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ASYMPTOTIC SPECTRAL DISTRIBUTIONS OF DISTANCE k-GRAPHS OF LARGE-DIMENSIONAL HYPERCUBES

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Abstract. We derive the asymptotic spectral distribution of the distance k-graph of N-dimensional hypercube as $N \to \infty$.

1. Introduction. For a given graph $G = (V, E)$ and a positive integer k the *distance k-graph* is defined to be a graph $G^{[k]} = (V, E^{[k]})$ with

$$E^{[k]} = \{\{x, y\} : x, y \in V,\ \partial_G(x, y) = k\},$$

where $\partial_G(x, y)$ is the graph distance. In this paper we focus on the asymptotic spectral distribution of the distance k-graphs of the N-dimensional hypercube as $N \to \infty$. The results are viewed as concrete examples of limit distributions obtained along with quantum probability theory [5].

The N-dimensional hypercube is a graph $G^{(N)} = (V^{(N)}, E^{(N)})$, where

$$V^{(N)} = \{x = (\xi_1, \xi_2, \dots, \xi_N) : \xi_i \in \{0, 1\}\},$$
$$E^{(N)} = \{\{x, y\} : \partial(x, y) = 1\},$$

and $\partial(x, y)$ is the Hamming distance defined by

$$\partial(x, y) = \bigl|\{1 \le i \le N : \xi_i \ne \eta_i\}\bigr|,$$
$$x = (\xi_1, \xi_2, \dots, \xi_N), \quad y = (\eta_1, \eta_2, \dots, \eta_N) \in V^{(N)}.$$

The N-dimensional hypercube is also called the Hamming graph $H(N, 2)$. For $1 \le k \le N$, let $G^{(N,k)} = (V^{(N)}, E^{(N,k)})$ be the distance k-graph of the N-dimensional hyper-

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cube $G^{(N)}$. We see easily that $G^{(N,k)}$ is a regular graph with degree $\binom{N}{k}$. Note also that $G^{(N,k)}$ is not necessarily connected.

Let $A^{(N,k)}$ denote the adjacency matrix of $G^{(N,k)} = (V^{(N)}, E^{(N,k)})$. We are interested in the spectral distribution (eigenvalue distribution) of the normalized adjacency matrix:

$$\binom{N}{k}^{-1/2} A^{(N,k)}$$

and its limit distributions as $N \to \infty$. The main result of this paper is the following

Theorem 1.1. *For $k = 1, 2, \dots$ let μ_k be the probability distribution of the random variable defined by*

$$\frac{1}{\sqrt{2^k k!}}\, H_k\Big(\frac{X}{\sqrt{2}}\Big)$$

where $H_k(x)$ is the k-th Hermite polynomial and X is a random variable obeying the standard normal distribution $N(0,1)$. Then

$$\lim_{N\to\infty} \binom{N}{k}^{-m/2} \varphi_{\mathrm{tr}}\big((A^{(N,k)})^m\big) = \int_{-\infty}^{+\infty} x^m\, \mu_k(dx), \qquad k, m = 1, 2, \dots,$$

where φ_{tr} is the normalized trace.

Setting $k = 2$, we obtain the following

Corollary 1.2. *The normalized asymptotic spectral distribution of the distance 2-graph of the N-dimensional hypercube as $N \to \infty$ is given by*

$$\mu_2(dx) = \frac{1}{\sqrt{\pi(\sqrt{2}\,x + 1)}} \exp\Big(-\frac{\sqrt{2}\,x + 1}{2}\Big) 1_{(-1/\sqrt{2}, +\infty)}(x)\, dx,$$

i.e., the normalized χ_1^2-distribution.

The result in Corollary 1.2 was shown first by Kurihara–Hibino [6] by means of quantum decomposition but the result for an arbitrary $k \ge 3$ has not been yet obtained. Theorem 1.1 answers this question. Our proof is based on direct computation of the spectral distribution of the N-dimensional hypercube. It was also shown in [6] that the asymptotic spectral distribution of $A^{(N,N-1)}$ as $N \to \infty$ is the Gaussian distribution. This type of asymptotics is different from that of Theorem 1.1. In this connection it seems interesting to investigate the asymptotic spectral distribution of $A^{(N,k)}$ as $N \to \infty$, $k \to \infty$ with $k/N \to \lambda$.

