Computing Diffusion State Distance using Green’s Function and Heat Kernel on Graphs

Edward Boehnlein\(^1\), Peter Chin**\(^2\), Amit Sinha\(^3\), and Linyuan Lu\(^4\)**

\(^{1}\) University of South Carolina, Columbia, SC 29208, USA, boehnlei@email.sc.edu
\(^{2}\) Boston University, Boston, MA 02215, USA, spchin@cs.bu.edu
\(^{3}\) Boston University, Boston, MA 02215, USA, amits@bu.edu
\(^{4}\) University of South Carolina, Columbia, SC 29208, USA, lu@math.sc.edu

Abstract. The diffusion state distance (DSD) was introduced by Cao-Zhang-Park-Daniels-Crovella-Cowen-Hescott [PLoS ONE, 2013] to capture functional similarity in protein-protein interaction networks. They proved the convergence of DSD for non-bipartite graphs. In this paper, we extend the DSD to bipartite graphs using lazy-random walks and consider the general \(L_q\)-version of DSD. We discovered the connection between the DSD \(L_q\)-distance and Green’s function, which was studied by Chung and Yau [J. Combinatorial Theory (A), 2000]. Based on that, we computed the DSD \(L_q\)-distance for Paths, Cycles, Hypercubes, as well as random graphs \(G(n, p)\) and \(G(w_1, \ldots, w_n)\). We also examined the DSD distances of two biological networks.

1 Introduction

Recently, the diffusion state distance (DSD, for short) was introduced in [3] to capture functional similarity in protein-protein interaction (PPI) networks. The diffusion state distance is much more effective than the classical shortest-path distance for the problem of transferring functional labels across nodes in PPI networks, based on evidence presented in [3]. The definition of DSD is purely graph theoretic and is based on random walks.

Let \(G = (V, E)\) be a simple undirected graph on the vertex set \(\{v_1, v_2, \ldots, v_n\}\). For any two vertices \(u\) and \(v\), let \(He^{(k)}(u, v)\) be the expected number of times that a random walk starting at node \(u\) and proceeding for \(k\) steps, will visit node \(v\). Let \(He^{(k)}(u)\) be the vector \((He^{(k)}(u, v_1), \ldots, He^{(k)}(u, v_n))\). The diffusion state distance (or DSD, for short) between two vertices \(u\) and \(v\) is defined as

\[
DSD(u, v) = \lim_{k \to \infty} \left\| He^{(k)}(u) - He^{(k)}(v) \right\|_1
\]

\(^*\) This author is supported in part by NSF grant DMS 1222567 as well as AFOSR grant FA9550-12-1-0136.

\(**\) Research supported in part by NSF grant DMS 1300547 and ONR grant N00014-13-1-0717.
provided the limit exists (see [3]). Here the $L_1$-norm is not essential. Generally, for $q \geq 1$, one can define the DSD $L_q$-distance as

$$DSD_q(u, v) = \lim_{k \to \infty} \left\| H e^{(k)}(u) - H e^{(k)}(v) \right\|_q$$

provided the limit exists. (We use $L_q$ rather than $L_p$ to avoid confusion, as $p$ will be used as a probability throughout the paper.)

In [3], Cowen et al. showed that the above limit always exists whenever the random walk on $G$ is ergodic (i.e., $G$ is connected non-bipartite graph). They also prove that this distance can be computed by the following formula:

$$DSD(u, v) = \| (1 - 1) (I - D^{-1} A + W)^{-1} \|_1$$

where $D$ is the diagonal degree matrix, $A$ is the adjacency matrix, and $W$ is the constant matrix in which each row is a copy of $\pi$, $\pi = \frac{1}{\sum_{i=1}^n d_i} (d_1, \ldots, d_n)$ is the unique steady state distribution.

A natural question is how to define the diffusion state distance for a bipartite graph. We suggest to use the lazy random walk. For a given $\alpha \in (0, 1)$, one can choose to stay at the current node $u$ with probability $\alpha$, and choose to move to one of its neighbors with probability $(1 - \alpha)/d_u$. In other words, the transitive matrix of the $\alpha$-lazy random walk is

$$T_\alpha = \alpha I + (1 - \alpha) D^{-1} A.$$

Similarly, let $H e^{(k)}_{\alpha}(u, v)$ be the expected number of times that the $\alpha$-lazy random walk starting at node $u$ and proceeding for $k$ steps, will visit node $v$. Let $H e^{(k)}_{\alpha}(u)$ be the vector $(H e^{(k)}_{\alpha}(u, v_1), \ldots, H e^{(k)}_{\alpha}(u, v_n))$. The $\alpha$-diffusion state distance $L_q$-distance between two vertices $u$ and $v$ is

$$DSD^\alpha_q(u, v) = \lim_{k \to \infty} \left\| H e^{(k)}_{\alpha}(u) - H e^{(k)}_{\alpha}(v) \right\|_q.$$

**Theorem 1.** For any connected graph $G$ and $\alpha \in (0, 1)$, the $DSD^\alpha_q(u, v)$ is always well-defined and satisfies

$$DSD^\alpha_q(u, v) = (1 - \alpha)^{-1} \| (1 - 1) G \|_q.$$

Here $G$ is the matrix of Green’s function of $G$.

