Circulant Preconditioners for Hermitian Toeplitz Systems

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Abstract. We study the solutions of Hermitian positive definite Toeplitz systems $Ax = b$ by the preconditioned conjugate gradient method for three families of circulant preconditioners C. The convergence rates of these iterative methods depend on the spectrum of $C^{-1}A$. For a Toeplitz matrix A with entries which are Fourier coefficients of a positive function f in the Wiener class, we establish the invertiblity of C, and that the spectrum of the preconditioned matrix $C^{-1}A$ clusters around one. We prove that if f is $(l+1)$-times differentiable, with $l > 0$, then the error after $2q$ conjugate gradient steps will decrease like $((q-1)!)^{-2l}$. We also show that if C copies the central diagonals of A, then C minimizes $||C - A||_1$ and $||C - A||_\infty$.

Abbreviated Title. Hermitian Toeplitz Systems

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1. Introduction.

In this paper we discuss the solutions to a class of Hermitian positive definite Toeplitz systems $Ax = b$ by the preconditioned conjugate gradient method. Direct methods that are based on the Levinson recursion formula are in constant use; see for instance, Levinson [10] and Trench [12]. For an n by n Toeplitz matrix A_n, these methods require $O(n^2)$ operations. Faster algorithms that require $O(n \log^2 n)$ operations have been developed, see Bitmead and Anderson [1] and Brent, Gustavson and Yun [2]. The stability properties of these direct methods for symmetric positive definite matrices are discussed in Bunch [3].

In [11], Strang proposed using preconditioned conjugate gradient method with circulant preconditioners for solving symmetric positive definite Toeplitz systems. The number of operations per iteration is of order $O(n \log n)$ as circulant systems can be solved efficiently by the Fast Fourier Transform. R. Chan and Strang [4] then considered using a circulant preconditioner S_n that is obtained by copying the central diagonals of A_n and bringing them around to complete the circulant. In that paper, we proved that if the underlying generating function f, the Fourier coefficients of which give the entries of A_n, is a positive function in the Wiener class, then for n sufficiently large, S_n and S_n^{-1} are uniformly bounded in the l_2 norm and that the eigenvalues of the preconditioned matrix $S_n^{-1}A_n$ cluster around 1. We note that f is an even function since the matrices A_n are symmetric.

In this paper, we extend these results to Hermitian positive definite Toeplitz systems. More precisely, we show in §2 that if the generating function f is a real-valued positive function in the Wiener class, then the spectrum of $S_n^{-1}A_n$ is clustered around 1. We remark that the proof given in R. Chan and Strang [4] cannot be readily generalized to cover this case. In fact, for Hermitian A_n, the Hankel matrices $H_{n/2}$ used in the proof in [4] are not Hermitian, and the Circulant-Toeplitz eigenvalue problem cannot be split into two similar Toeplitz-Hankel eigenvalue problems. In §3, we establish the superlinear convergence rate of the conjugate gradient method when applied to these preconditioned systems. In particular, we show that if f is $(l+1)$-times differentiable, with $l > 0$, then the error after $2q$ conjugate gradient steps will decrease like $((q-1)!)^{-2l}$.

In §4, we discuss other viable preconditioners for the same problem. We show that the preconditioned systems for these preconditioners also have clustered spectra around 1 for large n and that they all have the same asymptotic convergence rate. In §5, we show that the preconditioner that copies the central diagonals of A_n is optimal in the sense that it minimizes $||C_n - A_n||_1 = ||C_n - A_n||_\infty$ over all Hermitian circulant matrices C_n. Finally, numerical results are given in §6.

2. The Spectrum of the Preconditioned Matrix.

Let us first assume that the Hermitian Toeplitz matrices A_n are finite sections of a fixed singly infinite positive definite matrix A_∞, see R. Chan and Strang [4]. Thus the (i,j)-th entries of A_n and A_∞ are a_{i-j}, with $a_k = \bar{a}_{-k}$ for all k. We associate with A_∞ the real-valued generating function

$$f(\theta) = \sum_{-\infty}^{\infty} a_k e^{-ik\theta},$$

defined on $[0, 2\pi)$. We will assume that f is a positive function and is in the Wiener class, i.e. the sequence $\{a_k\}_{k=-\infty}^{\infty}$ is in l_1. It then easily follows that the A_n are Hermitian positive definite matrices for all n, see for instance, Grenander and Szegö [8]. Moreover, if

