Finding the Smallest Eigenvalue by the Inverse Monte Carlo Method with Refinement^{*}

Vassil Alexandrov¹ and Aneta Karaivanova²

¹ School of Systems Engineering, University of Reading, Reading RG6 6AY, UK
v.n.alexandrov@rdg.ac.uk

<http://www.cs.reading.ac.uk/people/V.Alexandrov.htm>

² IPP - BAS, Acad. G. Bonchev St., Bl.25A, 1113 Sofia, Bulgaria
anet@parallel.bas.bg
<http://parallel.bas.bg/~anet/>

Abstract. Finding the smallest eigenvalue of a given square matrix A of order n is computationally very intensive problem. The most popular method for this problem is the Inverse Power Method which uses LU -decomposition and forward and backward solving of the factored system at every iteration step. An alternative to this method is the Resolvent Monte Carlo method which uses representation of the resolvent matrix $[I - qA]^{-m}$ as a series and then performs Monte Carlo iterations (random walks) on the elements of the matrix. This leads to great savings in computations, but the method has many restrictions and a very slow convergence.

In this paper we propose a method that includes fast Monte Carlo procedure for finding the inverse matrix, refinement procedure to improve approximation of the inverse if necessary, and Monte Carlo power iterations to compute the smallest eigenvalue. We provide not only theoretical estimations about accuracy and convergence but also results from numerical tests performed on a number of test matrices.

Keywords: Monte Carlo methods, eigenvalues, Markov chains, parallel computing, parallel efficiency.

1 Introduction

Let A be a real symmetric matrix. Consider the problem of evaluating the eigenvalues of A , i.e. the values of λ for which

$$Au = \lambda u \tag{1}$$

holds. Suppose, the n eigenvalues of A are ordered as follows $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_{n-1}| > |\lambda_n|$.

^{*} Supported by the Ministry of Education and Science of Bulgaria under Grant No. I1405/04.

It is known that the problem of calculating the smallest eigenvalue of A is more difficult from numerical point of view than the problem of evaluating the largest eigenvalue. Nevertheless, for many applications in physics and engineering it is important to estimate the smallest one, because it usually defines the most stable state of the system which is described by the considered matrix.

2 Background

2.1 Inverse Power Method

One of the most popular methods for finding extremal eigenvalues is the power method ([6], [8]) which for a given matrix A is defined by the iteration

$$x^{new} = Ax^{old}.$$

Except for special starting points, the iterations converge to an eigenvector corresponding to the eigenvalue of A with largest magnitude (**dominant eigenvalue**). The least squares solution μ to the overdetermined linear system

$$\mu x_k = x_{k+1}$$

is an estimate for λ_1 which is called the **Raleigh quotient**.

$$\mu = \frac{x_k^T x_{k+1}}{x_k^T x_k}.$$

Suppose that we want to compute the eigenvector corresponding to the eigenvalue of A of smallest magnitude. Letting (λ_1, e_1) through (λ_n, e_n) denote the eigenpairs of A , the corresponding eigenpairs of $C = A^{-1}$ are $(1/\lambda_1, e_1)$ through $(1/\lambda_n, e_n)$. If λ_n is the eigenvalue of A of smallest magnitude, then $1/\lambda_n$ is C 's eigenvalue of largest magnitude and the power iteration $x^{new} = A^{-1}x^{old}$ converges to the vector e_n corresponding to the eigenvalue $1/\lambda_n$ of $C = A^{-1}$. When implementing the inverse power method, instead of computing the inverse matrix A^{-1} we multiply by A to express the iteration $x^{new} = A^{-1}x^{old}$ in the form $Ax^{new} = x^{old}$. Replacing A by its LU factorization yields

$$(LU)x^{new} = x^{old}. \quad (2)$$

In each iteration of the inverse power method, the new x is obtained from the old x by forward and back solving the factored system (2). This scheme is computationally more efficient. With k iterations, the number of arithmetic operations is $O(kn^2)$ for Power method and $O(n^3 + kn^2)$ for Inverse Power Method.