Observe that $(1 - \alpha) DSD^\alpha_q(u, v)$ is independent of the choice of $\alpha$. Naturally, we define the DSD $L_q$-distance of any graph $G$ as:

$$DSD_q(u, v) := \lim_{\alpha \to 0} (1 - \alpha) DSD^\alpha_q(u, v) = \| (1 - 1) G \|_q.$$

This definition extends the original definition for non-bipartite graphs.

With properly chosen $\alpha$, $\| H e^{(k)}_{\alpha}(u) - H e^{(k)}_{\alpha}(v) \|_q$ converges faster than $\| H e^{(k)}(u) - H e^{(k)}(v) \|_q$. This fact leads to a faster algorithm to estimate a single distance $DSD_q(u, v)$ using random walks. We will discuss it in Remark [1].
Green’s function was introduced in 1828 by George Green \[17\] to solve some partial differential equations, and it has found many applications (e.g. \[1\], \[5\], \[9\], \[16\], \[19\], \[24\]).

The Green’s function on graphs was first investigated by Chung and Yau \[5\] in 2000. Given a graph \(G = (V, E)\) and a given function \(g : V \to \mathbb{R}\), consider the problem to find \(f\) satisfying the discrete Laplace equation

\[
Lf = \sum_{y \in V} (f(x) - f(y))p_{xy} = g(x).
\]

Here \(p_{xy}\) is the transition probability of the random walk from \(x\) to \(y\). Roughly speaking, Green’s function is the left inverse operator of \(L\) (for the graphs with boundary). It is closely related to the Heat kernel of the graphs (see also \[15\]) and the normalized Laplacian.

In this paper, we will use Green’s function to compute the DSD \(L_q\)-distance for various graphs. The maximum DSD \(L_q\)-distance varies from graphs to graphs. The maximum DSD \(L_q\)-distance for paths and cycles are at the order of \(\Theta(n^{1+1/q})\) while the \(L_q\)-distance for some random graphs \(G(n, p)\) and \(G(w_1, \ldots, w_n)\) are constant for some ranges of \(p\). The hypercubes are somehow between the two classes. The DSD \(L_1\)-distance is \(\Omega(n)\) while the \(L_q\)-distance is \(\Theta(1)\) for \(q > 1\). Our method for random graphs is based on the strong concentration of the Laplacian eigenvalues.

The paper is organized as follows. In Section 2, we will briefly review the terminology on the Laplacian eigenvalues, Green’s Function, and heat kernel. The proof of Theorem \[1\] will be proved in Section 3. In Section 4, we apply Green’s function to calculate the DSD distance for various symmetric graphs like paths, cycles, and hypercubes. We will calculate the DSD \(L_2\)-distance for random graphs \(G(n, p)\) and \(G(w_1, w_2, \ldots, w_n)\) in Section 5. In the last section, we examined two brain networks: a cat and a Rhesus monkey. The distributions of the DSD distances are calculated.

## 2 Notation and background

In this paper, we only consider undirected simple graph \(G = (V, E)\) with the vertex set \(V\) and the edge set \(E\). For each vertex \(x \in V\), the neighborhood of \(x\), denoted by \(N(x)\), is the set of vertices adjacent to \(x\). The degree of \(x\), denoted by \(d_x\), is the cardinality of \(N(x)\). We also denote the maximum degree by \(\Delta\) and the minimum degree by \(\delta\).

Without loss of generalization, we assume that the set of vertices is ordered and assume \(V = [n] = \{1, 2, \ldots, n\}\). Let \(A\) be the adjacency matrix and \(D = \text{diag}(d_1, \ldots, d_n)\) be the diagonal matrix of degrees. For a given subset \(S\), let the volume of \(S\) to be \(\text{vol}(S) := \sum_{i \in S} d_i\). In particular, we write \(\text{vol}(G) = \text{vol}(V) = \sum_{i=1}^n d_i\).
Let $V^*$ be the linear space of all real functions on $V$. The discrete Laplace operator $L: V^* \to V^*$ is defined as

$$L(f)(x) = \sum_{y \in N(x)} \frac{1}{d_x} (f(x) - f(y)).$$

The Laplace operator can also be written as a $(n \times n)$-matrix:

$$L = I - D^{-1}A.$$

Here $D^{-1}A$ is the transition probability matrix of the (uniform) random walk on $G$. Note that $L$ is not symmetric. We consider a symmetric version

$$\mathcal{L} := I - D^{-1/2}AD^{-1/2} = D^{1/2}LD^{-1/2},$$

which is so called the normalized Laplacian. Both $L$ and $\mathcal{L}$ have the same set of eigenvalues. The eigenvalues of $\mathcal{L}$ can be listed as

$$0 = \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n-1} \leq 2.$$

The eigenvalue $\lambda_1 > 0$ if and only if $G$ is connected while $\lambda_{n-1} = 2$ if and only if $G$ is a bipartite graph. Let $\phi_0, \phi_1, \ldots, \phi_{n-1}$ be a set of orthogonal unit eigenvectors. Here $\phi_0 = \frac{1}{\sqrt{\text{vol}(G)}}(\sqrt{d_1}, \ldots, \sqrt{d_n})$ is the positive unit eigenvector for $\lambda_0 = 0$ and $\phi_i$ is the eigenvector for $\lambda_i$ ($1 \leq i \leq n-1$).

