An Investigation of Expanders and Ramanujan Graphs along Random Walks of Cubic Bipartite Graphs

PETER C. RICHTER*

May 11, 2001

Abstract

A numerical experiment is performed to observe whether or not the second largest eigenvalue $\lambda_1(X_N)$ of the random cubic bipartite graph X_N on N vertices appears to satisfy $\lambda_1(X_N) \to 2\sqrt{2}$ as $N \to \infty$ with probability 1. If so, then a family of random graphs $\{X_m\}_{m=1}^{\infty}$ satisfying $|X_m| \to \infty$ as $m \to \infty$ would be, with probability 1, an excellent family of "expanders" (highly-connected sparse graphs). More precisely, in the limit $m \to \infty$, the expanding constant of X_m would have the same optimal bound (in terms of the spectral gap of the graph) as that of the arithmetically constructed Ramanujan graph.

*Undergraduate Math. Lab., Princeton U., Princeton, NJ. prichter@princeton.edu

1 Expanders and Ramanujan Graphs

Given a graph $G = (V, E)$, the *boundary* ∂F of a subset $U \subseteq V$ is the set of edges connecting U to $\overline{U}$. The *expanding constant*, which gives a measure of the connectivity of G, is defined as follows:

$$h(G) := \inf\{\frac{|\partial U|}{\min\{|U|, |\overline{U}|\}} : U \subseteq V,\ 0 < |U| < \infty\} \tag{1.1}$$

Fix $k \geq 2$ and consider a family $\{G_m\}_{m=1}^{\infty}$ of finite connected k-regular graphs. Call $\{G_m\}$ a *family of expanders* if $|G_m| \to \infty$ as $m \to \infty$ and if there exists a positive constant $\epsilon > 0$ such that $h(G_m) \geq \epsilon$ for every $m \geq 1$. Expanders then are characterized by their *sparsity* (since the number of edges grows at most linearly with the number of vertices) and *high connectivity* (since the corresponding sequence of expanding constants has a positive lower bound).

It can be shown that if G is a k-regular graph with eigenvalues $\{\lambda_i\}_{i=0}^{|G|-1}$ listed in decreasing order, then (i) $\lambda_0 = k$, and (ii) $\lambda_0 > \lambda_1 \Leftrightarrow G$ is connected.[1] Moreover, if G is connected, then its eigenvalues are symmetric about zero if and only if G is bipartite. The Cheeger-Buser inequalities give upper and lower bounds for the expanding constant of a finite k-regular connected graph in terms of the spectral gap $k - \lambda_1$ of G:

$$\frac{k - \lambda_1}{2} \leq h(G) \leq 2\sqrt{2k(k - \lambda_1)} \tag{1.2}$$

Thus, a family $\{G_m\}$ of finite connected k-regular graphs with $|G_m| \to \infty$ as $m \to \infty$ is a family of expanders if and only if there exists a positive constant $\epsilon > 0$ such that $k - \lambda_1(G_m) \geq \epsilon$ for every $m \geq 1$.

We can obtain increasingly better expanders by raising the lower bound on the spectral gaps $k - \lambda_1$ of each of the graphs. However, this can only be done up to a point; Alon-Boppana, Burger, and Serre showed that for any family $\{G_m\}$ of finite connected k-regular graphs with $|G_m| \to \infty$ as $m \to \infty$,

$$\liminf_{m \to \infty} \lambda_1(G_m) \geq 2\sqrt{k - 1} \tag{1.3}$$

To maximize the lower bound on the spectral gap then, we want each graph G in the family $\{G_m\}$ of expanders to satisfy

[1] Most of the results in this section are proved and discussed in greater depth in G. Davidoff, P. Sarnak, and A. Valette [1].

$$\lambda_1(G) \leq 2\sqrt{k-1} \tag{1.4}$$

A graph G with this property is called *Ramanujan*. An infinite family $\{G_m\}_{m=1}^{\infty}$ of Ramanujan graphs is a family of expanders with optimal bounds on the expanding constant $h(G_m)$ in terms of the spectral gap $k - \lambda_1(G_m)$ for each $m \geq 1$. Such families have been constructed explicitly using sophisticated mathematical techniques. In this numerical experiment, we investigate whether, with probability 1, the random *simple* (single-bonds only) *cubic* (3-regular) connected bipartite graph X_N on N vertices satisfies

$$\lim_{N\to\infty} \lambda_1(X_N) = 2\sqrt{2} \tag{1.5}$$

If so, then with probability 1, the infinite family $\{X_N\}$ is an asymptotically optimal family of expanders with respect to λ_1.

