# Probability of graphs with large spectral gap by multicanonical Monte Carlo

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## Abstract

Graphs with large spectral gap are important in various fields such as biology, sociology and computer science. In designing such graphs, an important question is how the probability of graphs with large spectral gap behaves. A method based on multicanonical Monte Carlo is introduced to quantify the behavior of this probability, which enables us to calculate extreme tails of the distribution. The proposed method is successfully applied to random 3-regular graphs and large deviation probability is estimated.

Keywords: random graph; spectral gap; Ramanujan graph; multicanonical Monte Carlo; large deviation

# 1. Introduction

Random graphs often appear and have been studied in various fields of natural science and engineering. A recent interest in their applications is generating expander graphs [1], regular graphs that shows high connectivity and homogeneity. Such graphs have important applications in designing networks of computers [2], infrastructures [3], and real and artificial neurons [4, 5].

A way to define and generate expanders is maximization of the spectral gap g, which is defined as the difference between the largest eigenvalue and the second largest eigenvalue of the adjacency matrix of a graph. Donetti et al. [5, 6] numerically maximized the spectral gap by simulated annealing and generated examples of these graphs. However, in designing networks, we are also interested in quantitative properties; specifically how the probability of large spectral gap graphs behaves when the size N of graphs increases.

In this paper we apply a method based on multicanonical Monte Carlo [7, 8] to the calculation of large deviations in the spectral gap of random graphs. The method can be regarded as an extension of the method introduced in [9]; in [9], large deviations in the largest eigenvalue of random matrices are computed by a similar method.

Multicanonical Monte Carlo enables us to estimate tails of the distribution whose probability is very small and cannot be computed by naive random sampling. By using the proposed method, we estimate the distribution of the spectral gap of random 3-regular graphs and quantify the probability  $P(g > \xi)$  that the spectral gap is larger than a given  $\xi$ ; when  $\xi \gtrsim 0.18$ , it is shown that  $P(g > \xi) \sim \exp(-N^2\Phi(\xi))$  for large N.

# 2. Spectral Gaps

An undirected graph is described by the corresponding adjacency matrix  $A_{ij}$ , whose entries are defined by

$$A_{ij} = \begin{cases} 1 & i \text{ and } j \text{ are connected,} \\ 0 & \text{otherwise.} \end{cases}$$
 (1)

Here we denote eigenvalues of the adjacency matrix by  $\{\lambda_i\}$ . In the case of k-regular graphs,  $A_{ij}$  has the trivial largest eigenvalue  $\lambda_1 = k$ , therefore we assume

$$k = \lambda_1 \ge \lambda_2 \ge \dots \ge \lambda_N. \tag{2}$$

The difference  $\lambda_1 - \lambda_2$  between the largest eigenvalue and the largest non-trivial eigenvalue of  $A_{ij}$  is called "spectral gap" and takes a non-zero value if the corresponding graph is connected. We are interested in tails of the distribution of the spectral gap. In the case of regular graphs, Alon and Boppana (see [10]) proved an asymptotic lower bound of the largest non-trivial eigenvalue  $\lambda_2$  as

$$\liminf_{N \to \infty} \lambda_2 \ge 2\sqrt{k-1}.$$
(3)

Assuming that the limit exists, this gives an asymptotic upper bound for the spectral gap as  $\lim_{N\to\infty}g\le k-2\sqrt{k-1}$ . Graphs with  $g\ge k-2\sqrt{k-1}$  are called "Ramanujan graphs" [11]. On the other hand, Friedman [12] proved that for  $k\ge 3$  and for any constant  $\epsilon>0$  "most" random k-regular graphs have  $\lambda_2$  that satisfies  $\lambda_2\le 2\sqrt{k-1}+\epsilon$  as  $N\to\infty$ . These results indicate that the peak of the distribution of  $\lambda_2$  is located near  $2\sqrt{k-1}$  for large N. Miller  $et\ al.$  [13] studied the distribution around this peak using naive random sampling. None of these studies, however, discusses extreme tails of the distribution of  $\lambda_2$  or g, which is the main subject of this paper.

