

1           **REVIVING CIRCULANT PRECONDITIONERS FOR ADAPTIVE**  
2           **MESH REFINEMENT \***

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4           In collaboration with: James Adler, Xiaozhe Hu, Misha Kilmer,

5           **Abstract.** A preconditioner for solving fractional partial differential equations (PDEs) is pre-  
6           sented. In our method the fractional PDE is discretized on an adaptive grid, resulting in a Hierarchi-  
7           cal matrix representation. The stiffness matrix has Toeplitz blocks along the diagonal and low-rank  
8           approximations off the diagonal. Our preconditioner expands on previously developed methods of  
9           conditioning Toeplitz systems with circulant matrices. We show how these methods can be applied  
10           cheaply on the adaptive mesh and prove that the spectrum of the resulting system is well-clustered.  
11           In order to prove these results, we must take special consideration of how the low-rank blocks perturb  
12           the eigenvalues of the Toeplitz block-diagonal system. We validate our results for various fractional  
13           orders and inspect any assumptions through numerical tests.

14           Preconditioning on adaptive grid, theoretical and numerical results for eigenvalue clustering

15           **Key words.** Preconditioner, Toeplitz, Circulant

16           **1. Introduction.** fPDEs FEM and GMG, appearnace of Toeplitz matrices, cir-  
17           culant preconditioning for krylov methods

- circulant preconditioning
- AMR and low-rank approx in hierarchical matrices
- fractional PDEs

21           There has long been interest in solving Toeplitz systems efficiently. An  $n \times n$   
22           matrix is called Topelitz if  $a_{ij} = a_{i-j}$  (constant diagonals). Since a Toeplitz system  
23           has just order  $n$  entires is can be solved directly in  $\mathcal{O}(n^2)$  time, as opposed to an  
24           arbitrary matrix with  $n^2$  entries solved in  $\mathcal{O}(n^3)$  time.

25           Solving large Toeplitz systems, particularly those that are positive definite, has  
26           been made even faster by the use of circulant preconditioners. Def circulant. These  
27           preconditioners can be thought of as coming from Kernels of displacement operators.  
28           Cite Kalaith and Chan-Yeung. These SPD Toepltiz matrices are common in PDE  
29           discretization, singal processing, and control theory.

30           Toepltiz PDEs arise from uniform grids.

31           Further, multilevel

32           is multilevel the right word?

33           Topelitz systems naturally arise from PDEs solved on adaptive meshes. Adaptive  
34           mesh refinement is sued to solve system that need different orders of granularity  
35           in different parts of the domain. To avoid the expensive grid refinement on the  
36           whole domain, only certain subsets of the domain are refined. Each part of the  
37           domain is refined only until the desired level of error is met. Int his setting we  
38           no longer have a uniform mesh on the whole domain, but every point on the mesh  
39           is part of a *locally uniform* mesh. Each locally uniform subdomain corresponds to a  
40           Toeplitz block in the stiffness matrix. Blocks have different sizes. Geometric multigrid,  
41           hierarchical matrices, off diagonal low rank blocks. In the case of a system of purely  
42           Toeplitz blocks the preconditioning and theoretical results about spectral clustering

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43 are straightforward, we must also deal with how the off diagonal blocks perturb the  
 44 spectrum. Weak and strong interactions.

45 In this paper we investigate how to precondition such systems using circulant  
 46 matrices. Our investigation is focused on hierarchical matrices from GMG cite Xiaozhe,  
 47 but the same methods could be used on any multilevel Toeplitz system. We prove  
 48 spectral clustering around 1 and show numerical results with superlinear convergence.

## 49 2. Background.

### 50 applications for fpDEs

51 One of the most common approaches to numerically solving PDEs is the finite  
 52 element method (FEM). FEM requires the domain be broken into a grid or mesh.  
 53 When each piece of the domain, or element, is the same size we say it is an uniform  
 54 mesh.

