

Preconditioned GMRES Method for the Solution of Non-Symmetric Real Toeplitz Systems

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Introduction

Toeplitz Matrices

An $n \times n$ Toeplitz matrix T_n , is of the form:

$$T_n = \begin{bmatrix} t_0 & t_{-1} & t_{-2} & \cdots & t_{-(n-2)} & t_{-(n-1)} \\ t_1 & t_0 & t_{-1} & \cdots & t_{-(n-3)} & t_{-(n-2)} \\ t_2 & t_1 & t_0 & \cdots & t_{-(n-4)} & t_{-(n-3)} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ t_{n-2} & t_{n-3} & t_{n-4} & \cdots & t_0 & t_{-1} \\ t_{n-1} & t_{n-2} & t_{n-3} & \cdots & t_1 & t_0 \end{bmatrix}.$$

We define as $T_n(f)$ the Toeplitz matrix generated by the function f . The entries of a Toeplitz matrix $T_n(f)$ are the coefficients of the Fourier expansion of a function f :

$$t_{jk} = t_{j-k} = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-i(j-k)x} dx, \quad i^2 = -1, \quad 1 \leq j, k \leq n.$$

We note that properties of the generating function f correspond to specific properties of $T_n(f)$.

f

- Real
- Real & positive
- Real & non-negative
- Real & even
- Complex

 $T_n(f)$

- Hermitian
- Hermitian, positive definite & well conditioned
- Hermitian, positive definite & ill conditioned
- Real & symmetric
- Complex

f

- Real
- Real & positive
- Real & non-negative
- Real & even
- Complex

$$\kappa(A) < c,$$

$c > 0$ independent of n

$T_n(f)$

- Hermitian
- Hermitian, positive definite & well conditioned
- Hermitian, positive definite & ill conditioned
- Real & symmetric
- Complex

$$\kappa(A) = \|A\| \|A^{-1}\|$$

f

- Real
- Real & positive
- Real & non-negative
- Real & even
- Complex

~~$\kappa(A) < c,$~~

~~$c > 0$ independent of n~~

 $T_n(f)$

- Hermitian
- Hermitian, positive definite & well conditioned
- Hermitian, positive definite & ill conditioned
- Real & symmetric
- Complex

f

- Real
- Real & positive
- Real & non-negative
- Real & even
- Complex
- Complex with $\text{Re}(f)$: even & $\text{Im}(f)$: odd

 $T_n(f)$

- Hermitian
- Hermitian, positive definite & well conditioned
- Hermitian, positive definite & ill conditioned
- Real & symmetric
- Complex
- Real & non-symmetric

GMRES

- Krylov subspace Methods

$$K_m(A, b) = \text{span}\{b, Ab, A^2b, \dots, A^{m-1}b\}$$

- Non-symmetric systems
- Generalized Minimal Residual Method (GMRES) (Saad and Schultz 1986)
- GMRES Converges to the solution at most in n iterations
- GMRES Converges Efficiently when $\text{Re}(\lambda_i(A)) > 0$ and $|\lambda_i(A)| < \infty$

Theoretical Background

Definition 1 (Tyrtshnikov¹)

A set $\Phi \subset \mathbb{R}$ is called a general eigenvalue cluster for a hermitian matrix A_n , if for all $\epsilon > 0$ and Φ_ϵ being an ϵ -extension of Φ :

$$\lim_{n \rightarrow \infty} \frac{\gamma_n(\epsilon)}{n} = 0,$$

where $\gamma_n(\epsilon)$ is the number of eigenvalues of A_n , that lie outside of Φ_ϵ . Φ is called a proper cluster if $\gamma_n(\epsilon) \leq c(\epsilon)$, where $c(\epsilon)$ is independent of n .

