Journal of Applied Mathematics, Statistics and Informatics (JAMSI), **6** (2010), No. 2

ON COMPUTING DOMINANT EIGENPAIR BY MARKOV CHAIN MONTE CARLO METHOD

BEHROUZ FATHI VAJARGAH, FARSHID MEHRDOUST AND KIANOUSH FATHI VAJARGAH

Abstract

In this paper we introduce a Markov chain Monte Carlo(MCMC) approach for calculating dominant eigenpair of symmetric matrices. The algorithm is tested on large randomized symmetric matrices.

Mathematics Subject Classification 2000: 34L16, 60J65

Additional Key Words and Phrases: Markov chain, Monte Carlo, Matrix computations, eigenpair

1. INTRODUCTION

Matrix eigenvalue problems arise in a large number of disciplines of sciences and engineering[5]. For example, Physics and chemistry provide numerous problems where obtaining largest eigenpair is important. It is known that Monte Carlo (MC) algorithms give statistical estimates for bilinear forms by performing random sampling of a certain random variable, whose mathematical expectation is the desired solution[1]. We are interested in the bilinear form of matrix powers since it is a basic task for many matrix computations

$$(v, A^k h). \tag{1}$$

Here, we consider the following problem of calculating eigenvalues performed by,

$$Ax = \lambda x \tag{2}$$

where the pair (λ, x) for $x \neq 0$, is called an eigenpair of $A \in \Re^{n\times n}$ matrix.

2. POWER METHOD

The power method gives us an estimate for the dominant eigenvalue λ_1. Suppose $A \in \Re^{n\times n}$ is a symmetric matrix and also

$$\lambda_{min} = \lambda_n < \lambda_{n-1} \leq \cdots \leq \lambda_2 < \lambda_1 = \lambda_{max}$$

then the dominant eigenvalue can be obtained using the iteration process for large value of i,

$$\lambda_1 \approx \frac{< h, A^i f >}{< h, A^{i-1} f >}. \tag{3}$$

3. MONTE CARLO IMPLEMENTATION

Consider matrix $A \in \Re^{n \times n}$ and two vectors $f, h \in \Re^n$. Consider the following Markov chain T_i with length i

$$T_i : k_0 \to k_1 \to \cdots \to k_i$$

where for $j = 1, \cdots, i$; $k_j \in \{1, 2, \cdots, n\}$. The statistical nature of constructing the chain (2) follow as

$$p(k_0 = \alpha) = p_\alpha, \quad p(k_j = \beta | k_{j-1} = \alpha) = p_{\alpha\beta}$$

where p_α and $p_{\alpha\beta}$ show the probability of starting chain at α and transition probability from state α to β, respectively.
Now, define the random variable W_j using the following recursion for

$$W_0 = 1 \quad , \quad W_j = W_{j-1} \frac{a_{k_{j-1}k_j}}{p_{k_{j-1}k_j}} \quad , j = 1, 2, ..., i \tag{4}$$

From all possible permissible densities, we choose the following

$$\begin{aligned} p_\alpha &= \frac{|h_\alpha|}{\sum_{\alpha=1}^{n} |h_\alpha|} \\ p_{\alpha\beta} &= \frac{|a_{\alpha\beta}|}{\sum_{\beta=1}^{n} |a_{\alpha\beta}|} \qquad \alpha = 1, 2, ..., n \end{aligned}$$

The choice of the initial density vector and the transition probability matrix leads to an Almost Optimal Monte Carlo algorithm.

THEOREM 3.1. *Using the above choice $p = \{p_\alpha\}_{\alpha=1}^{n}$ and $P = \{p_{\alpha\beta}\}_{\alpha,\beta=1}^{n}$ the variance of the unbiased estimator for obtaining the inverse matrix is minimized.*

Proof. See[2].

THEOREM 3.2. *Under above assumption we have*

$$E[W_i f_{k_i}] =< h, A^i f > \quad i = 1, 2, \cdots \tag{5}$$

Proof. See [3].

