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The First Eigenvalue of (c, d)-Regular Graph

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#### Abstract

We show a phase transition of the first eigenvalue of random (c, d)-regular graphs, whose instance of them consists of one vertex with degree c and the other vertices with degree d for c > d. We investigate a reduction from the first eigenvalue analysis of a general (c, d)-regular graph to that of a tree, and prove that, for any fixed c and d, and for a graph G chosen from the set of all (c, d)-regular graphs with n vertices uniformly at random, the first eigenvalue of G is approximately max  $\{d, c/\sqrt{c-d+1}\}$  with high probability.

# **1** Introduction

Spectral analysis of graphs plays key roles in various fields of mathematical sciences, such as information science, combinatorics, statistics, physics, economics and sociology [2, 7, 5, 3, 9]. This is in general to analyze eigenvalues and eigenvectors of matrices related to graphs expressing certain relations; in particular, the first (largest) eigenvalue and its corresponding eigenvector are important for understanding the typical structure of graphs. In many contexts, it has been important to analyze random symmetric matrices defined as adjacency matrices of random graphs.

Motivated by such needs, the first eigenvalue of random symmetric matrices has been studied in depth; (see e.g. [5] and references herein); however, the analysis is still not sufficient, in particular, for sparse random matrices that are important for constructing approximate solutions of various combinatorial problems [9]. One of the important questions is to understand the influence of the fluctuation of degrees. For example, one may naturally expect that the first eigenvalue (and its corresponding eigenvector) would be affected if there are some vertices with large degree; but how much is it affected? Understanding such influence would reveal the meaning of "hub node" in a network in various situations.

As a first step for understanding this question, Kabashima and Takahashi proposed [6] to study a random graph ensemble that typically generates, e.g., almost *d*-regular graph with one exception vertex that has much larger degree c, and among several results, they heuristically and asymptotically analyzed the influence of the large degree vertex to the first eigenvalue of the adjacency matrices of such random graphs. The purpose of this paper is to give a rigorous analysis to what they derived by the statistical mechanical method.

Now we state our results precisely. Throughout this paper, we identify a graph and its adjacency matrix. For a graph G, the notation G is also used to denote G's adjacency matrix; thus, we denote by  $\lambda_1(G)$  the first eigenvalue of the adjacency matrix of graph G. For two graphs G and G', we consider them equivalent iff they have the same adjacency matrices under a fixed indexing of vertices. We consider in this paper random (c, d)-graphs G defined below and analyze the eigenvalue of their



Figure 1: Asymptotic behavior of  $\lambda_1(G)$  for a fixed *d*.

adjacency matrices G. For any c > d, a graph is called (c, d)-regular graph if it consists of one vertex with degree c and the other vertices with degree d. We use  $\mathcal{G}_{n,c,d}$  to denote the set of all simple (c, d)regular graphs with n vertices. Note that  $\mathcal{G}_{n,c,d}$  may be empty for some combinations of c, d, and n; but in this paper, we consider only the case where  $\mathcal{G}_{n,c,d}$  is not empty.

It is clear that the first eigenvector of any *d*-regular graph is  $\mathbf{1} = (1, 1, ..., 1)^{T}$  and the first eigenvalue is *d*. Now how much is it affected with one vertex with larger degree *c*? By the statistical mechanical method, Kabashima and Takahashi [6] heuristically showed that

$$\lambda_1(G) \approx \max\left\{d, \frac{c}{\sqrt{c-d+1}}\right\} = \begin{cases} d & \text{if } c \le d(d-1), \\ \frac{c}{\sqrt{c-d+1}} & \text{if } c > d(d-1). \end{cases}$$
(1)

holds for a typical graph  $G \in \mathcal{G}_{n,c,d}$  (see Fig. 1). In this paper, we give both lower and upper bounds on  $\lambda_1(G)$  that asymptotically match to (1) for a random graph G uniformly chosen from  $\mathcal{G}_{n,c,d}$  with  $n \ge 1$  and  $c > d \ge 3$  (if such a graph exists).

Here is the outline of our analysis. We first show lower and upper bounds of  $G \in \mathcal{G}_{n,c,d}$  where it contains a (c, d, k)-complete tree, a tree defined as a rooted tree which consists of the root with degree c and nodes with degree d and leaves with degree 1, and all leaves have depth k (defined in Definition 2.1).

**Theorem 1.1.** For any fixed c and d, if a graph  $G \in \mathcal{G}_{n,c,d}$  contains a (c,d,k)-complete tree as a subgraph and  $k \to \infty$  when  $n \to \infty$ , then we have

$$\max\left\{d, \ \frac{c}{\sqrt{c-d+1}}\right\} \le \lambda_1(G) \le \max\left\{d, \ \frac{c}{\sqrt{c-d+1}}\right\} + o(1)$$

This theorem states that the upper bound tends to the lower bound, which is the same as (1), as a sequence of (c, d)-regular graphs with *n* vertices contains a sequence of (c, d, k)-complete tree with increasing *k*.

Next, we show that, for fixed *c* and *d*, a sequence of (c, d)-regular graphs *G* chosen from  $\mathcal{G}_{n,c,d}$  uniformly at random contains a sequence of (c, d, k)-complete trees with increasing *k* with high probability. This together with Theorem 1.1 proves our main result stated as follows.

**Theorem 1.2.** For any fixed c and d, and for a graph G chosen from  $\mathcal{G}_{n,c,d}$  uniformly at random,

$$\max\left\{d, \ \frac{c}{\sqrt{c-d+1}}\right\} \le \lambda_1(G) \le \max\left\{d, \ \frac{c}{\sqrt{c-d+1}}\right\} + o(1)$$

*holds with probability greater than* 1 - o(1)*,* 

This paper is organized as follows. In Section 2, we define some notations and technical terms, including "regularized (c, d, k)-complete tree", the main technical tool of our analysis. In Section 3, we analyze an asymptotic value of the first eigenvalue of the regularized (c, d, k)-complete tree. In Section 4, we relate the first eigenvalue of a general (c, d)-regular graph to that of the regularized (c, d, k)-complete tree. In Section 5, we show that a sequence of random (c, d)-regular graphs with *n* vertices contains a sequence of (c, d, k)-complete trees with increasing *k* with high probability. The final section is devoted to summaries of this paper and additional researches. In this paper, we explain some details of derivations in Appendix.

## 2 Preliminaries

For an integer  $n \ge 1$ , we use the notation  $[n] := \{1, 2, ..., n\}$ , and the notations of vectors  $\mathbf{0} := (0, 0, ..., 0)^{\mathrm{T}}$  and  $\mathbf{1} := (1, 1, ..., 1)^{\mathrm{T}}$  for any dimension.

For a vector v, let  $v_x$  denote the *x*-th element of v, and ||v|| denote the Euclid norm of v. For a matrix *A*, let  $A_{xy}$  denote the (x, y)-element of *A*, and for a symmetric matrix *A*, let  $\lambda_i(A)$  denote the *i*-th largest eigenvalue of *A*. Note that all matrices we consider in this paper are symmetric.

For a graph G, we use V(G) and E(G) to denote respectively the set of vertices and that of edges of G. For a graph which contains self-loops, we consider that contribution of one self-loop to the degree of each vertex is one. A graph G is called *simple* if G has neither self-loop nor multiple edge. Recall that we identify a graph and its adjacency matrix.

Let  $\mathcal{G}_{n,c,d}$  denote the set of all simple (c, d)-regular graphs with *n* vertices as we introduced above, we use  $\widetilde{\mathcal{G}}_{n,c,d}$  to denote the set of all (c, d)-regular graphs with *n* vertices which may not be simple. For a graph  $\widetilde{\mathcal{G}}_{n,c,d}$ , we denote V(G) by  $\{v_1, v_2, \ldots, v_n\}$  where  $v_1$  is the vertex with degree *c* and  $v_2, \ldots, v_n$  are vertices with degree *d*.

We define the depth of a vertex on  $G \in \widetilde{\mathcal{G}}_{n,c,d}$  as follows:

**Definition 2.1.** For a vertex  $v \in V(G)$ , the depth of v, denoted by dp(v), is defined by the minimum path length from  $v_1$  to v.

In particular, the depth in  $T_k$  takes values from 0 to k, the root has depth 0, nodes have depth 1 to k - 1, and leaves have depth k. Note that the number of vertices in depth h is  $c(d')^{h-1}$ .

For fixed *c* and *d*, we use  $T_k$  to denote the (c, d, k)-complete tree, and d' := d - 1 to denote the number of children of nodes of the  $T_k$ .

We define a certain modification of a (c, d, k)-complete tree that is used in our analysis.

**Definition 2.2.** The regularized (c, d, k)-complete tree is a (c, d)-regular graph constructed by adding d' self-loops to all leaves of (c, d, k)-complete tree.



Figure 2: (c, d, k)-complete tree  $T_k$  and regularized (c, d, k)-complete tree  $\hat{T}_k$  for c = 4, d = 3, k = 2.

