SCIENTIFIC APPLICATIONS OF ITERATIVE TOEPLITZ SOLVERS

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ABSTRACT - Recent research on using the preconditioned conjugate gradient method as an iterative method for solving Toeplitz systems has brought much attention. One of the main important results of this methodology is that the complexity of solving a large class of Toeplitz systems can be reduced to $O(n \log n)$ operations as compared to the $O(n \log^2 n)$ operations required by fast direct Toeplitz solvers, provided that a suitable preconditioner is chosen under certain conditions on the Toeplitz operator. In this paper, we survey some applications of iterative Toeplitz solvers to Toeplitz-related problems arising from scientific applications. These applications include partial differential equations, queueing networks, signal and image processing, integral equations, and time series analysis.

Key words. Toeplitz matrices, preconditioners, preconditioned conjugate gradient methods, differential equations, signal and image processing, time series, queueing problems, integral equations

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1. Introduction

An n-by-n matrix A is said to be *Toeplitz* if A is constant along its diagonals. The name Toeplitz originates from the work of Otto Toeplitz [60] in the early 1900's on bilinear forms related to Laurent series, see Grenander and Szegö [28] for details. Toeplitz systems arise in a variety of applications in mathematics and engineering, see Bunch [3] and the references therein. These applications

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have motivated both mathematicians and engineers to develop specific algorithms catering to solving Toeplitz systems. We will call these algorithms *Toeplitz solvers*. Most of the early works on Toeplitz solvers were focused on direct methods. Since n-by-n Toeplitz matrices are determined by only $(2n-1)$ entries rather than n^2 entries, it is expected that the solution of Toeplitz systems can be obtained in less than $O(n^3)$ operations. In the literature, there are a number of fast Toeplitz solvers and superfast Toeplitz solvers with complexity $O(n^2)$ and $O(n\log^2 n)$ operations respectively, see [3], [42] and the references therein.

Recent research on using the preconditioned conjugate gradient method as an iterative method for solving Toeplitz systems has brought much attention, see the survey paper by Chan and Ng [13]. In this methodology, we solve the preconditioned system $C^{-1}Ax = C^{-1}b$ instead of the original system $Ax = b$. In each iteration, it requires two inner products of n-vectors and two matrix-vector products Ay and $C^{-1}y$. With circulant matrices as preconditioners, in each iteration, we have to solve a circulant system. Since circulant matrices can be diagonalized by discrete Fourier matrices [22, p.73], and hence the inversion of n-by-n circulant systems can be done in $O(n\log n)$ operations by using Fast Fourier Transforms (FFTs) of size n. The matrix-vector multiplications Ay can also be computed by FFTs by first embedding A into a $2n$-by-$2n$ circulant matrix, i.e.,

$$\begin{bmatrix} A & \times \\ \times & A \end{bmatrix} \begin{bmatrix} y \\ 0 \end{bmatrix} = \begin{bmatrix} Ay \\ \dagger \end{bmatrix},$$

see [13], and then carrying out the multiplication by using the decomposition of circulant matrices. The matrix-vector multiplication thus requires $O(2n\log(2n))$ operations. It follows that the total number of operations per iteration is of $O(n\log n)$ operations.

Several successful circulant preconditioners have been proposed and analyzed, see [13]. One of the successful circulant preconditioners is T. Chan's circulant preconditioner. For an n-by-n Toeplitz matrix A, T. Chan's circulant preconditioner $c(A)$ is defined to be the minimizer of

$$(1.1)\quad ||C-A||_F$$

over all n-by-n circulant matrices C, see T. Chan (1988) [18]. Here $\|\cdot\|_F$ denotes the Frobenius norm. In [18], the matrix $c(A)$ is called an *optimal* circulant preconditioner because it minimizes (1.1). The diagonals of $c(A)$ are just the average of the diagonals of A, with the diagonals being extended to length n by a wrap-around. It has been shown in [17] that if the Toeplitz matrix A is assumed to be generated by a 2π-periodic continuous function f, i.e. the diagonals of A are given by the Fourier coefficients of f, then these circulant preconditioned systems converge superlinearly. When A is not a Toeplitz matrix, the circulant minimizer $c(A)$ of (1.1) can still be obtained easily by taking the arithmetic average of the entries of A.

The main important results of the circulant preconditioned conjugate method is that the complexity of solving a large class of n-by-n Toeplitz systems can be reduced to $O(n \log n)$ operations as compared to the $O(n \log^2 n)$ operations required by superfast Toeplitz solvers, provided that a suitable preconditioner is chosen under certain conditions on the Toeplitz operator. In the following sections, we will discuss some applications of these iterative Toeplitz solvers to Toeplitz-related systems arising from partial differential equations, queueing networks, signal and image processing, integral equations, and time series analysis.