2.2 Resolvent Monte Carlo Method

Given a matrix A , consider an algorithm based on Monte Carlo iterations by the resolvent matrix $R_q = [I - qA]^{-1} \in \mathbb{R}^{n \times n}$. The following representation

$$[I - qA]^{-m} = \sum_{i=0}^{\infty} q^i C_{m+i-1}^i A^i, \quad |q\lambda| < 1 \quad (3)$$

is valid because of behaviors of binomial expansion and the spectral theory of linear operators. Let remind that the eigenvalues of the matrices R_q and A are connected by the equality $\mu = \frac{1}{1-q\lambda}$, and the eigenvectors coincide. The following expression (see [4])

$$\mu^{(m)} = \frac{([I - qA]^{-m} f, h)}{([I - qA]^{-(m-1)} f, h)} \xrightarrow{m \rightarrow \infty} \mu = \frac{1}{1 - q\lambda}, \quad f \in \mathbb{R}^n, h \in \mathbb{R}^n, \quad (4)$$

is valid (f and h are vectors in $\mathbb{R}^n$). For negative values of q , the largest eigenvalue μ_{max} of R_q corresponds to the smallest eigenvalue λ_{min} of the matrix A .

Moreover, if $|\lambda'_{max}| < 1$ where λ'_{max} is the largest eigenvalue of the matrix $A' = \{|a_{ij}|\}_{i,j=1}^n$, the following statement holds, [4], [2]:

$$([I - qA]^{-m} f, h) = E \left\{ \sum_{i=0}^{\infty} q^i C_{m+i-1}^i (A^i f, h) \right\}.$$

Now we can construct Monte Carlo method. Define Markov chain $k_0 \rightarrow k_1 \rightarrow \dots \rightarrow k_i$ ($1 \leq k_j \leq n$ are natural numbers) with initial and transition densities, $Pr(k_0 = \alpha) = p_\alpha$, $Pr(k_j = \beta | k_{j-1} = \alpha) = p_{\alpha\beta}$, (see [4],[2]). Now define the random variables W_j using the following recursion formula:

$$W_0 = \frac{h_{k_0}}{p_{k_0}}, \quad W_j = W_{j-1} \frac{a_{k_{j-1}k_j}}{p_{k_{j-1}k_j}}, \quad j = 1, \dots, i. \quad (5)$$

Than it can be proven that (see [4], [2]):

$$\begin{aligned} \lambda_{min} &\approx \frac{1}{q} \left(1 - \frac{1}{\mu^{(m)}} \right) = \frac{(A[I - qA]^{-m} f, h)}{([I - qA]^{-m} f, h)} = \\ &= \frac{E \sum_{i=1}^{\infty} q^{i-1} C_{i+m-2}^{i-1} W_i f_{x_i}}{E \sum_{i=0}^{\infty} q^i C_{i+m-1}^i W_i f_{x_i}} = \frac{E \sum_{i=0}^l q^i C_{i+m-1}^i W_{i+1} f_{x_i}}{E \sum_{i=0}^l q^i C_{i+m-1}^i W_i f_{x_i}}, \end{aligned} \quad (6)$$

where $W_0 = \frac{h_{k_0}}{p_{k_0}}$ and W_i are defined by (5). The coefficients C_{i+m}^n are calculated using the presentation $C_{i+m}^i = C_{i+m-1}^i + C_{i+m-1}^{i-1}$.

This method has strong requirements about matrices for which it can be applied. The systematic error consists of two parts:

- an error from the Power method applied on the resolvent matrix $[I - qA]^{-1}$ which determines the value of the parameter m in the following way: The rate of convergence is

$$O\left(\left(\frac{1 + |q|\lambda_n}{1 + |q|\lambda_{n-1}}\right)^m\right).$$

The parameter m has to be chosen such that $(\frac{\mu_2}{\mu_1})^m < \varepsilon$.

- an error which comes from the series expansion of the resolvent matrix - it determines the value of the parameter l (length of each random walk). Considering the presentation

$$([I - qA]^{-m} f, g) \approx \sum_{i=0}^l q^i C_{m+i-1}^i (A^i f, g) = \sum_{i=1}^l u_i,$$

the parameter l has to be chosen such that $|u_{l+1}| < \varepsilon_2$.