#### 3. Methods

Here, we will give a brief explanation of multicanonical Monte Carlo. The aim of this method is to estimate the density of states  $\Omega(g)$  defined by

$$\Omega(g) = \int \delta(g(A) - g) \, dA,\tag{4}$$

where  $\delta$  is the Dirac  $\delta$ -function and  $\int dA$  denotes a multiple integral in the space of matrix A. We define the weight by w(g) as a function of g, a key quantity of this method. When a weight function w(g) is given, we can generate samples from the distribution defined by the weight using the Metropolis algorithm [14, 15]. The essential idea is to tune the weight function w(q) so as to produce a flat histogram of q. After we find a appropriate weight function  $w^*(q)$  that gives a flat histogram, an approximate value of the density of states is estimated by  $1/w^*(q)$ . To obtain this  $w^*(g)$ , we modify the weight function step-bystep through the Metropolis simulation using the current guess of the weight function w(g). There are several ways to modify the function w(g). Among them, a method proposed by Wang and Landau [16] is most successful and used in this study. For a more accurate estimate of the density of states, we calculate a histogram  $h^*(g)$  by performing a long simulation with fixed  $w^*(q)$ . Then  $\Omega(q)$  is estimated by  $\Omega(g) \propto h^*(g)/w^*(g)$  and the probability distribution p(g) of g is obtained by  $p(g) = \Omega(g) / \sum_{g} \Omega(g)$ . Practically, we calculate the density p(g) only in a prescribed interval  $g^{min} < g < g^{max}$ .

Details of the implementation of the Metropolis algorithm are as follows. The simulation starts from an arbitrary k-regular graph with the desired number of vertices N. In each step, a candidate  $A^{new}$  is generated by rewiring edges in the way used in [4, 6, 17], where the degree k of each vertex is not changed; a pair of links ij and kl that satisfy  $A_{ij} = A_{kl} = 1$ ,  $A_{ik} = A_{jl} = 0$  is selected and rewired as  $A_{ij} = A_{kl} = 0$ ,  $A_{ik} = A_{jl} = 1$ . Then the spectral gap g of a candidate is calculated by the Householder method and accept/reject decision of the transition from the current state  $A^{old}$  to  $A^{new}$  is made by comparing the Metropolis ratio

$$\alpha = \frac{w(g(A^{new}))}{w(g(A^{old}))}. (5)$$

with a random number uniformly distributed in (0,1]. A candidate with g=0, indicating a disconnected graph, is always rejected, hence an ensemble of connected random k-regular graphs is sampled.

#### 4. Results

Using the proposed method, we estimate the distribution of the spectral gap of random 3-regular graphs with the number of vertices  $N \leq 128$ . Figure 1 shows graphs with the largest spectral gap for N = 16,32 and 64 found

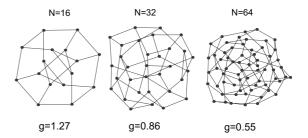


Figure 1: 3-regular graphs with the largest spectral gap found in the simulation.

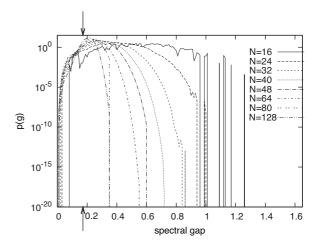


Figure 2: The estimated probability density p(g) of the spectral gap of random 3-regular graphs. The density at g plotted in the vertical axis is obtained from the probability in a small bin around g of a fixed width; the values of them depend on the bin width in the right tail of the distribution, because discreteness of the spectra becomes relevant there. The arrows indicate  $g = 3 - 2\sqrt{3 - 1}$ ; graphs whose g is above this value are Ramanujan.

in the simulations. In Figure 2, we show p(g) of random 3-regular graphs with the number of vertices  $16 \le N \le 128$ ; the computational time is 7 hours for N=16 and 251 hours for N=128 using a core of Intel Xeon X5365. As N increases, the probability density becomes sharper and the peak becomes closer to around  $3-2\sqrt{3-1}=0.172$ , which is consistent with a theoretical estimate [12] and a numerical experiment [13]. Specifically, the probability of graphs with large g decreases drastically for large N.