$$0 < f_{\min} < f < f_{\max} < \infty,$$

then the spectrum $\sigma(A_n)$ of A_n satisfies

$$\sigma(A_n) \subseteq [f_{\min}, f_{\max}]. \tag{1}$$

Let S_n be the Hermitian circulant preconditioner that copies the central diagonals of A_n. More precisely, the entries $s_{ij} = s_{i-j}$ of S_n are given by

$$s_k = \begin{cases} a_k & 0 \le k \le m, \\ a_{k-n} & m < k < n, \\ \bar{s}_{-k} & 0 < -k < n. \end{cases} \tag{2}$$

For simplicity, we are assuming here and in the following that $n = 2m+1$. The case where $n = 2m$ can be treated similarly, and in that case, we define $s_m = (a_m + a_{-m})/2$, see (17) below.

We will show that $S_n^{-1}A_n$ has a clustered spectrum. We first note that

Theorem 1. *Suppose f is positive and is in the Wiener class. Then for large n, the circulants S_n and S_n^{-1} are uniformly bounded in the l_2 norm. In fact, for large n, the spectrum $\sigma(S_n)$ of S_n satisfies*

$$\sigma(S_n) \subseteq [f_{\min}, f_{\max}]. \tag{3}$$

The proof of this Theorem is similar to the proof of Theorem 1 of R. Chan and Strang [4], and we therefore omit it.

Next we show that $A_n - S_n$ has a clustered spectrum:

Theorem 2. *Let f be a positive function in the Wiener class, then for all $\epsilon > 0$, there exist M and $N > 0$ such that for all $n > N$, at most M eigenvalues of $S_n - A_n$ have absolute values exceeding ϵ.*

Proof: Clearly $B_n = S_n - A_n$ is a Hermitian Toeplitz matrix with entries $b_{ij} = b_{i-j}$ given by

$$b_k = \begin{cases} 0 & 0 \le k \le m, \\ a_{k-n} - a_k & m < k < n, \\ \bar{b}_{-k} & 0 < -k < n. \end{cases} \tag{4}$$

Since f is in the Wiener class, for all given $\epsilon > 0$, there exists an $N > 0$, such that $\sum_{k=N+1}^{\infty} |a_k| < \epsilon$. Let $U_n^{(N)}$ be the n by n matrix obtained from B_n by replacing the $(n-N)$ by $(n-N)$ leading principal submatrix of B_n by the zero matrix. Then $\text{rank}(U_n^{(N)}) \le 2N$. Let $W_n^{(N)} \equiv B_n - U_n^{(N)}$. The leading $(n-N)$ by $(n-N)$ block of $W_n^{(N)}$ is the leading $(n-N)$ by $(n-N)$ principal submatrix of B_n, hence this block is a Toeplitz matrix, and it is easy to see that the maximum absolute column sum of $W_n^{(N)}$ is attained at the first column (or the $(n-N-1)$-th column). Thus

$$||W_n^{(N)}||_1 = \sum_{k=m+1}^{n-N-1} |b_k| = \sum_{k=m+1}^{n-N-1} |a_{k-n} - a_k| \le \sum_{k=N+1}^{n-N-1} |a_k| < \epsilon. \tag{5}$$

Since $W_n^{(N)}$ is Hermitian, we have $||W_n^{(N)}||_\infty = ||W_n^{(N)}||_1$. Thus

$$||W_n^{(N)}||_2 \le (||W_n^{(N)}||_1 \cdot ||W_n^{(N)}||_\infty)^{\frac{1}{2}} < \epsilon.$$

Hence the spectrum of $W_n^{(N)}$ lies in $(-\epsilon, \epsilon)$. By Cauchy Interlace Theorem, see Wilkinson [13], we see that at most $2N$ eigenvalues of $B_n = S_n - A_n$ have absolute values exceeding ϵ. $\square$

Combining Theorems 1 and 2, and using the fact that

$$S_n^{-1}A_n = I_n + S_n^{-1}(A_n - S_n),$$

we have

Corollary. *Let f be a positive function in the Wiener class, then for all $\epsilon > 0$, there exist N and $M > 0$, such that for all $n > M$, at most N eigenvalues of $S_n^{-1}A_n - I_n$ have absolute values larger than ϵ.*

Thus the spectrum of $S_n^{-1}A_n$ is clustered around one for large n.