Let $O = (\phi_0, \ldots, \phi_{n-1})$ and $A = \text{diag}(0, \lambda_1, \ldots, \lambda_{n-1})$. Then $O$ is an orthogonal matrix and $\mathcal{L}$ be diagonalized as

$$\mathcal{L} = OAO'. \quad (2)$$

Equivalently, we have

$$L = D^{-1/2}OAO'D^{1/2}. \quad (3)$$

The Green’s function $\mathcal{G}$ is the matrix with its entries, indexed by vertices $x$ and $y$, defined by a set of two equations:

$$\mathcal{G} L(x, y) = I(x, y) - \frac{d_y}{\text{vol}(G)}, \quad (4)$$

$$\mathcal{G} 1 = 0. \quad (5)$$

(This is the so-called Green’s function for graphs without boundary in [5].)

The normalized Green’s function $\mathcal{G}$ is defined similarly:

$$\mathcal{G} \mathcal{L}(x, y) = I(x, y) - \frac{\sqrt{d_x d_y}}{\text{vol}(G)}.$$

The matrices $\mathcal{G}$ and $\mathcal{G}$ are related by

$$\mathcal{G} = D^{1/2} \mathcal{G} D^{-1/2}. $$
Alternatively, $G$ can be defined using the eigenvalues and eigenvectors of $L$ as follows:

$$G = O \Lambda^{(-1)} O',$$

where $\Lambda^{(-1)} = \text{diag}(0, \lambda_1^{-1}, \ldots, \lambda_{n-1}^{-1})$. Thus, we have

$$G(x, y) = \sum_{l=1}^{n-1} \frac{1}{\lambda_l} \sqrt{\frac{d}{d_x}} \phi_l(x) \phi_l(y).$$

(6)

For any real $t \geq 0$, the heat kernel $H_t$ is defined as

$$H_t = e^{-t L}.$$  

Thus,

$$H_t(x, y) = \sum_{l=0}^{n-1} e^{-\lambda_l t} \phi_l(x) \phi_l(y).$$

The heat kernel $H_t$ satisfies the heat equation

$$\frac{d}{dt} H_t f = -L H_t f.$$  

The relation of the heat kernel and Green’s function is given by

$$G = \int_0^\infty H_t dt - \phi'_0 \phi_0.$$  

The heat kernel can be used to compute Green’s function for the Cartesian product of two graphs. We will omit the details here. Readers are directed to [5] and [6] for the further information.

### 3 Proof of main theorem

**Proof (Proof of Theorem 1):** Rewrite the transition probability matrix $T_\alpha$ as

$$T_\alpha = \alpha I + (1 - \alpha) D^{-1} A.$$  

$$= D^{-1/2}(\alpha I + (1 - \alpha) D^{-1/2} A D^{-1/2}) D^{1/2}.$$  

$$= D^{-1/2}(\alpha I + (1 - \alpha) (I - L)) D^{1/2}.$$  

$$= D^{-1/2}(I - (1 - \alpha) L) D^{1/2}.$$  

For $k = 0, 1, \ldots, n-1$, let $\lambda^*_k = 1 - (1 - \alpha) \lambda_k$ and $\Lambda^* = \text{diag}(\lambda^*_0, \ldots, \lambda^*_{n-1}) = I - (1 - \alpha) A$. Applying Equation (3), we get

$$T_\alpha = D^{-1/2} O \Lambda^* O' D^{1/2} = (O' D^{1/2})^{-1} \Lambda^* O' D^{1/2}.$$
Then for any $t \geq 1$, the $t$-step transition matrix is $T^t = (OD^{1/2})^{-1}A^{t}OD^{1/2} = D^{-1/2}OA^{t}OD^{1/2}$. Denote $p^{(t)}_\alpha(u,j)$ as the $(u,j)^{th}$ entry in $T^t$.

\[
p^{(t)}_\alpha(u,j) = \sum_{l=0}^{n-1} (\lambda^*)^t \sqrt{\frac{d_j}{d_u}} \phi_l(u)\phi_l(j)
= \frac{d_j}{\text{vol}(G)} + \sum_{l=1}^{n-1} (\lambda^*)^t \sqrt{\frac{d_j}{d_u}} \phi_l(u)\phi_l(j).
\]

Thus,

\[
He^{(k)}_\alpha(u,j) - He^{(k)}_\alpha(v,j) = \sum_{t=0}^{k} \sum_{l=1}^{n-1} (\lambda^*)^t d_j^{1/2} \phi_l(j)(d_u^{-1/2} \phi_l(u) - d_v^{-1/2} \phi_l(v)).
\]

