EIGENVALUE SPACINGS FOR REGULAR GRAPHS

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Abstract. We carry out a numerical study of fluctuations in the spectra of regular graphs. Our experiments indicate that the level spacing distribution of a generic k-regular graph approaches that of the Gaussian Orthogonal Ensemble of random matrix theory as we increase the number of vertices. A review of the basic facts on graphs and their spectra is included.

1. Introduction

A regular graph is a combinatorial structure consisting of a set V of $|V|$ vertices, connected by edges. Two vertices are called neighbors if they are connected by an edge; the graph is k-regular if each vertex has exactly k neighbors. To such a graph one associates a combinatorial Laplacian, which operates on functions on the vertices by giving the sum of the differences between the values of a function f at a vertex and its neighbors:

$$\Delta f(x) = kf(x) - \sum_{y \sim x} f(y)$$

the sum being over all neighbors of the vertex x. The $|V|$ eigenvalues $0 = E_0 \leq E_1 \leq \cdots \leq E_{|V|-1}$ lie in the interval between 0 and $2k$. If we take a sequence of graphs with the number of vertices $|V| \to \infty$, then under certain conditions (see Section 2) there is a limiting density of states analogous to Weyl's law. This gives a mean counting function $\bar{N}(E)$, the expected number of levels below E, which we can use to measure the fluctuation properties of the eigenvalues in a large graph. If we "unfold" the sequence of eigenvalues (for instance by setting $\widehat{E}_j = \bar{N}(E_j)$), then we get a sequence $\hat{E}_j$ with mean spacing unity: $s_j := \widehat{E}_{j+1} - \widehat{E}_j \sim 1$. The distribution function of the spacings $\{s_i\}$ – $P_N(s) = \frac{1}{N}\sum \delta(s - s_i)$ – is called the *level spacing distribution* of the graph. It is one of several quantities used to

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measure the statistical fluctuations of a spectrum. We wish to examine it in the limit as we increase the number of vertices to infinity.

Our motivation for studying these spectral fluctuations comes from the theory of Quantum Chaos, where one studies fluctuations of energy levels of dynamical systems, for instance the spectrum of the Laplacian of a manifold (where the classical motion is the geodesic flow). It has been conjectured that generically there is a remarkable dichotomy:

1. If the classical dynamics are **completely integrable**, then Berry and Tabor [2] conjectured that the fluctuations are the same as those of an uncorrelated sequence of levels, and in particular $P(s) = e^{-s}$ is Poissonian.
2. If the classical dynamics are **chaotic** then Bohigas, Giannoni and Schmit [4], [5] conjectured that the fluctuations are modeled by the eigenvalues of a large random symmetric matrix - the Gaussian Orthogonal Ensemble (GOE)[1].

That is, the statistics of the spectral fluctuations are **universal** in each of the two classes.

While some obvious counter-examples exist, such as the sphere in the integrable case (the levels are $k(k+1)$ with multiplicity $2k+1$), and more subtle examples in the chaotic case, such as the modular surface (the quotient of the upper half-plane by the modular group $SL(2, \mathbf{Z})$), where the spacings appear to be Poissonian [1], [6], [7], [14], there is sufficient numerical evidence for us to believe that these universality conjectures hold in the generic case.

In the hope of gaining some extra insight into this matter we checked fluctuation properties of the spectrum of a regular graph. Graphs, for us, will occupy an intermediate step between quantizations of genuine chaotic dynamical systems and the statistical models of Random Matrix Theory. While we have no direct interpretation of graphs in terms of classical mechanics, an analogy is the random walk on a graph: Starting with an initial probability distribution, a particle at a given vertex moves to one its its neighbors with equal probability. This substitute for dynamics is **chaotic** in the following sense: The walk is recurrent if the graph is connected (which we interpret as ergodicity), and in that case is mixing if the graph is not bipartite. In the bipartite case, the set of vertices is a union of two

[1] Assuming the dynamics are invariant under time reversal.

disjoint sets (inputs and outputs) so that inputs can only be connected to outputs and vice-versa. Thus if we start from an input vertex and walk any even number of steps then we will only be able to land on another input, never on an output.