For fixed *c* and *d*, we use  $\hat{T}_k$  to denote the regularized (c, d, k)-complete tree and we use the notation  $\lambda_{\rm T}(k) := \lambda_1(\hat{T}_k)$ . We also use terms "root", "node" and "leaf" for  $\hat{T}_k$  as well as  $T_k$ ; the root of  $\hat{T}_k$  is the vertex with degree *c*, a leaf of  $\hat{T}_k$  is a vertex whose depth is *k*, and nodes are other vertices of  $\hat{T}_k$ . The adjacency matrix  $\hat{T}_k$  is written as follows;  $(\hat{T}_k)_{vv} = d'$  if *v* is a leaf, and  $(\hat{T}_k)_{vv'} = (T_k)_{vv'}$  otherwise.

In this article, vertices of  $\hat{T}_k$  as indices for vectors and matrices are arranged in increasing order of their depths, from the root to leaves.

For  $G \in \mathcal{G}_{n,c,d}$ , we define two numbers  $\delta(G)$  and  $\Delta(G)$ ;  $\delta(G)$  is the maximum number of k such that G contains a (c, d, k)-complete tree, and  $\Delta(G) := \max_{v \in V(G)} dp(v)$ .

In this paper, we use the big-O notation and the small-o notation (with respect to *n*) as follows: for non-negative functions f(n) and g(n) which are defined for infinite non-negative numbers,

$$f(n) \le O(g(n)) \Leftrightarrow \exists \eta > 0; \exists v \ge 0; \forall n \ge v; f(n) \le \eta g(n),$$
  
$$f(n) \le o(g(n)) \Leftrightarrow \forall \eta > 0; \exists v \ge 0; \forall n \ge v; f(n) \le \eta g(n).$$

We always consider that c and d used for degrees are constant.

# **3** Spectral analysis of (c, d, k)-regular tree $\hat{T}_k$

In this section, we prove our lower and upper bounds of  $\lambda_{T}(k)$  for any fixed *c* and *d*. Throughout this section, big-O and small-o notation is used with respect to *k*. We state the main result of this section:

**Theorem 3.1.** For any fixed c and d, we have

$$\max\left\{d, \ \frac{c}{\sqrt{c-d+1}}\right\} \le \lambda_{\mathrm{T}}(k) \le \max\left\{d, \ \frac{c}{\sqrt{c-d+1}}\right\} + o(1).$$

To avoid complicated notation, we use notations  $\hat{T} := \hat{T}_k$  and  $\lambda_T := \lambda_T(k)$ . Let f be the eigenvector of  $\hat{T}$  corresponding to  $\lambda_T$ .

We use the following special structure of f, this property is called as f is *spherically symmetric* (around  $v_1$ );

**Lemma 3.2.** For any pair  $v, v' \in V(\hat{T})$  where dp(v) = dp(v'), we have  $f_v = f_{v'}$ .

See the survey [4] for detail.

For all  $h, 0 \le h \le k$ , we define  $f_h := f_v$  for any  $v \in V(\hat{T})$  such that dp(v) = h. This notation is well-defined according to the above lemma. Then f is described by k + 1 numbers  $f_0, f_1, \ldots, f_k$ . For a vertex v in depth h, the element of  $\hat{T}$  at v is written by

$$(\hat{T}f)_{v} = \begin{cases} cf_{1} & \text{for } k = 0, \\ f_{h-1} + d'f_{h+1} & \text{for } 1 \le h \le k-1, \\ f_{k-1} + d'f_{k} & \text{for } h = k. \end{cases}$$
(2)

Note that the vector  $\hat{T}f$  is also spherically symmetric. Then, the equation  $\lambda_T f = \hat{T}f$  are written by the following recursion:

$$\lambda_{\rm T} f_0 = c f_1, \tag{3}$$

$$\lambda_{\rm T} f_h = f_{h-1} + d' f_{h+1}$$
 for  $1 \le h \le k - 1$ , (4)

$$\lambda_{\mathrm{T}} f_k = f_{k-1} + d' f_k. \tag{5}$$

If we set  $f_k$  to any positive number, then all  $f_h$  for  $0 \le h \le k - 1$  are determined by (4) and (5) and  $f_h > 0$  for all  $0 \le h \le k - 1$ . By Perron's Theorem, this implies that f is the unique eigenvector corresponding to  $\lambda_T$ .

#### **3.1** Lower bound of $\lambda_{\rm T}$

We prove our lower bound of  $\lambda_{\rm T}$ :

#### Lemma 3.3.

$$\lambda_{\rm T} \ge \max\left\{d, \ \frac{c}{\sqrt{c-d'}}\right\}.$$
 (6)

*Proof.* Since all sums of rows are not less than *d*, we have  $\lambda_T \ge d$ . Thus, we show  $\lambda_T \ge c/\sqrt{c-d'}$  for c > dd' below. Recall that *f* is the eigenvector of  $T_k$  corresponding to  $\lambda_T$ . We set  $f_k := 1$ , then *f* is determined by the recursion (4) and (5). By standard calculation, we have an explicit formula for  $f_h$  as

$$f_h = \frac{\beta^{k-h+1} - \alpha^{k+h-1}}{\beta - \alpha} - d' \frac{\beta^{k-h} - \alpha^{k-h}}{\beta - \alpha}$$
(7)

where  $\alpha + \beta = \lambda_T$  and  $\alpha\beta = d'$  (see Appendix A.5.1). We assume  $\alpha \leq \beta$ , then we have

$$\alpha = \frac{\lambda_{\rm T} - \sqrt{\lambda_{\rm T}^2 - 4d'}}{2} \quad \text{and} \quad \beta = \frac{\lambda_{\rm T} + \sqrt{\lambda_{\rm T}^2 - 4d'}}{2}.$$
(8)

Since  $\lambda_{\rm T} \ge d \ge 3$  implies  $\lambda_{\rm T} - 4d' \ge 1$ , it is easy to see that  $0 < \alpha < 1$  and  $\beta > d'$ , hence the denominator of (7) can not be 0 for  $d \ge 3$  (see Appendix A.5.2). Let  $\sigma_h = \sum_{i+j=h} \alpha^i \beta^j$ ; then we have  $\sigma_h = \beta \sigma_{h-1} + \alpha^h$ . Using this, (7) can be written as

$$f_h = \beta \sigma_{k-h-1} + \alpha^{k-h} - d' \sigma_{k-h-1}.$$
 (9)

(See Appendix A.5.3). Substituting this to (3) and by  $\beta \sigma_{h-1} = \sigma_h - \alpha^h$ , we have

$$\partial_{\mathrm{T}}(\beta - d' + \gamma_k) = c(1 - \alpha + \gamma_k)$$

where  $\gamma_h = \alpha^h / \sigma_{h-1}$ . Hence

$$\lambda_{\rm T} = \frac{c(1 - \alpha + \gamma_k)}{\beta(1 - \alpha + \gamma_k/\beta)},\tag{10}$$

(see Appendix A.5.4) then, we have

$$\frac{c}{\beta} \le \lambda_T \le \frac{c}{\beta} \left( 1 + \frac{\gamma_k}{1 - \alpha} \right). \tag{11}$$

Now by substituting (8) to (11), we restate the above lower bound as

$$\lambda_{\rm T}^2 + \lambda_{\rm T} \sqrt{\lambda_{\rm T}^2 - 4d'} - 2c \ge 0.$$

Let  $\phi(\lambda_T)$  denote the LHS formula of this inequality. Note that the function  $\phi(x)$  is increasing for  $x \ge 2\sqrt{d'}$ , hence  $\phi(\xi) = 0$  for some  $\xi \ge 2\sqrt{d'}$  implies  $\lambda_T \ge \xi$ . Under the assumption  $c > dd' \ge 2d'$ , we have

$$\phi\left(\frac{c}{\sqrt{c-d'}}\right) = \frac{c}{c-d'} \left(\sqrt{(c-2d')^2} - c + 2d'\right)$$
$$= \frac{c}{c-d'} \left(|c-2d'| - (c-2d')\right) = 0,$$

and  $2\sqrt{d'} \le c/\sqrt{c-d'}$  (see Appendix A.5.5). Thus, we have  $\lambda_T \ge c/\sqrt{c-d'}$ , which is our desired bound.

#### **3.2** Upper bound of $\lambda_{\rm T}$

First, we prove our upper bound of  $\lambda_T$  in the case c > dd' by modifying the proof of the above lower bound.

**Lemma 3.4.** For  $c \ge dd' + 1$ , we have

$$\lambda_{\rm T} \le \frac{c}{\sqrt{c-d'}} \left( 1 + O\left( (d')^{-k} \right) \right). \tag{12}$$

*Proof.* We analyze the upper bound of the upper side of inequalities (11). For this, we give a more precise upper bound of  $1/(1 - \alpha)$ , that is

$$\frac{1}{1-\alpha} \le 2(d')^2. \tag{13}$$

We derive this bound in Appendix.