2. Applications to Partial Differential Equations

2.1. Elliptic Problems

Consider the elliptic problem

$$-(a(x,y)u_x)_x - (b(x,y)u_y)_y = g(x,y) \tag{2.1}$$

on the unit square $[0,1] \times [0,1]$ with Dirichlet boundary conditions. After discretization with a mesh-size of $1/(n+1)$, such a problem reduces to the solution of an n^2-by-n^2 linear system of the form $Ax = b$. With a standard 5-point stencil and lexicographical ordering, the discretization matrix A is a block tridiagonal matrix, where the diagonal blocks are tridiagonal matrices and the off-diagonal blocks are diagonal matrices. R. Chan and T. Chan [7] proposed two choices of circulant preconditioners for these discretization matrices A. The first one is $C_P = c(A) + \rho n^{-2} I$. The diagonals of this point-circulant preconditioner is thus obtained as the simple averages of the coefficients $a(x,y)$ and $b(x,y)$ over the whole grid. The second choice is a block-circulant-circulant-block preconditioner which preserves the block structure of A and is defined as $C_B = c_2(A) + \rho n^{-2} I$, where $c_2(A)$ is the optimal circulant approximation within each block and also on each block level, see [19]. Thus, the diagonals are obtained as the simple averages of the coefficients along the lines of the grid. The constant ρn^{-2} added to the main diagonal is to minimize the condition number of the resulting preconditioned systems. We note that the product $C_B^{-1} y$ can be computed by using $2n$ FFTs of size n and the solution of n intermediate circulant tridiagonal systems, each requiring $O(n)$ complexity, whereas $C_P^{-1} y$ requires two FFTs of size n^2. Similar circulant preconditioners can be defined for more general elliptic operators with more complicated difference stencils and also in higher dimensions.

R. Chan and T. Chan [7] proved that if $0 < c_{\min} \le a(x,y), b(x,y) \le c_{\max}$ in (2.1) for some constants $c_{\min}$ and $c_{\max}$, then the condition numbers of $C_B^{-1} A$ and $C_P^{-1} A$ are $O(n)$ and $O(n \log n)$ respectively. We remark that for second-order elliptic problems, the condition number $\kappa(A)$ of A is $O(n^2)$. It follows from the above theorem that the condition number of the system is reduced from $O(n^2)$ to $O(n)$ by circulant preconditioning. Works in this direction can be found in Huckle [37] where skew circulant preconditioners are used for these discretization matrices. Finally, we note that the application of the circulant preconditioners

requires $O(n^2 \log n)$ flops per iteration, which is slightly more expensive than the $O(n^2)$ flops for the incomplete LU-type preconditioners studied in [30]. However, FFTs can be computed in $O(\log n)$ parallel steps with $O(n^2)$ processors, whereas the incomplete LU preconditioners require at least $O(n)$ steps regardless of how many processors are available. The computation (based on averaging of the coefficients of the elliptic operator) of these circulant preconditioners is also highly parallelizable across a wide variety of architectures.

One can view the circulant preconditioners as approximations to the original given equation, but with the given boundary conditions being replaced by periodic ones. It is thus natural to consider using other optimal fast transform based preconditioners to precondition elliptic problems, see [24, 16]. The discrete sine transform matrix Ψ [61] diagonalizes all symmetric tridiagonal Toeplitz matrices, in particular the 1-dimensional discrete Laplacian with Dirichlet boundary conditions. In [16], R. Chan and Wong proposed using the optimal sine transform based preconditioners for matrices A that come from the discretization of second-order elliptic operators. For simplicity, we let $(\Gamma + \Sigma)\Sigma^{-1}(\Gamma^* + \Sigma)$ be the block Cholesky factorization of A with lower block triangular matrix Γ and diagonal block matrix Σ. For such factorizations, the preconditioner is defined to be the matrix $P = (\hat{\Gamma} + \Phi)\Phi^{-1}(\hat{\Gamma}^* + \Phi)$ with block diagonal matrix Φ and lower block triangular matrix $\hat{\Gamma}$. Here the diagonal blocks of Φ and the subdiagonal blocks of $\hat{\Gamma}$ are respectively the optimal sine transform approximations to the diagonal blocks of Σ and the subdiagonal blocks of Γ. R. Chan and Wong showed that for 2-dimensional domains, the construction cost of P and the cost for each iteration of the preconditioned conjugate gradient algorithm are of $O(n^2 \log n)$. For rectangular regions, the condition number of the preconditioned system $P^{-1}A$ is proved to be of $O(1)$. In contrast, the system preconditioned by the modified incomplete LU factorization (MILU), MINV, and optimal circulant preconditioners are of $O(n)$. We remark that a similar construction of optimal circulant approximations on L-shaped domains has recently been considered by Lirkov, Margenov and Vassilevski [48].

