Multicanonical sampling of rare events in random matrices

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A method based on multicanonical Monte Carlo is applied to the calculation of large deviations in the largest eigenvalue of random matrices. The method is successfully tested with the Gaussian orthogonal ensemble (GOE), sparse random matrices, and matrices whose components are subject to uniform density. Specifically, the probability that all eigenvalues of a matrix are negative is estimated in these cases down to the values of \( \sim 10^{-200} \), a region where naive random sampling is ineffective. The method can be applied to any ensemble of matrices and used for sampling rare events characterized by any statistics.

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I. INTRODUCTION

Rare events caused by rare realization of impurities often govern the properties of random systems and play an essential role in their study. Numerical computation of the probabilities of rare events is, however, computationally expensive. When the probability takes very small values, say, \( 10^{-15} \) or less, it is virtually impossible to calculate the correct probability value by naive random sampling.

Recently, approaches based on dynamic Monte Carlo (Markov chain Monte Carlo) \cite{1, 2} have been shown to be useful for sampling rare events and calculating large deviations in the corresponding statistics. The novelty of the approach is that a dynamic Monte Carlo algorithm is used for calculating sample averages over configurations of impurities, instead of computing thermal averages. Successful examples in physics include applications in spin glass \cite{3, 4}, diluted magnets \cite{5}, and directed random walks in random media \cite{6}. Some references \cite{7-10} also discuss applications in information processing and other engineering problems.

The aim of this paper is to apply the method to sample rare events in random matrices. Random matrices have been a classical subject with a number of applications in physics and other fields \cite{11-13}. Specifically, large deviations in the maximum eigenvalue of random matrices is a subject of recent interest in various fields such as ecology \cite{14}, cosmology \cite{15}, mathematical statistics \cite{16}, and information compression \cite{17}. The tail of the distribution of the maximum eigenvalue is important because it gives the probability of all eigenvalues being negative, which is often related to the stability condition of complicated systems \cite{14, 15}.

A well-known study by Tracy and Widom established the celebrated “1/6 law” \cite{18} on small deviations in the maximum eigenvalue of random matrices. On the other hand, analytical studies \cite{19-21} of large deviations give estimations of the tails of probabilities in special cases such as the Gaussian orthogonal ensemble (GOE) and ensemble of random Wishart matrices. However, the techniques based on the Coulomb gas representation are difficult to generalize to ensembles with other distributions of the components. Other results by mathematicians and physicists are also limited to special ensembles and/or give only the upper bound of the probabilities \cite{17}. Thus, an efficient numerical approach that enables exploration of extreme tails of density is necessary.

We propose a method based on multicanonical Monte Carlo \cite{22-23} as a promising approach to the problem. As we will show in this study, quantitative results are obtained in examples of sparse random matrices and matrices whose components are subject to the uniform density. A similar method is used in \cite{10} to calculate large deviations in the growth ratio of matrices. The paper \cite{10}, however, focuses on applications in numerical analysis and does not compute large deviations in the largest eigenvalues.

The organization of this paper is as follows: In Sec. \ref{sec:multicanonical}, we summarize the multicanonical Monte Carlo algorithm. In Sec. \ref{sec:results}, we discuss how multicanonical Monte Carlo is used to calculate large deviations and show the results of
numerical experiments on the tails of the distribution of the largest eigenvalues. Sec. IV covers the computation of the probability that all eigenvalues are negative; as noted above, this is a typical application of the proposed method. In Sec. V, sparse matrices are treated. In Sec. VI concluding remarks are given.

II. MULTICANONICAL MONTE CARLO

Let us summarize the idea of multicanonical Monte Carlo. Assuming the energy $E(x)$ of a state $x$, our task is to calculate the density $D(E)$ of states defined by

$$D(E) = \int \delta(E(x) - E) \, dx,$$

where $\delta$ is the Dirac $\delta$-function, and $\int \cdots dx$ denotes a multiple integral in the space of states $x$.