3. Superlinear Convergence Rate.

It follows easily from the Corollary of the last section that the conjugate gradient method, when applied to the preconditioned system $S_n^{-1}A_n$, converges superlinearly. More precisely, for all $\epsilon > 0$, there exists a constant $C(\epsilon) > 0$ such that the error vector e_q at the q-th iteration satisfies

$$||e_q|| \le C(\epsilon)\epsilon^q||e_0||, \tag{6}$$

where $||x||^2 \equiv x^* S_n^{-\frac{1}{2}} A S_n^{-\frac{1}{2}} x$, see R. Chan and Strang [4] for a proof. Thus the number of iterations to achieve a fixed accuracy remains bounded as the matrix order n is increased. Since each iteration requires $O(n \log n)$ operations using the Fast Fourier Transform, see Strang [11], the work of solving the equation $A_n x = b$ to a given accuracy δ is $c(f, \delta) n \log n$, where $c(f, \delta)$ is a constant that depends on f and δ only.

We note that if extra smoothness conditions are imposed on f, we can get a more precise bound on the convergence rate:

Theorem 3. *Let f be a $(l+1)$-times differentiable function with its $(l+1)$-th derivative of f in $L^1[0,2\pi)$, $l>0$. Then for large n,*

$$||e_{2q}|| \leq \frac{c^q}{((q-1)!)^{2l}} ||e_0||, \tag{7}$$

for some constant c that depends on f and l only.

Proof: We remark that from the standard error analysis of the conjugate gradient method, we have

$$||e_q|| \leq [\min_{P_q} \max_{\lambda} |P_q(\lambda)|]\ ||e_0||, \tag{8}$$

where the minimum is taken over polynomials of degree q with constant term 1 and the maximum is taken over the spectrum of $S_n^{-1}A_n$, or equivalently, the spectrum of $S_n^{-\frac{1}{2}}A_nS_n^{-\frac{1}{2}}$, see for instance, Golub and van Loan [7]. In the following, we will try to estimate that minimum.

We first note that the assumptions on f imply that

$$|a_j| \leq \frac{\hat{c}}{|j|^{l+1}} \quad \forall j,$$

where $\hat{c} = ||f^{(l+1)}||_{L^1}$, see, for instance, Katznelson [9]. Hence

$$\sum_{j=k+1}^{n-k-1} |a_j| \leq \hat{c} \sum_{j=k+1}^{n-k-1} \frac{1}{|j|^{l+1}} \leq \hat{c} \int_k^{\infty} \frac{dx}{x^{l+1}} \leq \frac{\hat{c}}{k^l}, \quad \forall k \geq 1. \tag{9}$$

As in Theorem 2, we write

$$B_n = W_n^{(k)} + U_n^{(k)}, \quad \forall k \geq 1,$$

where $U_n^{(k)}$ is the matrix obtained from B_n by replacing its $(n-k)$ by $(n-k)$ principal submatrix of B_n by a zero matrix. Using the arguments in Theorem 2, cf (5) and (9), we see that $\text{rank}(U_n^{(k)}) \leq 2k$ and $||W_n^{(k)}||_2 \leq \hat{c}/k^l$, for all $k \geq 1$. Now consider

$$S_n^{-\frac{1}{2}}B_nS_n^{-\frac{1}{2}} = S_n^{-\frac{1}{2}}W_n^{(k)}S_n^{-\frac{1}{2}} + S_n^{-\frac{1}{2}}U_n^{(k)}S_n^{-\frac{1}{2}} \equiv \tilde{W}_n^{(k)} + \tilde{U}_n^{(k)}.$$

By Theorem 1, we have, for large n, $\mathrm{rank}(\tilde{U}_n^{(k)}) \le 2k$ and

$$||\tilde{W}_n^{(k)}||_2 \le ||S_n^{-1}||_2 ||W_n^{(k)}||_2 \le \frac{\tilde{c}}{k^l}, \quad \forall k \ge 1, \tag{10}$$

with $\tilde{c} = \hat{c}/f_{\min}$.