2.2. Domain Decomposition

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with a piecewise smooth boundary $\partial\Omega$. Given $f \in L^2(\Omega)$, we are interested in finding the weak solution $u \in H^1(\Omega)$ of the following Neumann problem:

$$a(u, v) = \int_\Omega f v dx, \quad \forall v \in H^1(\Omega)$$

where

$$a(u, v) = \int_\Omega \left(\sum_{i,j=1}^{2} a_{ij}(x) \frac{\partial u}{\partial x_i} \frac{\partial v}{\partial x_j} + c(x) uv \right) dx$$

and $a_{ij}(x), c(x) \in L^\infty(\Omega)$. We assume that the bilinear form $a(u,v)$ is symmetric and there exist positive constants α_1, α_2 such that

$$\alpha_1 \|v\|^2_{H^1(\Omega)} \le a(u,v) \le \alpha_2 \|v\|^2_{H^1(\Omega)}.$$

Suppose that Ω is a disjoint union of two subdomains Ω_1 and Ω_2, and that a fast solver is available on each subdomain. Domain decomposition methods for elliptic problems defined on union of subdomains have been studied in many papers, see for instance [63]. The idea of substructuring is to reduce the problem in Ω to one on the interface $\partial\Omega_1 \cap \partial\Omega_2$. Let $H^{1/2}(\partial\Omega_k)$ be the Sobolev space of order one half on the boundary $\partial\Omega_k$, $k = 1, 2$, with weighted norm:

$$\begin{aligned} ||v||_{H^{1/2}(\partial\Omega_k)} \equiv & \int_{\partial\Omega_k}\int_{\partial\Omega_k} \frac{|v(x(s),y(s)) - v(x(r),y(r))|^2}{||(x(s),y(s)) - (x(r),y(r))||^2} ds dr + \\ & \frac{1}{d_k}\int_{\partial\Omega_k} |v(x(s),y(s))|^2 ds \end{aligned} \tag{2.2}$$

where $\|\cdot\|$ is the Euclidean distance in $\mathbb{R}^2$. In [44, 45], Kiss and Molnárka proposed using circulant matrices as preconditioners for these elliptic problems. Their idea is to approximate the Euclidean norm $||\cdot||$ in (2.2) by $|s-r|_k \equiv \min\{|s-r|, \text{length}(\partial\Omega_k) - |s-r|\}$. It turns out that the matrix representation C of the resulting approximated bilinear form is circulant and for the Neumann problem it is a good approximation. Kiss and Molnárka [45, 44] proved that for the Neumann problem, the original bilinear form and the approximated one are spectrally equivalent, and hence $\kappa(C^{-1}A) = O(1)$. We remark that Dirichlet and mixed boundary problems have also been considered in [44, 45].

2.3. Hyperbolic and Parabolic Problems

The idea of circulant preconditioners has also been applied to systems arising from implicit time-marching methods for first-order hyperbolic equations of the form

$$\frac{\partial u}{\partial t} + a(x,y)\frac{\partial u}{\partial x} + b(x,y)\frac{\partial u}{\partial y} = g(x,y),$$

see Holmgren and Otto [33, 34, 35, 36] and Otto [56]. For such problems, the discretization matrix A is non-symmetric and often highly non-diagonally dominant, and hence many classical preconditioning techniques are not effective (and sometimes not well-defined). For these problems, the circulant preconditioners are often the only ones that work.

In [33], comparisons of circulant and block-circulant-circulant-block (BCCB) preconditioners with incomplete LU (ILU) and block ILU are done. Some of the circulant-type preconditioners are obtained by changing the boundary conditions from Dirichlet type to periodic ones. It is found that if β, the ratio between the time-step and the spatial mesh size is large, then ILU-type preconditioners fail to

converge, while the rate of convergence for circulant-type preconditioners remains constant independent of the mesh size. In [34], a framework of circulant-block (CB) and BCCB preconditioners is developed, and an analysis of the convergence rate for a BCCB preconditioner is performed for problems that have both periodic and Dirichlet boundary conditions. Analysis of a circulant-block preconditioner for problems with only Dirichlet boundary conditions is done in [56], which also includes a Fourier analysis of ILU, MILU, and block-MILU preconditioned systems. The analysis indicates that the condition number of the MILU preconditioned system remains $O(\beta)$, whereas the convergence rate of the circulant-block preconditioned systems remains independent of β and mesh size h. The convergence analysis was later extended to include a time-independent equation with a weak artificial viscosity, see [35]. Applications of circulant-type preconditioners to the computation of flow in a driven cavity governed by the Navier-Stokes equations can be found in [36].