The limit $\lim_{k \to \infty} He^{(k)}_\alpha(u,j) - He^{(k)}_\alpha(v,j)$ forms the sum of $n$ geometric series:

\[
\sum_{t=0}^{\infty} \sum_{l=1}^{n-1} (\lambda^*)^t d_j^{1/2} \phi_l(j)(d_u^{-1/2} \phi_l(u) - d_v^{-1/2} \phi_l(v)).
\]

Note each geometric series converges since the common ratio $\lambda^* \in (-1,1)$. Thus,

\[
\lim_{k \to \infty} \left( He^{(k)}_\alpha(u,j) - He^{(k)}_\alpha(v,j) \right) = \sum_{t=0}^{\infty} \sum_{l=1}^{n-1} (\lambda^*)^t d_j^{1/2} \phi_l(j)(d_u^{-1/2} \phi_l(u) - d_v^{-1/2} \phi_l(v))
= \sum_{t=1}^{n-1} \frac{1}{1-\lambda^*} d_j^{1/2} \phi_l(j)(d_u^{-1/2} \phi_l(u) - d_v^{-1/2} \phi_l(v))
= \frac{1}{1-\alpha} \sum_{t=1}^{n-1} \frac{1}{\lambda^*} d_j^{1/2} \phi_l(j)(d_u^{-1/2} \phi_l(u) - d_v^{-1/2} \phi_l(v))
= \frac{1}{1-\alpha} (\mathcal{G}(u,j) - \mathcal{G}(v,j)).
\]

We have

\[
\lim_{k \to \infty} He^{(k)}_\alpha(u) - He^{(k)}_\alpha(v) = \frac{1}{1-\alpha}(1_u - 1_v)\mathcal{G}.
\]

**Remark 1.** Observe that the convergence rate of $He^{(k)}_\alpha(u) - He^{(k)}_\alpha(v)$ is determined by $\lambda^* := \max \{1 - (1-\alpha)\lambda_1, (1-\alpha)\lambda_{n-1} - 1\}$. It is critical that we assume $\alpha \neq 0$. When $\alpha = 0$ then $\lambda^* < 1$ holds only if $\lambda_{n-1} < 2$, i.e. $G$ is a non-bipartite graph (see [3]).

When $\lambda_1 + \lambda_{n-1} > 2$, $\lambda^*$ (as a function of $\alpha$) achieves the minimum value $\frac{\lambda_{n-1} - \lambda_1}{\lambda_{n-1} + \lambda_1}$ at $\alpha = 1 - \frac{2}{\lambda_1 + \lambda_{n-1}}$. This is the best mixing rate that the $\alpha$-lazy random
walk on $G$ can achieve. Using the $\alpha$-lazy random walks (with $\alpha = 1 - \frac{2}{\lambda_1 + \lambda_{n-1}}$) to approximate the DSD $L_q$-distance will be faster than using regular random walks.

Equation (6) implies $\|G\|_2 \leq \frac{1}{\lambda_1} \sqrt{\frac{2}{\delta}}$. Combining with Theorem 1, we have

**Corollary 1.** For any connected simple graph $G$, and any two vertices $u$ and $v$, we have $DSD_2(u, v) \leq \frac{\sqrt{2}}{\lambda_1} \sqrt{\frac{2}{\delta}}$.

Note that for any connected graph $G$ with diameter $m$ (Lemma 1.9, [6])

$$\lambda_1 > \frac{1}{m \text{ vol}(G)}.$$  

This implies a uniform bound for the DSD $L_2$ distances on any connected graph $G$ on $n$ vertices.

$$DSD_2(u, v) \leq \sqrt{\frac{2\Delta}{\delta} m \text{ vol}(G)} < \sqrt{2}n^{3.5}.$$  

This is a very coarse upper bound. But it does raise an interesting question “How large can the DSD $L_q$-distance be?”

## 4 Some examples of the DSD distance

In this section, we use Green’s function to compute the DSD $L_q$-distance (between two vertices of the distance reaching the diameter) for paths, cycles, and hypercubes.

### 4.1 The path $P_n$

We label the vertices of $P_n$ as $1, 2, \ldots, n$, in sequential order. Chung and Yau computed the Green’s function $G$ of the weighed path with no boundary (Theorem 9, [5]). It implies that Green’s function of the path $P_n$ is given by: for any
\(u \leq v,\)

\[
G(u, v) = \frac{\sqrt{d_u d_v}}{4(n-1)^2} \left( \sum_{z \leq u} (d_1 + \cdots + d_z)^2 + \sum_{v \leq z} (d_{z+1} + \cdots + d_n)^2 \right)
- \sum_{u \leq z < v} (d_1 + \cdots + d_z)(d_{z+1} + \cdots + d_n)
\]

\[
= \frac{\sqrt{d_u d_v}}{4(n-1)^2} \left( \sum_{z=1}^{u-1} (2z-1)^2 + \sum_{z=v}^{n-1} (2n-2z-1)^2 - \sum_{z=u}^{v-1} (2z-1)(2n-2z-1) \right)
\]

\[
= \frac{\sqrt{d_u d_v}}{4(n-1)^2} \left( \sum_{z=1}^{n-1} (2z-1)^2 + \sum_{z=v}^{n-1} (2n-2)(2n-4z) - \sum_{z=u}^{v-1} (2z-1)(2n-2) \right)
\]

\[
= \frac{\sqrt{d_u d_v}}{2(n-1)} \left( \frac{(2n-1)(2n-3)}{12} \right) + \frac{\sqrt{d_u d_v}}{2(n-1)} \left( \sum_{z=v}^{n-1} (2n-4z) - \sum_{z=u}^{v-1} (2z-1) \right)
\]

\[
= \frac{\sqrt{d_u d_v}}{2(n-1)} \left( (u-1)^2 + (n-v)^2 - \frac{2n^2 - 4n + 3}{6} \right)
\]

