Numerical Experiments with Monte Carlo Methods and SPAI Preconditioner for Solving System of Linear Equations

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Abstract. In this paper we present the results of experiments comparing the performance of the mixed Monte Carlo algorithms and SPAI preconditioner with BICGSTAB. The experiments are carried out on a Silicon Graphics ONYX2 machine. Based on our experiments, we conclude that these techniques are comparable from the point of view of robustness and rates of convergence, with the Monte Carlo approach performing better for some general cases and SPAI approach performing better in case of very sparse matrices.

Keywords: Sparse Linear Systems, Preconditioned iterative methods, approximate inverse, SPAI, Monte Carlo methods.

1 Introduction

Consider a system of linear algebraic equations (SLAE) presented in the form:

$$Ax = b \tag{1}$$

where A is a real square $n \times n$ matrix, $x = (x_1, x_2, \dots, x_n)^t$ is a $1 \times n$ solution vector and $b = (b_1, b_2, \dots, b_n)^t$.

There are now quite a few deterministic methods based on Krylov subspace methods for solving general linear systems such as GMRES, BI-CGSTAB and QMR. In order to be effective these methods must be combined with a good preconditioner, and it is generally agreed that the choice of the preconditioner is even more crucial than the choice of the Krylov subspace iteration. The search for effective preconditioners is an active research topic in scientific computing. Several potentially successful methods have been proposed in the literature, and the SPAI preconditioner is regarded as one of the most promising approaches [4–6]. However Monte Carlo methods are coming to play a role in finding a rough approximate inverse and few efficient parallel Monte Carlo approaches for MI have been presented in the past few years [7, 1]. Nowadays, parallel Monte Carlo

methods can be one of the most promising approaches for solving SLAE and also be an efficient preconditioner. We tested the algorithms solving general systems of linear equations, where the corresponding matrices were generated by simple generator constructing general dense and sparse matrices, which were stored in a row-packed format. Some matrices from the matrix market have also been used. We used Silicon Graphics ONYX2 machine to carry out the experiments.

The ideas of Monte Carlo for Matrix Computation are presented in Section 2, the main algorithm is described in Section 3 and the parallel approach and some numerical experiments are presented in Section 4.

2 Monte Carlo for Matrix Computation

Let us assume that we need to solve a general SLAE in form (1). Consider the general case when $\|I - A\| \geq 1$. We consider the splitting $A = B_n - B_1$, where the off-diagonal elements of B_n are the same as A . The diagonal elements of B_n are defined as $b_{ii} = a_{ii} + \gamma_i \|A\|$, choosing in most cases $\gamma_i > 1, i = 1, 2, \dots, n$. We then split $B_n = M - K$, where M is diagonal matrix of B_n . We could transform system (1) to

$$x = Cx + f \quad (2)$$

where $C = B_n^{-1}B_1$ and $f = B_n^{-1}b$. The multipliers γ_i are chosen so that they reduce the norm of C and reduce the number of Markov chains required to reach a given precision, in a similar way as proposed in [3]. Therefore we consider two possibilities, first, finding the solution of $x = Cx + f$ using Monte Carlo (MC) method and, second, finding A^{-1} and obtaining the solution via $x = A^{-1}f$. In this paper we are more interested in the second idea as a general goal, where we compute the approximate inverse of B_n with MC, then retrieve A^{-1} via a function that will be introduced in the next section.

Consider firstly the stochastic approach. Assume that the system is transformed to its iterative form (2). Consider now the Markov Chain given by:

$$s_0 \rightarrow s_1 \rightarrow \dots \rightarrow s_k \quad (3)$$

where the $s_i, i = 1, 2, \dots, k$, belongs to the state space $S = \{1, 2, \dots, n\}$. Then for $\alpha, \beta \in S, p_0(\alpha) = p(s_0 = \alpha)$ is the probability that the Markov chain starts at state α and $p(s_{j+1} = \beta | s_j = \alpha) = p_{\alpha\beta}$ is the transition probability from state α to state β . The set of all probabilities $p_{\alpha\beta}$ defines a transition probability matrix $P = \{p_{\alpha\beta}\}_{\alpha, \beta=1}^n$ [7] [8]. We say that the distribution $(p_1, \dots, p_n)^t$ is acceptable for a given vector g , and that the distribution $p_{\alpha\beta}$ is acceptable for matrix C , if $p_\alpha > 0$ when $g_\alpha \neq 0$, and $p_\alpha \geq 0$, when $g_\alpha = 0$, and $p_{\alpha\beta} > 0$ when $C_{\alpha\beta} \neq 0$, and $p_{\alpha\beta} \geq 0$ when $C_{\alpha\beta} = 0$ respectively. We assume $\sum_{\beta=1}^n p_{\alpha\beta} = 1$, for all $\alpha = 1, 2, \dots, n$. Generally, we define

$$W_0 = 1, W_j = W_{j-1} \frac{C_{s_{j-1}s_j}}{p_{s_{j-1}s_{j-1}}} \quad (4)$$

for $j = 1, 2, \dots, n$.