- rounding errors - to maintain them at a low level the condition $(\max_{1 \leq i \leq l} |u_i|) \varepsilon < \alpha \mu$ must be satisfied, where $\alpha < 1$ represents the requested precision and ε is the machine precision parameter.

Unfortunately, the parameter l can not be relatively large because the binomial coefficients C_{m+l-1}^l grow exponentially with l . This is serious restriction for using the resolvent Monte Carlo.

The Resolvent Monte Carlo method computes the smallest eigenvalue with only $O(lN)$ operations, where l is the average length of the Markov chains and N is the number of walks. But this method has a lot of restrictions, and, also, gives very rough approximation.

3 Inverse Monte Carlo with Refinement

Here we propose a method that includes fast Monte Carlo scheme for matrix inversion, refinement of the inverse matrix (if necessary) and Monte Carlo power iterations for computing the largest eigenvalue of the inverse (the smallest eigenvalue of the given matrix).

3.1 Monte Carlo for Computing the Inverse Matrix

To find the inverse $A^{-1} = C = \{c_{rr'}\}_{r,r'=1}^n$ of some matrix A , we must first compute the elements of matrix $M = I - A$, where I is the identity matrix. Clearly, the inverse matrix is given by

$$C = \sum_{i=0}^{\infty} M^i, \tag{7}$$

which converges if $\|M\| < 1$ (sufficient condition).

To estimate the element $c_{rr'}$ of the inverse matrix C , we define Markov chain $s_0 \rightarrow s_1 \rightarrow \dots \rightarrow s_k$, 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 $P = \{p_{\alpha\beta}\}_{\alpha, \beta=1}^n$.

We then can use the following Monte Carlo method (see, for example, [11], [3]) for calculating elements of the inverse matrix C :

$$c_{rr'} \approx \frac{1}{N} \sum_{s=1}^N \left[\sum_{(j|s_j=r')} W_j \right], \quad (8)$$

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

$$W_j = \frac{M_{rs_1} M_{s_1 s_2} \dots M_{s_{j-1} s_j}}{p_{rs_1} p_{s_1 s_2} \dots p_{s_{j-1} s_j}} \quad (9)$$

for which $s_j = r'$ are included in the sum (8).

Since W_j is included only into the corresponding sum for $r' = 1, 2, \dots, n$, then 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.

Furthermore, if necessary we transform matrix A to matrix D where D is diagonally dominant matrix, we find its inverse and after that apply a filter procedure in order to find A^{-1} [5].

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 $\bar{\theta}$ [11].

3.2 Refinement

Given a square nonsingular matrix A , Monte Carlo gives fast but very rough estimation of the elements of the inverse matrix C_0 . Under the condition $\|R_0\| \leq \delta < 1$ where $R_0 = I - AC_0$, the elements of A^{-1} may be computed to whatever degree of accuracy is convenient using the iterative process: $C_m = C_{m-1}(I + R_{m-1})$, $R_m = I - AC_m$ for $m = 1, 2, \dots$. It can be shown that

$$\|C_m - A^{-1}\| \leq \|C_0\| \frac{\delta^{2^m}}{1 - \delta}.$$

It follows that once we have an initial approximation C_0 of the inverse such that $\|I - AC_0\| \leq k < 1$ we can use the above iterative scheme and than the number of correct digits increases in geometric progression.

If we have inverted matrix D then we need to apply the filter procedure to obtain the A^{-1} using the formula

$$A_k^{-1} = A_{k+1}^{-1} + \frac{A_{k+1}^{-1} S_{i+1} A_{k+1}^{-1}}{1 - \text{trace}(A_{k+1}^{-1} S_{i+1})}, i = k-1, k-2, \dots, 1, 0.$$

3.3 Evaluation of the Smallest Eigenvalue

Once we have the matrix $C = A^{-1}$ we apply the Monte Carlo power iterations to find its largest eigenvalue performing random walks on the elements of the matrix C :

$$\lambda_{max}(C) \approx \frac{E\{W_m f_{k_i}\}}{E\{W_{m-1} f_{k_{i-1}}\}}.$$

Here $W_j = \frac{C_{k_0 k_1} C_{k_1 k_2} \dots C_{k_{j-1} k_j}}{p_{k_0 k_1} p_{k_1 k_2} \dots p_{k_{j-1} k_j}}$, and m is sufficiently large to ensure the convergence of the power method which is $O(\frac{\lambda_n}{\lambda_{n-1}})^m$.