Definition 2

A set $\Phi \subset \mathbb{R}^+$ is called a general singular value cluster for a matrix A_n , if:

$$\lim_{n \rightarrow \infty} \frac{\gamma_n(\epsilon)}{n} = 0,$$

where $\gamma_n(\epsilon)$ is the number of singular values of A_n , that lie outside of Φ_ϵ . Φ is called a proper cluster if $\gamma_n(\epsilon) \leq c(\epsilon)$, where $c(\epsilon)$ is independent of n .

¹Tyrtshnikov, E. E. (1996). A unifying approach to some old and new theorems on distribution and clustering. *Linear Algebra and its Applications*, 232, 1-43.

Theorem 3 (Tilli²)

Let $f \in L^2([-\pi, \pi])$ be the generating function of $T_n(f)$. Then, the set $[\min |f|, \max |f|]$ is a general singular value cluster for $T_n(f)$.

It is proven that all the singular values are less than $\max |f|$ and at most $o(n)$ singular values of $T_n(f)$ are smaller than $\min |f|$.

²Tilli, P. (1998). Singular values and eigenvalues of non-Hermitian block Toeplitz matrices. *Linear algebra and its applications*, 272(1-3), 59-89.

Theorem 4

Let $f \in L^2([-\pi, \pi])$ and p be a trigonometric polynomial such that $\operatorname{Re} \left(\frac{f}{p} \right) > 0$ and:

$$0 < \alpha = \min_{-\pi \leq x \leq \pi} \left| \frac{f(x)}{p(x)} \right| \leq \max_{-\pi \leq x \leq \pi} \left| \frac{f(x)}{p(x)} \right| = \beta < \infty.$$

Then the interval $[\alpha, \beta]$ is a general cluster of the singular values of the preconditioned matrix $T_n^{-1}(p)T_n(f)$.

We prove here that at most $o(n)$ singular values of $T_n^{-1}(p)T_n(f)$ are smaller than α and at most a constant number of singular values are greater than β .

Proof

- The singular values are the square roots of the eigenvalues of the preconditioned system of the normal equations:

$$\begin{aligned}(T_n^{-1}(\rho) T_n(f))^H T_n^{-1}(\rho) T_n(f) &= T_n^H(f) T_n^{-H}(\rho) T_n^{-1}(\rho) T_n(f) \\ &= T_n(\bar{f}) T_n^{-1}(\bar{\rho}) T_n^{-1}(\rho) T_n(f)\end{aligned}$$

Proof

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- This matrix is similar with:

$$A_n(f, \rho) = T_n^{-1}(\rho) T_n(f) T_n(\bar{f}) T_n^{-1}(\bar{\rho})$$

Proof

$$\begin{aligned}
A_n(f, \rho) &= T_n^{-1}(\rho) T_n(f) T_n(\bar{f}) T_n^{-1}(\bar{\rho}) \\
&= T_n^{-1}(\rho) \left(T_n(\rho) T_n\left(\frac{f}{\rho}\right) + E_n \right) \left(T_n\left(\frac{\bar{f}}{\bar{\rho}}\right) T_n(\bar{\rho}) + E_n^H \right) T_n^{-1}(\bar{\rho}) \\
&= T_n\left(\frac{f}{\rho}\right) T_n\left(\frac{\bar{f}}{\bar{\rho}}\right) + R_n \leq T_n\left(\frac{f\bar{f}}{\rho\bar{\rho}}\right) + R_n = T_n\left(\left|\frac{f}{\rho}\right|^2\right) + R_n,
\end{aligned}$$

where R_n is a low rank matrix, with rank at most $2d - 2$, where d is the bandwidth of the band Toeplitz matrix $T_n(\rho)$.

From Tilli's Theorem, the general cluster is achieved.

Moreover, since of the low rank matrix R_n , at most a constant number of singular values may be greater than β .

Construction of the Preconditioner

Approximation of f

We construct the Band Toeplitz Preconditioner $T_n(p)$, generated by the trigonometric polynomial p , in order to obtain a cluster of the singular values of the preconditioned matrix $T_n(p)^{-1}T_n(f)$ in a small interval around 1, as well as to obtain a good cluster of its eigenvalues in a small bounded region of the right halfplane around 1.