Next we note that $W_n^{(k)} - W_n^{(k+1)}$ can be written as the sum of two rank one matrices of the form:

$$W_n^{(k)} - W_n^{(k+1)} = u_k v_k^* + v_k u_k^* = \frac{1}{2}(w_k^+ w_k^{+*} - w_k^- w_k^{-*}), \quad \forall k \ge 0.$$

Here u_k is the $(n-k)$-th unit vector, $v_k = (b_{n-k-1}, \cdots, b_1, b_0/2, 0, \cdots, 0)$, with b_j given by (4), and $w_k^{\pm} = u_k \pm v_k$. Hence by letting $z_k^{\pm} = S_n^{-\frac{1}{2}} w_k^{\pm}$ for $k \ge 0$, we have

$$\begin{aligned} S_n^{-\frac{1}{2}} B_n S_n^{-\frac{1}{2}} &= \tilde{W}_n^{(0)} = \tilde{W}_n^{(k)} + \frac{1}{2}\sum_{j=0}^{k-1}(z_j^+ z_j^{+*} - z_j^- z_j^{-*}), \\ &= \tilde{W}_n^{(k)} + V_k^+ - V_k^-, \quad \forall k \ge 1, \end{aligned} \tag{11}$$

where $V_k^{\pm} \equiv \frac{1}{2}\sum_{j=0}^{k-1} z_j^{\pm} z_j^{\pm *}$ are positive semi-definite matrices of rank k. Let us order the eigenvalues of $\tilde{W}_n^{(0)}$ as

$$\mu_0^- \le \mu_1^- \le \cdots \le \mu_1^+ \le \mu_0^+.$$

By applying Cauchy Interlace Theorem to (11) and using the bound of $||\tilde{W}_n^{(k)}||_2$ in (10), we see that for all $k \ge 1$, there are at most k eigenvalues of $\tilde{W}_n^{(0)}$ lying to the right of $\tilde{c}/k^l$, and there are at most k of them lying to the left of $-\tilde{c}/k^l$. More precisely, we have

$$|\mu_k^{\pm}| \le ||\tilde{W}_n^{(k)}||_2 \le \frac{\tilde{c}}{k^l}, \quad \forall k \ge 1.$$

Using the identity

$$S_n^{-\frac{1}{2}} A_n S_n^{-\frac{1}{2}} = I_n + S_n^{-\frac{1}{2}} B_n S_n^{-\frac{1}{2}} = I_n + \tilde{W}_n^{(0)},$$

we see that if we order the eigenvalues of $S_n^{-\frac{1}{2}} A_n S_n^{-\frac{1}{2}}$ as

$$\lambda_0^- \le \lambda_1^- \le \cdots \le \lambda_1^+ \le \lambda_0^+,$$

then $\lambda_k^\pm = 1 + \mu_k^\pm$ for all $k \geq 0$ with

$$1 - \frac{\tilde{c}}{k^l} \leq \lambda_k^- \leq \lambda_k^+ \leq 1 + \frac{\tilde{c}}{k^l}, \quad \forall k \geq 1. \tag{12}$$

For $\lambda_0^\pm$, the bounds are obtained from (1) and (3):

$$\frac{f_{\min}}{f_{\max}} \leq \lambda_0^- \leq \lambda_0^+ \leq \frac{f_{\max}}{f_{\min}}. \tag{13}$$

Having obtained the bounds for $\lambda_k^\pm$, we can now construct the polynomial that will give us a bound for (8). Our idea is to choose P_{2q} that annihilates the q extreme pairs of eigenvalues. Thus consider

$$p_k(x) = (1 - \frac{x}{\lambda_k^+})(1 - \frac{x}{\lambda_k^-}), \quad \forall k \geq 1.$$

Between those roots $\lambda_k^\pm$, the maximum of $|p_k(x)|$ is attained at the average $x = \frac{1}{2}(\lambda_k^+ + \lambda_k^-)$, where by (12), we have

$$\max_{x \in [\lambda_k^-, \lambda_k^+]} |p_k(x)| = \frac{(\lambda_k^+ - \lambda_k^-)^2}{4\lambda_k^+\lambda_k^-} \leq (\frac{2\tilde{c}}{k^l})^2 \cdot (\frac{f_{\max}}{2f_{\min}})^2 = (\frac{\tilde{c}f_{\max}}{f_{\min}})^2 \cdot \frac{1}{k^{2l}}, \quad \forall k \geq 1,$$