In [31], Hemmingsson has considered using Toeplitz-block and block-Toeplitz-Toeplitz-block (BTTB) preconditioners for the same first-order hyperbolic PDE. The Toeplitz blocks are obtained by minimization as is done in (1.1), except that the minimization is now taken over a restricted set of Toeplitz matrices. The convergence rate of the resulting preconditioned methods is also favorable and thoroughly analyzed in [32].

Circulant preconditioners for second-order hyperbolic equations have been considered by Jin and R. Chan [41]. In [41], the equation

$$u_{tt} = (a(x,y)u_x)_x + (b(x,y)u_y)_y + g(x,y)$$

is considered. The coefficient matrix, obtained from an implicit time-marching scheme, has condition number of $O(\kappa^2) + O(h^{-2})$. With circulant-type preconditioners, Jin and R. Chan [41] proved that the condition number is reduced to $O(\kappa) + O(h^{-1})$. The same idea of proof can also be applied to parabolic equations, see [40]. In [36], Holmgren and Otto investigated circulant-type solvers for mixed hyperbolic-parabolic equations. The second-order terms were considered small or used as artificial viscosity, such as for the discretized Euler equations in computational fluid dynamics.

3. Applications to Queueing Problems

3.1. Overflow Queueing Networks

Consider a 2-queue Markovian network with overflow permitted only from queue 1 to queue 2 when queue 1 is full, see [43]. We are interested in finding the steady-state probability distribution vector of the network. Let λ_i, μ_i, n_i, and s_i be the input rate, output rate of a single server, buffer size and number of servers for queue i, respectively. If the traffic density, defined as $\lambda_i/(s_i\mu_i)$ is close to 1, then the queueing problem resembles a second-order elliptic equation on a rectangle with an oblique boundary condition on one side (the side with overflow) and Neumann boundary conditions on the others, see [4].

The SOR method is one of the standard methods for solving this problem, see [43]. However, in [4], the preconditioned conjugate gradient method has also been considered, with the preconditioner being constructed by changing the oblique boundary condition to Neumann boundary condition. The convergence rate of the preconditioned conjugate gradient method with this preconditioner is much better than the SOR method, ranging from 10 times faster for small n_i to about 100 times faster for $n_i = 128$. However, inversion of these preconditioners is expensive when the number of servers $s_i > 1$, see [4]. Since the 1-dimensional discrete Laplacian with Neumann boundary conditions can be diagonalized by the cosine transform matrix, one is naturally lead to consider optimal cosine transform based preconditioners [10] for such queueing systems. By using FFTs, each inversion of the preconditioner requires $O(n_1 n_2 \log(n_1 n_2))$ operations independent of s_i. Thus, the cost per iteration is comparable to the $O(n_1 n_2)$ operations required by the SOR method. Numerical results in R. Chan, Ching, and Wong [10] show that the optimal cosine transform based preconditioner performs even better than the preconditioner constructed by changing the oblique boundary condition to Neumann boundary condition.

3.2. Queueing Networks with Batch Arrivals

Queueing systems with batch arrivals occur in many applications, such as the telecommunication networks [55] and the loading dock models [59]. Again we are interested in finding the stationary distribution vector of the network. It will be the normalized null-vector of the generator matrix of the problem. For this problem, the generator matrix can be written as a sum of a Toeplitz matrix and a rank s matrix, where s is the number of servers. Since the generator matrix is singular, the Toeplitz matrix will have a generating function f that has zeros. We remark that if $f_{\min} = 0$, then the circulant preconditioners fail because they cannot match the zeros of the given f, while the band-Toeplitz preconditioners proposed in [5] give only linear convergence because the preconditioned matrices do not have clustered spectra. In R. Chan and Ching [9], they considered using products of circulant matrices and band-Toeplitz matrices as preconditioners for Toeplitz systems generated by non-negative functions. The singularity of the generator matrix is canceled by the band-Toeplitz part of the preconditioner, and the circulant part of the preconditioner is used to speed up the convergence of the algorithm. They proved superlinear convergence of the method when s is independent of n, the size of the queue. Numerical results in [9] verified the fast convergence for small s, and show moreover that the convergence is still linear when $s = n$.