There are examples (such as some Cayley graphs, see [3], [13]) where there are systematic multiplicities in the spectrum and the level spacing distribution at best exists only in some singular limit. For instance in the case of Cayley graphs of the cyclic group $\mathbf{Z}/n\mathbf{Z}$ the appropriate limit gives a **rigid** spectrum: $\widehat{E}_n = n$, so that $P(s) = \delta(s-1)$ is a Dirac delta function. Another special example, analogous to the modular surface, seems to have Poisson spacings (numerical evidence by Lafferty and Rockmore [12]). These examples have certain symmetries or degeneracies. We tested a number of families of generic (pseudo)-random k-regular graphs (see section 4 for the details of the generation algorithm). The numerical evidence we accumulated, described in Section 5, indicates that the resulting family of graphs have GOE spacings. This should be compared with the numerical investigations by Evangelou [9] and the discussion by Mirlin and Fyodorov [17] which suggest that in the case of **sparse** random symmetric matrices the spacings are GOE. We are thus led to conjecture that for a fixed degree $k \geq 3$, the eigenvalues of the generic k-regular graph on a large number of vertices have fluctuations which tend to those of GOE (see Section 5 for a more precise statement).

The purpose of our paper is not only to describe our experimental results, but also to give a brief survey of the theory of Quantum Chaos for graph theorists, and of a bit of relevant graph theory for experts in Quantum Chaos. Accordingly, we included a survey of background material on graphs and their spectra in Section 2 , and a brief overview of Random Matrix Theory in Section 3. In section 4 we present the method used for generating graphs, and in section 5 the results of our experiments.

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2. Graphs and their spectra

A *graph* G consists of a set V of *vertices* and a set E of *edges* connecting pairs of vertices. Two vertices v and w are called *adjacent* or *neighboring* (denoted $v \sim w$) if they are joined by an edge. An ordering (v, w) of the endpoints of an edge e gives e an *orientation*; the second vertex is often called the *head* of e (denoted e_+), the first one is called the *tail* (denoted e_-). A graph G is *directed* if every edge of G is given an orientation. We shall mostly consider undirected graphs, where orientations are not specified.

Several edges connecting the same two vertices are called *multiple* edges; a graph with multiple edges is sometimes called a *multigraph*[2]. An edge with coinciding endpoints is called a *loop*; we shall generally consider graphs without loops or multiple edges. The *degree* (or *valency*) of a vertex is the number of edges meeting at that vertex; G is called *k-regular* if the degree of every vertex is equal to k. A *walk* in G is a sequence $(v_0, v_1, \dots, v_s)$ of vertices such that $v_i \sim v_{i+1}$; it is *closed* if $v_0 = v_s$. G is *connected* if every two vertices can be joined by a walk.

Associated to every graph is its *adjacency matrix* A. It is a square matrix of size $n = |V|$ whose (i, j)-th entry is equal to the number of edges joining vertices v_i and v_j of G. For loopless graphs the diagonal entries of A are zero. The *Laplacian* Δ is an operator acting on functions on the set of vertices of G. It is defined by

$$(\Delta f)(v) \;=\; \sum_{w \sim v} (f(v) - f(w)) \tag{2.1}$$

Denote by B the diagonal matrix whose i-th entry is the degree of v_i; then

$$\Delta \;=\; B - A$$

For regular graphs this gives

$$\Delta \;=\; k \cdot \mathrm{Id} - A \tag{2.2}$$

To motivate the analogy with the Laplace-Beltrami operator on Riemannian manifolds, we first define the *incidence mapping* D. To do that, orient all edges of G in some way. D maps functions on the set of vertices to functions on the set of edges by the formula

$$Df(e) \;=\; f(e_+) - f(e_-)$$

[2]The terminology varies: occasionally what we call a graph is called a *simple graph*, while what we call a multigraph is simply called a graph.

If $|V| = n$ and $|E| = m$, the matrix of D (called the *incidence matrix*) is an n-by-m matrix whose elements are 0 and ± 1; $D_{ij} = +1$ if v_i is the head of e_j, to -1 if it is the tail and to 0 otherwise. The Laplacian matrix satisfies

$$\Delta = DD^t. \tag{2.3}$$

One may consider the set $\mathcal{E}$ of all directed edges ($|\mathcal{E}| = 2|E|$) and think of directed edges one of whose endpoints is v as a tangent space to G at v; D can then be interpreted as a combinatorial analog of exterior differentiation d. The adjoint D^* of D acts on functions $g : \mathcal{E} \to \mathbf{R}$ by

$$D^* g(v) = \sum_{e \in \mathcal{E} : e_+ = v} g(e)$$

Then $\Delta = D^* D$, analogously to $\Delta = d^* d$ on manifolds.