Similarly, for $k = 0$, we have, by using (13),

$$\max_{x \in [\lambda_0^-, \lambda_0^+]} |p_0(x)| = \frac{(\lambda_0^+ - \lambda_0^-)^2}{4\lambda_0^+\lambda_0^-} \leq \frac{(f_{\max}^2 - f_{\min}^2)^2}{4f_{\min}^4}.$$

Hence the polynomial $P_{2q} = p_0 p_1 \cdots p_{q-1}$, which annihilates the q extreme pairs of eigenvalues, satisfies

$$|P_{2q}(x)| \leq \frac{c^q}{((q-1)!)^{2l}}, \tag{14}$$

for some constant c that depends only on f and l. This holds for all $\lambda_k^\pm$ in the inner interval between λ_{q-1}^- and λ_{q-1}^+, where the remaining eigenvalues are. Equation (7) now follows directly from (8) and (14). $\Box$

4. Other Circulant Preconditioners.

The proof of Theorem 2 suggests that there are many other viable preconditioners that can give us the same asymptotic convergence rate. One example is given by the circulant matrix T_n proposed by T. Chan [6]. It is obtained by averaging the corresponding diagonals of A_n with the diagonals of A_n being extended to length n by a wrap-around. More precisely, the entries $t_{ij} = t_{i-j}$ of T_n are given by

$$t_k = \begin{cases} \frac{1}{n}\{k a_{k-n} + (n-k)a_k\} & 0 \le k < n, \\ \bar{t}_{-k} & 0 < -k < n, \end{cases}$$

where a_n is taken to be 0. He proved that such T_n minimizes the Frobenius norm $||T_n - A_n||_F$ over all possible circulant matrices T_n. The entries $b_{ij} = b_{i-j}$ of $T_n - A_n$ are given by

$$b_k = \begin{cases} \frac{k}{n}(a_{k-n} - a_k) & 0 \le k < n, \\ \bar{b}_{-k} & 0 < -k < n. \end{cases}$$

As in Theorem 2, we let $W_n^{(N)}$ to be the matrix obtained from $T_n - A_n$ by replacing the last N rows and N columns of $T_n - A_n$ by zero vectors. We see that

$$||W_n^{(N)}||_1 \le 2 \sum_{k=0}^{n-N-1} |b_k| \le 2 \sum_{k=0}^{N} \frac{k}{n}|a_k| + 4 \sum_{k=N+1}^{n} |a_k|. \tag{15}$$

Now let $M > N$ be such that $\frac{1}{M}\sum_{k=0}^{N} k|a_k| < \epsilon$. Then for all $n > M$, we have $||W_n^{(N)}||_1 < 6\epsilon$. Hence the eigenvalues of $T_n - A_n$ are clustered around zero, except for at most $2N$ of them. We remark that by using results in R. Chan [5], we can show that $\lim_{n\to\infty} ||S_n - T_n||_2 = 0$ and that the convergence rate of $S_n^{-1}A_n$ and $T_n^{-1}A_n$ are the same for large n. In particular, both will converge superlinearly.

As another example, let us consider the circulant matrix R_n with entries $r_{ij} = r_{i-j}$ given by

$$r_k = \begin{cases} a_{k-n} + a_k & 0 \le k < n, \\ \bar{r}_{-k} & 0 < -k < n, \end{cases}$$

where a_n is again taken to be 0. The entries $b_{ij} = b_{i-j}$ of $R_n - A_n$ are given by

$$b_k = \begin{cases} a_{k-n} & 0 \le k < n, \\ \bar{b}_{-k} & 0 < -k < n. \end{cases}$$

It is easily seen that the conclusion of Theorem 2 holds for this preconditioner too, cf (5) and (15). Similar to the case of T_n, we can also show that $\lim_{n\to\infty} ||S_n - R_n||_2 = 0$ and that the convergence rate of $S_n^{-1}A_n$ and $R_n^{-1}A_n$ are the same for large n, see R. Chan [5]. Numerical results in §6 indeed show that the three preconditioners R_n, S_n and T_n behave almost the same for large n.