2 Numerical Experiment

In this numerical experiment, the second-largest eigenvalue $\lambda_1(X_N)$ was computed at each step of a random walk in the space of simple cubic connected bipartite graphs X_N on N vertices. The objective was to gain some insight into the behavior of the probability distribution for $\lambda_1(X_N)$ as N increases, and to perhaps arrive at a prediction of whether or not

$$\lim_{N\to\infty} \lambda_1(X_N) = 2\sqrt{2} \tag{2.1}$$

The random walk is determined as follows. First, an initial bipartite graph with independent sets of vertices $\{v_0, ..., v_{N/2-1}\}$ and $\{v_{N/2}, ..., v_{N-1}\}$ is chosen, by randomly permuting each of 3 arrays V_1, V_2, V_3 of length $N/2$ and constructing an edge between vertices v_j and v_k if and only if $V_i[j] = k$ for some $i : 1 \leq i \leq 3$. In the event that this produces a graph which is not both simple and connected, the process is repeated until such a graph is produced. At each step along the walk, two randomly chosen edges (v_j, w_j) and (v_k, w_k) satisfying $(v_j, w_k) \notin E$ and $(v_k, w_j) \notin E$ are switched, i.e., (v_j, w_j) and (v_k, w_k) are destroyed and (v_j, w_k) and (v_k, w_j) are constructed.

For each graph X_N along the random walk, the eigenvalue $\lambda_1(X_N)$ of the adjacency matrix A of X_N is computed using an eigenvalue routine based on the following power method variant:

$x \leftarrow x_0$
$while\ (|\lambda_{new} - \lambda_{old}| \geq \epsilon\ or\ \theta(\lambda_{new}, A, x) \geq |\lambda_{new} - 2\sqrt{2}|)$
$\quad y \leftarrow x - \frac{1}{N}[\sum_{i=0}^{N-1} x_i]\xi_0 - \frac{1}{N}[\sum_{i=0}^{N/2-1} x_i - \sum_{i=N/2}^{N-1} x_i]\xi_{N-1}$
$\quad z \leftarrow y/\|y\|_2$
$\quad x \leftarrow A(Az)$
$\quad \lambda_{old} \leftarrow \lambda_{new}$
$\quad \lambda_{new} \leftarrow \sqrt{x^T z}$

For any non-pathological initial vector x_0, λ_{new}^2 converges to the eigenvalue $\lambda_1^2 = \lambda_{N-2}^2$ of the real symmetric matrix A^2 and x converges to a corresponding eigenvector ϕ (a linear combination of the eigenvectors ξ_1 and ξ_{N-2} of A^2).[2] The methodology is as follows: Write x_0 as a linear combination $\sum_{i=0}^{N-1} c_i\xi_i$. (Since A^2 is real symmetric, its eigenvectors $\{\xi_i\}_{i=0}^{N-1}$ form an orthonormal basis for $\Re^N$.) Then after $m \geq 1$ iterations of the loop, we have $x = x^{(m)}$ where

$$\begin{aligned} x^{(m)} &= (A^2 \sum_{i=1}^{N-2} c_i \lambda_i^{2(m-1)} \xi_i) \ / \ \| \sum_{i=1}^{N-2} c_i \lambda_i^{2(m-1)} \xi_i \|_2 \\ &= (\sum_{i=1}^{N-2} c_i \lambda_i^{2m} \xi_i) \ / \ \| \sum_{i=1}^{N-2} c_i \lambda_i^{2(m-1)} \xi_i \|_2 \end{aligned} \tag{2.2}$$