The computational cost of power Monte Carlo is mN , where m is determined by the convergence of the power iterations and N is the number of walks.

3.4 Restrictions of the Method and How to Avoid Them

Suppose that $\lambda_n < \lambda_{n-1}$; in this case the power method is convergent. The only possible restriction in the above scheme is the requirement $\|M\| < 1$ for the convergence of the Monte Carlo inversion. This can easily be avoided using the presented bellow algorithm for inverting general type matrices using Monte Carlo:

Algorithm: Finding A^{-1} .

1. **Initial data:** Input matrix A , parameters γ and ϵ .
2. **Preprocessing:**
 - 2.1 **Split** $A = D - (D - A)$, where D is a diagonally dominant matrix.
 - 2.2 **Set** $D = B - B_1$ where B is a diagonal matrix $b_{ii} = d_{ii}$ $i = 1, 2, \dots, n$.
 - 2.3 **Compute** the matrix $T = B^{-1}B_1$.
 - 2.4 **Compute** $\|T\|$, the Number of Markov Chains $N = (\frac{0.6745}{\epsilon} \cdot \frac{1}{(1-\|T\|)})^2$.
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 $nextpoint$.
 - 3.1.3 **If** $T[point][nextpoint]! = 0$.
 - LOOP**
 - 3.1.3.1 **Compute** $W_j = W_{j-1} \frac{T[point][nextpoint]}{P[point][nextpoint]}$.
 - 3.1.3.2 **Set** $Point = nextpoint$ and $SUM[i] = SUM[i] + W_j$.
 - 3.1.3.3 **If** $|W_j| < \gamma$, $t_k = t_k + 1$
 - 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 $V = (I - T)^{-1}$.
6. **Therefore** $D^{-1} = VB^{-1}$.
7. **Compute** the MC inversion $D^{-1} = B(I - T)^{-1}$.
8. **Set** $D_0 = D^{-1}$ (approximate inversion) and $R_0 = I - DD_0$.
9. **use filter procedure** $R_i = I - DD_i$, $D_i = D_{i-1}(I + R_{i-1})$, $i = 1, 2, \dots, m$, where $m \leq k$.
10. **Consider the accurate inversion of D** by step 9 given by $D_0 = D_k$.
11. **Compute** $S = D - A$ where S can be any matrix with all non-zero elements in diagonal and all of its off-diagonal elements are zero.
12. **Main function** for obtaining the inversion of A based on D^{-1} step 9:
 - 12.1 **Compute** the matrices S_i , $i = 1, 2, \dots, k$, where each S_i has just one element of matrix S .
 - 12.2 **Set** $A_0 = D_0$ and $A_k = A + S$
 - 12.3 **Apply** $A_k^{-1} = A_{k+1}^{-1} + \frac{A_{k+1}^{-1}S_{i+1}A_{k+1}^{-1}}{1 - \text{trace}(A_{k+1}^{-1}S_{i+1})}$, $i = k - 1, k - 2, \dots, 1, 0$.
13. **Print** the inversion of matrix A.
14. **End** of algorithm.

4 Parallel Implementation and Numerical Tests

The method presented in this paper consists of 3 procedures:

- Monte Carlo inversion
- Refinement
- Power Monte Carlo iterations

We study the convergence and the parallel behaviour of each of the above procedures separately in order to have the overall picture.