5. The Optimality of S_n.

From the discussion in §§2 and 4, we know that it is interesting to obtain the Hermitian circulant matrix C_n that minimizes the norm $||C_n - A_n||_1 = ||C_n - A_n||_\infty$. The minimum is attained by S_n:

Theorem 4. *The circulant matrix S_n whose entries are given by (2) minimizes $||C_n - A_n||_1 = ||C_n - A_n||_\infty$ over all possible Hermitian circulant matrices C_n.*

Proof: Let us construct the circulant matrix C_n that minimizes the absolute column sums of $C_n - A_n$. Let the (i,j)-th entries of C_n be $c_{ij} = c_{i-j}$. Since C_n is Hermitian and circulant, we have $c_k = \bar{c}_{n-k}$ for $k = 1, \ldots, m$, where $m = (n-1)/2$. Hence C_n is determined by $\{c_k\}_{k=0}^m$. For $j = 0, \ldots, n-1$, the j-th absolute column sum u_j of $C_n - A_n$ is given by

$$u_j = \sum_{k=0}^{n-1-j} |a_k - c_k| + \sum_{k=1}^{j} |\bar{a}_k - \bar{c}_k|. \tag{16}$$

We note that $u_{n-1-j} = u_j$ for $0 \le j < n$. Hence it suffices to consider u_j for $0 \le j \le m$. The term involving c_0 in (16) is $|a_0 - c_0|$ which has its minimum at $c_0 = a_0$. For $k = 1, \ldots, m$, the terms involving c_k in (16) are either of the form

$$\text{(a)} \quad |a_k - c_k| + |\bar{a}_k - \bar{c}_k| = 2|a_k - c_k|,$$

$$\text{or (b)} \quad |a_k - c_k| + |a_{n-k} - c_{n-k}| = |a_k - c_k| + |\bar{a}_{n-k} - c_k|.$$

In case (a), the minimum is at $c_k = a_k$. In case (b), the minimum occurs at any c_k lying on the line segment joining a_k and $\bar{a}_{n-k}$. In particular, (a) and (b) attain their minima at $c_k = a_k$. Thus C_n so constructed is the same as the S_n given by (2).

Now for any other Hermitian circulant matrix H_n, the j-th absolute column sum v_j of $H_n - A_n$ will satisfy $u_j \leq v_j$, for $j = 0, \ldots, n-1$. Hence,

$$||S_n - A_n||_1 = \max_j u_j \leq \max_j v_j = ||H_n - A_n||_1. \quad \square$$

Remark: When $n = 2m$ is even, c_m is real since C_n is both Hermitian and circulant. The term involving c_m in u_j takes the form $|a_m - c_m|$ or $|\bar{a}_m - c_m|$. Since $u_j = u_{n-1-j}$ for $j = 0, \cdots, n-1$, we see that c_m should be chosen such that both terms are minimized, i.e,

$$c_m = \frac{1}{2}(a_m + \bar{a}_m). \tag{17}$$

6. Numerical Results.

To test the convergence rates of the preconditioners, we have applied the preconditioned conjugate gradient method to $A_n x = b$ with

$$a_k = \begin{cases} \dfrac{1+\sqrt{-1}}{(1+k)^{1.1}} & k > 0, \\ 2 & k = 0, \\ \bar{a}_{-k} & k < 0. \end{cases}$$

The underlying generating function f is given by

$$f(\theta) = 2\sum_{k=0}^{\infty} \frac{\sin(k\theta) + \cos(k\theta)}{(1+k)^{1.1}}.$$

Clearly f is in the Wiener class. The spectra of A_n, $R_n^{-1}A_n$, $S_n^{-1}A_n$ and $T_n^{-1}A_n$ for $n = 32$ are represented in Figure 1. Table 1 shows the number of iterations required to make $||r_q||_2/||r_0||_2 < 10^{-7}$, where r_q is the residual vector after q iterations. The right hand side b is the vector of all ones and the zero vector is our initial guess. We see that as n increases, the number of iterations increases like $O(\log n)$ for the original matrix A_n, while it stays almost the same for the preconditioned matrices. Moreover, all preconditioned systems converge at the same rate for large n.

n	A_n	$R_n^{-1}A_n$	$S_n^{-1}A_n$	$T_n^{-1}A_n$
16	13	7	8	7
32	15	6	7	6
64	18	7	7	7
128	19	7	7	7
256	21	7	7	7

Table 1. Number of Iterations for Different Systems

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