3.3. Markov Modulated Poisson Processes

Markov-modulated Poisson process (MMPP) is a generalization of Poisson process and is commonly used in modeling the input process of communication

systems such as data traffic systems and Asynchronous Transfer Mode (ATM) networks. An MMPP is a Poisson process whose instantaneous rate is itself a stationary random process which varies according to an irreducible n-state Markov chain. Consider a queueing system with $(q+1)$ trunks, where each trunk has m waiting spaces and s multiple exponential servers. The analysis of these queueing systems can be used to determine call congestions in teletraffic networks with alternate routing, see Hellstern [49]. A call will overflow to other trunks if its first destination trunk is full and will be blocked from the system if all the trunks are full. The analysis of these queueing systems can be decomposed into the study of each trunk independently, see Hellstern [49]. For each trunk, the overflow from other trunks is modeled by a 2^q-state MMPP which is a superposition of q independent 2-state MMPPs, i.e. each trunk is an (MMPP/M/s/$s+m$) queue. The generator matrices of these processes are $(s+m+1)2^q \times (s+m+1)2^q$ tridiagonal block matrices with each diagonal block being a sum of tensor product of matrices. The problem is to find the steady state probability distributions of the queues which are the normalized null-vectors of the generator matrices.

Usually classical iterative methods, such as the block Gauss-Seidel method, are used to solve for the steady state probability distribution. They are easy to implement, but their convergence rates are slow in general. Ching, Chan and Zhou [21] proposed to use the preconditioned conjugate gradient method with preconditioners constructed by taking circulant approximation of the tensor blocks of the generator matrix. They proved that the preconditioned system has singular values clustered around 1 independent of the size of the waiting spaces m. Hence the conjugate gradient method will converge very fast when employed to solving the preconditioned system for large m. The numerical method developed for the queueing networks above is well suitable for solving the steady state probability distribution for these processes. Moreover, the analysis of the MMPP queueing systems can be applied to the production planning of manufacturing systems of multiple parallel machines producing one type of product, see [21].

4. Applications to Signal and Image Processing

4.1. Image Restorations

Image restoration refers to the removal or reduction of degradations (or blur) in an image using a priori knowledge about the degradation phenomena; see for instance [39]. When the quality of the images is degraded by blurring and noise, important information remains hidden and cannot be directly interpreted without numerical processing. In operator notation, the form of the image restoration problem is given as $b = \mathcal{A}x + \eta$, where the operator $\mathcal{A}$ represents the degradation, b is the observed image and η represents an additive noise. Given b and $\mathcal{A}$, and possibly, the statistics of the noise vector η, the problem is to compute an approximation to the original signal x. In many practical applications, the degradation is *spatially invariant*, i.e., it acts uniformly across the image and object planes.

In this case, the discretization of $\mathcal{A}$ is just a BTTB matrix.

Because of the ill-conditioning of $\mathcal{A}$, naively solving $\mathcal{A}x = b$ will lead to extreme instability with respect to perturbations in b, see [39]. The method of *regularization* can be used to achieve stability for these problems [1]. In the classical *Tikhonov regularization* [29], stability is attained by introducing a regularization functional R, which restricts the set of admissible solutions. Since this causes the regularized solution to be biased, a scalar μ, called a regularization parameter, is introduced to control the degree of bias. More specifically, the regularized solution is computed as

$$\min_{x(\mu)} \|\mathcal{A}x(\mu) - b\|_2^2 + \mu R(x(\mu))) \tag{4.1}$$

where $R(\cdot)$ is a certain functional which measures the irregularity of x in a certain sense.

When $R(f) = \|f\|_2^2, \|\mathcal{D}_k f\|_2^2$, where D is a kth order differential operator, it forces the solution to small kth order derivative. Notice that if the discretization of the differential operator is a Toeplitz matrix, then in digital implementation, (4.1) reduces to a block-Toeplitz least squares problem. For these Toeplitz least squares problems, R. Chan, Nagy, and Plemmons [11, 12] and R. Chan, Ng and Plemmons [14] considered different preconditioners based on the circulant approximations. In [14, 50], restoration of real images by using the circulant preconditioned conjugate gradient algorithm has been carried out.

The algorithms for deblurring and noise removal have been based on least squares. The output of these least squares based algorithms will be a continuous or smooth function, which cannot obviously be a good approximation to original image if it contains edges. To overcome this difficulty, a technique based on the minimization of the *"total variation norm"* subject to some noise and blurring constraints is proposed by Rudin, Osher and Fatemi [57]. They proposed to use as regularization function the so-called Total Variation norm:

$$TV(f) = \int_\Omega |\nabla f| \, dxdy = \int_\Omega \sqrt{\left(\frac{\partial f}{\partial x}\right)^2 + \left(\frac{\partial f}{\partial y}\right)^2} \, dxdy.$$

The solution to (4.1) for $R(f) = TV(f)$ can have discontinuities, thus allowing us to recover the edges of the original image from the blurred and noisy data. Since the gradient equation of (4.1) is nonlinear, Vogel and Oman [62] employed the fixed point (FP) iteration to solve this nonlinear gradient equation. The FP iteration will produce a sequence of approximations x_k to the solution x and can be expressed as

$$(A^*A + \mu L(x_k))x_{k+1} = A^*b, \quad k = 0, 1, \ldots$$

The coefficient matrix will correspond to a sum of a convolution operator A^*A and an elliptic operator L. In [8], R. Chan, T. Chan and C. Wong used the optimal cosine transform based preconditioner to precondition the linear system.