When \(u > v\), we have

\[
G(u, v) = G(v, u) = \frac{\sqrt{d_u d_v}}{2(n-1)} \left( (v-1)^2 + (n-u)^2 - \frac{2n^2 - 4n + 3}{6} \right)
\]

Applying \(G(u, v) = \sqrt{d_u d_v} G(u, v)\), we get

\[
G(u, v) = \begin{cases} 
\frac{d_v}{2(n-1)} \left((u-1)^2 + (n-v)^2 - \frac{2n^2 - 4n + 3}{6}\right) & \text{if } u \leq v; \\
\frac{d_u}{2(n-1)} \left((v-1)^2 + (n-u)^2 - \frac{2n^2 - 4n + 3}{6}\right) & \text{if } u > v.
\end{cases}
\]

We have

\[
G(1,1) = \frac{4n^2 - 8n + 3}{12(n-1)};
\]

\[
G(1,j) = \frac{1}{n-1} \left((n-j)^2 - \frac{2n^2 - 4n + 3}{6}\right) \quad \text{for } 2 \leq j \leq n-1;
\]

\[
G(1,n) = -\frac{2n^2 - 4n + 3}{12(n-1)};
\]

\[
G(n,1) = -\frac{2n^2 - 4n + 3}{12(n-1)};
\]

\[
G(n,j) = \frac{1}{n-1} \left((j-1)^2 - \frac{2n^2 - 4n + 3}{6}\right) \quad \text{for } 2 \leq j \leq n-1;
\]

\[
G(n,n) = \frac{4n^2 - 8n + 3}{12(n-1)}.
\]
Thus,
\[ G(1, j) - G(n, j) = \begin{cases} 
\frac{n-1}{2} & \text{if } j = 1; \\
n + 1 - 2j & \text{if } 2 \leq j \leq n - 1; \\
-\frac{n+1}{2} & \text{if } j = n.
\end{cases} \] (7)

**Theorem 2.** For any \( q \geq 1 \), the DSD \( L_q \)-distance of the Path \( P_n \) between 1 and \( n \) satisfies
\[ DSD_q(1, n) = (1 + q)^{-1/q} n^{1+1/q} + O(n^{1/q}). \]

**Proof.**
\[ DSD_q(1, n) = \left( 2 \left( \frac{n-1}{2} \right)^q + \sum_{j=2}^{n-1} |n + 1 - 2j|^q \right)^{1/q} 
= \left( \frac{1}{1 + q} n^{1+q} + O(n^q) \right)^{1/q} 
= (1 + q)^{-1/q} n^{1+1/q} + O(n^{1/q}). \]

For \( q = 1 \), we have the following exact result:
\[ DSD_1(1, n) = \sum_{j=1}^{n} |G(1, j) - G(n, j)| = \begin{cases} 
2k^2 - 2k + 1 & \text{if } n = 2k \\
2k^2 & \text{if } n = 2k + 1.
\end{cases} \]

### 4.2 The cycle \( C_n \)

Now we consider Green’s function of cycle \( C_n \). For \( x, y \in \{1, 2, \ldots, n\} \), let \( |x - y|_c \) be the graph distance of \( x, y \) in \( C_n \). We have the following Lemma.

**Lemma 1.** For even \( n = 2k \), Green’s function \( G \) of \( C_n \) is given by
\[ G(x, y) = \frac{1}{2k} (k - |x - y|_c)^2 - \frac{k}{6} - \frac{1}{12k}. \]

For odd \( n = 2k + 1 \), Green’s function \( G \) of \( C_n \) is given by
\[ G(x, y) = \frac{2}{2k + 1} \left( k + 1 - |x - y|_c \right) - \frac{k^2 + k}{3(2k + 1)}. \]