Since $\lambda_1^2 = \lambda_{N-2}^2$ is the eigenvalue of largest modulus in the in the iteration above (the eigenvectors $\xi_0 = (1, ..., 1)$ and $\xi_{N-1} = (1, ..., 1, -1, ..., -1)$ corresponding to the eigenvalue $\lambda_0^2 = \lambda_{N-1}^2$ are projected out of $x^{(m)}$ at each step), $c_1\lambda_1^{2m}\xi_1$ and $c_{N-2}\lambda_{N-2}^{2m}\xi_{N-2}$ dominate the sum above in the limit $m \to \infty$. Thus, $x^{(m)} \to \lambda_1(c_1\xi_1 + c_{N-2}\xi_{N-2})\ /\ \|c_1\xi_1 + c_{N-2}\xi_{N-2}\|_2$ and $(\lambda_{new}^2)^{(m)} \to \lambda_1^2$ as $m \to \infty$.

For best performance, the multiplication of the vector z by the matrix A^2 in the pseudocode above should be performed by multiplying z twice by the sparse matrix A rather than once by the square matrix A^2. This way, matrix-vector multiplication will take $O(N)$ time provided that A is stored as an adjacency list. In this particular experiment, performance can also be improved by using the value of x computed in the last call to the eigenvalue routine as the initial vector x_0 in the next call, since successive graphs in our walk are quite similar and often have similar eigenvalues and eigenvectors.

Since we want our program to determine definitively for each graph X_N whether $\lambda_1(X_N)$ is smaller or larger than $2\sqrt{2}$ (to get an accurate count

[2] The power method will not converge to nontrivial eigenvalue/eigenvector pairs of A because the eigenvalues of A occur in +/- pairs; instead, we apply it to A^2 and take the square root of the computed eigenvalue to get the corresponding eigenvalue of A.

of the number of Ramanujan graphs found in a particular walk), we must iterate until the θ-neighborhood of λ_{new} does not contain $2\sqrt{2}$, where θ is the error bound on the approximate eigenvalue λ_{new}. This bound is computed using A and the approximate eigenvector x of A^2 as follows:

$$\begin{aligned}
&y \leftarrow x/\|x\|_2 \\
&z \leftarrow A(Ay) \\
&\zeta \leftarrow z - \lambda_{new}^2 y \\
&\theta \leftarrow \sqrt{\|\zeta\|_2}
\end{aligned}$$

This error bound procedure is based on the fact that the for any approximate eigenvalue/eigenvector pair (μ, v) of a real symmetric matrix A with $\|v\|_2 = 1$, the vector $\zeta := Av - \mu v$ satisfies

$$\min_i |\lambda_i - \mu| \leq \|\zeta\|_2 \tag{2.3}$$

This result is easily derived: Replace A^2 by its eigenvalue decomposition $S\Lambda S^{-1}$. Then we have

$$\begin{aligned}
\zeta &= S\Lambda S^{-1}v - \mu v = S(\Lambda - \mu I)S^{-1}v \\
\Rightarrow v &= S(\Lambda - \mu I)^{-1}S^{-1}\zeta \qquad (2.4)
\end{aligned}$$

Taking norms and recalling that $\|v\|_2 = \|S\|_2 = \|S^{-1}\|_2 = 1$, it follows that

$$\begin{aligned}
1 &\leq \|(\Lambda - \mu I)^{-1}\|_2 \|\zeta\|_2 \\
\Rightarrow \|\zeta\|_2 &\geq \|(\Lambda - \mu I)^{-1}\|_2^{-1} = (\max_i \frac{1}{|\lambda_i - \mu|})^{-1} = \min_i |\lambda_i - \mu| \qquad (2.5)
\end{aligned}$$

The computer procedure above calculates the error bound on the approximate eigenvalue λ_{new}^2 of A^2 using this prescription, then takes the square root to get the error bound on the approximate eigenvalue λ_{new} of A.