### 55 Prove uniform mesh gives toeplitz here

56 If the mesh is not fine enough to give the desired accuracy the initial approach  
 57 may be to increase  $n$  and make each element smaller, keeping a uniform mesh. Alternatively,  
 58 when different levels of granularity are required across the domain to achieve  
 59 desired accuracy, adaptive meshes can be employed. This approach only increases the  
 60 mesh size in certain subdomains. While the entire mesh is no longer uniform, each  
 61 element is part of a locally uniform mesh.

### 62 toeplitz blocks

63 fractional PDEs mean all elements interact, though some weaker some stronger.  
 64 Weak and strong interaction guiding a natural splitting. Good for low-rank approxi-  
 65 mation. Summary of matrix structure, spsd?

66 Toeplitz matrices have many unique properties that give rise to efficient algo-  
 67 rithms (see for example [?]). For our purposes we focus on their connection to func-  
 68 tions in the Wiener class. This will allow us to take our problem from matrix operator  
 69 theory to function theory. Suppose we have a singly infinite, symmetric Toeplitz ma-  
 70 trix,

$$71 \quad A = \begin{bmatrix} a_0 & a_1 & a_2 & & \\ a_1 & a_0 & a_1 & & \ddots \\ a_2 & a_1 & a_0 & & \ddots \\ & \ddots & \ddots & \ddots & \ddots \end{bmatrix}.$$

72 Assume  $\sum_{k=-\infty}^{\infty} |a_k| < \infty$ . Then the function  $a(z) = \sum_{k=-\infty}^{\infty} a_k z^k$  is real, positive,  
 73 and in the Wiener class for  $|z| = 1$ . It will be convenient to define the corresponding  
 74 truncated function for a finite subsection of the infinite matrix:

75 **DEFINITION 2.1.** *The  $m \times m$  finite subsection of the singly infinite matrix  $A$  is  
 76 denoted  $A_m$  and defined as*

$$77 \quad A_m = \begin{bmatrix} a_0 & a_1 & \cdots & a_{m-1} \\ a_1 & a_0 & \cdots & a_{m-2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m-1} & a_{m-2} & \cdots & a_0 \end{bmatrix}.$$

78 *Similarly this matrix induces a function from the truncated series,  $a_m(z) = \sum_{k=-m}^m a_k z^k$ .* ■

boundaries is the problem always (not infinite, block division)

- FEM, adaptive mesh and GMG
- Hierarchical matrices
- Hankel
- circulant and DFT/FFT (displacement kernel's)
- discrete convolution for exact solution and the boundary problem

**3. Preconditioner.** A good preconditioner for an iterative method must in general decrease the total number of iterations without increasing the cost of a single iteration. We borrow Kailath's [?] criteria for preconditioners, though similar criteria has been established since Bini and Benedetto [?]:

1. Complexity of constructing applying  $\tau$  should be  $\mathcal{O}(m \log m)$ .
2. A linear system with  $\tau$  should be solved in  $\mathcal{O}(m \log m)$  operations.
3. The spectrum of  $\tau^{-1}A$  should be clustered around 1

We can make this last point more precise.

**DEFINITION 3.1** (Eigenvalue Clustering). *For any  $\varepsilon > 0$  we say the eigenvalues of a matrix  $\tau^{-1}A_m$  are clustered around 1 if there exists  $N_1$  and  $N_2$  such that for all  $m > N_1$  there are at most  $N_2$  eigenvalues of  $\tau^{-1}A_m$  that do not lie within  $[1-\varepsilon, 1+\varepsilon]$ .*

The use of circulant preconditioners for Toeplitz systems originates from TODO. Kailath showed how both Strang and Chan type preconditioners come from the kernel of displacement operators, they further detail eight specific preconditioners for each form of the discrete sine and cosine transforms.