Substituting (13) to (11) and by  $\gamma_k \leq \alpha^k / \beta^{k-1} \leq 1/(d')^{k-1}$ , we have

$$\lambda_{\rm T} \le \frac{c}{\beta} \left\{ 1 + 2(d')^2 \gamma_k \right\} \le \frac{c}{\beta} \left\{ 1 + \frac{2}{(d')^{k-3}} \right\}.$$
 (14)

Let  $\rho = 1 + 2/(d')^{k-3}$ , this inequality is restated as

$$\lambda_{\rm T}^2 + \lambda_{\rm T} \sqrt{\lambda_{\rm T}^2 - 4d'} - 2c\rho \le 0.$$
<sup>(15)</sup>

(See Appendix A.5.6). using (8). Let  $\psi(\lambda_T)$  be the LHS formula of this inequality. Note that the function  $\psi(x)$  is increasing for  $x \ge 2\sqrt{d'}$ . Hence  $\psi(\xi) = 0$  for some  $\xi \ge 2\sqrt{d'}$  implies  $\lambda_T \le \xi$ .

We determine  $\xi \ge 2\sqrt{d'}$  such that  $\psi(\xi) = 0$ . By reforming the equation, we have a necessary condition of  $\xi$  as

$$\left(\xi^2 - 2c\rho\right)^2 = \xi^2 \left(\xi^2 - 4d'\right).$$
(16)

(See Appendix A.5.7). By calculation, we have

$$(2\sqrt{d'})^2 \le \frac{c^2}{c-d'} \le \xi^2 \le \frac{c^2 \rho^2}{c-d'},\tag{17}$$

(see Appendix A.5.8), hence

$$\lambda_{\mathrm{T}} \leq \frac{c\rho}{\sqrt{c-d'}} \leq \frac{c}{\sqrt{c-d'}} \left( 1 + O\left( (d')^{-k} \right) \right)$$

Next, we prove an upper bound in the case  $c \leq dd'$ , that is done by a different way to the previous proof.

**Lemma 3.5.** For  $c \leq dd'$ , we have

$$\lambda_{\mathrm{T}} \le d + O\left( (d')^{-k} \right) \qquad \qquad if \quad c \le dd' - 1, \tag{18}$$

$$\lambda_{\rm T} \le d + O\left((d')^{-k/2}\right) \qquad \qquad if \quad c = dd'. \tag{19}$$

To prove this, we introduce another matrix *B* and its characteristic polynomial  $\Phi(x)$ . Let *B* be a (k + 1)-dimensional matrix, defined by  $B = (B_{ij})_{i,j=0}^k$  such that

$$B_{01} = B_{10} = \sqrt{c},\tag{20}$$

$$B_{i,i+1} = B_{i+1,i} = \sqrt{d'}$$
 for  $1 \le i \le k - 1$ , (21)

$$B_{kk} = d', (22)$$

$$B_{ij} = 0$$
 otherwise. (23)

Note that *B* is a symmetric and tridiagonal matrix.

We first show that  $\hat{T}$  and B have the same first eigenvalue. See Appendix for the proof.

**Lemma 3.6.**  $\lambda_1(B) = \lambda_T$ .

Let  $\Phi(x) = \det(xI - B)$  be the characteristic polynomial of *B*. It is known that the characteristic polynomial of a tridiagonal matrix is determined by a 3-term recursion, which is derived by recursive row expansion of determinant. That is

$$\Phi(x) = x\Phi_k(x) - c\Phi_{k-1}(x) \tag{24}$$

where the sequence of polynomials  $\Phi_h(x)$  is defined by

$$\Phi_0(x) = 1, \tag{25}$$

$$\Phi_1(x) = x - d',\tag{26}$$

$$\Phi_h(x) = x \Phi_{h-1}(x) - d' \Phi_{h-2}(x)$$
 for  $2 \le h \le k$  (27)

(see Appendix A.5.9).

As shown below, the eigenvalue of *B* that is greater than *d* is only the first one  $\lambda_T$ ; that is, others are smaller than *d*, which is stated as follows. See Appendix for the proof.

**Lemma 3.7.**  $\lambda_2(B) < d$ .

**Corollary 3.8.** For any  $\xi > 2\sqrt{d'}$  such that  $\Phi(\xi) \ge 0$ , we have  $\lambda_T \le \xi$ .

*Proof.* Let  $\xi \ge 2\sqrt{d'}$  be a number that satisfies  $\Phi(\xi) \ge 0$ . By the recursion of  $\Phi$ , we have  $\Phi_h(d) = 1$  for all  $0 \le h \le k$ , and  $\Phi(d) = d - c < 0$ . Hence there exists a root  $x_0$  of  $\Phi(x)$  on the interval  $d \le x \le \xi$ . Lemma 3.7 implies that  $x_0$  is exactly  $\lambda_T$ .

*Proof of Lemma 3.5.* We show a small number  $\eta > 0$  such that  $\Phi(d + \eta) \ge 0$ . This implies that  $d \le \lambda_T \le d + \eta$ .

Let  $a_h = \Phi_h(d + \eta)$  for  $1 \le h \le k$ , then  $\Phi(d + \eta) = (d + \eta)a_k - ca_{k-1}$ . Now we determine explicit formulas of  $a_0, a_1, \ldots, a_k$  by the following recursion:

$$a_0 = 1,$$
  
 $a_1 = 1 + \eta,$   
 $a_h = (d + \eta)a_{h-1} - d'a_{h-2}.$ 

By similar calculation to derive (7), we have an explicit formula for  $a_h$  as

$$a_h = (1+\eta)\frac{\nu^h - \mu^h}{\nu - \mu} - \mu \nu \frac{\nu^{h-1} - \mu^{h-1}}{\nu - \mu}$$
(28)

where  $\mu + \nu = d + \eta$  and  $\mu\nu = d'$  (see Appendix A.5.10). We assume that  $\mu \le \nu$ , then we have

$$\mu = \frac{d + \eta - \sqrt{(d + \eta)^2 - 4d'}}{2} \quad \text{and} \quad \nu = \frac{d + \eta + \sqrt{(d + \eta)^2 - 4d'}}{2}$$

Again, it is easy to see that  $0 < \mu < 1$  and  $\nu > d'$ , hence the denominator (28) can not be 0. Let  $\tau_h = \sum_{i+j=h} \mu^i \nu^j$ ; then we have  $\tau_h = \nu \tau_{h-1} + \mu^h$ . Using this, (28) can be written as

$$a_h = (1 + \eta - \mu)\tau_{h-1} + \mu^h.$$
<sup>(29)</sup>

(See Appendix A.5.11).

Then, we can rewrite  $\Phi(d + \eta)$  as

$$\Phi(d+\eta) = (1+\eta-\mu) \left( \frac{dd'-c\mu}{d'} + \eta \right) \tau_{k-1} - (c-d-\eta)\mu^k.$$
(30)

See Appendix for this technical calculation. Since  $\mu < 1$  and  $\tau_{k-1} \ge \nu^{k-1} > (d')^{k-1}$  and  $dd' - c \ge 0$ , we have

$$\Phi(d+\eta) \ge \eta \left(\frac{dd'-c}{d'} + \eta\right) (d')^{k-1} - (c-d-\eta)\mu^k.$$
(31)

Now we prove (18) by (31). Suppose c < dd', we have

$$\Phi(d+\eta) \ge \eta (dd'-c)(d')^{k-2} - (c-d-\eta)\mu^k.$$

Hence, if we set

$$\eta = \frac{c - d}{(dd' - c)(d')^{k-2}} \le O\left((d')^{-k}\right)$$

we have  $\Phi(d + \eta) \ge 0$ . Thus, by Corollary 3.8, (18) follows.

Next, we prove (19). Suppose c = dd', (31) can be written as

$$\Phi(d+\eta) \ge \eta^2 (d')^{k-1} - (c-d-\eta)\mu^k.$$

Hence, if we set

$$\eta = \frac{\sqrt{1 + 4(c - d)(d')^{k - 1}}}{2(d')^{k - 1}} \le O\left((d')^{-k/2}\right)$$

we have  $\Phi(d + \eta) \ge 0$ . Thus, by Corollary 3.8, (19) follows.

# **4** Reduction from graph to tree

We introduce a way to relate the above spectral analysis of trees to that of general (c, d)-regular graphs. For any graph  $G \in \mathcal{G}_{n,c,d}$ , we relate  $\lambda_1(G)$  to  $\lambda_T(k)$ . More specifically, we show the following lemma;

**Lemma 4.1.** For any  $G \in \mathcal{G}_{n,c,d}$ , we have

$$\lambda_{\mathrm{T}}(\Delta(G)) \le \lambda_{1}(G) \le \lambda_{\mathrm{T}}(\delta(G)). \tag{32}$$

Combining this lemma with Lemma 3.3, 3.4 and 3.5, we have our main technical result, Theorem 1.1.

We prove the lower and upper bounds of Lemma 4.1.