3 Experimental Results

The numerical experiment was performed as follows: For $N = 100, 200, ..., 1000$, $\lambda_1(X_N)$ was computed for each matrix X_N along 5 different random walks of length 1000. The table below lists, for each value of N: $\{R_i =$ the # of graphs X_N found to be Ramanujan in the i^{th} walk out of 5$\}$, $R_{avg} =$ the average # of graphs per walk found to be Ramanujan, $P_{avg} =$ the average proportion of graphs found to be Ramanujan, $(\lambda_1)_{avg} =$ the average value of $\lambda_1(X_N)$ over all graphs X_N (cf. $2\sqrt{2} \approx 2.8284$), and $\sigma =$ the standard deviation of the distribution of $\lambda_1(X_N)$.

N	$\{R_i\}_{i=1}^5$	R_{avg}	P_{avg}	$(\lambda_1)_{avg}$	σ
100	986, 973, 983, 993, 970	981	0.981	2.7686	0.0281
200	905, 955, 977, 969, 949	951	0.951	2.8010	0.0175
300	938, 963, 915, 874, 859	910	0.910	2.8088	0.0142
400	864, 953, 925, 905, 951	920	0.920	2.8128	0.0109
500	870, 932, 955, 937, 943	927	0.927	2.8139	0.0097
600	864, 969, 909, 875, 757	875	0.875	2.8182	0.0092
700	933, 927, 903, 917, 915	919	0.919	2.8187	0.0068
800	890, 764, 905, 887, 917	873	0.873	2.8206	0.0067
900	984, 758, 927, 890, 853	882	0.882	2.8208	0.0068
1000	983, 972, 905, 894, 805	912	0.912	2.8208	0.0062

The following 10 diagrams plot the probability distributions obtained experimentally for $\lambda_1(X_N)$ for the distinct values of N.