It is well known that Monte Carlo algorithms have high parallel efficiency. In fact, in the case where a copy of the non-zero matrix elements of A is sent to each processor, the execution time for computing an extremal eigenvalue on p processors is bounded by $O(lN/p)$ where N is the number of performed random walks and l is the mean value of the steps in a single walk. This result assumes that the initial communication cost of distributing the matrix, and the final communication cost of collecting and averaging the distributed statistics is negligible compared to the cost of generating the Markov chains and forming the chosen statistic.

The numerical tests presented include example with 128×128 matrix, where we have applied rough Monte Carlo estimate and no refinement. In this case, the procedure for finding the largest eigenvalue of the inverse matrix using power Monte Carlo iterations, has no convergence. After that we applied a refinement procedure to find more accurate inverses with $\epsilon = 10^{-6}$ and 10^{-8} . Applying power Monte Carlo iterations to find the largest eigenvalue of the refined inverse matrix gives the value $\lambda Inv_{max} = 3.3330$ which is closed enough to the value given by the MATLAB eigenvalue procedure which is 3.3062.

In addition to convergence test, we also performed parallel computations to empirically confirm the parallel efficiency of this Monte Carlo method. A lot of parallel tests concerning Monte Carlo inversion and refinement can be found in [1], here we test the Monte Carlo part for computing the desired eigenvalue. The parallel numerical test was performed on a Compaq Alpha parallel cluster with 8 DS10 processors each running at 466 megahertz using MPI to provide the parallel calls. Each processor executes the same program for N/p trajectories (here p is the number of processors), and at the end of the trajectory computations, a designated host processor collects the results of all realizations and computes the desired average values. The results shown in *Figure* that the high parallel efficiency of Monte Carlo methods is preserved for this problem as well.

Fig. 1. Computing the largest eigenvalue of the inverse matrix - Speedup vs number of processors

5 Conclusion

The Monte Carlo methods with refinement have been proposed and extensively tested for solving systems of linear algebraic equations (see, for example, [1, 5]). In this paper we propose a method that includes Monte Carlo procedure for finding the inverse matrix, refinement procedure to improve approximation of the inverse if necessary, and Monte Carlo power iterations to compute the smallest eigenvalue. This method gives better results than the Resolvent Monte Carlo.

References

1. V. N. Alexandrov, S. Branford, and C. Weihrauch, A New Parallel Hybrid Monte Carlo Algorithm for Matrix Computations', *Proc. Of PMAA 2004*, September 2004.
2. I. Dimov, V. Alexandrov, A. Karaivanova, Resolvent Monte Carlo Methods for Linear Algebra Problems, *Mathematics and Computers in Simulations*, Vol. . **55**, 2001, pp. 25-36.

3. I. Dimov, T. Dimov, T. Gurov, A new iterative Monte Carlo Approach for Inverse Matrix Problem, *J. of Comp. and Appl. Mathematics*, **92**, 1998, pp. 15-35.
4. I. Dimov, A. Karaivanova, Parallel computations of eigenvalues based on a Monte Carlo approach, *Journal of MC Methods and Appl.*, Vol.**4**, Num.1, 1998 pp.33-52.
5. B. Fathi, B. Liu and V. Alexandrov, Mixed Monte Carlo Parallel Algorithms for Matrix Computations, *Computational Science - ICCS2002*, LNCS **2330**, pp. 609-618, 2002.
6. G. H. Golub, C.F. Van Loon, *Matrix computations*, **The Johns Hopkins Univ. Press**, Baltimore, 1996.
7. J.H. Halton, Sequential Monte Carlo Techniques for the Solution of Linear Systems, *SIAM Journal of Scientific Computing*, Vol.**9**, pp. 213-257, 1994.
8. William W. Hager, *Applied Numerical Linear Algebra*, Prentice Hall International (UK) Limited, London, 1989.
9. J.M. Hammersley, D.C. Handscomb, *Monte Carlo methods*, **John Wiley & Sons, inc.**, New York, London, Sydney, Methuen, 1964.
10. G.A. Mikhailov, *Optimization of the "weight" Monte Carlo methods*, Nauka, Moscow, 1987.
11. I.M. Sobol *Monte Carlo numerical methods*, Nauka, Moscow, 1973.