The Laplacian is a non-negative and self-adjoint operator. A constant function on a connected component of G is an eigenfunction of Δ with eigenvalue 0; the multiplicity of 0 is equal to the number of the connected components of G (exactly as for the manifold Laplacian). In the sequel we will only deal with connected graphs. The spectrum of $A(G)$ for a k-regular graph G is clearly contained in $[-k, k]$; the spectrum of $\Delta(G)$ is contained in $[0, 2k]$. A graph is *bipartite* if the set V can be partitioned into disjoint subsets $V = V_1 \cup V_2$ such that all edges have one endpoint in V_1 and another in V_2. A k-regular graph is bipartite if and only if $2k$ is an eigenvalue of Δ, and in that case the spectrum of Δ has the symmetry $E \mapsto 2k - E$. Indeed, let G be a bipartite graph and f be an eigenfunction of $\Delta(G)$ with eigenvalue E. Then let $f'(v)$ be defined as follows:

$$f'(v) = \begin{cases} f(v), & v \in V_1 \\ -f(v), & v \in V_2 \end{cases}$$

It is not hard to check that f' is an eigenfunction of $\Delta(G)$ with eigenvalue $2k - E$.

Denote the eigenvalues of the adjacency matrix $A(G)$ of a k-regular graph G by

$$k = \lambda_1 > \lambda_2 \geq \ldots \geq \lambda_n \geq -k$$

The (i, j)-th entry of the matrix A^r is equal to the number of walks of length r starting at the vertex v_i and ending at v_j. Accordingly, the trace of A^r is equal to the number of closed walks of length r. On the other hand, $\operatorname{tr}(A^r) = \sum_{i=1}^n \lambda_i^r$ is (by definition) equal to n times the r-th moment of the *spectral density*

$$\frac{1}{n}\sum_{i=1}^{n}\delta(x-\lambda_i) \tag{2.4}$$

of A.

A closed walk $(v_0, v_1, \dots, v_r)$ is called a *cycle* if $v_1, \dots, v_r$ are distinct. The *girth* $\gamma(G)$ of G is the length of the shortest cycle of G; all closed walks of length less than $\gamma(G)$ necessarily involve backtracking (i.e. $v_{i+1} = v_{i-1}$ for some i). The number of closed walks of (necessarily even) length $2r < \gamma$ starting and ending at any vertex v of a k-regular graph G is equal to the number of such closed walks starting and ending at any vertex of the infinite k-regular tree T_k.

We denote by $G_{n,k}$ the set of k-regular graphs with n vertices. It is known [19] (and not hard to see) that for any fixed $r \geq 3$ the expected number $c_r(G)$ of r-cycles in a regular graph $G \in G_{n,k}$ approaches a constant as $n \to \infty$; accordingly, for "most" graphs $G \in G_{n,k}$ $c_r(G)/n \to 0$ as $n \to \infty$.

It is easy to show ([15, Lemma 2.2]) that the last condition implies that for each fixed r and for most graphs $G \in G_{n,k}$ the average number of closed walks of length r on G is asymptotic to that of the tree. Accordingly, the r-th moments of the spectral density (2.4) approach those of the spectral density of the of the infinite k-regular tree T_k as $n \to \infty$.

It follows ([15]) that the spectral density (2.4) for a general $G \in G_{n,k}$ converges to the tree density ([11]) given by

$$f_k(x) = \begin{cases} \dfrac{k(4(k-1)-x^2)^{1/2}}{2\pi(k^2-x^2)} & |x| \leq 2\sqrt{k-1} \\ 0 & |x| > 2\sqrt{k-1} \end{cases} \tag{2.5}$$

supported in $I_k = [-2\sqrt{k-1}, 2\sqrt{k-1}]$. We refer to (2.5) as *McKay's law*. It can be regarded as an analog for graphs of Weyl's law for manifolds, in that both give limiting distributions for spectral densities.

3. Random Matrix Theory

We give a brief overview of the Gaussian Orthogonal Ensemble (GOE) of Random Matrix Theory[3] - the statistical model relevant to graphs. It is the space of $N \times N$ real symmetric matrices $H = (H_{ij})$ with a probability measure $P(H)dH$ which satisfies

[3] The standard reference is Mehta's book [16].