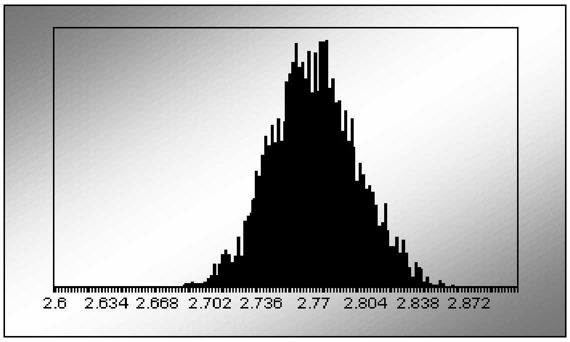

Figure 1: N=100

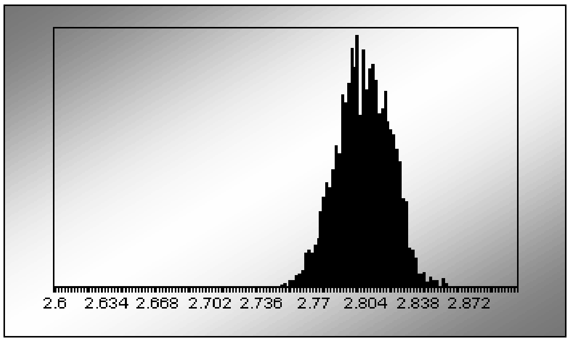

Figure 2: N=200

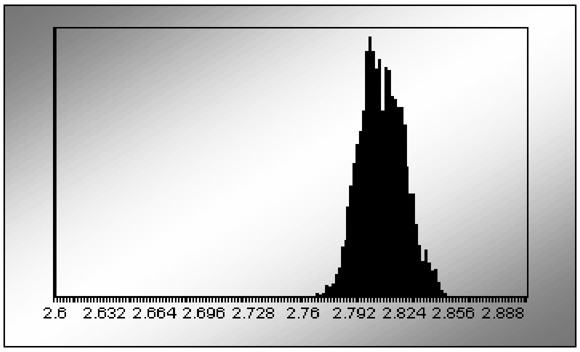

Figure 3: N=300

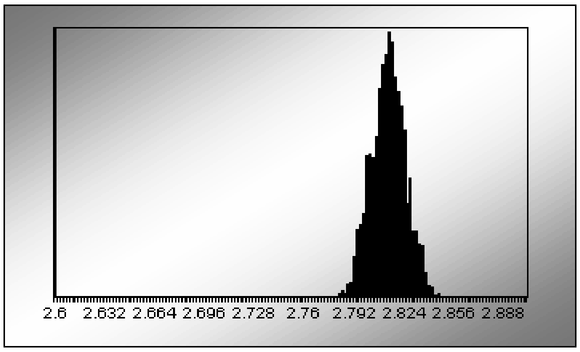

Figure 4: N=400

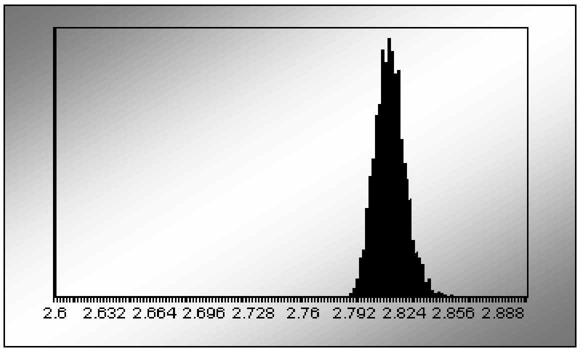

Figure 5: N=500

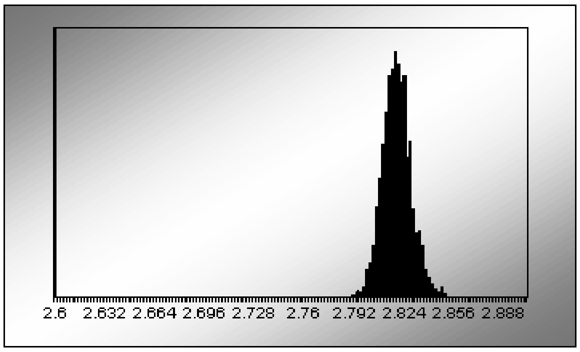

Figure 6: N=600

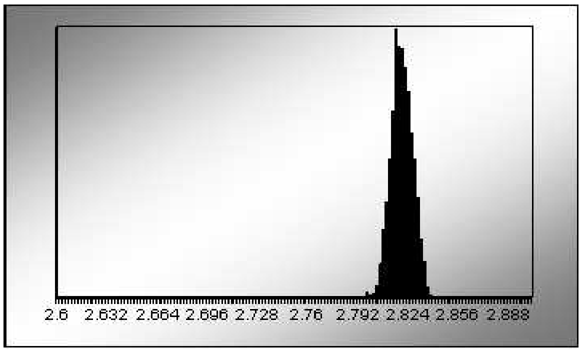

Figure 7: N=700

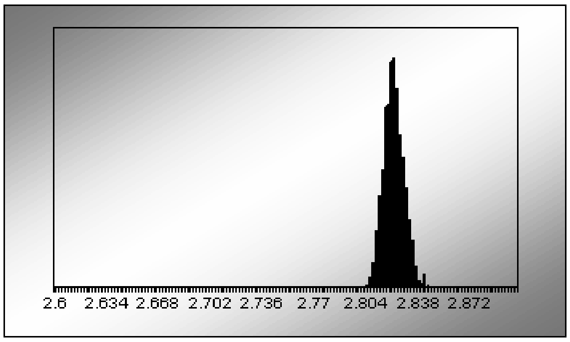

Figure 8: N=800

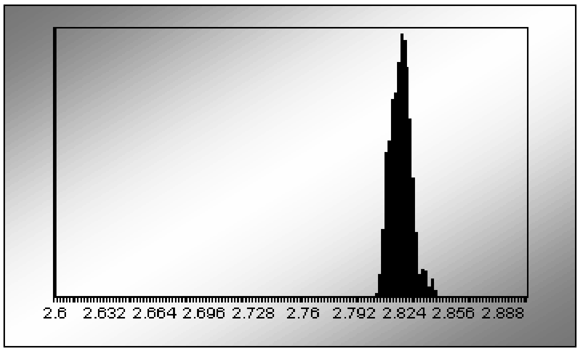

Figure 9: N=900

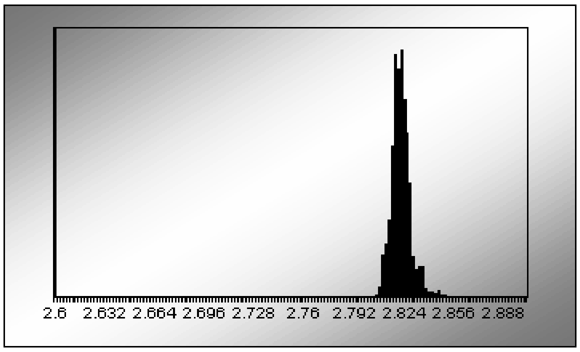

Figure 10: N=1000

4 Analysis and Interpretation

The proportion of graphs found to be Ramanujan, perhaps somewhat surprisingly, remained fairly constant as N was increased from 100 to 1000, hovering around the 90 percent range. It seems intuitively unlikely that the probability of the random cubic bipartite graph X_N being Ramanujan would tend to ~ 0.9 rather than, say, 0 or 1 as $N \to \infty$, so this phenomenon may well arise only because of the relatively small range of N. Unfortunately, as fast as the power method is at computing $\lambda_1(X_N)$, without the aid of parallel processing or a supercomputer it starts to become impractical to use for a random walk of length 1000 once $N > 1000$.

Nevertheless, it does appear likely that $\lambda_1(X_N)$ converges to the optimal value $2\sqrt{2}$ in the limit $N \to \infty$. This prediction is considerably well supported by the behavior of the distributions for $\lambda_1(X_N)$ for $N = 100$, 200, ..., 1000. (See the relavant table and plots beginning on page 6.) As N increases, the growth of the average value $(\lambda_1)_{avg}$ slows down (perhaps indicating that it is approaching $2\sqrt{2}$ asymptotically) and the standard deviation σ of $\lambda_1(X_N)$ appears to approach zero (indicating that as $N \to \infty$, the value of $\lambda_1(X_N)$ approaches $(\lambda_1)_{avg}$ with probability one). Thus, although the numerical evidence is far from definitive (and could never be truly definitive), it seems to indicate the strong possibility that with probability 1 the random simple cubic connected bipartite graph X_N on N vertices satisfies