A key quantity of multicanonical Monte Carlo is the weight function $f(E)$ of the energy $E$. Performing dynamic Monte Carlo sampling with the weight $f(E(x))$, we modify $f(E)$ step-by-step until the marginal density $q(E)$ of $E$ is almost flat in a prescribed interval $E_{\text{min}} < E < E_{\text{max}}$. The initial form of $f(E)$ is arbitrary, and we can start, for example, from a constant function. Several methods are proposed for optimizing a univariate function $f(E)$, among which a method proposed by Wang and Landau is most useful and used in this paper. After a weight function $f^*(E)$ that gives a sufficiently flat $q(E)$ is obtained, we compute an accurate estimate $q^*(E)$ of $q(E)$ by a long simulation run with the weight $f^*(E(x))$. Then, $D(E)$ is estimated by the relation

$$D(E) \propto \frac{q^*(E)}{f^*(E)}, \quad (E_{\text{min}} < E < E_{\text{max}}).$$

This simple algorithm has significant advantages over conventional methods for estimation of $D(E)$. First, it realizes accurate sampling of tails of $D(E)$ without estimating densities in the high-dimensional state space of $x$. Second, when we include the region of $E$ with large values of $D(E)$ in the interval $E_{\text{min}} < E < E_{\text{max}}$, the mixing of dynamic Monte Carlo is dramatically facilitated. This “annealing” effect is the reason that multicanonical Monte Carlo is successfully used to calculate thermal averages at low temperatures in the studies of spin glass and biomolecules.

III. LARGE DEVIATIONS IN THE LARGEST EIGENVALUES

An essential observation in the present approach is that the energy $E$ in multicanonical Monte Carlo need not be an energy in the ordinary sense. That is, we can substitute for $E$ any quantity for which we are interested in its rare fluctuations or large deviations from the average; similar approaches to other problems are found in [4, 5, 8, 10].

In this study, we regard the maximum eigenvalue $\lambda_1(x)$ of a matrix $x$ as a fictitious “energy” of the state $x$. Also, we can introduce an underlying density $p(x)$ that gives the probability of $x$ under random sampling. While $p(x)$ is the uniform density in statistical mechanics, $p(x)$ in the present case characterizes an ensemble of matrices. Hereafter, we assume the factorization $p(x) = \prod_{ij} p_{ij}(x_{ij})$. The normalized density $D(\lambda_1)$ of the states is written as

$$D(\lambda_1) = \int \delta(\lambda_1(x) - \lambda_1)p(x) \, dx,$$

where we replace $E(x)$ in (1) with $\lambda_1(x)$. $D(\lambda_1)$ is simply the probability distribution of $\lambda_1$, whose extreme tails we are interested in.

Now the application of multicanonical Monte Carlo is straightforward. We employ a Metropolis-Hastings algorithm to generate samples according to the weight $f(\lambda_1(x))p(x)$. A single component $x_{ij}$ of the random matrix $x$ is chosen and changed at each step; in ensembles of symmetric matrices, $x_{ij}$ should also be changed if $i \neq j$, which is necessary to keep the symmetry of the matrix. The candidate $x_{ij}^{\text{new}}$ of $x_{ij}$ is generated according to the proposal density $r_{ij}(x_{ij}^{\text{new}}|x_{ij}^{\text{old}})$, where $x_{ij}^{\text{old}}$ is the current value of $x$; $x_{ij}^{\text{new}}$ is accepted if and only if the Metropolis ratio

$$R = \frac{p_{ij}(x_{ij}^{\text{new}})}{p_{ij}(x_{ij}^{\text{old}})} \frac{r_{ij}(x_{ij}^{\text{new}}|x_{ij}^{\text{old}})}{r_{ij}(x_{ij}^{\text{old}}|x_{ij}^{\text{new}})} \frac{f(\lambda_1(x_{ij}^{\text{new}}))}{f(\lambda_1(x_{ij}^{\text{old}}))}$$

is smaller than a random number uniformly distributed in $(0, 1)$. Repeating this procedure, the function $f(\lambda_1)$ is tuned by the method of Wang-Landau. Once a weight function $f^*(\lambda_1)$ that gives a sufficiently flat $q(\lambda_1)$ is obtained, we estimate $D(\lambda_1)$ using the formula

$$D(\lambda_1) \propto \frac{q^*(\lambda_1)}{f^*(\lambda_1)}, \quad (\lambda_1^{\text{min}} < \lambda_1 < \lambda_1^{\text{max}}),$$

where $q^*(\lambda_1)$ is the density of $\lambda_1$ estimated by a long run with the fixed weight function $f^*(\lambda_1)$.