apply in  $n \log n$  time

In our numerical results we use type TODO, discussed in [?]. Though the results could be generalized to all eight forms. An important fact that we will use later:

eigenvalues as points on function

$A$  is Toeplitz block,  $H$  is "Hankel Correction"

$$A = \begin{bmatrix} a_0 & a_1 & a_2 & \cdots & a_{n-2} & a_{n-1} \\ a_1 & a_0 & a_1 & \cdots & a_{n-3} & a_{n-2} \\ a_2 & a_1 & a_0 & \cdots & a_{n-4} & a_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n-2} & a_{n-3} & a_{n-4} & \cdots & a_0 & a_1 \\ a_{n-1} & a_{n-2} & a_{n-3} & \cdots & a_1 & a_0 \end{bmatrix} H = \begin{bmatrix} a_2 & a_3 & a_4 & \cdots & a_{n-1} & 0 & 0 \\ a_3 & a_4 & a_5 & \cdots & 0 & 0 & 0 \\ a_4 & a_5 & a_6 & \cdots & 0 & 0 & a_{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a_5 & a_4 & a_3 \\ 0 & 0 & a_{n-1} & \cdots & a_4 & a_3 & a_2 \end{bmatrix}$$

$$\tau = A - H$$

We'll also utilize the common assumptions that  $a(z) = \sum_{k=-\infty}^{\infty} |a_k| < \infty$  and  $a(z) > 0$  for each Toeplitz block.

To apply the  $\tau$  preconditioner to our adaptive mesh we can think first of a block construction, (explicit) Identify Toeplitz blocks  $A_j$ , Build Hankel correction  $H_j$ , Con-

$$\text{struct little } \tau_j = A_j - H_j. \text{ Assemble big } \mathcal{T} = \begin{bmatrix} \tau_1 & & & \\ & \tau_2 & & \\ & & \ddots & \\ & & & \tau_m \end{bmatrix}$$

To apply it  $m \log m$  instead, (implicit) Get sizes of Toeplitz blocks  $n_j$ , calculate  $\lambda_i = c_i[S]_i$  for  $1 \leq i \leq n_j$ , apply  $S\Lambda^{-1}S$ .

- story of many
- SPSD with SPSD A

- 117 • how it works w multigrid

118 **4. Theoretical Results.** Story: we know how this works on one block, what  
119 about block diagonal, what about with things happening outside of block diagonal?

120 **4.1. Eigenvalue Bounds.**

LEMMA 4.1 (Weyl's Inequality).

Let  $M$  and  $E$  be Hermitian  $n \times n$  matrices. Then for  $A := M + E$  we have

$$|\lambda_k(A) - \lambda_k(M)| \leq \|E\|_2, 1 \leq k \leq n.$$

121 That is the eigenvalues of  $A$  are at most  $\|E\|_2$  away from the eigenvalues of  $M$ .

122 **4.1.1. Kailath-Olshevsky Proof rewritten.** Fix  $\varepsilon > 0$ . Assumptions:

1. Generating function is in the Wiener Class,

$$a(z) = \sum_{k=-\infty}^{\infty} a_k z^k, \quad \sum_{k=-\infty}^{\infty} |a_k| < \infty.$$

2. Generating function is bounded away from zero on unit circle,

$$a(z) > 2\varepsilon, |z| = 1.$$

123 LEMMA 4.2. Let  $a_m(z)$  be the truncated generating function with  $2m - 1$  terms,  
124  $\sum_{k=-(m-1)}^{m-1} a_k z^k$ . Then for each  $\lambda_k(S_Q(A))$  there exists  $z_k$  on the unit circle such  
125 that  $\lambda_k = a_m(z_k)$ .

126 LEMMA 4.3. Choose  $m$  and  $N < m$  big enough so that  $\sum_{N+1}^{\infty} |a_k| < \varepsilon$ . Then  
127 assumption 2 implies that  $a_m(z)$  is positive on the unit circle.