Remark 3.3. By simulating N random paths

$$T_i^s : k_0^{(s)} \to k_1^{(s)} \to \cdots \to k_i^{(s)}$$

we can find

$$\Theta_k^{(s)}(h) = \frac{h_{k_0}}{p_{k_0}^{(s)}} W_k^{(s)} f_{k_i} \quad , \quad s = 1, ..., N$$

The Monte Carlo estimation can be evaluated by

$$\Theta_k = \frac{1}{N} \sum_{s=1}^{N} \Theta_k^{(s)}(h)$$

which is an unbiased estimator of $< h, A^i f >$. Therefore, from 3 and 5 we have

$$\lambda_1 \approx \frac{E[W_i f_{k_i}]}{E[W_{i-1} f_{k_{i-1}}]} \tag{6}$$

Remark 3.4. By setting $h = e(r) = (0, ..., 0, 1, 0, ..., 0)^T$, the r^{th} canonical unit vector, for $r = 1, ..., n$ the above random variable has expected value equal to the r^{th} component of the dominant eigenvector.

4. NUMERICAL EXAMPLES

In this section, the experimental results for obtaining dominant eigenpair of a randomized symmetric matrix $A_{100\times100}$ are given in the following table.

Table 1: Monte Carlo error to obtain eigenpair for randomized symmetric matrix

Number of trajectory	Eigenvector error	Eigenvalue error	Time(sec.)
100	0.7928	0.0061	0.98
200	0.6214	0.0036	2.05
400	0.5479	0.0020	4.07
800	0.4740	3.3759×10^{-4}	8.05
1600	0.4201	0.0022	16.1
3200	0.4093	0.0020	32.18
6400	0.4031	0.0019	64.53

5. CONCLUDING REMARKS

We have presented a iterative MCMC algorithm that enables the determination of the dominant eigenpair of a very large matrices. Experimental results show that the linear dependency between number of Markov chains and computational times in proposed MCMC method (Fig. 2). This method can be extended for finding more than one eigenpair. Also, The studied algorithm is easily programmable and parallelization.

REFERENCES

[1] Dimov, I. and Karaivanova, A., A power method with Monte Carlo iteration,Recent advances in numerical methods and application 1999, 239-247.

[2] Fathi Vajargah, B. and Fathi Vajargah, K., Parallel Monte Carlo computation for solving SLAE with minimum communication, Applied Mathematics and computation, 2006, 1-9.

[3] B. Fathi Vajargah and F. Mehrdoust, New Monte Carlo algorithm for obtaining three dominant eigenvalues, International journal of applied mathematics, 22(2009)553-559.

[4] Rubinstein R.Y. , Simulation and the Monte Carlo Method, John Wiley & Sons, New York , 1981.

[5] Saad Y. , Numerical methods for large eigenvalue problems, Manchester University Press, 1991.

Behrouz Fathi Vajargah
Department of Mathematics
University of Guilan, Iran,
e-mail: behrouz.fathi@gmail.com

Farshid Mehrdoust
Department of Mathematics
University of Guilan, Iran,
e-mail: fmehrdoust@guilan.ac.ir

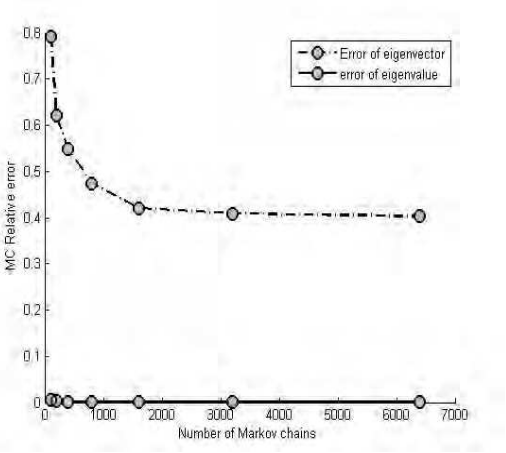

Fig. 1. Curve of relative error for various number of Markov chians

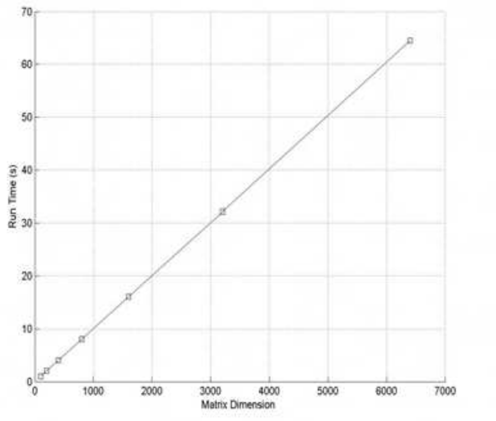

Fig. 2. Curve of CPU time for various number of matrices

Guilan, Iran and Kianoush Fathi Vajargah
Department of Stistics,
Islamic Azad University,
North Branch, Tehran, Iran
e-mail:fathi@guilan.ac.ir, fathi-kia10@yahoo.com

Received August 2010