2. Adjacency matrices. The N-dimensional hypercube $G^{(N)}$ is isomorphic to the N-fold direct product of the complete graph with two vertices:

$$G^{(N)} = K_2 \times \ldots \times K_2 \quad (N\text{-times}).$$

Since the adjacency matrix of K_2 is given by

$$R = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

the adjacency matrix of $G^{(N)}$ is expressed as

$$A = \sum_{i=1}^{N} I \otimes \ldots \otimes I \otimes R \otimes I \otimes \ldots \otimes I \tag{1}$$

where R sits at the i-th position and I denotes the identity matrix. Similarly, for $k = 1, 2, \ldots, N$ the adjacency matrix of $G_N^{(k)}$ is expressed as

$$A^{(N,k)} = \sum_{1 \le i_1 < i_2 < \ldots < i_k \le N} I \otimes \ldots \otimes I \otimes R \otimes I \otimes \ldots \otimes I \otimes R \otimes I \otimes \ldots \otimes I,$$

where R appears k times and sits at the i_1-th, i_2-th, $\ldots$, i_k-th positions. Whenever there is no confusion, we write for simplicity

$$A^{(k)} = A^{(N,k)}, \quad A = A^{(1)} = A^{(N,1)}, \quad I = A^{(0)} = A^{(N,0)}.$$

Lemma 2.1. *For a fixed $N \ge 1$*

$$\begin{aligned} &A^{(0)} = I, \quad A^{(1)} = A, \\ &AA^{(k)} = (k+1)A^{(k+1)} + (N-k+1)A^{(k-1)}, \qquad k = 1, 2, \ldots, N-1. \end{aligned}$$

Proof. By direct computation. We need only to note that $R^2 = I$. ∎

3. Krawtchouk polynomials. Following the standard notation [2, 3], for an integer $N \ge 1$ and $0 < p < 1$ we define the *Krawtchouk polynomials* $k_n^{(N,p)}(x)$ by

$$\begin{aligned} k_n^{(N,p)}(x) &= \sum_{k=0}^{n} \frac{(x-N)_{n-k}(x-k+1)_k}{(n-k)!k!}\, p^{n-k}(1-p)^k \\ &= (-p)^n \binom{N}{n} \sum_{k=0}^{n} \frac{(-n)_k(-x)_k}{(-N)_k k!}\, p^{-k} = \frac{1}{n!}\, x^n + (\text{lower}), \qquad n = 0, 1, 2, \ldots, N. \end{aligned}$$

It is known that $\{k_n^{(N,p)}(x) : n = 0, 1, 2, \ldots, N\}$ are the orthogonal polynomials with respect to the binomial distribution $B(N,p)$, i.e.,

$$\sum_{x=0}^{N} k_m^{(N,p)}(x) k_n^{(N,p)}(x) \binom{N}{x} p^x (1-p)^{N-x} = \binom{N}{n} p^n (1-p)^n \delta_{mn}\,.$$

Moreover, the three-term recurrence relation holds:

$$\begin{aligned} k_0^{(N,p)}(x) &= 1, \\ k_1^{(N,p)}(x) &= x - pN \\ xk_n^{(N,p)}(x) &= (n+1)k_{n+1}^{(N,p)}(x) \\ &\qquad + (pN + n - 2pn)k_n^{(N,p)}(x) + p(1-p)(N-n+1)k_{n-1}^{(N,p)}(x). \end{aligned}$$

Now we set

$$K_n^{(N)}(x) = 2^n n!\, k_n^{(N,1/2)}\Big(\frac{x+N}{2}\Big), \qquad n = 0, 1, 2, \ldots, N.$$