$$\lim_{N \to \infty} \lambda_1(X_N) = 2\sqrt{2} \tag{4.1}$$

5 Conclusion

If indeed the random simple cubic bipartite graph X_N approaches with probability 1 the Ramanujan condition, i.e., $\lambda_1(X_N) \to 2\sqrt{2}$ as $N \to \infty$, then a family of random graphs $\{X_m\}_{m=1}^{\infty}$ with $|X_m| \to \infty$ as $m \to \infty$ is, with probability 1, a family of expanders with optimally large bounds on the expanding constant $h(X_m)$ in terms of the spectral gap $k - \lambda_1(X_m)$ in the limit $m \to \infty$. Such a result would be a significant illustration of the power of randomization in constructing highly-connected sparse graphs and could potentially have applications to the design of networks. Perhaps future numerical experiments could be performed to investigate graphs of greater regularity, i.e., k-regular graphs where $k > 3$, or *weighted* graphs with costs assigned to the edges.

6 Bibliography

For a good introduction to expanders and arithmetically constructed Ramanujan graphs, consult G. Davidoff, P. Sarnak, and A. Valette [1]. A discussion of the power method for computing the dominant eigenvalue of a matrix can be found in G. Dahlquist and A. Bjorck [2]. The derivation of the error bound (2.3) of an approximate eigenvalue is given in B. Noble [3].

References

[1] G. Davidoff, P. Sarnak, and A. Valette. *An Elementary Approach to Ramanujan Graphs.* Not yet published.

[2] G. Dahlquist and A. Bjorck. *Numerical Methods.* Prentice-Hall, Englewood Cliffs, N.J., 1974. Translated by Ned Anderson.

[3] B. Noble. *Applied Linear Algebra.* Prentice-Hall, Englewood Cliffs, N.J., 1969.