Numerical results showed that the performance of these preconditioners works very well.

4.2. Signal and Image Reconstruction

One of the principal problem in signal analysis is the reconstruction or approximation of a signal from its discrete samples, see [39]. In many applications, one is forced to sample signals at nonuniformly spaced points. In [23], Feichtinger, Gröchenig and Strohmer reformulated the problem as a Toeplitz system with the adaptive weights method. They found that if the signal is sampled near the critical density or if there are many large gaps in the sampling set, it may happen that even the conjugate gradient method converges rather slow. To remedy this problem, they turns to the circulant preconditioned systems. Numerical results showed that their method needs considerably less computation time.

Image reconstruction from projections is an important tool in medical imaging. Computer tomography have been studied in details, see [39]. In [58], Roux, Lise, Zerbib and Foguet showed that if the measured data are the values of samples of the projections and the projections are band-limited, the optimal reconstructed image is the solution of a 2-dimensional convolution equation $Ax = b$ where A is a large Toeplitz-block-block-Toeplitz matrix and b is a first image reconstructed through 1-dimensional filtering and backprojection. They used a conjugate gradient method where the matrix-vector products are performed in the frequency domain. This avoids interpolations in the spatial domain. The idea is similar to preconditioning with circulant preconditioners. Their reconstruction method is very well in the case of noisefree images.

5. Applications to Integral Equations

5.1. Inverse Heat Problem in $\mathbb{R}^m$

The inverse heat problem in $\mathbb{R}^m$ is the problem of recovering the initial data $\Upsilon(y)$ for all $y \in \mathbb{R}^m$ in

$$u(x,t) = \frac{1}{\sqrt{4\pi t}} \int_{\mathbb{R}^m} \exp\left(\frac{-(x-y)^2}{4t}\right) \Upsilon(y) dy,$$

when for some $t > 0$, $u(x,t)$ is given for all $x \in \mathbb{R}^m$. Using discrete time and spatial sampling of the domain and sinc expansion for approximating the initial data, the problem is reduced to solving a linear system with block Toeplitz coefficient matrices: $(A \otimes A \otimes \cdots \otimes A)\Upsilon = u$, where A is a Toeplitz matrix, see Gilliam, Martin, and Lund [25]. In [6], the system is preconditioned by $C \otimes C \otimes \cdots \otimes C$ with circulant preconditioners C. Numerical results in [6] show that for solving block Toeplitz systems of order 65536, the time required by using the circulant preconditioned conjugate gradient method is half the time required by the direct Toeplitz solver available in the IMSL package [38].

5.2. Wiener-Hopf Equations

Half-line Wiener-Hopf integral equations

$$(5.1)\quad y(t) + \int_0^\infty a(t-s)y(s)ds = g(t), \quad 0 \le t < \infty,$$

in which $a(t) \in L_1(\mathbb{R})$ and $g(t) \in L_2[0,\infty)$ are given functions, arise in a variety of practical applications in mathematics and engineering, such as linear prediction problems for stationary stochastic processes, diffusion problems and scattering problems. One way of solving (5.1) is by the projection method [26], where the solution $y(t)$ of (5.1) is approximated by the solution $y_\tau(t)$ of the finite-section equation

$$(5.2)\quad y_\tau(t) + \int_0^\tau a(t-s)y_\tau(s)ds = g(t), \quad 0 \le t \le \tau.$$

The finite-section equation (5.2) can be solved numerically by either direct or iterative methods. For a fixed τ, the finite-section operator $\mathcal{A}_\tau$ defined by

$$(5.3)\quad (\mathcal{A}_\tau x)(t) = \begin{cases} \displaystyle\int_0^\tau a(t-s)x(s)ds, & 0 \le t \le \tau, \\ 0, & t > \tau. \end{cases}$$

is a compact operator. Therefore, the spectrum of the Wiener-Hopf operator $\mathcal{I} + \mathcal{A}_\tau$ (where $\mathcal{I}$ is the identity operator) is clustered around 1, and hence solving (5.2) by iterative methods such as the conjugate gradient method is less expensive than direct methods. However, as τ tends to ∞, the spectrum of this finite-section operator $\mathcal{A}_\tau$ becomes dense in the spectrum of the half-line operator defined by (5.1), and hence the convergence rate of the conjugate gradient method deteriorates, see the numerical results in [27] for instance. A standard way of speeding up the convergence rate of the conjugate gradient method is to apply a preconditioner. Thus, instead of solving (5.2), one solves a preconditioned operator equation. We remark that there is a close relation between Wiener-Hopf integral equations and semi-infinite Toeplitz operators, see Gohberg and Fel'dman [26, p.5]. The methodology of preconditioning "discrete" Toeplitz systems can be modified and applied to the "continuous" Wiener-Hopf equations.