A simple choice of the proposal density is $r_{ij}(x_{ij}^{\text{new}}|x_{ij}^{\text{old}}) = p_{ij}(x_{ij}^{\text{new}})$, which results in a simple form of the Metropolis ratio

$$R = \frac{f(\lambda_1(x_{ij}^{\text{new}}))}{f(\lambda_1(x_{ij}^{\text{old}}))}.$$
The proposed strategy also allows us to calculate the probability $P(\forall i, \lambda_i < 0)$ that all eigenvalues of a random matrix are negative, which is important in applications in a variety of fields [14, 15]. Using the relation $\forall i, \lambda_i \leq \lambda_1$, this probability is calculated by

$$P(\forall i, \lambda_i < 0) = \int_{\lambda_{\text{min}}^\lambda}^0 D(\lambda_1) \, d\lambda_1.$$  

Here we assume that the density $D(\lambda_1)$ of the maximum eigenvalue is estimated in an interval $[\lambda_{\text{min}}^\lambda, \lambda_{\text{max}}^\lambda]$ by the proposed method. The probabilities $P(\lambda_1 < \lambda_{\text{min}}^\lambda)$ and $P(\lambda_{\text{min}}^\lambda < \lambda_1 < \lambda_{\text{max}}^\lambda)$ are also assumed to be negligibly smaller than $P(\lambda_{\text{min}}^\lambda < \lambda_1 < 0)$ and $P(\lambda_{\text{min}}^\lambda < \lambda_1 < \lambda_{\text{max}}^\lambda)$, respectively.

The probability that all eigenvalues are positive can also be calculated with a similar way; it coincides with the probability that all eigenvalues are negative when the distribution of components is symmetric with respect to the origin.

First, we test the proposed method with GOE, where the asymptotic behavior of $P(\forall i, \lambda_i < 0)$ for large $N$ is given by Dean and Majumdar [16, 20] as

$$P(\forall i, \lambda_i < 0) \sim \exp \left( -aN^2 \right),$$

where $a = \tfrac{\ln 3}{4} = 0.274653 \cdots$. This expression is derived by interpreting the eigenvalues as a Coulomb gas, a method that obviously does not apply general distribution of components of matrices.

Confirming the result by numerical methods is difficult because we should sample very rare events to estimate the tails of the distribution. Dean and Majumdar [16, 20] (and Aazami and Easther [15]) provided numerical results by naive random sampling, but their results are limited to small $N$, such as $N = 7$ in [15, 20] ($N = 8$ with an additional assumption [20]). Dean and Majumdar also did numerical computation up to $N = 35$ based on the Coulomb gas representation; their computation does not, however, provide an independent check to the theory and cannot be generalized to an arbitrary ensemble.

Fig. 2 shows our numerical results for GOE. We can treat matrices up to $N = 40$, which is not treated by naive random sampling. Here we use the random walk scheme $r_{ij}(x_{ij}^{\text{new}} | x_{ij}^{\text{old}}) = p_{ij}(x_{ij}^{\text{new}} - x_{ij}^{\text{old}})$ and the total number of matrix diagonalizations is $3 \times 10^9$ for $N = 4 \sim 20$ and $4.5 \times 10^9$ for $N = 22 \sim 40$. The results for $N \leq 7$ coincide with those by naive random sampling. They are also consistent with the fit $-0.272N^2 - 0.493N + 0.244$ of the numerical results calculated in [20] with the Coulomb gas representation. Hence, probabilities as tiny as $\sim 10^{-200}$ are estimated by the proposed method and agree well with the known results.