Proof of Lemma 4.1 (Lower bound). We use the notation  $\Delta := \Delta(G)$  and  $\lambda_T := \lambda_T(\Delta)$  in this proof. Let f be the eigenvector of  $\hat{T}_{\Delta}$  corresponding to  $\lambda_T$ . For  $0 \le h \le \Delta$ ,  $f_h := f_v$  for  $v \in V(\hat{T}_{\Delta})$  such that dp(v) = h.

We can see  $\{f_h\}$  is non-increasing sequence, i.e.  $f_{\Delta} \leq f_{\Delta-1} \leq \cdots \leq f_0$  by the following induction

$$f_{\Delta-1} = \lambda_{\mathrm{T}} f_{\Delta} - d' f_{\Delta} \ge f_{\Delta}$$
  
$$f_{h-1} = \lambda_{\mathrm{T}} f_h - d' f_{h+1} \ge df_h - d' f_{h+1}$$
  
$$= f_h - d' (f_h - f_{h+1}) \quad (1 \le h \le \Delta - 1)$$

For all  $h, 0 \le h \le \Delta$ , define  $L_h \subset V(G)$  by

$$L_h = \{ v \in V(G) \mid \mathrm{dp}(v) = h \}.$$

Note  $L_0 = \{v_1\}$  and  $L_{\Delta} \neq \emptyset$ . By the definition of dp and  $L_h$ , every  $v \in L_h$  has edges only to vertices in  $L_{h-1} \cup L_h \cup L_{h+1}$ ; thus every  $L_h$  for  $0 \le h \le \Delta$ , is not empty.

Let g be a |V(G)|-dimensional vector, indexed by vertices in V(G), defined by  $g_v := f_h$  for  $v \in L_h$ . We show below that  $g^T G g \ge \lambda_T ||g||^2$ , which is sufficient for the lemma because  $\lambda_1(G) = \max_{\boldsymbol{v} \neq \boldsymbol{0}} \boldsymbol{v}^T G \boldsymbol{v} / ||\boldsymbol{v}||^2$ .

Consider any vertex v of G, and let h be the index such that  $v \in L_h$ . At first, consider the case that h is neither 0 nor  $\Delta$ . Then v has edges to vertices in  $L_{h-1} \cup L_h \cup L_{h+1}$  and v is connected at least one vertex in  $L_{h-1}$ , hence we have

$$(Gg)_v = (d - (p + q)) \cdot f_{h+1} + q \cdot f_h + p \cdot f_{h-1}$$

for some  $p \ge 1$  and  $q \ge 0$ . Since  $\{f_h\}$  is non-increasing sequence, we have

$$(G\boldsymbol{g})_v = (d - (p + q)) \cdot f_{h+1} + q \cdot f_h + p \cdot f_{h-1}$$
  
$$\geq d' f_{h+1} + f_{h-1} = \lambda_{\mathrm{T}} f_h = \lambda_{\mathrm{T}} \boldsymbol{g}_v.$$

Similar arguments hold for the case h = 0 or  $h = \Delta$ . Thus, we have  $(Gg)_v \ge \lambda_T g_v$  for all vertices v. Hence,

$$\boldsymbol{g}^{\mathrm{T}} \boldsymbol{G} \boldsymbol{g} = \sum_{v \in V(G)} \boldsymbol{g}_{v} (\boldsymbol{G} \boldsymbol{g})_{v} \geq \lambda_{\mathrm{T}} \sum_{v \in V(G)} \boldsymbol{g}_{v}^{2} = \lambda_{\mathrm{T}} ||\boldsymbol{g}||^{2},$$

which is our desired bound.

Proof of Lemma 4.1 (Upper bound). Let  $k = \delta(G)$ , T be the (c, d, k)-complete tree contained in G, and  $\hat{T}$  be the tree constructed as  $\hat{T}_k$  from  $T_k$  on the same vertex set V(T). We define a graph H as follows; (1) V(H) := V(G), (2) the set of vertices V(T) on H has same connection to that of  $\hat{T}$ , (3) all other vertices are isolated and have d self-loops. The adjacency matrix of H is written as  $H_{vv'} = \hat{T}_{vv'}$  for  $v, v' \in V(T)$  and  $H_{vv} = d$  for  $v \in V(H) \setminus V(T)$  and  $H_{vv'} = 0$  otherwise. Since each of V(T) and  $\{v\}$  for  $v \in V(H) \setminus V(T)$  forms a connected component on H, we have  $\lambda_1(H) = \max\{\lambda_T(k), d\} = \lambda_T(k)$ .

We introduce a kind of edge-elimination transform  $\mathcal{E}_{vv'}$  for  $v, v' \in V(G)$  to construct H from G. We show below that  $\mathcal{E}_{vv'}$  does not decrease the first eigenvalue of a graph.  $\mathcal{E}_{vv'}$  is defined as this: remove the edge (v, v') and add a self-loop for each of v and v' (see Fig. 2.) Note that each transform  $\mathcal{E}_{vv'}$  for  $(v, v') \in V(G) \times V(G)$  is commutative. Let  $L \subset V(T)$  be the set of all leaves of T. We obtain H by applying  $\mathcal{E}_{vv'}$  for all  $v \in L$  and  $v' \in V(G) \setminus V(T)$ , and for all  $v, v' \in V(G) \setminus V(T)$ .

We show that the transform  $\mathcal{E}_{vv'}$  does not decrease the first eigenvalue of a graph. Let  $G_1$  be any graph, which may have self-loops and multiple-edges, and  $G_2 = \mathcal{E}_{vv'}(G_1)$ . In respect to adjacency matrix, the transform  $G_1 \rightarrow G_2$  is described as addition  $G_1 \rightarrow G_1 + D_{vv'}$  where  $D_{vv'}$  is a matrix defined by  $D_{vv} = D_{v'v'} = 1$ ,  $D_{vv'} = D_{v'v} = -1$  and other elements are 0. It is easy to see that  $D_{vv'}$  has eigenvalues  $\lambda_1(D_{vv'}) = 2$  and  $\lambda_i(D_{vv'}) = 0$  for  $i \ge 2$ ; hence  $D_{vv'}$  is positive semi-definite. This implies  $\lambda_1(G_1) \le \lambda_1(G_2)$ . Therefore, we have  $\lambda_1(G) \le \lambda_1(H) = \lambda_T(k)$ 



Figure 3:  $\mathcal{E}_{vv'}$ 

See the text for definition and meaning of symbols. **Outline:** Generate a wiring *W* uniformly at random from  $\mathcal{W}_{n,c,d}$  and output g(W).

#### **Generation of Wiring:**

Fix a rule function  $r : \mathcal{P} \to [2m]$  such that  $r(P) \notin U(P)$  for all  $P \in \mathcal{P}$ . 1.  $P_0 := \emptyset$ . 2. For  $t := 1 \sim m$ , do the following: (a)  $a := r(P_{t-1})$ ; (b) choose  $b \in [2m] \setminus (U(P_{t-1}) \cup \{a\})$  uniformly at random; (c)  $P_t := P_{t-1} \cup \{a, b\}$ ; 3. Output wiring  $P_m$ .

#### **Rule Function:**

 $r(P) := \min R(P)$ 

i iguie il olupii generation mettoa	Figure 4:	Graph	generation	method
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# **5** Tree depth of random (*c*, *d*)-regular graphs

Finally, in this section, we give our spectral analysis of a random (c, d)-regular graph, thereby showing our main theorem, Theorem 1.2. For this, it suffices to show that a random graph in  $\mathcal{G}_{n,c,d}$  contains a tree with sufficient large depth w.h.p. Here we first specify a method of generating a graph in  $\mathcal{G}_{n,c,d}$ uniformly at random, and analyze the tree depth of generated graphs.

#### 5.1 Random graph generation method

First, we explain a method to generate a random graph in  $\mathcal{G}_{n,c,d}$  for given *n*, *c* and *d*. This method generates a simple graph uniformly, and this fact will be proved in the following. Figure 4 shows its outline.

We introduce some notions and notations that are used in this section. We fix *n*, *c* and *d*, then the number of edges of any  $G \in \mathcal{G}_{n,c,d}$  is also fixed to m = (c + (n-1)d)/2. Let  $V_1$  be the set  $\{1, \ldots, c\}$  and for each  $i \in \{2, \ldots, n\}$ , let  $V_i$  be the set  $\{c + d(i-2) + 1, \ldots, c + d(i-1)\}$ . We identify each set  $V_i$  as vertex  $v_i$  of the generated graph. Note that  $|\bigcup_{i=1}^n V_i| = 2m$ . For any  $a \in [2m]$ , we use  $\ell(a)$  to denote the index of  $V_i$  to which it belongs; that is,  $a \in V_{\ell(a)}$  and  $\ell(a) = \max\{0, \lceil (a-c)/d \rceil\} + 1$ .