128 *Proof.* First notice  $\varepsilon > \sum_{N+1}^{\infty} |a_k| > \sum_m^{\infty} |a_k|$ . Now

$$\begin{aligned} a(z) &= a_m(z) + \sum_{-\infty}^{-m} a_k z^k + \sum_m^{\infty} a_k z^k \\ &\implies a_m(z) = a(z) - \sum_{-\infty}^{-m} a_k z^k - \sum_m^{\infty} a_k z^k \\ &\implies a(z) - 2\varepsilon < a_m(z) \\ &0 < a(z) - 2\varepsilon < a_m(z) \end{aligned}$$

□

134 COROLLARY 4.4. The matrices  $S_Q(A_m)$  and  $S_Q(A_m)^{-1}$  are positive definite.

135 First we present the proof for a single Toeplitz matrix/block, adapted from [?].  
136 This will be used in the proof of the full matrix spectral clustering.

137 Lemma statement

138 (4.1)  $S_Q(A) = A + H + B$

139 (4.2)  $A = S_Q(A) - (H + B)$

Where  $A$  is Toeplitz (given),  $H$  is Hankel, and  $B$  is ‘border’ matrix, at most nonzero  
in exterior rows and columns. Thus

$$S_Q(A)^{-1} A = I - S_Q(A)^{-1}(H + B).$$

141 So it suffices to show the spectrum of  $S_Q(A)^{-1}(H + B)$  is clustered around zero.  
 142 Let  $\varepsilon > 0$  and choose  $N$  such that  $\sum_{N+1}^{\infty} |a_k| < \varepsilon$ . We can then split  $H + B$  into  
 143 the sum of a low-rank matrix  $A_{lr}$  and a small norm matrix  $A_{sn}$ . Here  $A_{lr}$  contains  
 144 the diagonals with entries  $a_0, \dots, a_N$ . Let  $s := \text{rank}(A_{lr}) \ll m$ . Now  $A_{sn} :=$   
 145  $(H + B) - A_{lr}$  is a hermitian  $m \times m$  matrix with at most two copies of  $a_{N+1}, \dots, a_m$   
 146 in each row/column. Thus  $\|A_{sn}\|_2 = \sqrt{\|A_{sn}\|_1 \|A_{sn}\|_{\infty}} = \|A_{sn}\|_1 < 2\varepsilon$ . Hence by  
 147 Weyl's Inequality at least  $m - s$  of the eigenvalues of  $H + B$  are clustered within  $2\varepsilon$   
 148 of zero.

149 Now we use the min-max theorem to bound the eigenvalues of  $S_Q(A)^{-1}(H + B)$ .

$$\begin{aligned} 150 \quad \lambda_k(S_Q(A)^{-1}(H + B)) &= \min_{\dim V=k} \max_{x \in V} \left( \frac{((H + B)x, x)}{(S_Q(A)x, x)} \right) \\ 151 \quad &\leq \min_{\dim V=k} \left[ \max_{x \in V} \left( \frac{((H + B)x, x)}{(x, x)} \right) \max_{x \in V} \left( \frac{(x, x)}{(S_Q(A)x, x)} \right) \right] \\ 152 \quad &\leq \left[ \min_{\dim V=k} \max_{x \in V} \left( \frac{((H + B)x, x)}{(x, x)} \right) \right] \max_{x \in \mathbb{R}^n} \left( \frac{(x, x)}{(S_Q(A)x, x)} \right) \\ 153 \quad &= \lambda_k(H + B) \max_{x \in \mathbb{R}^n} \left( \frac{(x, x)}{(S_Q(A)x, x)} \right) \\ 154 \quad &\leq \lambda_k(H + B) \frac{1}{\lambda_{\min}(S_Q(A))} \\ 155 \quad &= \lambda_k(H + B) \frac{1}{a_m(z_{\min})} \\ 156 \quad &\leq \lambda_k(H + B) \frac{1}{\min_{|z|=1} a_m(z)} \\ 157 \end{aligned}$$

158 Can be simplified with  $B = \mathbf{0}$  Actual condition:  $a(z) > 2\varepsilon$ .

## 159 4.2. Full Matrix Proof.

160 **4.2.1. setup.** A single block preconditioner is  $\tau$  the block diagonal precondi-  
 161 tioner is  $T$ .