Consider now the random variable $\theta[g] = \frac{g_{s_0}}{p_{s_0}} \sum_{i=1}^{\infty} W_i f_{s_i}$. We use the following notation for the partial sum:

$$\theta_i[g] = \frac{g_{s_0}}{p_{s_0}} \sum_{j=0}^i W_j f_{s_j}. \quad (5)$$

Under the condition $\|C\| < 1$, the corresponding Neumann series converges for any given f , and $E\theta_i[g]$ tends to (g, x) as $i \rightarrow \infty$. Thus, $\theta_i[g]$ can be considered as an estimate of (g, x) for i sufficiently large. To find an arbitrary component of the solution, for example, the r^{th} component of x , we should choose,

$$g = e(r) = \underbrace{(0, \dots, 1, 0, \dots, 0)}_r \text{ such that}$$

$$e(r)_\alpha = \delta_{r\alpha} = \begin{cases} 1 & \text{if } r = \alpha \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

It follows that

$$(g, x) = \sum_{\alpha=1}^n e(r)_\alpha x_\alpha = x_r. \quad (7)$$

The corresponding Monte Carlo method is given by

$$x_r = \hat{\theta} = \frac{1}{N} \sum_{s=1}^N \theta_i[e(r)]_s$$

where N is the number of chains and $\theta_i[e(r)]_s$ is the approximate value of x_r in the s^{th} chain. It means that using Monte Carlo method, we can estimate only one, few or all elements of the solution vector. We consider Monte Carlo with uniform transition probability (UM) $p_{\alpha\beta} = \frac{1}{n}$ and Almost optimal Monte Carlo method (MAO) with $p_{\alpha\beta} = \frac{|C_{\alpha\beta}|}{\sum_{\beta=1}^n |C_{\alpha\beta}|}$, where $\alpha, \beta = 1, 2, \dots, n$. Monte Carlo MI is obtained in a similar way [7, 1].

To find the approximate inverse $Q^{-1} = \{q_{rr'}\}_{r, r'=1}^n$ of some matrix T , we must first compute matrix

$$F = I - T, \quad (8)$$

where I is the identity matrix. Clearly, the inverse matrix is given by

$$Q = \sum_{i=0}^{\infty} F^i, \quad (9)$$

which converges if $\|F\| < 1$.

To estimate the element $q_{rr'}$ of the inverse matrix Q , we let the vector f be the following unit vector

$$f_{r'} = e(r'). \quad (10)$$

We then can use the following Monte Carlo method for calculating elements of the inverse matrix Q :

$$q_{rr'} \approx \frac{1}{N} \sum_{s=1}^N \left[\sum_{(j|s_j=r')} W_j \right], \quad (11)$$

where $(j|s_j = r')$ means that only

$$W_j = \frac{F_{rs_1} F_{s_1 s_2} \cdots F_{s_{j-1} s_j}}{p_{rs_1} p_{s_1 s_2} \cdots p_{s_{j-1} s_j}} \quad (12)$$

for which $s_j = r'$ are included in the sum (11).

Since W_j is included only in the corresponding sum of $r' = 1, 2, \dots, n$, the same set of N chains can be used to compute a single row of the inverse matrix, which is one of the inherent properties of MC making them suitable for parallelization.

The *probable error* of the method, is defined as $r_N = 0.6745\sqrt{D\theta/N}$, where $P\{|\bar{\theta} - E(\theta)| < r_N\} \approx 1/2 \approx P\{|\bar{\theta} - E(\theta)| > r_N\}$, if we have N independent realizations of random variable (r.v.) θ with mathematical expectation $E\theta$ and average $\bar{\theta}$ [8].

3 The parallel approximate methods

It is well-known that Monte Carlo (MC) methods are efficient for solving systems of linear algebraic equations. Initially MC methods have been applied to SLAEs with $\|I - A\| < 1$. In the further developments [7, 3, 2] MC methods have been applied to solve SLAE with diagonally dominant and M-matrices. To use Monte Carlo algorithms for solving general systems of linear equations, we developed a new mixed algorithm, where for the system (1), firstly, we construct a diagonal dominant matrix B_n whose off-diagonal elements are the same as those of A , then, secondly we compute the approximate inverse matrix of B_n [3] using the algorithm below.