In [27], Gohberg, Hanke, and Koltracht proposed using *circulant integral operators* to precondition (5.2). Circulant integral operators are operators of the form

$$(5.4)\quad (\mathcal{C}_\tau x)(t) = \int_0^\tau c_\tau(t-s)x(s)ds, \quad 0 \le t \le \tau,$$

where c_τ is a τ-periodic conjugate symmetric function in $L_1[-\tau,\tau]$. We remark that $\mathcal{C}_\tau$ is a compact, self-adjoint operator on $L_2[-\tau,\tau]$. The preconditioned equation is given by

$$(5.5)\quad (\mathcal{I} + \mathcal{C}_\tau)^{-1}(\mathcal{I} + \mathcal{A}_\tau)y_\tau(t) = (\mathcal{I} + \mathcal{C}_\tau)^{-1}g(t), \quad 0 \le t \le \tau.$$

It has been shown in [27] that for large τ, the spectra of the circulant preconditioned operators $(\mathcal{I}+\mathcal{C}_\tau)^{-1}(\mathcal{I}+\mathcal{A}_\tau)$ are clustered around 1.

When (5.2) is discretized with the rectangular quadrature rule, we get an n-by-n matrix system $Ay = g$, where A is a Toeplitz matrix. Here n is the number of quadrature points used in the discretization. We note that if the rectangular quadrature rule is used to discretize (5.5), then we get a matrix system:

$$(5.6)\quad (I+C)^{-1}(I+A)y = (I+C)^{-1}g,$$

where the matrices $(I+C)$ and $(I+A)$ are n-by-n circulant and Toeplitz matrices, respectively. We see that (5.6) is basically a circulant-preconditioned Toeplitz system, which requires only $O(n\log n)$ operations in each iteration.

One main drawback of using the rectangular rule is that the order of accuracy of the discretized solution y depends only linearly on the number of quadrature points. Thus, in order to obtain a reasonably accurate solution for (5.2), a small step-size has to be used and hence the dimension of the resulting matrix system will be large. In order to obtain high order of accuracy, one can use higher order quadrature rules such as the trapezoidal rule or Simpson's rule, which have second and fourth order of accuracy, respectively. In these cases, the discretization matrices of the Wiener-Hopf integral operators are *non-Toeplitz* matrices. Moreover, the corresponding discretization matrices of the circulant integral operators are in general *not* circulant, and therefore their inversion cannot be computed by using FFT. Hence, the cost per iteration of the preconditioned conjugate gradient method exceeds $O(n\log n)$ operations.

Instead of constructing matrix preconditioners for these discretization matrices, we can consider preconditioners from the operator point of view. In [46, 47], Lin, Ng, and R. Chan constructed preconditioners $\mathcal{B}_\tau$ for (5.2) such that the preconditioned operators $(\mathcal{I}-\mathcal{B}_\tau)(\mathcal{I}+\mathcal{A}_\tau)$ have clustered spectra and that only $O(n\log n)$ operations are required in each iteration of the preconditioned conjugate gradient method, even when higher order quadrature rules are employed. The performance of their proposed preconditioner for Simpson's rule is the best one in terms of the accuracy and the computational work.

5.3. Boundary Integral Equations

Consider the solution of the potential equation

$$(5.7)\quad \begin{cases} \Delta w(x) = 0, & x \in \Omega, \\ w(x) = g(x), & x \in \partial\Omega, \end{cases}$$

where $\partial\Omega$ is a smooth closed curve in $\mathbb{R}^2$ and Ω is either the bounded interior region with boundary $\partial\Omega$ or the unbounded exterior region with boundary $\partial\Omega$. In the boundary integral equation approach, see for instance Chen and Zhou [20, §6.12], The harmonic function $w(x)$ is represented as a single-layer potential generated by a source distribution $\sigma(x)$ over $\partial\Omega$, with the potential satisfying the boundary

condition $g(x)$ prescribed for $w(x)$. More precisely, we write

$$(5.8)\quad w(x) = -\frac{1}{2\pi}\int_{\partial\Omega} \log|x-y|\sigma(y)dS_y + \eta, \qquad x \in \Omega$$

where S_y is the arc length variable corresponding to y and η is a constant to be determined. The limit of (5.8), as x is taken to $\partial\Omega$, gives the integral equation on the boundary:

$$(5.9)\quad g(x) = -\frac{1}{2\pi}\int_{\partial\Omega} \log|x-y|\sigma(y)dS_y + \eta, \quad x \in \partial\Omega.$$