A wiring W is a set of unordered pairs such that

- (i)  $W = \{w \mid w = \{a, b\}, a, b \in [2m]\}$ , and
- (ii) each  $i \in [2m]$  appears exactly once over all  $w \in W$

Let  $W_{n,c,d}$  be the set of all wirings. A subset *P* of some wiring  $W \in W_{n,c,d}$  is called a *partial wiring*, and let  $\mathcal{P}$  be the set of all partial wirings. For  $P \in \mathcal{P}$ , let U(P) denote the set defined by  $U(P) = \bigcup_{w \in P} w$ . Note that U(W) = [2m] for any wiring  $W \in W_{n,c,d}$  Intuitively, each (partial) wiring defines a graph as illustrated in Figure 5. Precisely, we use a function *g* that maps a partial wiring *P* to some subgraph of  $\widetilde{\mathcal{G}}_{n,c,d}$ . Let *g* denote the function defined by g(P) = A (recalling that we identify a graph and its adjacency matrix), where

$$A_{ij} = |\{\{a, b\} \in P \mid \{\ell(a), \ell(b)\} = \{i, j\}\}|.$$

Below, we sometimes treat  $V_i$  as a vertex  $v_i$ ; and use, e.g.,  $dp(V_i)$ .



An example of partial wiring. Here  $P = \{\{1, 8\}, \{2, 12\}, \{6, 14\}, \{9, 16\}, \{10, 15\}\}$  is illustrated, where one example pair  $\{6, 14\}$  is focused by a heavy line.

Figure 5: A partial wiring and the corresponding graph

We generate a wiring by adding wires incrementally. At each step  $t \ge 1$ , we add one wire to so far constructed partial wiring  $P_{t-1}$ . For this, in our method, we use some rule function r to pick one element  $a \in [2m]$  that has not been used by  $P_{t-1}$ ; that is,  $r(P_{t-1}) \in [2m] \setminus U(P_{t-1})$ . Then choose b randomly from remaining elements, i.e.,  $b \in [2m] \setminus (U(P_{t-1}) \cup \{a\})$ .

For our analysis, we need a generation method that is easy to calculate the depth of the regularized (c, d)-complete tree in g(W), and for this, we would like to generate a partial wiring as a tree grows from  $v_1$ . Our rule function r is defined for this motivation. For any  $P \in \mathcal{P}$ , let R(P) be the set of all  $v \in [2m] \setminus U(P)$  such that  $dp(V_{\ell(v)}) \leq dp(V_{\ell(u)})$  for any  $u \in [2m] \setminus U(P)$ . Then we define the rule function r as  $r(P) = \min R(P)$  (see Fig. 6 for an example).

We now show that the method of Figure 4 generates simple graph uniformly. This fact is immediate from the following two lemmas.

Lemma 5.1. "Generation of Wiring" in Figure 4 generates wiring uniformly.



An example of the rule function. Here  $R(P) = \{6, 11, 14\}$ , and the rule function chooses smallest one i.e. 6



*Proof.* To prove this lemma, we show that the probability of generating W is the same for all  $W \in W_{n,c,d}$ .

For any fixed  $W \in W_{n,c,d}$ , we discuss the probability that our method generates  $P_0, P_1, \ldots, P_m$  such that  $P_m = W$ . Note that this event holds iff  $P_t \subseteq W$  for all  $t \in [m]$ .

Note first that  $\Pr[P_0 \subseteq W] = 1$  since  $P_0 = \emptyset$ . Consider any  $t \ge 0$ , and we analyze  $\Pr[P_{t+1} \subseteq W | P_t \subseteq W]$ . Thus, suppose that  $P_t \subseteq W$ . Let  $\{a, b\}$  be a wiring added to  $P_t$  to have  $P_{t+1} = P_t \cup \{a, b\}$ . Recall that the method determines a by  $a = r(P_t)$ . Then b should be uniquely determined in order to have  $\{a, b\} \in W$  (and hence  $P_{t+1} \subseteq W$ ), because every element of [2m] appears exactly once in W. Thus, the probability that  $P_{t+1} \subseteq W$  is that of the event that this particular b is chosen from 2m - 2t - 1 elements; hence,  $\Pr[P_{t+1} \subseteq W | P_t \subseteq W] = 1/(2m - 2t - 1)$ .

Thus it follows that the probability that W is chosen by the generation method of wiring is

$$\prod_{t=0}^{m-1} \Pr[P_{t+1} \subseteq W \mid P_i \subseteq W] = \prod_{t=1}^m \frac{1}{2t-1}.$$

Clearly, this probability is the same for all  $W \in W_{n,c,d}$ .

**Lemma 5.2.** Any simple graph corresponds to the same number of wirings. More precisely, for any simple graph  $G \in \mathcal{G}_{n,c,d}$ , there are

$$\prod_{k\in[n]} |V_k|! = c!(d!)^{n-1}$$

wirings mapped identically to G by function g.

*Proof.* Consider any graph fixed, and enumerate all of its edges in the lexicographic order  $e_1, e_2, \ldots, e_m$ . We count inductively the number of wiring corresponding to this sequence of edges. Consider any  $s \ge 0$  where the correspondence has been fixed for  $e_1, \ldots, e_s$ ; let  $e_{s+1} = \{v_i, v_j\}$ . Then, there are  $|V'_i| \cdot |V'_j|$  wirings  $\{a, b\}$  such that  $a \in V'_i$  and  $b \in V'_j$ . where  $V'_i$  (resp.  $V'_j$ ) is the set of element of  $V_i$ 

(resp.  $V_j$ ) that are not used by  $e_1, \ldots, e_s$ . From this observation, it is easy to see that the number of wiring corresponds to  $e_1, \ldots, e_m$  is  $\prod_{i=1}^n |V_i|! = (c!)(d!)^{n-1}$ .

**Corollary 5.3.** For every simple graph  $G \in \mathcal{G}_{n,c,d}$ , the probability that the generation method of Figure 4 outputs G is the same.

#### 5.2 Tree depth analysis

We show that a random graph generated as Figure 4 contains a (c, d, k)-complete tree with some increasing function k w.r.t. n with probability 1 - o(1). For this, we first consider a graph  $g(W) \in \widetilde{\mathcal{G}}_{n,c,d}$  for a random wiring generated by our method and analyze the probability that it contains a (c, d, k)-complete tree. Let PT(G) and SG(G) denote respectively the event that G contains (c, d, k)-complete tree and the event that G is a simple graph.

**Lemma 5.4.** Define k by  $k = \lfloor \log_{d'} n^{1/4} - \log_{d'} c + 1 \rfloor$ . For any n, and c > d, let W denote a random wiring uniformly chosen from  $W_{n,c,d}$ . Then we have

$$\Pr_{W}[\Pr(g(W))] \ge 1 - o(1).$$

*Proof.* Let *W* be a random wiring uniformly chosen from  $W_{n,c,d}$ . From Lemma 5.1, we may assume that *W* is generated by the method of Figure 4. Thus, consider the process of generating *W*, and let  $P_0, P_1, \ldots P_m$  (= *W*) be the partial wirings generated at each iteration.

Let  $m_k = \sum_{h=0}^k c(d')^{h-1}$  be the number of edges of (c, d, k)-complete tree, and  $m' := 2\lceil n^{1/4} \rceil$ , then we have  $m_k \le m'$  by our choice of k. Then, from the choice of our rule function, we can see that if  $g(P_{m'})$  is a tree, then it should contain a (c, d, k)-complete tree. Therefore, for the lemma, it suffices to show that  $g(P_{m'})$  is a tree.

For any  $t \in [m]$ , we analyze the probability that  $g(P_t)$  has no cycle, where by "cycle" we allow it is formed by self-loops or multiple edges. Note that the connectivity of  $g(P_t)$  is guaranteed by our choice of r provided  $g(P_t)$  has no cycle. Now we assume that  $g(P_{t-1})$  has no cycle and estimate the probability that no cycle is formed by  $P_t := P_{t-1} \cup \{a, b\}$  at the t-th iteration. Recall that a is fixed as  $r(P_{t-1})$  and the choice of b determines whether a cycle is formed. It is easy to see that cycle is formed if and only if  $V_{\ell(b)} \cap (U(P_{t-1}) \cup \{a\}) \neq \emptyset$ , and that there are at most c + d'(t-1) ways to choose b such that  $V_{\ell(b)} \cap (U(P_{t-1}) \cup \{a\}) \neq \emptyset$  holds. Hence, we have

$$\leq \frac{c+d'(t-1)}{2m-2t-1} = \frac{c+d'(t-1)}{c+d(n-1)-2t-1}$$
  
$$\leq \frac{c+d'(t-1)+(2t+1)}{c+d(n-1)-2t-1+(2t+1)}$$
  
$$\leq \frac{c+d(t-1)+t+1}{c+d(n-1)} \leq \frac{d(t+c/d)+t+1}{d(n+c/d)}$$
  
$$\leq \frac{d(t+c/d)+dt}{d(n+c/d)} = \frac{2t+c/d}{n+c/d}.$$

using the relation that  $x/y \le (x+z)/(y+z)$  for any  $y \ge x > 0$  and  $z \ge 0$ .