To do this, we have to choose p as a good approximation of f :

Let $f = f_1 + if_2$, where $\begin{cases} f_1: \text{even} \\ f_2: \text{odd} \end{cases}$

Let $f_1 > 0$. We can approximate f :

- 1 Best uniform trigonometric approximation
 - $f_1 \leftarrow$ even trigonometric polynomial of degree d_1
 - $f_2 \leftarrow$ odd trigonometric polynomial of degree d_2
 - Remez exchange algorithm
 - Nodes: k Chebyshev points of the first kind mapped on $[0, \pi]$
- 2 Analogous by trigonometric interpolation

The singular values of $T_n^{-1}(p)T_n(f)$ behave as the function $\left|\frac{f}{p}\right|$:

$$f_1(x) = p_1(x) + e_1(x) \text{ and } f_2(x) = p_2(x) + e_2(x),$$

where e_1 and e_2 , the error functions and $\|e_1\|_\infty = \epsilon_1$ and $\|e_2\|_\infty = \epsilon_2$, the approximation errors. Then,

$$\begin{aligned} \frac{f}{p} &= \frac{f_1 + if_2}{p_1 + ip_2} = \frac{p_1 + e_1 + i(p_2 + e_2)}{p_1 + ip_2} = 1 + \frac{e_1 + ie_2}{p_1 + ip_2} \Rightarrow \\ \left|\frac{f}{p} - 1\right| &= \left|\frac{e_1 + ie_2}{p_1 + ip_2}\right| = \left(\frac{e_1^2 + e_2^2}{p_1^2 + p_2^2}\right)^{\frac{1}{2}} \\ &\leq \max_{-\pi \leq x \leq \pi} \left(\frac{2}{p_1^2(x) + p_2^2(x)}\right)^{\frac{1}{2}} \max\{\epsilon_1, \epsilon_2\} = M\epsilon. \end{aligned} \quad (1)$$

The errors ϵ_1 and ϵ_2 , reduce as the degrees d_1 and d_2 increase. Thus, for a prescribed $\epsilon > 0$, we can choose d_1 and d_2 , such that $\max\{\epsilon_1, \epsilon_2\} \leq \epsilon$. This means that

$$\frac{f}{p} \in [1 - M\epsilon, 1 + M\epsilon]$$

Thus, from Tilli's Theorem, the interval $[1 - M\epsilon, 1 + M\epsilon]$ is a general singular value cluster of $T_n(p)^{-1}T_n(f)$.

Remark

The approximation above gives also a kind of cluster of the shape $\frac{f}{p}$ in a small region of the complex plane around $\mathbf{1}$.

This results that the eigenvalues of $T_n(p)^{-1}T_n(f)$ are clustered in an analogous region, as we will see in a variate of numerical experiments.

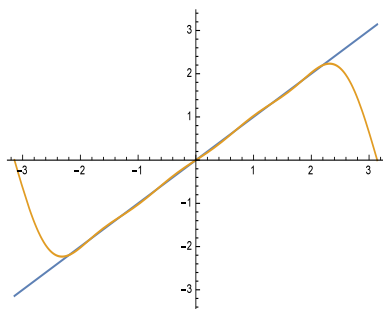
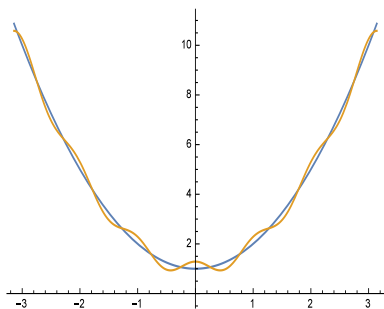
Numerical Results