1. $P(H)dH$ is invariant under all orthogonal changes of basis:

$$P(XHX^{-1})dH = P(H)dH, \qquad X \in O(N)$$

2. Different matrix elements are statistically independent.

These requirements force P to be of the form

$$P(H) = \exp(-a\,\mathrm{tr}(H)^2 + b\,\mathrm{tr}(H) + c)$$

for suitable constants $a > 0$, b, c. After shifting the origin and normalizing one finds that the joint probability distribution of the eigenvalues λ_j, $j = 1, \dots, N$ of H is given by

$$P_N(\lambda_1 \dots, \lambda_N)d\lambda = C_N \prod_{i<j} |\lambda_i - \lambda_j| \exp(-\sum_j \lambda_j^2) \prod_{j=1}^N d\lambda_j. \tag{3.1}$$

There is an expected limiting density for the eigenvalues of a large $N \times N$ matrix as $N \to \infty$, given by *Wigner's semi-circle law*:

$$R_1(x) = \begin{cases} \frac{1}{\pi}\sqrt{2N - x^2}, & |x| \le \sqrt{2N} \\ 0, & |x| > \sqrt{2N} \end{cases} \tag{3.2}$$

Near the top of the semi-circle, at $x = 0$, the density is $\sqrt{2N}/\pi$. Thus if we "unfold" the eigenvalues by setting $x_j := \lambda_j \sqrt{2N}/\pi$, we will get a sequence of numbers $\{x_j\}$ whose mean spacing is unity, as $N \to \infty$.

RMT studies spectral fluctuation of the unfolded spectrum $\{x_j\}$ as $N \to \infty$, such as the probability distribution of the nearest neighbor spacing $s_n := x_{n+1} - x_n$. For each $N \times N$ matrix H, form the probability measure

$$p(s, H) = \frac{1}{N} \sum_{n=1}^N \delta(s - s_n)$$

Then as $N \to \infty$, there is an expected limiting distribution (called the *level spacing distribution*) given by

$$P(s) = \lim_{N \to \infty} \int p(s, H) P(H) dH$$

called the *level spacing distribution.* It was expressed by Gaudin and Mehta in terms of a Fredholm determinant. For small s, $P(s) \sim \frac{\pi^2}{6} s$.

An approximation derived by Wigner before the Gaudin-Mehta formula was known, on basis of the $N = 2$ case, is the *Wigner surmise*

$$P_W(s) = \frac{\pi}{2} s e^{-\pi s^2/4}$$

which gives a surprisingly good fit (see [16], Figure 1.5).

It is worth emphasizing that the utility of RMT lies in that the predicted level spacing distribution $P(s)$ and correlation functions are model-independent and appear in many instances, both probabilistic and deterministic, independent of features such as the level density (3.2). For instance, numerical studies indicate that *sparse* random matrices have GOE spacings [9], and the experiments described in the following section indicate that the same is true for eigenvalues of random regular graphs.

4. Random graph generation

We generated random k-regular graphs using a method described in [20]. It is easy to implement and extremely efficient for the small (≤ 6) values of k of current interest to us. On the other hand, the running time of the algorithm grows exponentially with the degree k, and (at least in our implementation) was found impractical for $k > 7$ on the hardware[4] which we used. It should be noted that in the same paper [20], Wormald describes an algorithm which scales well with k, but is much more cumbersome to implement and slower for small k.

Wormald's algorithm is easiest explained in terms of generating random bipartite graphs with prescribed vertex degrees. Assume that we wish to generate a random bipartite graph G with M_b blue vertices, named $b_1, \dots, b_{M_b}$, and M_r red vertices, named $r_1, \dots, r_{M_r}$. We would like the vertex b_i to have degree v_i, while the vertex r_j to have degree w_j. Evidently, we must have $\sum_i v_i = \sum_j w_j = |E(G)|$.

We now construct an array $\mathcal{A}$ of size $|E(G)|$. The first w_1 cells of $\mathcal{A}$ contain r_1, the next w_2 contain r_2, and so on. Now, we permute the $E(G)$ cells of $\mathcal{A}$ by a random permutation in $S_{E(G)}$, to get another array $\mathcal{A}'$. The array $\mathcal{A}'$ defines a bipartite (multi)graph G' as follows: The neighbors of b_1 are the first v_1 entries of $\mathcal{A}'$, the neighbors of b_2 are the next v_2 entries, and so on. It is possible that G' is a multigraph, since two of the neighbors of some b_i might well be the same. If that turns out to be the case, we scrap $\mathcal{A}'$, and generate another random permutation, and thus another random array $\mathcal{A}''$, and corresponding multigraph G'', and so on, until we have a true bipartite graph. It is clear that if the valences v_i and v_j are small, this process has a good chance of converging in reasonable time, and it should

[4] A 100Mhz Pentium processor PC running Linux.

also be intuitively fairly clear that each bipartite graph with prescribed degrees is equally likely to appear. Both statements are proved in [20].