To quantify decreasing rate of the tails of the distribution, we define the probability  $P(g > \xi)$  that g is larger than  $\xi$  by

$$P(g > \xi) = \int_{\xi}^{g^{max}} p(g) dg.$$
 (6)

Here, we assume the probability  $P(g>g^{max})$  is negligibly smaller than  $P(\xi \leq g \leq g^{max})$ . In Figure 3, estimated  $P(g>\xi)$ s are shown as functions of N. For each  $\xi$ ,  $P(g>\xi)$  is well fitted by a quadratic functions of N, when  $\xi \gtrsim 0.18$ . This result indicates that  $P(g>\xi)$  decreases for large N as

$$P(g > \xi) \sim \exp(-N^2 \Phi(\xi)), \tag{7}$$

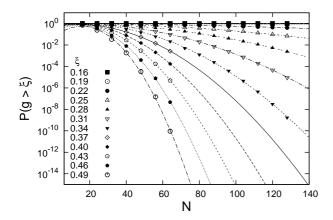


Figure 3: Estimated  $P(g > \xi)$ s are shown as functions of N. Each curve corresponds to different values of  $\xi$ . Data are well fitted by quadratic functions when  $\xi \gtrsim 0.18$ .

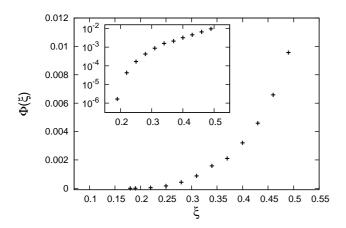


Figure 4: The rate function  $\Phi(\xi)$  is plotted. The inset shows semilog plot of  $\Phi(\xi)$ . In the region  $\xi>0.18$ ,  $\Phi(\xi)$  exponentially increases as  $\xi$  increases.  $\xi=0.18$  is the point that  $\Phi(\xi)$  becomes negative.

where the rate function  $\Phi(\xi)$  is shown in Figure 4. In the region  $\xi \lesssim 0.16$ ,  $P(g > \xi)$  is no longer a monotonic decreasing function of N and asymptotically approaches to unity for large N.

## 5. Concluding Remarks

A method based on multicanonical Monte Carlo is introduced to the estimation of large deviations in the spectral gap of random graphs. By using this method, we calculate the distribution of the spectral gap g and the probability  $P(g>\xi)$  for random 3-regular graphs. While naive random sampling provides reasonable estimates of  $P(g>\xi)$  only when  $\xi$  is around the peak of the distribution p(g), the proposed method enables us to estimate  $P(g>\xi)$  in a wide region of  $\xi$  including extreme tails of the distribution. We find that  $P(g>\xi)$  behaves as  $P(g>\xi) \sim \exp(-N^2\Phi(\xi))$  for large N, when  $\xi \gtrsim 0.18$ .

Our preliminary results indicate that a similar behavior is also seen in the case of random 4- and 5-regular graphs, suggesting that it is a general feature of random k-regular graphs. The proposed method can be applied to calculations of large deviations in any statics of any ensemble of random graphs. In the case of non-regular graphs, the spectral gap are defined as the smallest non-trivial eigenvalue of the Laplacian matrix L [5, 6]; hence we sample matrices L instead of A by using multicanonical Monte Carlo.

Recent studies on Gaussian or Wishart random matrices [18, 19] showed that the probability of all eigenvalues being negative decreases as  $\sim \exp(-N^2 \times \text{const})$  when the size N of the matrices is large. Our results are regarded as an extension of these results to the spectral gap of random graphs.

## 6. Acknowledgments

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