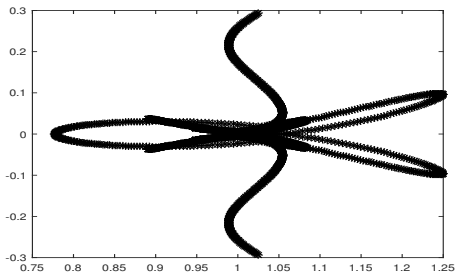
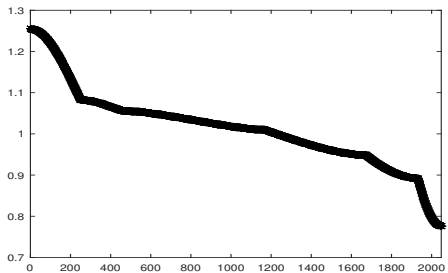
- MATLAB
- We solve $T_n(f)x = b$ by PGMRES method
- $x_0 = 0$
- Stopping criterion: $\frac{\|r^{(k)}\|_2}{\|r^{(0)}\|_2} \leq 10^{-6}$

$r^{(k)}$: residual vector of k iteration and $r^{(0)} = b$

$$x^2 + 1 + ix$$

n	I_n	$R_{4,4}$	$R_{6,4}$	$CGN_{4,4}$
256	37	8	7	11
512	36	8	7	11
1024	35	8	7	11
2048	34	8	7	11





Root at $x_0 = 0$

When f has roots, we have first to eliminate the roots and then to form the approximation technique, described above.

First we study the case where the root is at zero.

Let m_1, m_2 be the multiplicities of the root of f_1 and f_2 , respectively. We separate the following cases:

- 1 $m_1 < m_2$
- 2 $m_1 > m_2$

Obviously, in the first case the multiplicity of the root depends on m_1 , while in the second case on m_2 .

1. Root at $x_0 = 0$, with $m_1 < m_2$

Following the technique proposed by Raymond Chan³ we eliminate the root of f_1 , dividing by the trigonometric polynomial :

$$g = (2 - 2 \cos(x))^{\left(\frac{m_1}{2}\right)}.$$

Thus, we obtain the function

$$\hat{f} = \frac{f}{g} = \frac{f_1 + if_2}{g} = \frac{f_1}{g} + i\frac{f_2}{g} = \hat{f}_1 + i\hat{f}_2.$$

for which: $\hat{f}_1 > 0$.

³Chan, R. H. (1991). Toeplitz preconditioners for Toeplitz systems with nonnegative generating functions. IMA journal of numerical analysis, 11(3), 333-345.

Now, we form the previous technique to approximate \hat{f}_1 and \hat{f}_2 by the trigonometric polynomials q_1 and q_2 , respectively.

Then, $q = q_1 + iq_2$ is the associated approximation of \hat{f} .

Dividing by q , we get :

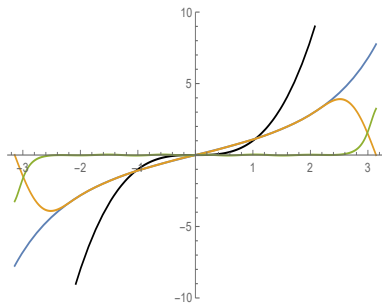
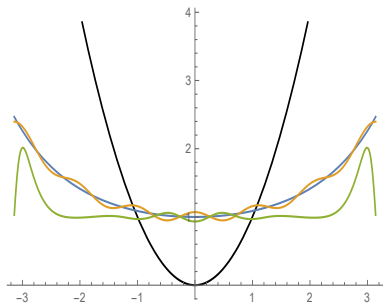
$$\frac{\hat{f}}{q} = \frac{f}{g} = \frac{f_1 + if_2}{q_1 + iq_2} = \frac{f_1 + if_2}{gq_1 + igq_2} = \frac{f}{p} \quad (2)$$