1. **Initial data:** Input matrix B_n , parameters δ and ϵ .
2. **Preprocessing:**
 - 2.1 **Split** $B_n = M - K$ where M is a diagonal matrix $m_{ii} = b_{ii}$ $i = 1, 2, \dots, n$.
 - 2.2 **Compute** the matrix $C = M^{-1}K$.
 - 2.3 **Compute** $\|C\|$ and the Number of Markov Chains $N = \left(\frac{0.6745}{\epsilon}, \frac{1}{(1-\|C\|)}\right)^2$.
3. **For** $i=1$ to n ;
 - 3.1 **For** $j=1$ to $j=N$;

Markov Chain Monte Carlo Computation:

 - 3.1.1 **Set** $t_k = 0$ (stopping rule), $W_0 = 1$, $SUM[i] = 0$ and $Point = i$.
 - 3.1.2 **Generate** an uniformly distributed random number giving *nextpoint*.
 - 3.1.3 **If** $C[point][netxpoint]! = 0$.

LOOP

- 3.1.3.1 **Compute** $W_j = W_{j-1} \frac{C[\text{point}][\text{netxpoint}]}{P[\text{point}][\text{netxpoint}]}$.
- 3.1.3.2 **Set** $\text{Point} = \text{nextpoint}$ and $SUM[i] = SUM[i] + W_j$.
- 3.1.3.3 **If** $|W_j| < \delta$, $t_k = t_k + 1$
- 3.1.3.4 **If** $t_k \geq n$, end LOOP.
- 3.1.4 **End If**
- 3.1.5 **Else** go to step 3.1.2.
- 3.2 **End of loop j.**
- 3.3 **Compute** the average of results.
4. **End of loop i.**
5. **Obtain** The matrix $Z = (I - C)^{-1}$. then the expecting approximate matrix $Y_n = Z \times M^{-1}$.

Finally we retrieve the inversion matrix of A via the following function [2]:

$$Y_{n-1} = Y_n + \frac{Y_n S_n Y_n}{1 - \text{trace}(Y_n S_n)}, \quad (13)$$

where Y_n is the computed approximate inverse of B , $S_n = B_n - \text{diag}(A)$, n is a sequence of integers ranging from one to the size of the matrix A . It is obvious that the approximate solution vector can be obtained by $A^{-1} * b$. Indeed, before we retrieve A^{-1} we also can apply the following refinement function

$$Y_n^{\text{new}} = Y_n^{\text{old}} (2 \times I - Y_n^{\text{old}} B_n), \quad (14)$$

where I denotes the identity matrix. Clearly the precision of the approximate solution vector can be controlled using the refinement function with just 1 or 2 steps. From the experimental work is evident that the number of steps required to obtain almost exact solution is at most 3 or 4.

On the other hand we studied the SPAI preconditioner, which is based on the idea of Frobenius norm minimization. The approximate inverse matrix of A is computed as matrix M which minimizes $\|I - MA\|$ (or $\|I - AM\|$ for the right preconditioning) subject to some sparsity constraints, see [4, 5]. Once the approximate inverse matrix of A is known, SPAI applies BICGSTAB to solve (1) (see <http://www.sam.math.ethz.ch/~grote/spai/>)

Now we have introduced both algorithms in brief. We will use both of them to solve general SLAEs.

4 Parallel Implementation and Numerical Results

The Monte Carlo code is written in C using PVM and the SPAI code is written in C using MPI. To test the two approaches we consider matrices from the Matrix Market (<http://math.nist.gov/MatrixMarket/>) and some general matrices randomly generated by the generator we provide. The generator generates random numbers for the matrices with predefined sparsity. The experiments are carried out on a Silicon Graphics ONYX2 parallel machine with 12 processors (four 195 MHZ and eight - 400 MHZ), with 5120 Mbytes main memory and 32 Kbytes

cache in total. We run both algorithms with the corresponding parameters. The computing time of the Monte Carlo calculation and the SPAI preconditioner are shown separately. The full time required to solve the SLAEs for mixed algorithms and SPAI with BICGSTAB is also shown. Some of the test matrices used in this experiment are given below.

- **BWM200.MTX** size $n=200$, with $nz=796$ nonzero elements, from Matrix Market web site;
- **CAVITY03.MTX** size $n=327$, with $nz=7327$ nonzero elements, from Matrix Market web site;
- **GEN200_DENSE.MC** size $n=200$, dense, from the generator;
- **GEN200_60SPAR.MC** size $n=200$, with $nz=16000$ nonzero elements, from the generator;
- **GEN800_DENSE.MC** size $n=800$, dense, from the generator;
- **GEN800_70SPAR.MC** size $n=800$, with $nz=192000$ nonzero elements, from the generator;
- **GEN2000_99SPAR.MC** size $n=2000$, with $nz=40000$ nonzero elements, from the generator;
- **GEN500_90SPAR.MC** size $n=500$, with $nz=25000$ nonzero elements, from the generator;
- **GEN1000_95SPAR.MC** size $n=1000$, with $nz=50000$ nonzero elements, from the generator;

The default parameters we set up in Monte Carlo methods are

1. $\epsilon = 0.05$ denotes a given stochastic error;
2. $\delta = 0.01$ denotes the accuracy of Monte Carlo approximation;
3. $step = 1$ denotes how many steps are spent on the refinement function, in each single step of using the refinement function two matrix-by-matrix multiplications are computed.