**Proof.** We only prove the even case here. The odd case is similar and will be left to the readers.

For \( n = 2k \), it suffices to verify that \( G \) satisfies Equations (4) and (5). To verify Equation (4), we need show
\[ G(x, y) - \frac{1}{2} G(x, y - 1) - \frac{1}{2} G(x, y + 1) = \begin{cases} 
-\frac{1}{n} & \text{if } x \neq y; \\
1 - \frac{1}{n} & \text{if } x = y.
\end{cases} \]
Let \( z = \frac{k}{6} + \frac{1}{12k} \) and \( i = |x - y|_c \). For \( x \neq y \), we have
\[
G(x, y) - \frac{1}{2}G(x, y - 1) - \frac{1}{2}G(x, y + 1) \\
= \left( \frac{1}{2k} (k - i)^2 - z \right) - \frac{1}{2} \left( \frac{1}{2k} (k - i - 1)^2 - z \right) - \frac{1}{2} \left( \frac{1}{2k} (k - i + 1)^2 - z \right) \\
= -\frac{1}{2k} \\
= -\frac{1}{n}.
\]
When \( x = y \), we have
\[
G(x, y) - \frac{1}{2}G(x, y - 1) - \frac{1}{2}G(x, y + 1) \\
= \frac{1}{2k} k^2 - z - \frac{1}{2} \left( \frac{1}{2k} (k - 1)^2 - z \right) - \frac{1}{2} \left( \frac{1}{2k} (k - 1)^2 - z \right) \\
= \frac{2k - 1}{2k} \\
= 1 - \frac{1}{n}.
\]
To verify Equation (5), it is enough to verify
\[
1^2 + 2^2 + \cdots + (k - 1)^2 + k^2 + (k - 1)^2 + \cdots + 1^2 = \frac{2k^3 + k}{3} = n^2 z.
\]
This can be done by induction on \( k \).

**Theorem 3.** For any \( q \geq 1 \), the DSD \( L_q \)-distance of the Cycle \( C_n \) between 1 and \( \lfloor \frac{n}{2} \rfloor + 1 \) satisfies
\[
DSD_q(1, \lfloor \frac{n}{2} \rfloor + 1) = \left( \frac{4}{1 + q} \right)^{1/q} \left( \frac{n}{4} \right)^{1+1/q} + O(n^{1/q}).
\]

**Proof.** We only verify the case of even cycle here. The odd cycle is similar and will be omitted.

For \( n = 2k \), the difference of \( G(1, j) \) and \( G(1 + k, j) \) have a simple form:
\[
G(1, j) - G(1 + k, j) = \frac{1}{2k} ((k - i)^2 - i^2) = \frac{k}{2} - i,
\]
where \( i = |j - 1|_c \). Thus,
\[
DSD_q(1, 1 + k) = \left( \sum_{i=0}^{k-1} \left| \frac{k}{2} - i \right| \right)^{1/q} \\
= \left( \frac{4}{1 + q} \left( \frac{k}{2} \right)^{1+q} + O(k^q) \right)^{1/q} \\
= \left( \frac{4}{1 + q} \left( \frac{n}{4} \right)^{1+1/q} + O(n^{1/q}) \right).
\]
4.3 The hypercube \( Q_n \)

Now we consider the hypercube \( Q_n \), whose vertices are the binary strings of length \( n \) and whose edges are pairs of vertices differing only at one coordinate. Chung and Yau \([5]\) computed the Green’s function of \( Q_n \): for any two vertices \( x \) and \( y \) with distance \( k \) in \( Q_n \),

\[
G(x, y) = 2^{-2n} \left( \sum_{j<k} \binom{n}{j} \binom{n}{j+1} \cdots \binom{n}{n} + \sum_{k<j} \frac{(n-1)^2}{(n-1)_j} \right)
\]

\[
= 2^{-2n} \sum_{j=0}^{n-1} \binom{n}{j+1} \binom{n}{n} - 2^{-n} \sum_{j<k} \binom{n}{j+1} \binom{n}{n}.
\]

We are interested in the DSD distance between a pair of antipodal vertices. Let \( 0 \) denote the all-0-string and \( 1 \) denote the all-1-string. For any vertex \( x \), if the distance between \( 0 \) and \( x \) is \( i \) then the distance between \( 1 \) and \( x \) is \( n - i \). We have

\[
G(0, x) - G(1, x) = -2^{-n} \sum_{j<k} \binom{n}{j+1} \binom{n}{n} + 2^{-n} \sum_{j<n-k} \binom{n}{j+1} \binom{n}{n} = 2^{-n} \sum_{j=k}^{n-k-1} \binom{n}{j+1} \binom{n}{n}.
\]

Here we use the convention that \( \sum_{j=b}^{a} c_j = -\sum_{j=a}^{b} c_j \) for \( b > a \).

**Theorem 4.** For any \( q \geq 1 \), the DSD \( L_q \)-distance of the hypercube \( Q_n \) between \( 0 \) and \( 1 \) satisfies

\[
DSD_q(0, 1) = \left( \sum_{k=0}^{n} \binom{n}{k} \left( 2^{-n} \sum_{j=k}^{n-k-1} \binom{n}{j+1} \binom{n}{n} \right)^q \right)^{1/q} \quad (9)
\]

In particular, \( DSD_q(0, 1) = \Theta(1) \) when \( q > 1 \) while \( DSD_1(0, 1) = \Omega(n) \).

**Proof.** Equation (9) follows from the definition of DSD \( L_q \)-distance and Equation (8).

Let \( a_k = \binom{n}{k} \left( 2^{-n} \sum_{j=k}^{n-k-1} \binom{n}{j+1} \binom{n}{n} \right)^q \).