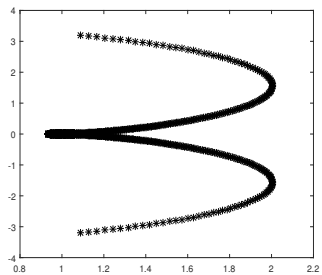
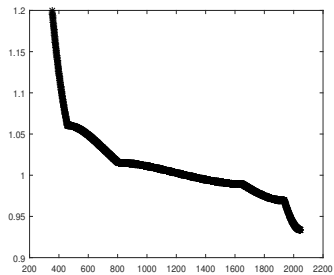
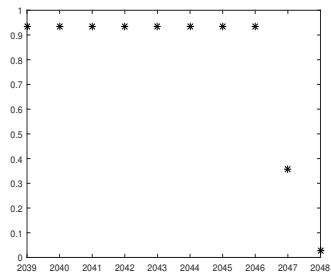
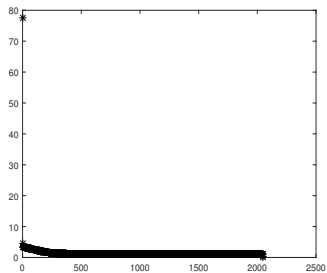
We choose the band Toeplitz matrix $T_n(p)$ as a preconditioner, where $p = gq_1 + igq_2$.

The root of f_2 is not eliminated, but it does not matter.

$$f(x) = x^2 + ix^3$$

n	I_n	B	$R_{4,4}$	$R_{6,6}$	$CGN_{6,6}$
256	256	67	24	22	38
512	512	70	27	26	45
1024	1022	69	28	27	50
2048	2029	68	28	27	55





2. Root at $x_0 = 0$, with $m_1 > m_2$

If we try to eliminate the root of f_1 , using the same technique, the imaginary term will tend to infinity at zero.

If we try to eliminate the root of f_2 dividing by:

$$i(\sin(x))^{m_2},$$

then the imaginary part of f becomes the real part of \hat{f} and the real part of f becomes the imaginary part of \hat{f} . It also holds: $\text{Re}(\hat{f}) > 0$.

The **problem** that arises in this case is that:

$$\lim_{x \rightarrow \pm\pi} \text{Re}(\hat{f}) = +\infty.$$

To avoid this **problem** we divide by the sum of both functions that eliminate the roots:

$$g = g_1 + ig_2 = (2 - 2 \cos(x))^{\frac{m_1}{2}} + i(\sin(x))^{m_2}$$

Then we get the function:

$$\hat{f} = \frac{f_1 + if_2}{g_1 + ig_2} = \frac{f_1g_1 + f_2g_2}{g_1^2 + g_2^2} + i\frac{f_2g_1 - f_1g_2}{g_1^2 + g_2^2} = \hat{f}_1 + i\hat{f}_2.$$

To avoid this **problem** we divide by the sum of both functions that eliminate the roots:

$$g = g_1 + ig_2 = (2 - 2 \cos(x))^{\frac{m_1}{2}} + i(\sin(x))^{m_2}$$

Then we get the function:

$$\hat{f} = \frac{f_1 + if_2}{g_1 + ig_2} = \frac{f_1g_1 + f_2g_2}{g_1^2 + g_2^2} + i\frac{f_2g_1 - f_1g_2}{g_1^2 + g_2^2} = \hat{f}_1 + i\hat{f}_2.$$

- $\hat{f}_1 > 0$
- $|\hat{f}| < \infty$
- $\hat{f}_2(0) = 0$

To avoid this **problem** we divide by the sum of both functions that eliminate the roots:

$$g = g_1 + ig_2 = (2 - 2 \cos(x))^{\frac{m_1}{2}} + i(\sin(x))^{m_2}$$

Then we get the function:

$$\hat{f} = \frac{f_1 + if_2}{g_1 + ig_2} = \frac{f_1g_1 + f_2g_2}{g_1^2 + g_2^2} + i\frac{f_2g_1 - f_1g_2}{g_1^2 + g_2^2} = \hat{f}_1 + i\hat{f}_2.$$

- $\hat{f}_1 > 0$
- $|\hat{f}| < \infty$
- $\hat{f}_2(0) = 0$

Now we are allowed to approximate the function \hat{f} .