The first five are given by

$$
\begin{aligned}
K_0^{(N)}(x) &= 1,\\
K_1^{(N)}(x) &= x,\\
K_2^{(N)}(x) &= x^2 - N,\\
K_3^{(N)}(x) &= x^3 - (3N-2)x,\\
K_4^{(N)}(x) &= x^4 - (6N-8)x^2 + 3N(N-2).
\end{aligned}
$$

LEMMA 3.1. $\{K_n^{(N)}(x)\}$ *are the orthogonal polynomials with respect to*

$$
\beta_N = \sum_{j=0}^{N} \binom{N}{j} \frac{1}{2^N}\, \delta_{-N+2j}\,. \tag{2}
$$

Here $\mathrm{mean}(\beta_N) = 0$ *and* $\mathrm{var}(\beta_N) = N$.

Proof. Straightforward by variable change. ■

LEMMA 3.2. $\{K_n^{(N)}(x)\}$ *fulfil the three-term recurrence relation*:

$$
\begin{gathered}
K_0^{(N)}(x) = 1, \quad K_1^{(N)}(x) = x,\\
xK_n^{(N)}(x) = K_{n+1}^{(N)}(x) + (N-n+1)nK_{n-1}^{(N)}(x).
\end{gathered}
$$

Therefore, the Jacobi parameters of $\{K_n^{(N)}(x)\}$*, or equivalently, of* β_N *are given by*

$$
\begin{aligned}
\omega_n &= (N-n+1)n, & 1 \le n \le N,\\
\alpha_n &= 0, & 1 \le n \le N+1.
\end{aligned}
$$

Proof. Straightforward from the three-term recurrence relations of $k_n^{(N,p)}(x)$ mentioned above. ■

LEMMA 3.3. *The adjacency matrix of the distance k-graph of the N-dimensional hypercube $G^{(N)}$ is given by*

$$
A^{(N,k)} = \frac{1}{k!}\, K_k^{(N)}(A), \qquad k = 0, 1, 2, \ldots, N,
$$

where A in the right-hand side is the adjacency matrix of $G^{(N)}$.

Proof. Straightforward from Lemmas 2.1 and 3.2. ■

4. Proof of the main result.

We start with

LEMMA 4.1. *Let $N \ge 1$ be a natural number. Let $A = A^{(1)} = A^{(N,1)}$ be the adjacency matrix of the N-dimensional hypercube $G^{(N)}$. Then the eigenvalue distribution of A coincides with β_N. Therefore,*

$$
\varphi_{\mathrm{tr}}(A^m) = \int_{-\infty}^{+\infty} x^m\, \beta_N(dx), \qquad m = 1, 2, \ldots. \tag{3}
$$

Proof. Since the eigenvalues of $R = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ are ± 1, we see from (1) that $-N+2j$ is an eigenvalue of A with multiplicity $\binom{N}{j}$. The assertion is then obvious. ■

Combining Lemmas 3.3 and 4.1, we obtain

$$\varphi_{\mathrm{tr}}\big((A^{(N,k)})^m\big) = \int_{-\infty}^{+\infty} \Big\{\frac{1}{k!}\, K_k^{(N)}(x)\Big\}^m \beta_N(dx), \qquad m = 1, 2, \dots. \tag{4}$$

Let $\tilde{\beta}_N$ be the normalization of β_N, i.e.,

$$\tilde{\beta}_N = \sum_{j=0}^{N} \binom{N}{j} \frac{1}{2^N}\, \delta_{-\sqrt{N}+2j/\sqrt{N}}\,.$$

Note that $\operatorname{mean}(\tilde{\beta}_N) = 0$ and $\operatorname{var}(\tilde{\beta}_N) = 1$. Then, after the change of variable (4) becomes

$$\begin{aligned}
&\binom{N}{k}^{-m/2} \varphi_{\mathrm{tr}}\big((A^{(N,k)})^m\big) \\
&= \{k!N(N-1)\dots(N-k+1)\}^{-m/2} \int_{-\infty}^{+\infty} \big\{K_k^{(N)}(x)\big\}^m \beta_N(dx) \\
&= \{k!N(N-1)\dots(N-k+1)\}^{-m/2} \int_{-\infty}^{+\infty} \big\{K_k^{(N)}(\sqrt{N}\,x)\big\}^m \tilde{\beta}_N(dx).
\end{aligned} \tag{5}$$

Our task is now to compute the limit as $N \to \infty$.