Thus,

$$\Pr_{W}[\Pr(g(W))] \ge \Pr[g(P_{m'}) \text{ is a tree }]$$

$$\ge \prod_{t=1}^{m'} \left(1 - \frac{2t + c/d}{n + c/d}\right) \ge \left(1 - \frac{2m' + c/d}{n + c/d}\right)$$

$$\ge 1 - \frac{m'(2m' + c/d)}{n + c/d}$$

By substituting  $m' = 2\lceil n^{1/4} \rceil$ , the last term is  $O(1/\sqrt{n})$ , hence we have  $\Pr_W[\Pr(g(W))] \ge 1 - o(1)$  as desired.

Now, we consider the case that a simple graph generated uniformly. Here we use *G* and *W* to denote a random (c, d)-regular simple graph and a random wiring under the corresponding uniform distributions. To be specific, by, e.g. "Pr<sub>*G*</sub>[*event*]" we mean the probability that the event holds when a graph *G* is chosen from  $\mathcal{G}_{n,c,d}$  uniformly at random.

**Lemma 5.5.** Define k by  $k = \lfloor \log_{d'} n^{1/4} - \log_{d'} c + 1 \rfloor$ . For any n, and c > d, let G denote a random simple graph in  $\mathcal{G}_{n,c,d}$  generated uniformly at random. Then we have

$$\Pr_G[\Pr(G)] \ge 1 - o(1).$$

*Proof.* We assume that there exists a positive number  $\epsilon_1$  such that

$$\Pr_G[\Pr(G)] \le 1 - \epsilon_1,$$

for infinitely many *n* (where  $\mathcal{G}_{n,c,d} \neq \emptyset$ ), say  $\{n_i\}_i$ , and derive a contradiction.

We first show that  $\Pr_W[SG(g(W))] \ge \epsilon_2$  for some constant  $\epsilon_2$ . The result of Bender and Canfield (see remarks on page 297 of [1]) is used here. Among other results, they show that the number of simple graphs in  $\mathcal{G}_{n,c,d}$ ; more specifically, as a special case of their analysis, we can show that the number of simple (c, d)-regular graphs with *n* vertices (which is denoted as G(J - I, (c, d, ..., d), 1) by their notation) is

$$\frac{(2m)!}{2^m m!} e^{-b^2 - b} \cdot \frac{1}{c!(d!)^{n-1}} + o(1), \tag{33}$$

m

where

$$b = \frac{c(c-1) + (n-1)d(d-1)}{2(c+(n-1)d)}$$
$$= \frac{d-1}{2} \left\{ 1 + \frac{c(c-d)}{c(d-1) + (n-1)d(d-1)} \right\} \le \frac{d-1}{2} + o(1).$$

Then, since each simple graph with degree sequence (c, d, ..., d) corresponds to  $c!(d!)^{n-1}$  wirings (see Lemma 5.2), the number of wirings W such that g(W) becomes a simple graph is

$$(33) \times c!(d!)^{n-1} = \frac{(2m)!}{2^m m!} e^{-b^2 - b} + o(1) \times c!(d!)^{n-1}.$$
(34)

On the other hand, the total number of wirings is

$$\prod_{j=1}^m \binom{2j}{2} / m! = \frac{(2m)!}{2^m m!},$$

which is larger than  $c!(d!)^{n-1}$ .

Hence, we have

$$\Pr_{W}[SG(g(W))] = e^{-b^{2}-b-o(1)} + o(1) \times c!(d!)^{n-1} \cdot \frac{2^{m}m!}{(2m)!}$$
$$= \exp\left\{-\frac{(d-1)^{2}}{4} - \frac{d-1}{2} - o(1)\right\} + o(1).$$

Therefore, there exists an positive constant  $\epsilon_2$  such that  $\Pr_W[SG(g(W))] \ge \epsilon_2$ .

Then we have

$$\begin{aligned} &\Pr_{W}[\neg \text{PT}(g(W))] \\ &\geq &\Pr_{W}[\neg \text{PT}(g(W)) \land \text{SG}(g(W))] \\ &= &\Pr_{W}[\neg \text{PT}(g(W)) \mid \text{SG}(g(W))] \times \Pr_{W}[\text{SG}(g(W))] \\ &\geq &\Pr_{G}[\neg \text{PT}(G)] \times \epsilon_{2} \geq \epsilon_{1}\epsilon_{2}. \end{aligned}$$

That is, with at least some constant probability, g(W) does not contain (c, d, k)-complete tree for all n of the infinite sequence  $\{n_i\}_i$ . This contradicts to Lemma 5.4.

# 6 Concluding Remarks

We prove that, for any fixed *c* and *d*, and for a graph *G* chosen from the set of all (c, d)-regular graphs with *n* vertices uniformly at random, the first eigenvalue of *G*, denoted by  $\lambda_1(G)$ , is approximately max  $\{d, c/\sqrt{c-d+1}\}$  with high probability. To prove this, we introduce and analyze the first eigenvalue of the regularized (c, d, k)-complete tree, denoted by  $\lambda_T(k)$ , and relate  $\lambda_1(G)$  to  $\lambda_T(k)$ , and show that, for fixed *c* and *d*, a sequence of (c, d)-regular graphs *G* chosen from  $\mathcal{G}_{n,c,d}$  uniformly at random contains a sequence of (c, d, k)-complete trees with increasing *k* with high probability. More precisely, the bounds of  $\lambda_T(k)$  is divided into the following three cases,

(i) 
$$d \leq \lambda_{\mathrm{T}}(k) \leq d + O((d')^{-k})$$
 if  $c \leq dd' - 1$ ,  
(ii)  $d \leq \lambda_{\mathrm{T}}(k) \leq d + O((d')^{-\frac{k}{2}})$  if  $c = dd'$ ,  
(iii)  $\frac{c}{\sqrt{c-d'}} \leq \lambda_{\mathrm{T}}(k) \leq \frac{c}{\sqrt{c-d'}} \left(1 + O((d')^{-k})\right)$  if  $c \geq dd' + 1$ .

Thus, our main results Theorem 1.1 and 1.2 can be stated more precisely by considering these three cases.

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# Appendix Technical analysis

Here we give some technical analysis omitted in the main text.

#### **A.1** The calculation to derive (13)

Since  $c \ge dd' + 1$ , we have  $\lambda_{\rm T} \ge \frac{dd'+1}{\sqrt{(d')^2+1}}$ , and since  $\lambda_{\rm T} \ge d$ ,  $\alpha = d'/\beta$  and  $\beta$  is increasing with respect to  $\lambda_{\rm T}$ . Hence, by substituting  $\lambda_{\rm T} = \frac{dd'+1}{\sqrt{(d')^2+1}}$ , we have

$$\begin{aligned} \alpha &\leq \frac{1}{2} \left\{ \frac{dd'+1}{\sqrt{(d')^2+1}} - \sqrt{\frac{(dd'+1)^2}{(d')^2+1}} - 4d' \right\} \\ &= \frac{1}{2} \left\{ \frac{dd'+1}{\sqrt{(d')^2+1}} - \sqrt{\frac{(dd'+1)^2 - 4d'((d')^2+1)}{(d')^2+1}} \right\} \\ &= \frac{1}{2\sqrt{(d')^2+1}} \left\{ dd'+1 - \sqrt{(dd')^2 + 2dd'+1} - 4(d')^3 - 4d' \right\} \\ &= \frac{1}{2\sqrt{(d')^2+1}} \left\{ dd'+1 - \sqrt{(dd'-2d'+1)^2} \right\} \end{aligned}$$
(35)  
$$&= \frac{1}{2\sqrt{(d')^2+1}} \left\{ dd'+1 - \left| dd'-2d'+1 \right| \right\} \\ &= \frac{1}{2\sqrt{(d')^2+1}} \left( dd'+1 - \left| dd'-2d'+1 \right| \right) \\ &= \frac{1}{2\sqrt{(d')^2+1}} \left( dd'+1 - dd'+2d'-1 \right) \end{aligned}$$
(36)  
$$&= \frac{d'}{\sqrt{(d')^2+1}} = \sqrt{\frac{(d')^2}{(d')^2+1}} = \sqrt{1 - \frac{1}{(d')^2}} \\ &\leq \sqrt{1 - \frac{1}{(d')^2} + \frac{1}{4((d')^2)^2}} = 1 - \frac{1}{2(d')^2} \end{aligned}$$

where (35) follows by the equality:

$$(dd' - 2d' + 1)^{2}$$
  
=  $(dd')^{2} - 2d(d')^{2} + dd'$   
 $- 2d(d')^{2} + 4(d')^{2} - 2d' + dd' - 2d' + 1$   
=  $(dd')^{2} - 4d(d')^{2} + 4(d')^{2} + 2dd' - 4d' + 1$   
=  $(dd')^{2} - 4(d')^{3} + 2dd' - 4d' + 1$ ,

and (36) follows by  $dd' - 2d' + 1 \ge 0$  for  $d \ge 3$ . Therefore, we have  $\frac{1}{1-\alpha} \le 2(d')^2$ .