Observe that \( a_k = a_{n-k} \), we only need to estimate \( a_k \) for \( 0 \leq k \leq n/2 \). Also we can throw away the terms in the second summation for \( j > n/2 \) since that part is at most half of \( a_k \). For \( k \leq j \leq n/2 \),

\[
\frac{1}{2} \leq 2^{-n} \left( \binom{n}{j+1} + \cdots + \binom{n}{n} \right) \leq 1.
\]
Thus $a_k$ has the same magnitude as $b_k := \binom{n}{k} \left( \sum_{j=k}^{n/2} \binom{n}{j} \right)^q$.

For $q > 1$, we first bound $b_k$ by $b_k \leq \binom{n}{k} \left( \frac{n}{k} \right)^q = O(n^{(1-q)k+q})$. When $k > \frac{q+2}{q-1}$, we have $b_k = O(n^{-2})$. The total contribution of those $b_k$’s is $O(n^{-1})$, which is negligible. Now consider the term $b_k$ for $k = 0, 1, \ldots, \lfloor \frac{q+2}{4} \rfloor$. We bound $b_k$ by $b_k \leq \binom{n}{k} \left( 1 + \frac{n/2}{(\frac{n}{k})^{k+1}} \right)^q = O(1)$.

This implies $\text{DSD}_1(0, 1) = O(1)$. The lower bound $\text{DSD}_q(0, 1) \geq 1$ is obtained by taking the term at $k = 0$. Putting together, we have $\text{DSD}_q(0, 1) = \Theta(1)$ for $q > 1$.

For $q = 1$, note that
$$b_k = \sum_{j=k}^{n/2} \frac{\binom{n}{j}}{\binom{n}{k}} > \frac{\binom{n}{k}}{\binom{n}{k-1}} = \frac{n}{n-k} > 1.$$

Thus, $\text{DSD}_1(0, 1) = \Omega(n)$.

5 Random graphs

In this section, we will calculate the DSD $L_q$-distance in two random graphs models. For random graphs, the non-zero Laplacian eigenvalues of a graph $G$ are often concentrated around 1. The following Lemma is useful to the DSD $L_q$-distance.

**Lemma 2.** Let $\lambda_1, \ldots, \lambda_{n-1}$ be all non-zero Laplacian eigenvalues of a graph $G$. Suppose there is a small number $\epsilon \in (0, 1/2)$, so that for $1 \leq i \leq n-1$, $|1 - \lambda_i| \leq \epsilon$. Then for any pair of vertices $u, v$, the DSD $L_q$-distance satisfies
\begin{align*}
|\text{DSD}_q(u, v) - 2^{1/q}| &\leq \frac{\epsilon}{1-\epsilon} \sqrt{\Delta_d + \Delta_{d'v}}, \quad \text{if } q \geq 2, \quad (10) \\
|\text{DSD}_q(u, v) - 2^{1/q}| &\leq \frac{\epsilon}{1-\epsilon} \sqrt{\Delta_d + \Delta_{d'v}}, \quad \text{for } 1 \leq q < 2. \quad (11)
\end{align*}

**Proof.** Rewrite the normalized Green’s function $\mathcal{G}$ as
$$\mathcal{G} = I - \phi_0 \phi_0' + \mathcal{Y}.$$ 

Note that the eigenvalues of $\mathcal{Y} := \mathcal{G} - I + \phi_0 \phi_0'$ are $0, \frac{1}{\lambda_1} - 1, \ldots, \frac{1}{\lambda_{n-1}} - 1$. Observe that for each $i = 1, 2, \ldots, n-1$, $|\frac{1}{\lambda_i} - 1| \leq \frac{\epsilon}{1-\epsilon}$. We have
$$\|\mathcal{Y}\| \leq \frac{\epsilon}{1-\epsilon}.$$
Thus,
\[
\text{DSD}_q(u, v) = \| (1 - \mathbf{I}^u \mathbf{I}^v D^{-1/2} G D^{1/2} \|_q \\
= \| (1 - \mathbf{I}^u \mathbf{I}^v (I - \phi'_0 \phi + \mathcal{Y}) D^{1/2} \|_q \\
\leq \| (1 - \mathbf{I}^u \mathbf{I}^v D^{-1/2} (I - \phi'_0 \phi) D^{1/2} \|_q + \| (1 - \mathbf{I}^u \mathbf{I}^v D^{-1/2} \mathcal{Y} D^{1/2} \|_q.
\]

Viewing \( \mathcal{Y} \) as the error term, we first calculate the main term.
\[
\| (1 - \mathbf{I}^u \mathbf{I}^v D^{-1/2} (I - \phi'_0 \phi) D^{1/2} \|_q \\
= \| (1 - \mathbf{I}^u \mathbf{I}^v (I - W) \|_q \\
= \| (1 - \mathbf{I}^u \mathbf{I}^v \|_q \\
= 2^{1/q}.
\]