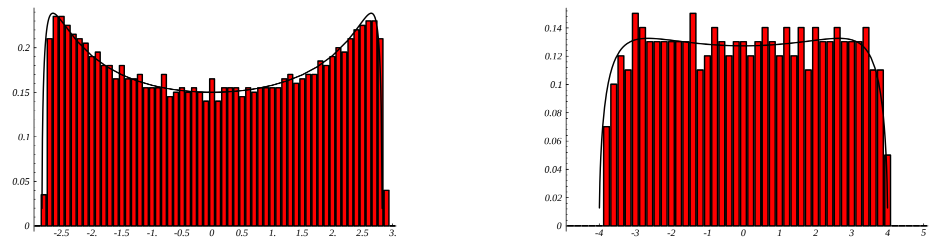
The problem of generating a random k-regular graph can, in effect, be reduced to the previous problem of generating a random bipartite graph. To wit, to each graph G we associate a bipartite graph B_G, such that $V(B_G) = V(G) \cup E(G)$, where the blue vertices of B_G correspond to the vertices of G, while the red vertices correspond to the edges of G. A vertex v is connected to e in B_G, whenever e is incident to v in G. A k-regular G gives rise to a graph B_G, where the blue vertices have degree k, while the red vertices have degree 2. On the other hand, not every bipartite H with degrees as above arises as B_G for some k-regular graph G, since if H has two red vertices r_1 and r_2 such that the blue neighbors of r_1 are the same as those of r_2, the corresponding G is, in actuality, a multigraph.

The algorithm can thus be summarized as follows: To generate a random k-regular graph with n vertices, first generate a random bipartite graph H with n blue vertices of degree k and $nk/2$ vertices of degree 2. If $H = B_G$ for some (obviously unique) graph G, then return G, else try again. The expected running time of this process is analyzed, and the uniformity of the results is proved in [20].

Remark. Evidently, this method is even better suited to generating random *bipartite* graphs with a prescribed degree sequence. We have used the algorithm to generate random 3-regular and 5-regular bipartite graphs. The experimental results were not substantively different from those for general regular graphs (as described below).

5. Experimental results

We computed the eigenvalues of graphs generated as above. The spectral densities of a couple of families – one of 3-regular graphs and another of 5-regular graphs – are displayed in Figures 1(a) and 1(b) against McKay's law (2.5).



(a) cubic graph on 2000 vertices; (b) 5-valent graph on 500 vertices.

Figure 1. Eigenvalue distributions of random graphs *vs* McKay's law

We then unfolded the spectrum by using McKay's law, and computed the level spacing distribution. The resulting plots compared with GOE showed a good fit – see Figure 2.

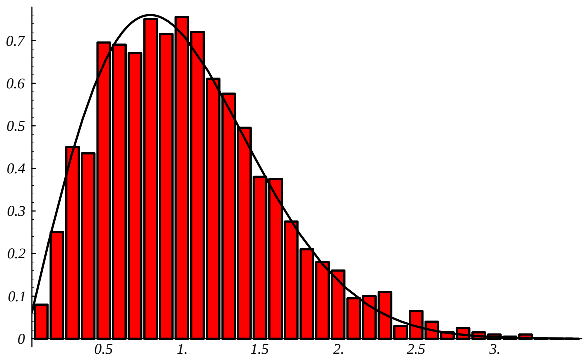


Figure 2. Level spacing distribution of a cubic graph on 2000 vertices *vs* GOE

We tested the matter further by using a variant of the Kolmogorov-Smirnov test. One compares an empirical, sample distribution to an expected answer by measuring the deviation of the cumulative distribution functions of the two. Recall that if s_i, $i = 1, \dots, N$ are random variables (the spacings, in our case), the empirical distribution function is $P_N(s) = \frac{1}{N}\sum_{i=1}^{N} \delta(s - s_i)$ and its cumulative distribution function is $C_N(s) = \frac{1}{N}\#\{i \mid s_i \leq s\}$. To test if the distribution function is given by a theoretical prediction $F(s)$, define the *discrepancy* $D(C_N, F)$ (or *Kolmogorov-Smirnov statistic*) to be the supremum of $|C_N(s) - F(s)|$ over $s > 0$. The discrepancy is small if and only if the two distributions are close to each other. In the case that the s_i are **independent**, identically distributed (definitely not the case at hand!) with cumulative distribution function $F(s)$, the discrepancy goes to zero almost surely as $N \to \infty$ and there is a limit law giving the the limiting distribution $L(z)$ of the normalized discrepancy $\sqrt{N}D(C_n, F)$ as $N \to \infty$:

$$L(z) := \lim_{N\to\infty} Pr\{\sqrt{N}D(C_N, F) \leq z\} = \sum_{j=-\infty}^{\infty} (-1)^j e^{-2j^2z^2}$$