On a single block we write  $\tau = A - H$ , but for the full adaptive matrix  $A$  includes off diagonal blocks. Denote the diagonal (Toeplitz blocks) as  $A_D$  and everything else  $A_E$  so that

$$A = A_D + A_E + B$$

162 . And thus the splitting as in [?] is expressed  $A_D = T + H$  and  $A = A_E + B + T + H$ .  
 163 So

$$164 \quad (4.3) \quad T^{-1}A = T^{-1}(T + H + A_E + B) = I + T^{-1}H + T^{-1}A_E + T^{-1}B$$

165 **4.2.2. Proof.** It suffices to show that  $T^{-1}H$ ,  $T^{-1}B$  and  $T^{-1}A_E$  have spectra  
 166 clustered around zero. First notice that  $T^{-1}H$  is block diagonal and the spectrum of  
 167 each block can be characterized using the former proof on each block.

since we don't really choose block size in practice the actual block size dictates  
 the size of  $\varepsilon$ . Over all the blocks we can take the max  $\varepsilon$  for a uniform bound, but  
 many will be clustered tighter than that. Supports argument that bigger Toeplitz  
 blocks = better clustering

Assume the off-diagonal-by-one blocks are low-rank. Let  $C$  be such a block with dimensions  $n_C \times n_C$  and rank  $r_C \ll n_C$ . Using the SVD we can split  $C$  as

$$C = \left( \sum_{i=1}^{r_C} \sigma_i^{(C)} \mathbf{u}_i^{(C)} \mathbf{v}_i^{(C)*} \right) + \left( \sum_{i=r_C+1}^{n_C} \sigma_i^{(C)} \mathbf{u}_i^{(C)} \mathbf{v}_i^{(C)*} \right).$$

With a slight abuse of notation, we can embed this decomposition in the appropriate “off-diagonal” position of an  $m \times m$  matrix. Doing this for all such off-diagonal blocks we write

$$\begin{aligned} B &= \sum_{C \in \text{off-diag}} \left[ \left( \sum_{i=1}^{r_C} \sigma_i^{(C)} \mathbf{u}_i^{(C)} \mathbf{v}_i^{(C)*} \right) + \left( \sum_{i=r_C+1}^{n_C} \sigma_i^{(C)} \mathbf{u}_i^{(C)} \mathbf{v}_i^{(C)*} \right) \right] \\ &= \left( \sum_{i=1}^{r_B} \sigma_i \mathbf{u}_i \mathbf{v}_i^* \right) + \left( \sum_{i=r_B+1}^{n_B} \sigma_i \mathbf{u}_i \mathbf{v}_i^* \right) \end{aligned}$$

where  $r_B = \max_{C \in \text{off-diag}} r_C$ .

We additionally split  $H$  by separating the anti-diagonals with coefficients  $a_0, \dots, a_N$  and the anti-diagonals comprising of  $a_{N+1}, \dots, a_m$ . So we have two splittings,

$$\begin{aligned} B &= \left( \sum_{i=1}^{r_B} \sigma_i \mathbf{u}_i \mathbf{v}_i^* \right) + \left( \sum_{i=r_B+1}^{n_B} \sigma_i \mathbf{u}_i \mathbf{v}_i^* \right) \\ H &= H|_{a_0, \dots, a_N} + H|_{a_{N+1}, \dots, a_m}. \end{aligned}$$

The first term in each sum can be thought of as our ‘low-rank’ equivalent from before and similarly the second term is our ‘small-norm’ summand.

### Bound on number of off diagonal blocks

Finally we can make the splitting  $A = A_{SN} + A_{LR}$  where

$$A_{SN} = H|_{a_{N+1}, \dots, a_m} + \sum_{i=r_B+1}^{n_B} \sigma_i \mathbf{u}_i \mathbf{v}_i^* + A_E$$

$$A_{LR} = H|_{a_0, \dots, a_N} + \sum_{i=1}^{r_B} \sigma_i \mathbf{u}_i \mathbf{v}_i^*.$$

$A_{LR}$  represent outliers, IE  $s := \text{rank}(A_{LR}) \leq N + r_B$  bounds the number of outliers.