#### A.2 The proof of Lemma 3.6

Proof of Lemma 3.6. Recall that the matrix B is the symmetric and tridiagonal matrix as

$$B = \begin{bmatrix} 0 & \sqrt{c} & & & \\ \sqrt{c} & 0 & \sqrt{d'} & O & \\ & \sqrt{d'} & 0 & & \\ & & \ddots & & \\ O & & 0 & \sqrt{d'} \\ & & & \sqrt{d'} & d' \end{bmatrix}$$

We define a transformation *C*. Let g be a  $|V(\hat{T})|$ -dimensional vector which is spherically symmetric as f and for  $0 \le h \le k$ , let  $g_h = g_v$  for any  $v \in V(\hat{T})$  such that dp(v) = h. Let *C* be a transform that maps the spherically symmetric vector g to the (k + 1)-dimensional vector  $g' = (g'_0, g'_1, \dots, g'_k)$  defined by  $g'_0 = g_0$  and  $g'_h = g_h \sqrt{c(d')^{h-1}}$  for  $1 \le h \le k$ . Note that *C* is invertible and isometric, i.e. ||g|| = ||g'||.

To prove the equality of this lemma, we use the fact

$$\lambda_{\rm T} = \frac{f^{\rm T}\hat{T}f}{||f||^2}.$$
(37)

By (2), we have

$$\boldsymbol{f}^{\mathrm{T}} \hat{\boldsymbol{T}} \boldsymbol{f} = f_0(cf_1) + \sum_{h=1}^{k-1} c(d')^{h-1} f_h(f_{h-1} + d'f_{h+1}) + c(d')^{k-1} f_k(f_{k-1} + d'f_k)$$
  
=  $2 \sum_{h=0}^{k-1} c(d')^h f_h f_{h+1} + c(d')^k f_k^2.$  (38)

Let f' = C(f), we can rewrite (38) as

$$2\sqrt{c}f'_0f'_1 + 2\sqrt{d'}\sum_{h=1}^{k-1}f'_hf'_{h+1} + d'(f'_k)^2 = (f')^{\mathrm{T}}Bf',$$

hence  $\lambda_{\rm T} = f^{\rm T} \hat{T} f / ||f||^2 = (f')^{\rm T} B f' / ||f'||^2$ .

The last term must achieve the maximum value of the Reighley quotient  $(g')^T Bg'/||g'||^2$  where  $g' \neq 0$ , and the maximum value is exactly  $\lambda_1(B)$ . If not, then  $g := C^{-1}(g')$  satisfies the inequality

$$\frac{\boldsymbol{f}^{\mathrm{T}}\hat{\boldsymbol{T}}\boldsymbol{f}}{\|\boldsymbol{f}\|^{2}} < \frac{\boldsymbol{g}^{\mathrm{T}}\hat{\boldsymbol{T}}\boldsymbol{g}}{\|\boldsymbol{g}\|^{2}} \leq \lambda_{\mathrm{T}},$$

which contradicts to (37). Therefore,  $\lambda_{\rm T} = \lambda_1(B)$ .

#### A.3 The proof of Lemma 3.7

We use Sturm's Theorem to count the number of roots of the characteristic polynomial  $\Phi$  on an interval [d, b] for an arbitrary large *b*. (See [8] for detail of this method.)

**Definition A.1.** Let [a, b] be any closed interval on the line of real numbers, a sequence of polynomials  $p = p_0, p_1, \ldots, p_l$  is called a Sturm sequence iff all of the following condition hold: (1)  $p_l(x) \neq 0$  for all  $x \in [a, b]$ , (2) for all  $1 \le i \le l - 1$  and all  $\xi \in [a, b]$ ,  $p_i(\xi) = 0$  implies  $p_{i-1}(\xi)p_{i+1}(\xi) < 0$ , (3) for all  $\xi \in [a, b]$ ,  $p_0(\xi) = 0$  implies  $p'_0(\xi)p_1(\xi) > 0$ .

For a Sturm sequence  $\{p_i\}$ , let  $N(\xi)$  denote the number of sign changes (zeros are not counted) over the sequence  $\{p_i(\xi)\}$ .

**Proposition A.2** (Sturm). For a polynomial p, if a sequence of polynomials  $p = p_0, p_1, ..., p_l$  forms a Sturm sequence on [a, b] and neither a nor b is a multiple root of p, then the number of distinct roots of p is N(a) - N(b).

We use the fact that for the tridiagonal matrix *B*, the sequence of polynomials  $\Phi$ ,  $\Phi_k$ ,  $\Phi_{k-1}$ , ...,  $\Phi_0$  forms Sturm sequence on any interval where  $\Phi$  is the characteristic polynomial of *B* and  $\Phi_h$  for  $0 \le h \le k$  are defined by (25)-(27).

*Proof of Lemma 3.7.* For sufficiently large  $b_0$ , we have N(b) = 0 for any  $b \ge b_0$  since the coefficients of the highest degree terms of  $\Phi$  and  $\Phi_h$  for  $1 \le h \le k$  are positive and  $\Phi_0(x) \equiv 1$ . The other side, we have N(d) = 1 since  $\Phi_h(d) = 1$  for all  $0 \le h \le k$  and  $\Phi(d) = d - c < 0$ . Therefore, there exists exactly one root of  $\Phi(x)$  not less than *d* by Sturm's theorem. This implies  $\lambda_2(B) < d$ .

#### **A.4** The calculation to derive (30)

$$\Phi(d+\eta) = (d+\eta)\left\{(1+\eta-\mu)\tau_{k-1}+\mu^k\right\} - c\left\{(1+\eta-\mu)\tau_{k-2}+\mu^{k-1}\right\}$$
$$= (d+\eta)\left\{(1+\eta-\mu)\tau_{k-1}+\mu^k\right\} - c\left\{(1+\eta-\mu)\left(\frac{\tau_{k-1}}{\nu}-\frac{\mu^{k-1}}{\nu}\right)+\mu^{k-1}\right\}$$
(39)

$$= (1 + \eta - \mu) \left\{ (d + \eta) - \frac{c}{\nu} \right\} \tau_{k-1} + (d + \eta)\mu^{k} + (1 + \eta - \mu)\frac{c\mu^{k-1}}{\nu} - c\mu^{k-1}$$

$$= (1 + \eta - \mu) \left\{ (d + \eta) - \frac{c\mu}{d'} \right\} \tau_{k-1} + (d + \eta)\mu^{k} + (1 + \eta - \mu)\frac{c\mu^{k}}{d'} - \frac{c\nu\mu^{k}}{d'} \qquad (40)$$

$$= (1 + \eta - \mu) \left\{ \frac{dd' - c\mu}{d'} + \eta \right\} \tau_{k-1} - \left\{ \frac{c(\mu + \nu - \eta - 1)}{d'} - (d + \eta) \right\} \mu^{k}$$

$$= (1 + \eta - \mu) \left\{ \frac{dd' - c\mu}{d'} + \eta \right\} \tau_{k-1} - (c - d - \eta)\mu^{k} \qquad (41)$$

(39) is derived by  $\nu \tau_{h-2} = \tau_{h-1} - \mu^{h-1}$ , and (40) and (41) are derived by  $\mu \nu = d'$  and  $\mu + \nu = d' + 1 + \eta$ .

#### A.5 Detail explanation for some technical points

Below we give detail explanations for technical points that we omitted due to space limit.

#### **A.5.1** derivation of (7)

By equation (4),

$$\lambda_T f_h = f_{h-1} + d' f_{h+1}$$

$$(\alpha + \beta) f_h = f_{h-1} + \alpha \beta f_{h+1} \quad \cdots \text{ substituting } \lambda_T = \alpha + \beta \text{ and } d' = \alpha \beta$$

$$f_{h-1} - \alpha f_h = \beta (f_h - \alpha f_{h+1})$$

$$f_{h-1} - \alpha f_h = \beta^{k-h} (f_{k-1} - \alpha f_k)$$

By equation (5),  $f_{k-1} = \lambda_T - d'$  where we choose  $f_k = 1$ . Therefore,

$$f_{h-1} - \alpha f_h = \beta^{k-h} (\lambda_T - d' - \alpha)$$
  
=  $\beta^{k-h} (\beta - d').$  (42)

Similarly, we have

$$f_{h-1} - \beta f_h = \alpha^{k-h} (\lambda_T - d' - \beta)$$
  
=  $\alpha^{k-h} (\alpha - d').$  (43)

By subtract (43) from (42), we have

$$\begin{aligned} (\beta - \alpha)f_h &= \beta^{k-h+1} - d'(\beta^{k-h}) - \alpha^{k-h+1} + d'(\alpha^{k-h}) \\ &= \beta^{k-h+1} - \alpha^{k-h+1} - d'(\beta^{k-h} - \alpha^{k-h}). \end{aligned}$$

#### **A.5.2** justification for $a \le 1$ and $\beta \ge d'$

We prove  $\beta \ge d'$ , and since  $d' = \alpha\beta$ , this clearly shows  $\alpha \le 1$ . By definition of  $\beta$ ,

$$\beta \ge \frac{1}{2}(d + \sqrt{(d'+1)^2 - 4d'}) = \frac{1}{2}(d + d' - 1) = d'.$$

Hence  $\beta \geq d'$ .