In the case that the s_i's are spacings of **uncorrelated** levels (hence certainly not independent!), the level spacing distribution is exponential $P(s) = e^{-s}$ as $N \to \infty$ and Pyke [18] derives a limit law for the normalized discrepancy.

In the case where the s_i's are spacings of certain models of RMT (not GOE, however), Katz and Sarnak [10] prove that the discrepancy goes to zero almost surely as $N \to \infty$ and conjecture that there is a limit law as in the case of Kolmogorov-Smirnov and Pyke.

Miller (work in progress) has investigated this distribution for random symmetric and hermitian matrices and has numerically discovered that, after being normalized by multiplying by $\sqrt{N}$, it approaches a limiting distribution which seems independent of the type of matrix involved. In Figure 3 we show this cumulative distribution function $L_{GOE}(z)$ of the normalized discrepancy for GOE (top plot) against the Kolmogorov-Smirnov "brownian bridge" $L(z)$ (bottom plot) and Pyke's distribution for spacings of uncorrelated levels (middle plot).

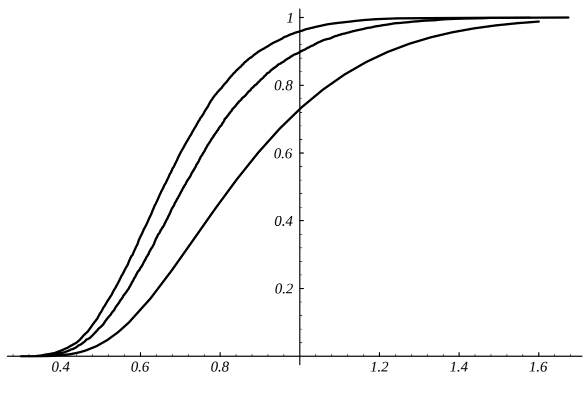


Figure 3. Cumulative distribution functions for normalized discrepancy.
Top plot: GOE. Middle plot: Pyke's limit law for spacings of uncorrelated levels.
Bottom plot: Kolmogorov-Smirnov limit law.

The numerical value of $L_{GOE}(z)$ can be used as a goodness-of-fit test to see if the eigenvalues of a large symmetric matrix have GOE spacings in the same way one uses the Kolmogorov-Smirnov test.

We computed the discrepancy for the eigenvalues of a large number of random graphs of particular types. Comparison of the normalized discrepancies to Miller's table gave good confidence that the spacings were indeed close to GOE. In Figure 4 we plot the distribution of the normalized discrepancies of a set of 4500 cubic graphs on 300 vertices against Miller's distribution (computed from a set of 5000 random symmetric 120×120 matrices). As the figure indicates, the two distributions are fairly close.

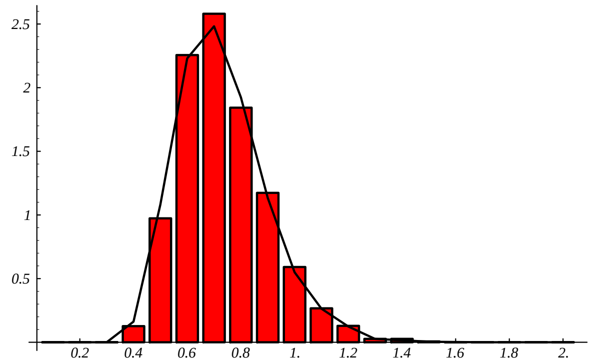


Figure 4. Distribution of normalized discrepancies for cubic graphs vs. GOE

Conclusion. The numerical evidence presented above leads us to believe that for a fixed valency $k \geq 3$, the eigenvalues of the generic k-regular graph on a large number of vertices have GOE fluctuations in the sense that as we increase the number N of vertices, for all but a vanishing fraction of these graphs the discrepancy between the level spacing distribution of the graph and the GOE distribution goes to zero.

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