Next, to show the flexibility of the proposed method, we calculate the probability $P(\forall i, \lambda_i < 0)$ for an ensem-
TABLE of REAL SYMMETRIC MATRICES Whose Entries are Independent and
DISTRIBUTED with the Uniform Distribution \( p_{ij}(x_{ij}) \) Defined by

\[
p_{ij}(x_{ij}) = \begin{cases} 
\frac{1}{2\sqrt{3}L}, & |x_{ij}| < \sqrt{\frac{3}{2}}L \text{ and } i = j, \\
\frac{1}{\sqrt{6}L}, & |x_{ij}| < \sqrt{\frac{3}{2}}L \text{ and } i \neq j, \\
0 & \text{else.}
\end{cases}
\]

Hereafter, the value of the parameter \( L \) is unity, which fits the variances of the components to those of the GOE. Results of the proposed method for this ensemble are shown in Fig. 2. The proposal density \( r_{ij}(x_{ij}^{\text{new}} | x_{ij}^{\text{old}}) = p_{ij}(x_{ij}^{\text{new}}) \) is used. Total number of matrix diagonalizations is \( 4.5 \times 10^9 \) for each value of \( N \); two third of which are used to optimize the weight. Fitting the results yields asymptotic behavior of the probability,

\[
P(\forall i, \lambda_i < 0) \sim \exp \left( -aN^2 - bN - c \right)
\]

for large \( N \), where \( a = 0.679 \), \( b = 4.76 \), and \( c = 17.31 \). As shown in Fig. 3, these probabilities significantly differ from that for the GOE with the same variance.

V. SPARSE RANDOM MATRICES

We also study ensembles of sparse random matrices. Once the matrices become sparse, the Coulomb gas approach is not applicable even in Gaussian cases. The proposed approach allows us to calculate the probability \( P(\forall i, \lambda_i < 0) \) in these cases. In this section, we use the proposal density \( r_{ij}(x_{ij}^{\text{new}} | x_{ij}^{\text{old}}) = p_{ij}(x_{ij}^{\text{new}}) \), but some of the results are also checked by random walk schemes.

Various ways of defining sparse random matrices are available. Among them, we consider two types of definitions in this study. The first is as follows: (1) The matrix is symmetric. (2) All diagonal entries are \(-1\). (3) Nonzero off-diagonal entries in the upper half of the matrix are mutually independent Gaussian variables with zero mean and unit variance. (4) Total number of nonzero entries is fixed at \( \gamma N \), where \( \gamma \) is the average number of nonzero entries per row. (5) The positions of nonzero off-diagonal entries in the upper half of the matrix are randomly chosen.

The total number of nonzero components should be preserved with this definition. Hence, the single component update in previous sections is replaced by a trial of exchanging zero and nonzero components with resampling of the nonzero component. Other parts of the algorithm remain essentially the same. An example of the density \( D(\lambda_i) \) computed by this modified method is shown in Fig. 4.

The probability \( P(\forall i, \lambda_i < 0) \) that all eigenvalues are negative is also successfully calculated by this algorithm for \( \gamma = 3, 4 \), and 5, as shown in Fig. 5. These results indicate that for sparse random matrices, the probability \( P(\lambda_i < 0 | \gamma) \) behaves as

\[
P(\forall i, \lambda_i < 0) \sim \exp \left( -a\gamma N \right)
\]

for large \( N \), where the estimated values of the constants \( a_\gamma \) are \( a_3 = 0.68 \), \( a_4 = 1.20 \), and \( a_5 = 1.81 \) for \( \gamma = 3, 4 \), and 5, respectively.

In the case of sparse matrices, the log-probability \( \log P(\forall i, \lambda_i < 0) \) is linear in \( N \), which is apparently different from the behavior proportional to \( N^2 \) seen in the previous two examples. However, if we plot the proba-
FIG. 4. Density $D(\lambda_1)$ in a case of sparse random matrices. The first definition is applied; results of the proposed method and the naive random sampling method are compared for $N = 30$ and $\gamma = 3$. The symbol $+$ appears only in the region where naive random sampling gives nonzero results.

FIG. 5. Probabilities $P(\forall i, \lambda_i < 0)$ for an ensemble of sparse random matrices estimated by the proposed method. The first definition is applied; the results with $\gamma = 3$, 4, and 5 versus size $N$ of the matrices are shown. The lines show linear fits of the data.