The functions $\sigma(y)$ and η can be obtained by solving the boundary integral equations

$$(5.10)\quad -\frac{1}{2\pi}\int_{\partial\Omega} \log|x-y|\sigma_i(y)dS_y = g_i(x), \qquad x \in \partial\Omega, \qquad i = 1, 2,$$

for $\sigma_1(y)$ and $\sigma_2(y)$ with $g_1(x) = g(x)$ and $g_2(x) \equiv 1$. Once $\sigma(y)$ and η are obtained, values of $w(x)$ in Ω can be computed from (5.8).

The well-known advantage of the boundary integral equation approach is that the dimension of the problem is reduced by one. The discrete matrix A_n associated with the integral equation (5.10) is only of size n-by-n for mesh size proportional to $1/n$. In contrast, the discrete matrix for the partial differential equation (5.7) will be of size n^2-by-n^2. However, the major drawback of the approach is that A_n is a dense matrix. Hence solving the problem with a direct method will require $O(n^3)$ operations which will be too expensive for practical, large scale numerical computations. In [15], Chan et al. considered the use of circulant integral operators as preconditioners for integral equations of the first kind as given in (5.10). Their integral equations are not of convolution-type and are ill-conditioned. They proved that the preconditioned systems will become well-conditioned and therefore the convergence rate is linear. Numerical results for two types of regions: the ellipses and the dumb-bell shape regions, illustrate the fast convergence of their method.

5.4. Applications to Time Series Analysis

Least squares estimations have been used extensively in a wide variety of scientific applications, see for instance [2]. In these applications, we usually need to estimate the transmitted signal from a sequence of received signal samples or to model an unknown system by using a linear system model. Let $x(i)$ be a discrete-time stationary zero-mean complex-valued process. A *finite impulse response* (FIR) linear filter of order n is of the form $\tilde{d}(i) = \sum_{k=1}^{n} b_k x(i-k+1)$, where $\tilde{d}(i)$ is the filter output based on the data $\{x(k)\}_{k=i}^{i-n+1}$ and $\{b_k\}_{k=1}^{n}$ are the impulse responses of the filter. The difference between the desired response $d(i)$ of the process and the filter output $\tilde{d}(i)$ is called the estimation error of order n. Since we are interested in estimating the desired response based on the

input measurements, the impulse responses $\{b_k\}_{k=1}^n$ should be chosen to make the estimation error as small as possible.

For the case of known statistics, i.e., the autocovariances of the stationary process are known, the optimal least mean squares predictor coefficients $\{b_k\}_{k=1}^n$ are given by the solution of the linear system of equations $Ab = d$. Here A is an n-by-n Hermitian Toeplitz matrix and its entries $\{a_j\}_{j=0}^{n-1}$ are the autocovariances of a discrete-time stationary process and are given by

$$a_k = \mathcal{E}[x(j)\overline{x(j-k)}],$$

where $\mathcal{E}$ is the expectation operator. The matrix A is called the covariance matrix of the stationary process, and the Toeplitz system is commonly called the Yule-Walker equations, see Yule [64]. If one assumes that the spectral density function of the stationary process exists and is positive (that can be guaranteed by the causality of the process) then the Yule-Walker equations can be solved in $O(n \log n)$ operations by using the preconditioned conjugate gradient method with T. Chan's circulant preconditioners, see [52].

We note that in practical cases, no prior knowledge is usually available on the autocovariances of the process. If m data samples have been taken, then all the information we have is contained in the finite number of data points $\{x(t)\}_{t=1}^m$. In this case, one can still formulate a well-defined least squares prediction problem by estimating the autocovariances from the data samples $\{x(t)\}_{t=1}^m$ with various types of windowing methods. The least squares estimators can then be found by solving for the n-vector b in $\min ||d - Ab||_2$. Here A is an m-by-n Toeplitz matrix with full column rank n, obtained by applying various types of windowing methods on the data samples $\{x(t)\}_{t=1}^m$. The solution b can be obtained by solving the normal equations $(A^*A)b = A^*d$. In [52], it has been shown that under certain practical assumptions in many signal processing applications, the spectra of the preconditioned matrices will be clustered around 1 with probability 1. We also remark that in [51, 53, 54], these techniques have been extended and applied to linear-phase least squares filtering, sliding window and exponentially-weighted recursive least squares filtering in signal processing applications.

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