#### A.5.3 derivation of (9)

By definition of  $\sigma_h$ , we have  $(\beta^h - \alpha^h)/(\beta - \alpha) = \sigma_{h-1}$ . Using this, (7) can be written as

$$f_h = \sigma_{k-h} - d'\sigma_{k-h-1}.$$

Since  $\sigma_h = \beta \sigma_{h-1} + \alpha^h$ , we have

$$f_h = \beta \sigma_{k-h-1} + \alpha^{k-h} - d' \sigma_{k-h-1}.$$

#### **A.5.4** derivation of (10)

Substituting (9) to (3), we have

$$\lambda_T(\beta\sigma_{k-1}+\alpha^k-d'\sigma_{k-1})=c(\beta\sigma_{k-2}+\alpha^{k-1}-d'\sigma_{k-2}).$$

We divide this equation by  $\sigma_{k-1}$ , then we have

$$\lambda_T \left( \beta - d' + \frac{\alpha^k}{\sigma_{k-1}} \right) = c \left( 1 - \frac{d'\sigma_{k-2} + \alpha^k - \alpha^k}{\sigma_{k-1}} \right)$$
$$= c \left( 1 - \frac{\alpha\beta\sigma_{k-2} + \alpha^k - \alpha^k}{\sigma_{k-1}} \right)$$
$$= c \left( 1 - \frac{\alpha(\beta\sigma_{k-2} + \alpha^{k-1})}{\sigma_{k-1}} + \frac{\alpha^k}{\sigma_{k-1}} \right)$$

Since  $\sigma_{k-1} = \beta \sigma_{k-2} + \alpha^{k-1}$ , we have

$$\lambda_T \left( \beta - d' + \frac{\alpha^k}{\sigma_{k-1}} \right) = c \left( 1 - \frac{\alpha(\beta \sigma_{k-2} + \alpha^{k-1})}{\beta \sigma_{k-2} + \alpha^{k-1}} + \frac{\alpha^k}{\sigma_{k-1}} \right)$$
$$= c \left( 1 - \alpha + \frac{\alpha^k}{\sigma_{k-1}} \right).$$

Therefore,

$$\lambda_T (\beta - d' + \gamma_k) = c(1 - \alpha + \gamma_k)$$
$$\lambda_T = \frac{c(1 - \alpha + \gamma_k)}{\beta(1 - \alpha + \frac{\gamma_k}{\beta})}$$

# **A.5.5** justification of $c/\sqrt{c-d'} \ge 2\sqrt{d'}$

Since  $c \ge dd'$ , we have

$$\frac{c}{\sqrt{c-d'}} \geq \frac{dd'}{\sqrt{dd'-d'}}$$
$$= \frac{dd'}{\sqrt{d'^2}}$$
$$= d = d' + 1 = \sqrt{d'^2 + 2d' + 1}.$$

Since  $d' \ge 2$ , we have  $\sqrt{d'^2 + 2d' + 1} \ge \sqrt{4d'} = 2\sqrt{d'}$ , and hence  $c/\sqrt{c - d'} \ge 2\sqrt{d'}$ .

## **A.5.6** derivation of (15)

Let  $\rho = 1 + 2/\sqrt{d'^{k-3}}$ , (14) is restated as,

$$\beta \lambda_T \leq c \rho.$$

By definition of  $\beta$ ,

$$\frac{\lambda_T^2 + \lambda_T \sqrt{\lambda_T^2 - 4d'}}{2} \leq c\rho$$

$$0 \geq -2c\rho + \lambda_T^2 + \lambda_T \sqrt{\lambda_T^2 - 4d'}$$

## A.5.7 derivation of (16)

The necessary condition of  $\psi(\xi) = 0$  is

$$c\rho - \frac{\xi^{2} + \xi \sqrt{\xi^{2} - 4d'}}{2} = 0$$
  

$$2c\rho = \xi^{2} + \xi \sqrt{\xi^{2} - 4d'}$$
  

$$2c\rho - \xi^{2} = \xi \sqrt{\xi^{2} - 4d'}$$
  

$$\left(\xi^{2} - 2c\rho\right)^{2} = \xi^{2}(\xi^{2} - 4d').$$

# **A.5.8** derivation of (17)

$$\begin{aligned} (\xi^2 - 2c\rho)^2 &= \xi^2(\xi^2 - 4d') \\ \xi^4 - 4c\rho\xi^2 + 4c^2\rho^2 &= \xi^4 - 4d'\xi^2 \\ -c\rho\xi^2 + c^2\rho^2 &= -d'\xi^2 \\ (c\rho - d')\xi^2 &= c^2\rho^2 \\ \xi^2 &= \frac{c^2\rho^2}{c\rho - d'} \end{aligned}$$

Since  $\rho \ge 1$ ,

$$\xi^2 \leq \frac{c^2 \rho^2}{c-d'}$$

#### A.5.9 derivation of (24)

We denote matrices  $B_0, \ldots, B_k$  iteratively as follows.

$$B_{1} = (d')$$

$$B_{2} = \begin{pmatrix} 0 & \sqrt{d'} \\ \sqrt{d'} & d' \end{pmatrix}$$

$$B_{i} = \begin{pmatrix} 0 & \sqrt{d'} & 0 & \cdots & 0 \\ \sqrt{d'} & & & & \\ 0 & & & B_{i-1} & \\ \vdots & & & & 0 \end{pmatrix}.$$

Using this, by definition of the matrix *B*, *B* can be written as

$$B = \begin{pmatrix} 0 & \sqrt{c} & 0 & \cdots & 0 \\ \sqrt{c} & & & \\ 0 & & & \\ \vdots & & & \\ 0 & & & & \end{pmatrix}$$

First, we show that  $\Phi_i(x) = \det(xI - B_i)$ . Since  $\Phi_1(x) = \det(xI - B_1)$ , we need to prove that for all *h*,  $2 \ge h \ge k$ ,

$$\det(xI - B_h) = x \det(xI - B_{h-1}) - d' \det(xI - B_{h-2})$$

is holds. We prove this by cofactor expansion.

$$det(xI - B_h) = \begin{pmatrix} x & -\sqrt{d'} & 0 & \cdots & 0 \\ -\sqrt{d'} & & & \\ 0 & & xI - B_{h-1} \\ \vdots & & \\ 0 & & \end{pmatrix}$$
$$= x det(xI - B_{h-1}) - (-\sqrt{d'} det \begin{pmatrix} -\sqrt{d'} & -\sqrt{d'} & 0 & \cdots & 0 \\ 0 & & & \\ \vdots & & xI - B_{h-2} \\ 0 & & & \end{pmatrix})$$
$$= x det(xI - B_{h-1}) - d' det(xI - B_{h-2}).$$

This implies  $\Phi_i(x) = \det(xI - B_i)$ . Similerly, we can derive that

$$\Phi(x) = \det(xI - B) = x \det(xI - B_k) - c \det(xI - B_{k-1}),$$

and since  $\Phi_i(x) = \det(xI - B_i)$ , we have

$$\Phi(x) = x\Phi_k(x) - c\Phi_{k-1}(x).$$

#### **A.5.10** derivation of (28)

substituting  $\mu$  and  $\nu$  to  $(d + \eta)a_{h-1} - d'a_{h-2}$ , we have

$$a_{h+1} - \mu a_h = \nu(a_h - \mu a_{h-1})$$
  
=  $\nu^h(a_1 - \mu a_0)$   
=  $\nu^h(1 + \eta - \mu).$ 

Similarly,

$$a_{h+1} - va_h = \mu^h (1 + \eta - v).$$

Therefore,

$$\begin{aligned} (\nu - \mu)a_h &= \nu^h (1 + \eta - \mu) - \mu^h (1 + \eta - \nu) \\ &= (1 + \eta)\nu^h - \mu\nu^h - (1 + \eta)\mu^h + \nu\mu^h \\ &= (1 + \eta)(\nu^h - \mu^h) - \mu\nu^h + \nu\mu^h. \end{aligned}$$

# A.5.11 derivation of (29)

By standard calculation, we have,

$$(\nu - \mu)a_h = (1 + \eta)(\nu^h - \mu^h) - \nu^h \mu + \mu^h \nu$$
  
=  $(1 + \eta)(\nu^h - \mu^h) - \nu^h \mu + \mu^h \nu + \mu^{h+1} - \mu^{h+1}$   
=  $(1 + \eta)(\nu^h - \mu^h) - \mu(\nu^h - \mu^h) + \mu^h(\nu - \mu).$  (44)

By definition of  $\tau_h$ , we have  $(\nu^h - \mu^h)/(\nu - \mu) = \tau_{h-1}$ . Using this, (44) can be written as

$$a_h = (1 + \eta)\tau_{h-1} - \mu\tau_{h-1} + \mu^h.$$

Therefore,

$$a_h = (1 + \eta - \mu)\tau_{h-1} + \mu^h$$