The first definition of sparse random matrices is given by assigning the probability $P(\forall i, \lambda_i < 0)$ with the number $M$ of nonzero components instead of the size $N$, the dependence is linear in all examples. Because $M \propto N$ in a sparse case and $M \propto N^2$ in a dense case, the obtained results are naturally explained.

The definition of sparse random matrices most frequent in the literature [27] differs from that given above. Here, a second definition of sparse random matrices is given by assigning the probability

$$p_{ij}(x_{ij}) = \left(1 - \frac{\gamma}{N}\right) \delta(x_{ij}) + \frac{\gamma}{N} \pi(x_{ij})$$

to all components $x_{ij}$, $(i \geq j)$, where $\delta$ and $\pi$ denote Dirac’s delta function and a Gaussian density with zero mean and unit variance, respectively; each component is assumed to be an independent sample from this distribution.

In this case, all components are mutually independent and the modification for keeping the number of nonzero components is not necessary. However, since the diagonal elements can vanish, singular behavior of the density $D(\lambda_1)$ of states appears at $\lambda_1 = 0$, which affects the efficiency of the proposed method.

Fortunately, when we are interested in $P(\forall i, \lambda_i < 0)$, this difficulty is easily treated; we use the fact that the condition that all diagonal elements are negative $\forall i, x_{ii} < 0$ is a necessary condition for $\forall i, \lambda_i < 0$. By using this condition, the following two-stage method is introduced. First, we calculate the conditional probability $P(\forall i, \lambda_i < 0 | \forall i, x_{ii} < 0)$. This conditional probability can be calculated with a multicanonical algorithm, in which we reject any state $\exists i, x_{ii} \geq 0$. The second step is to calculate the probability $P(\forall i, x_{ii} < 0)$. Elementary calculation shows that

$$P(\forall i, x_{ii} < 0) = \left(\frac{1}{2}\right)^N \times \left(\frac{\gamma}{N}\right)^N \quad (3)$$

Then, the probability $P(\forall i, \lambda_i < 0)$ is given by the product $P(\forall i, \lambda_i < 0 | \forall i, x_{ii} < 0) \times P(\forall i, x_{ii} < 0)$.

Fig. 6 shows examples of the probability $P(\forall i, \lambda_i < 0 | \forall i, x_{ii} < 0)$ calculated in the first step; it is linear in $N$ in the semi-log scale, as expected. The probability $P(\forall i, x_{ii} < 0)$ obtained from it is shown in Fig. 4. In this case, log $P(\forall i, x_{ii} < 0)$ is no longer linear in $N$ because of an $O(N \log N)$ term arising from (3). They are fitted as

$$P(\forall i, x_{ii} < 0) \sim \left(\frac{\gamma}{2N}\right)^N \exp(-a_N N),$$

where $a_3 = 0.845$, $a_4 = 1.14$, $a_5 = 1.44$, and $a_6 = 1.75$ for $\gamma = 3, 4, 5$, and 6, respectively.

VI. CONCLUDING REMARKS

A method based on multicanonical Monte Carlo is proposed and applied to the estimation of large deviations in the largest eigenvalue of random matrices. The method is successfully tested with the Gaussian orthogonal ensemble (GOE), an ensemble of matrices whose components are uniformly distributed in an interval, and an ensemble of sparse random matrices. The probabilities that all eigenvalues of a matrix are negative are successfully estimated in cases where naive random sampling is largely ineffective: the smallest values of the obtained probabilities are $\sim 10^{-200}$.

The method can be applied to any ensemble of matrices. Moreover, it enables sampling of rare events defined by any statistics. Hence, it will be interesting to apply the method to large deviations in other quantities, such
FIG. 6. Probabilities $P(\forall i, \lambda_i < 0 \mid \forall i, x_{ii} < 0)$ for an ensemble of sparse random matrices estimated by the proposed method. The second definition is applied; the results with $\gamma = 3$, 4, 5, and 6 versus size $N$ of the matrices are shown. The lines show linear fits to the data. The results of naive random sampling are also shown.

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