Let $q = q_1 + iq_2$ be the approximation of \hat{f} . Dividing by q we have:

$$\frac{\hat{f}}{q} = \frac{f}{g} = \frac{f}{gq} = \frac{f}{p},$$

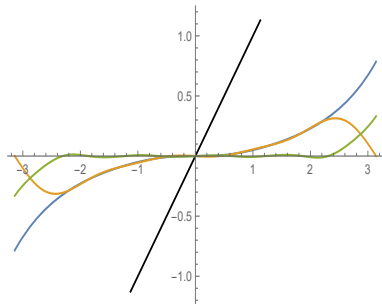
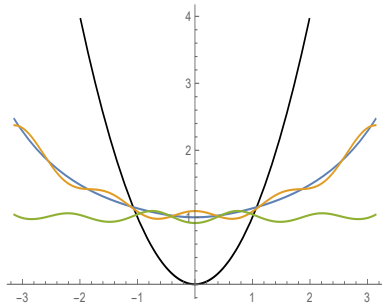
where:

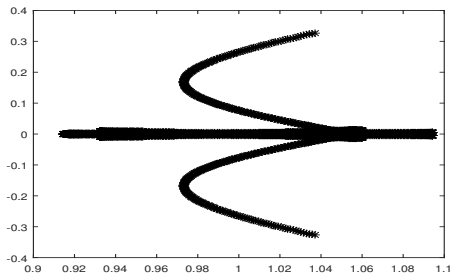
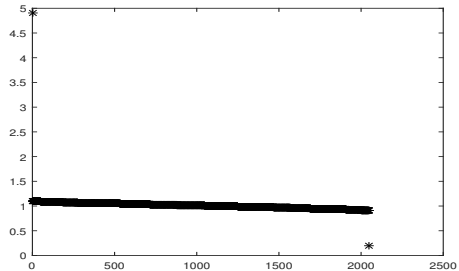
$$p = gq = (g_1 + ig_2)(q_1 + iq_2) = g_1q_1 - g_2q_2 + i(g_1q_2 + g_2q_1) = p_1 + ip_2.$$

Choosing the band Toeplitz matrix $T_n(p)$ as a preconditioner we achieve a singular value cluster.

$$f(x) = x^2 + ix$$

n	I_n	B	$R_{4,4}$	$CGN_{4,4}$
256	256	11	6	8
512	512	11	6	9
1024	1024	10	6	9
2048	2048	10	6	10





$$f(x_0) = 0, \text{ with } x_0 \neq 0$$

Suppose that f has a root at the point $x_0 \in [-\pi, \pi]$, $x_0 \neq 0$. Thus:

- $f_1(x_0) = 0$

- $f_2(x_0) = 0$

Let m_1 and m_2 , are the multiplicities of the root of f_1 and f_2 , respectively.

Since, f_1 : even and f_2 : odd, $-x_0$ is also a root with the same multiplicities

f_2 has an additional root at 0 with odd multiplicity m_0 .

The function f_1 should have the form:

$$f_1(x) = c_1(x)(x - x_0)^{m_1}(x + x_0)^{m_1} \quad (3)$$

in small regions of $\pm x_0$:

$$I_\epsilon = [-\epsilon - x_0, -x_0 + \epsilon] \cup [x_0 - \epsilon, x_0 + \epsilon],$$

where c_1 is a bounded function far from zero and conserves the sign in I_ϵ . We eliminate them dividing by:

$$\begin{aligned} & \text{sign}(c_1(x)) \left(\sin \left(\frac{x - x_0}{2} \right) \right)^{m_1} \left(\sin \left(\frac{x + x_0}{2} \right) \right)^{m_1} \\ &= \text{sign}(c_1(x)) \frac{1}{2^{\frac{m_1}{2}}} (\cos(x_0) - \cos(x))^{m_1}, \end{aligned}$$

or by the simplest form:

$$g_1(x) = \text{sign}(c_1(x)) (\cos(x_0) - \cos(x))^{m_1} \quad (4)$$

Following the same analysis for the function f_2 , its roots are eliminated by:

$$g_2(x) = \text{sign}(c_2(x)) (\cos(x_0) - \cos(x))^{m_2} (\sin(x))^{m_0}, \quad (5)$$

where c_2 plays the same role as c_1 .