As usual [2, 3], let $\{H_n(x)\}$ be the *Hermite polynomials* defined by the three-term recurrence relation:

$$H_0(x) = 1, \quad H_1(x) = 2x,$$
$$2xH_n(x) = H_{n+1}(x) + 2nH_{n-1}(x).$$

For normalization we set

$$\tilde{H}_n(x) = 2^{-n/2} H_n\Big(\frac{x}{\sqrt{2}}\Big), \qquad n = 0, 1, 2, \dots.$$

LEMMA 4.2. *$\{\tilde{H}_n(x)\}$ are the orthogonal polynomials with respect to the standard Gaussian distribution $N(0,1)$ and are normalized as $\tilde{H}_n(x) = x^n + (\text{lower})$. Moreover, the Jacobi parameters are given by $\omega_n = n$ and $\alpha_n = 0$, $n = 1, 2, \dots$.*

Proof. Easy. In fact, we have

$$\tilde{H}_0(x) = 1, \quad \tilde{H}_1(x) = 2x,$$
$$x\tilde{H}_n(x) = \tilde{H}_{n+1}(x) + n\tilde{H}_{n-1}(x),$$

from which the assertions are obvious. ∎

LEMMA 4.3. *For each $k = 0, 1, 2, \dots$*

$$\tilde{H}_k(x) = \lim_{N\to\infty} N^{-k/2} K_k^{(N)}(\sqrt{N}\,x).$$

Proof. Straightforward by comparison of the three-term recurrence relations satisfied by $\{\tilde{H}_k(x)\}$ and $\{K_k^{(N)}(x)\}$. ∎

LEMMA 4.4.

$$\lim_{N\to\infty} \int_{-\infty}^{+\infty} x^m\, \tilde{\beta}_N(dx) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} x^m e^{-x^2/2}\, dx, \qquad m = 1, 2, \dots.$$

Proof. This is a variant of the de Moivre–Laplace theorem (central limit theorem). ∎

We are now in a position to compute the limit of (5). By virtue of Lemmas 4.3 and 4.4 we obtain

$$
\begin{aligned}
&\lim_{N\to\infty} \binom{N}{k}^{-m/2} \varphi_{\mathrm{tr}}\big((A^{(N,k)})^m\big) \\
&= \lim_{N\to\infty} \{k!N(N-1)\dots(N-k+1)\}^{-m/2} \int_{-\infty}^{+\infty} \Big\{K_k^{(N)}(\sqrt{N}\,x)\Big\}^m \tilde{\beta}_N(dx) \\
&= (k!)^{-m/2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \{\tilde{H}_k(x)\}^m e^{-x^2/2}\, dx.
\end{aligned}
$$

Therefore, the probability distribution μ_k in the main theorem (Theorem 1.1) coincides with the distribution of

$$
(k!)^{-1/2}\tilde{H}_k(X) = (2^k k!)^{-1/2} H_k\Big(\frac{X}{\sqrt{2}}\Big),
$$

where X is a random variable obeying $N(0,1)$. Thus the proof of Theorem 1.1 is completed.

Remark 4.5. The probability distributions μ_k were obtained by Hora [4] in the study of asymptotic spectral distributions of the adjacency operators related to the infinite symmetric group. It is plausible that our result is generalized in terms of quotient spaces of the symmetric groups.

Remark 4.6. It is well known that the k-th distance matrix $A^{(k)}$ of a distance-regular graph is a polynomial of its adjacency matrix $A = A^{(1)}$, see e.g., [1]. In fact, the N-dimensional hypercube is a Hamming graph $H(N,2)$ so is distance-regular, and the polynomials are explicitly obtained in Lemma 3.3. From this aspect our argument in this paper is apparently applicable to a more general class of distance-regular graphs.

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