40	49	45	44	51	49
$T_{nm}(g)$	27	30	30	33	32	34	37	36

Theorem 1, is a good approximation of the eigenvector corresponding to λ_{nm} . Using this initial vector, we start the inverse power method and only a few iterations are required to get a good approximation $\tilde{\lambda}_{nm}$ of λ_{nm} . Finally, the approximation of the multiplicity is given by

$$2k_1 \approx \log_2(\tilde{s}_{nm}) = \log_2\left(\frac{\tilde{\lambda}_{n/4,m} - \tilde{\lambda}_{n/2,m}}{\tilde{\lambda}_{n/2,m} - \tilde{\lambda}_{nm}}\right)$$
(6)

Obviously, the multiplicity $2k_2$ (w.r.t. y) is approximated by following an analogous approach. Of course, if the function has a structure different from (3), then the reasoning is more complicated: however the information obtained in Step 2 is the key point for adapting the techniques to be used in Step 3. We perform two further numerical tests in order to show the effectiveness of our algorithm.

Numerical example 2: We consider the Toeplitz matrix $T_{nm}(f)$ generated by the symbol $f(x, y) = (x^2 + y^2)((x - 1)^2 + (y - 2)^2)$. It is obvious that the points (0,0) and (1,2) are roots of f with multiplicities 2 according to both variables. We applied the proposed method to the matrix $T_{nm}(f)$. Table II contains two parts: the first one refers to the root (0,0) and the second to (1,2). In the first column we give the dimension of the testing grid while in the second one the positions where the zeros of f have been estimated by the algorithm. In the third column, we give the approximated eigenvalues after 5 iterations of inverse power method. Finally, in the fourth column, the approximated multiplicities according to both axis are given. As it can be observed, our procedure approximates satisfactorily the multiplicity 2. We have implemented our approach to solve the Toeplitz system by PCG method and the numbers of iterations are given in Table III. In the first row, we report the dimensions of n and m while in the second one the required numbers of iterations of the iteration count of the PCG method is displayed. The preconditioner is the matrix $T_{nm}(\tilde{g})$, where the polynomial $\tilde{g}(x, y)$ has been computed by using the information in Table II. Finally, in the last row we report the number of iterations

Grid	(\tilde{x}, \tilde{y})	$\tilde{\lambda}_{nm}$	$\log_2(\tilde{s}_{nm})$	Grid	(\tilde{x}, \tilde{y})	$\tilde{\lambda}_{nm}$	$\log_2(\tilde{s}_{nm})$
(8,32)	(0.349,0.095)	0.1304		(32,8)	(0.095,0.349)	0.0730	
(16,32)	(0.185,0.095)	0.0362		(32, 16)	(0.095,0.185)	0.0146	
(32,32) (64,32)	(0.095,0.095) (0.048,0.095)	0.0097 0.0025	1.831 1.892	(32,32) (32,64)	(0.095,0.095) (0.095,0.048)	0.0097 0.0093	3.61 3.754

Table IV. Positions and multiplicities of the zeros: $f(x, y) = x^2 + y^4$.

of PCG method, where the preconditioner is the 'exact one', i.e. the matrix $T_{nm}(g)$ with $g(x, y) = (2 - 2\cos(x) + 2 - 2\cos(y))(2 - 2\cos(x - 1) + 2 - 2\cos(y - 2))$. We used as initial guess the null vector, as *b* the vector having all its components equal to 1, and as stopping criterion $||r_k||_2/||r_0||_2 \le 10^{-5}$, where r_k is the residual vector after *k* iterations. By comparing the last two rows, we observe that the preconditioner obtained by our procedure is very close to the 'exact' one. Indeed, it is clearly shown that the number of required iterations is independent of *n*, *m* and thus the corresponding PCG method is optimal.

Numerical example 3: We consider the Toeplitz matrix $T_{nm}(f)$ generated by $f(x, y) = x^2 + y^4$. In Table IV we have reported the same type of information as in Table II. The purpose of the choice of the latter function is to test the sensitivity of the proposed method when a zero has different multiplicity w.r.t. x and y. The results fully confirm the effectiveness of the algorithm.

Step 4: We finally focus our attention to the case where f has an infinite number of roots which form a curve of roots. If we have found (in Step 2) a sequence $z^{(k)}$, k = 1, 2, ..., of roots such that $||z^{(k+1)} - z^{(k)}|| \leq \varepsilon$, $k = 1, 2, ..., \varepsilon = \mathcal{O}(\max\{1/n, 1/m\})$, then we assume that these points represent an approximate sampling of a curve of roots. Consequently, we have to approximate the curve by using a method from approximation theory. The most useful of such methods are the Chebyshev approximation (L^{∞}) , least-squares approximation (L^2) and L^1 approximation. Let $C_f(x, y) = 2l\pi$, $(x, y) \in (-\pi, \pi]^2$, l an integer, be the approximate curve (in implicit form) of roots with multiplicity 2k and where $C_f(x, y)$ is a trigonometric polynomial. Let also $(\tilde{x}_i, \tilde{y}_i) \in (-\pi, \pi]^2$, i = 1, 2, ..., q, be distinct roots of even multiplicities $2k_{1_i}$ w.r.t. x and $2k_{2_i}$ w.r.t. y, respectively. Then the 2-level Toeplitz matrix $T_{nm}(\tilde{g})$ generated by the 2-variate trigonometric polynomial: $\tilde{g} = (2 - 2\cos(C_f))^k \prod_{i=1}^{q} ((2 - 2\cos(x - \tilde{x}_i))^{k_{1_i}} + (2 - 2\cos(y - \tilde{y}_i))^{k_{2_i}})$ can be used as preconditioner.

Numerical example 4: We apply the previous idea to the function $f(x, y) = (x - y)^2$ which vanishes in the line x - y = 0. In Figure 1 we show the exact line (solid line), the one estimated by our algorithm (approximated roots in the grid \mathcal{G}_{nm} , n = m = 32) and the line (dash line) obtained by least-squares approximation. It is clear that the two lines are very close each other: the result is nontrivial since the function f is not continuous when regarded as a 2π -periodic function and therefore the information provided by its Fourier coefficients (the entries of $T_{nm}(f)$) is quite poor.

Computational cost: We finally observe that the pre-computing computational cost (the one related to the analysis of the underlying generating function and to the construction of the preconditioner) is essentially given by few FFTs and therefore is dominated by any matrix vector product occurring in any single CG or PCG iteration. In fact, Step 1 is performed by using a bidimensional FFT ($O(nm(\log(n) + \log(m)))$ arithmetic operations (flops)), Step 2 has



Figure 1. Approximation of a curve of roots $f(x, y) = (x - y)^2$.

a linear cost in *nm* (and therefore is negligible w.r.t. the FFT cost), Step 3 is in principle very expensive since it involves the inverse power method, but it is performed on matrices of size constant w.r.t *n* and *m* and Step 4 could cost again $\mathcal{O}(nm(\log(n) + \log(m)))$ flops.

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