We have the following cases:

1 $m_1 \leq m_2$

We need to divide by:

$$g = g_1 = \text{sign}(c_1(x)) (\cos(x_0) - \cos(x))^{m_1}.$$

2 $m_1 > m_2$

We need to divide by the sum:

$$g = g_1 + ig_2 = \text{sign}(c_1(x)) (\cos(x_0) - \cos(x))^{m_1} + i \text{sign}(c_2(x)) (\cos(x_0) - \cos(x))^{m_2} (\sin(x))^{m_0}. \quad (6)$$

Following the same analysis for the function f_2 , its roots are eliminated by:

$$g_2(x) = \text{sign}(c_2(x)) (\cos(x_0) - \cos(x))^{m_2} (\sin(x))^{m_0}, \quad (5)$$

where c_2 plays the same role as c_1 .

We have the following cases:

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We need to divide by:

$$g = g_1 = \text{sign}(c_1(x)) (\cos(x_0) - \cos(x))^{m_1}.$$

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We need to divide by the sum:

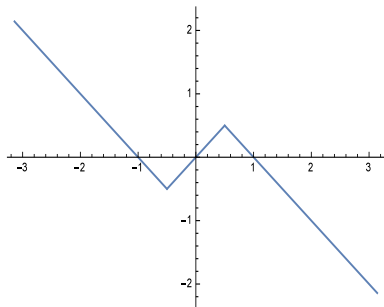
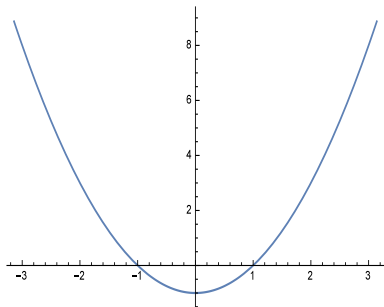
$$g = g_1 + ig_2 = \text{sign}(c_1(x)) (\cos(x_0) - \cos(x))^{m_1} + i \text{sign}(c_2(x)) (\cos(x_0) - \cos(x))^{m_2} (\sin(x))^{m_0}. \quad (6)$$

Then we follow the same technique to approximate $\hat{f} = \frac{f}{g}$ by a trigonometric polynomial and finally, the band Toeplitz preconditioner $T_n(\rho)$ will be generated by $\rho = gq$.

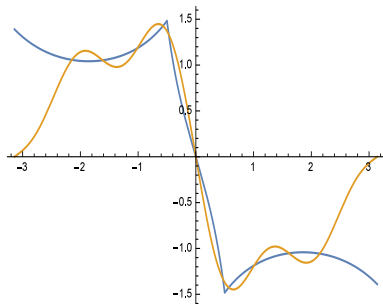
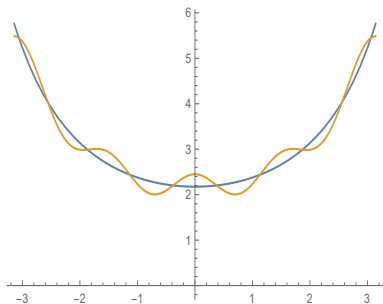
Example with $m_1 = m_2$

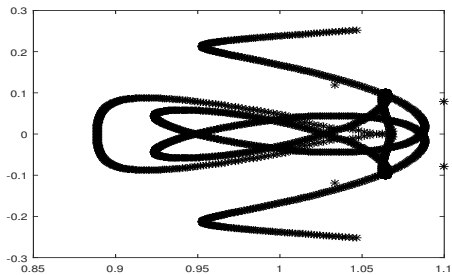
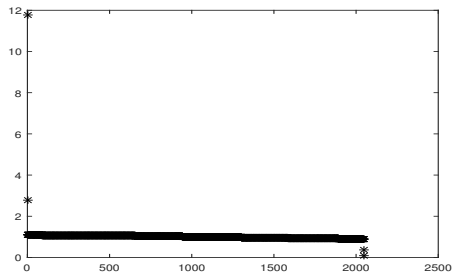
Let $f = f_1 + if_2$, where:

$$f_1(x) = x^2 - 1 \text{ and } f_2(x) = \begin{cases} -1 - x, & -\pi \leq x \leq -\frac{1}{2} \\ x & , -\frac{1}{2} \leq x \leq \frac{1}{2} \\ 1 - x & , \frac{1}{2} \leq x \leq \pi \end{cases} \quad (7)$$



n	I_n	B	$R_{4,4}$	$CGN_{4,4}$
256	256	15	6	11
512	512	15	6	12
1024	1024	16	6	13
2048	2047	15	6	15





Pathological case

- $f_1(\pm x_1) = 0$, with multiplicity m_1
- $f_2(\pm x_2) = 0$, with multiplicity m_2
- $f_2(0) = 0$, with multiplicity m_0

Pathological case

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In this case we could not find a trigonometric polynomial g , such that:

$$\operatorname{Re}\left(\frac{f}{g}\right) > 0 \quad \text{and} \quad 0 < \left|\frac{f}{g}\right| < \infty.$$

Pathological case

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$$\operatorname{Re}\left(\frac{f}{g}\right) > 0 \quad \text{and} \quad 0 < \left|\frac{f}{g}\right| < \infty.$$

This case will probably be covered by a different technique.

Roots at multiple points

Let $f_1(\pm x_i) = f_2(\pm x_i) = 0$, $i = 1, 2, \dots, k$ with multiplicities m_i and ℓ_i , respectively and $f_2(0) = 0$, with multiplicity ℓ_0 .

- $m_i \leq \ell_i$, $\forall i = 1, 2, \dots, k$

$$g = \prod_{i=1}^k \text{sign}(c_i(x)) (\cos(x_i) - \cos(x))^{m_i}$$

- $m_i > \ell_i$, $\forall i = 1, 2, \dots, k$

$$g = \prod_{i=1}^k \text{sign}(c_{1,i}(x)) (\cos(x_i) - \cos(x))^{m_i} \\ + i (\sin(x))^{\ell_0} \prod_{i=1}^k \text{sign}(c_{2,i}(x)) (\cos(x_i) - \cos(x))^{\ell_i}$$

- $\exists i, j$: $m_i \leq \ell_i$ and $m_j > \ell_j \rightarrow$ **Pathological case**

Extension to two-level nonsymmetric Toeplitz systems

This preconditioning technique can be extended to two-level nonsymmetric Toeplitz systems.

These matrices are Block Toeplitz with Toeplitz Blocks (BTTB) matrices and are generated by two variate functions:

$$f(x, y) = f_1(x, y) + if_2(x, y), \quad (x, y) \in [-\pi, \pi]^2,$$

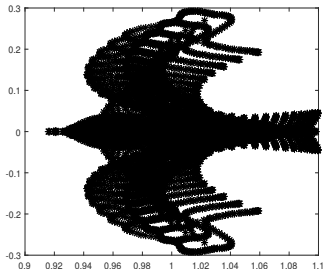
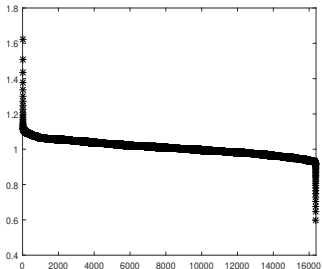
with f_1 : even and f_2 : odd, in both variables.

Difficulties:







- More Complicated Computations.
- There not exists Best Uniform Approximation. Instead, Trigonometric Polynomial Interpolation in two variables, is used.

$$f(x, y) = x^2 + y^2 + i(x + y)$$

$n \times m$	$R_{4,4}$
16 × 16	7
32 × 32	7
64 × 64	8
128 × 128	8



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**Thank you
for your attention**