We apply the appropriate parameters in SPAI and show the best performance with the best combination of these parameters. R-MC denotes the residual computing time of Monte Carlo approach which includes the time for the refinement procedure, the retrieval procedure and obtaining the approximate solution vector. MC denotes the time required for Monte Carlo algorithm only. Therefore, TOTAL-MC is the time required for the MC and R-MC. R-SPAI denotes the residual computing time of SPAI, which includes the time of BICGSTAB for obtaining the approximate solution vector (the block procedure and scalar-matrix procedure while using block algorithm). SPAI denotes the time required by the SPAI preconditioner. TOTAL-SPAI is the total time of SPAI and R-SPAI. ERROR denotes the absolute error of the approximate solution vector given below.

$$ERROR = \frac{\|x_{exact} - x_{approximate}\|_2}{\|x_{exact}\|_2} \quad (15)$$

Para	BL	SPAI	R-SPAI	TOTAL-SPAI	MC	R-MC	TOTAL-MC
0.5	1×1	0.9303448	85.6012096	86.5315544	2.186874	3.164163	5.351037
	3×3	0.9759936	75.2054016	76.1813952			
0.6	1×1	0.8856872	220.1436288	221.029316			
	3×3	0.9230960	150.3301808	151.2532768			
0.7	1×1	1.3930344	351.6003544	352.9933888			
	3×3	1.1148200	160.762056	161.876876			

Table 1. BW200.MTX Solution with parameters: ERROR = 10^{-4} and P=10 processors. SPAI is tested with different values of ϵ , and both blocked and non-blocked.

Para	BL	SPAI	R-SPAI	TOTAL-SPAI	MC	R-MC	TOTAL-MC
0.5	1×1	2.9910024	nan	nan	0.9338300	2.346462	3.280292
	3×3	1.1972320	nan	nan			
0.6	1×1	3.1077280	nan	nan			
	3×3	1.2565296	nan	nan			
0.7	1×1	2.6192136	nan	nan			
	3×3	0.9718288	nan	nan			

Table 2. GEN200_DENSE.MC Solution with parameters: ERROR = 10^{-4} and P=10 processors. SPAI is tested with different values of ϵ , and both blocked and non-blocked.

SPAI is run with the default parameter of iterations in BICGSTAB, 500, and nan means we can not obtain the results under the setting, or it is converging slowly.

P#	MC	TOTAL-MC	SPAI	TOTAL-SPAI
2	76.20574	85.813108	0.2917584	nan
5	36.16877	60.095253	0.5471512	nan
8	28.29067	46.830696	0.3889352	nan
12	21.07290	33.248477	1.3224760	nan

Table 3. CAVITY03.MTX ERROR= 10^{-4} and P=2, 5, 8, 12 processors respectively.

P#	MC	TOTAL-MC	SPAI	TOTAL-SPAI
2	156.1388	586.202544	130.6839168	nan
5	47.70701	385.626890	67.6120952	nan
8	36.74342	304.847875	24.0445288	nan
12	26.53539	294.639845	23.1435808	nan

Table 4. GEN800_70SPAR.MC ERROR= 10^{-4} and P=2, 5, 8, 12 processors respectively.

Matrix	MC	TATOL-MC	SPAI	TOTAL-SPAI
GEN200_60SPAR.MC	1.047589	4.720657	1.1548728	nan
GEN500_90SPAR.MC	7.730741	84.94246	4.1712408	nan
GEN800_DENSE.MC	24.32269	300.3137	29.000558	nan
GEN1000_95SPAR.MC	46.274798	746.9745	9.1504488	nan
GEN2000_99SPAR.MC	302.626325	4649.0219003	6.2901104	nan

Table 5. ERROR= 10^{-4} and P=10 processors

The examples show that for some cases MC converges much faster than SPAI. In case of some general matrices it can be seen that SPAI is converging

very slowly. There are also cases where SPAI is performing much better than MC. Further experiments are required to carry out detailed analysis.

5 Conclusion

We have presented the results of experiments comparing the efficiency of parallel SPAI preconditioner with BICGSTAB and parallel mixed Monte Carlo algorithms. The experiments are carried out on a Silicon Graphics ONYX2 machine. Based on our experiments, we conclude that these techniques are comparable from the point of view of robustness and rates of convergence, with the Monte Carlo approach being somewhat better for some general cases and SPAI approach performing better in case of very sparse matrices. We can also conclude that both techniques offer excellent potential for use on high performance computers.

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