### Is the N part of this bound true? 2N?

So the work is showing  $\|T^{-1}A_{SN}\|_2 \leq \varepsilon$ . Define  $\tilde{B} = \sum_{i=r_B+1}^{n_B} \sigma_i \mathbf{u}_i \mathbf{v}_i^*$  and  $\tilde{H} = H|_{a_{N+1}, \dots, a_m}$ , so that  $A_{SN} = \tilde{H} + \tilde{B} + A_E$ .

$$\|T^{-1}A_{SN}\|_2 \leq \|T^{-1}\tilde{H}\|_2 + \|T^{-1}\tilde{B}\|_2 + \|T^{-1}A_E\|_2$$

We can bound  $\|T^{-1}\tilde{H}\|_2$  as in [?]. We can bound  $\|T^{-1}A_E\|_2$  with Weyl’s inequality:

$$\|T^{-1}A_E\|_2 \leq \|T^{-1}\|_2 \|A_E\|_2 = \sigma_{\max}(T^{-1}) \sigma_{\max}(A_E) = \frac{\sigma_{\max}(A_E)}{\lambda_{\min}(T)}.$$

196 Finally we bound  $\|T^{-1}\tilde{B}\|_2$ .

$$\begin{aligned}
 197 \quad \lambda_k(T^{-1}\tilde{B}) &= \min_{\dim V=k} \max_{x \in V} \left( \frac{(\tilde{B}x, x)}{(Tx, x)} \right) \\
 198 \quad &\leq \min_{\dim V=k} \left[ \max_{x \in V} \left( \frac{(\tilde{B}x, x)}{(x, x)} \right) \max_{x \in V} \left( \frac{(x, x)}{(Tx, x)} \right) \right] \\
 199 \quad &\leq \left[ \min_{\dim V=k} \max_{x \in V} \left( \frac{(\tilde{B}x, x)}{(x, x)} \right) \right] \max_{x \in \mathbb{R}^n} \left( \frac{(x, x)}{(Tx, x)} \right) \\
 200 \quad &= \lambda_k(\tilde{B}) \max_{x \in \mathbb{R}^n} \left( \frac{(x, x)}{(Tx, x)} \right) \\
 201 \quad &\leq \lambda_k(\tilde{B}) \frac{1}{\lambda_{\min}(T)} \\
 202 \quad &= \lambda_k(\tilde{B}) \min_{n \in n_k} \min_{1 \leq i \leq n} \frac{\sin(\frac{\pi i}{n+1})}{\sum_{j=1}^n t_j \sin(\frac{\pi i j}{n+1})}
 \end{aligned}$$

204 Since  $\tilde{B}$  made of blocks that have form  $\sum_{i=r_B+1}^{n_B} \sigma_i \mathbf{u}_i \mathbf{v}_i *$  what can we say about  $\lambda_k$ ?

- 205 • Weyl's inequality vs min-max characterization – are they saying the same  
206 thing?
- 207 • for one-off blocks we can't write eigs as some point on  $a(z)$ , does this break  
208 things?
- 209 • Note on choosing  $m$  vs choosing  $\varepsilon$
- 210 • numerical test confirming off-diag low rank
- 211 • Explanation and tests showing off-off-diag are small norm
- 212 • For notation, do we like  $T$  as big  $\tau$ ?
- 213 • technically lots of  $1 \times 1$  blocks at boundaries, these get jacobi inverse treatment  
214 so are clustered around 1
- 215 • Comment - all problems come from boundaries
- 216 • Extend proof to different kinds of circulant preconditioner

## 217 5. Numerical Results.

- 218 • enough info to reproduce
- 219 • Single block clustering
- 220 • Adaptive clustering (what happens to smallest eigenvalue?)
- 221 • behavior for different  $\alpha$
- 222 • Verify assumptions from proof
- 223 • convergence of solving with PCG (superlinear convergence)

## 224 6. Conclusion.

225 Future work: how to build adaptive mesh to increase block size,  
other circulant preconditioners, tensor preconditioners, higher dimension domain