The \( L_2 \)-norm of the error term can be bounded by
\[
\| (1 - \mathbf{I}^u \mathbf{I}^v D^{-1/2} \mathcal{Y} D^{1/2} \|_2 \\
\leq \| (1 - \mathbf{I}^u \mathbf{I}^v D^{-1/2} \|_2 \| \mathcal{Y} \| D^{1/2} \| \\
\leq \sqrt{\frac{1}{d_u} + \frac{1}{d_v} - \epsilon \sqrt{\Delta}} \\
= \frac{\epsilon}{1 - \epsilon} \sqrt{\frac{\Delta}{d_u} + \frac{\Delta}{d_v}}.
\]

To get the bound of \( L_q \)-norm from \( L_2 \)-norm, we apply the following relation of \( L_q \)-norm and \( L_2 \)-norm to the error term. For any vector \( x \in \mathbb{R}^n \),
\[
\| x \|_q \leq \| x \|_2 \quad \text{for } q \geq 2.
\]

and
\[
\| x \|_q \leq n^{\frac{1}{q} - \frac{1}{2}} \| x \|_2 \quad \text{for } 1 \leq q < 2.
\]

The inequalities (10) and (11) follow from the triangular inequality of the \( L_q \)-norm and the upper bound of the error term.

Now we consider the classical Erdős-Renyi random graphs \( G(n, p) \). For a given \( n \) and \( p \in (0, 1) \), \( G(n, p) \) is a random graph on the vertex set \( \{1, 2, \ldots, n\} \) obtained by adding each pair \( (i, j) \) to the edges of \( G(n, p) \) with probability \( p \) independently.

There are plenty of references on the concentration of the eigenvalues of \( G(n, p) \) (for example, [12], [14], [21], and [22]). Here we list some facts on \( G(n, p) \).

1. For \( p > \frac{(1+\epsilon) \log n}{n} \), almost surely \( G(n, p) \) is connected.
2. For \( p \gg \frac{\log n}{n} \), \( G(n, p) \) is “almost regular”; namely for all vertex \( v \), \( d_v = (1 + o_n(1))np \).
3. For \( np(1 - p) \gg \log^4 n \), all non-zero Laplacian eigenvalues \( \lambda_i \)'s satisfy (see [22])
\[
| \lambda_i - 1 | \leq \frac{(3 + o_n(1))\sqrt{np}}{n^p}.
\]
Apply Lemma 2 with $\epsilon = \frac{(3+o_n(1))}{\sqrt{np}}$, and note that $G(n,p)$ is almost-regular. We get the following theorem.

**Theorem 5.** For $p(1-p) \gg \frac{\log^4 n}{n}$, almost surely for all pairs of vertices $(u,v)$, the DSD $L_q$-distance of $G(n,p)$ satisfies

$$DSD_q(u,v) = 2^{1/q} \pm O\left(\frac{1}{\sqrt{np}}\right) \quad \text{if } q \geq 2,$$

$$DSD_q(u,v) = 2^{1/q} \pm O\left(\frac{n^{\frac{q}{2} - \frac{1}{2}}}{\sqrt{np}}\right) \quad \text{if } 1 \leq q < 2.$$  

Now we consider the random graphs with given expected degree sequence $G(w_1, \ldots, w_n)$ (see [2], [7], [8], [9], [20]). It is defined as follows:

1. Each vertex $i$ (for $1 \leq i \leq n$) is associated with a given positive weight $w_i$.
2. Let $\rho = \frac{1}{\sum_{i=1}^{n} w_i}$. For each pair of vertices $(i,j)$, $ij$ is added as an edge with probability $w_i w_j \rho$ independently. $(i$ and $j$ may be equal so loops are allowed. Assume $w_i w_j \rho \leq 1$ for $i,j$.)

Let $w_{\text{min}}$ be the minimum weight. There are many references on the concentration of the eigenvalues of $G(w_1, \ldots, w_n)$ (see [10], [11], [12], [14], [22]). The version used here is in [22].

1. For each vertex $i$, the expected degree of $i$ is $w_i$.
2. Almost surely for all $i$ with $w_i \gg \log n$, then the degree $d_i = (1 + o(1))w_i$.
3. If $w_{\text{min}} \gg \log^4 n$, all non-zero Laplacian eigenvalues $\lambda_i$ (for $1 \leq i \leq n-1$),

$$|1 - \lambda_i| \leq \frac{3 + o_n(1)}{\sqrt{w_{\text{min}}}}.$$  

**Theorem 6.** Suppose $w_{\text{min}} \gg \log^4 n$, almost surely for all pairs of vertices $(u,v)$, the DSD $L_q$-distance of $G(w_1, \ldots, w_n)$ satisfies

$$DSD_q(u,v) = 2^{1/q} \pm O\left(\frac{1}{\sqrt{w_{\text{min}}}} \sqrt{\frac{w_{\text{max}}}{w_u} + \frac{w_{\text{max}}}{w_v}}\right) \quad \text{if } q \geq 2,$$

$$DSD_q(u,v) = 2^{1/q} \pm O\left(\frac{n^{\frac{q}{2} - \frac{1}{2}}}{\sqrt{w_{\text{min}}}} \sqrt{\frac{w_{\text{max}}}{w_u} + \frac{w_{\text{max}}}{w_v}}\right) \quad \text{if } 1 \leq q < 2.$$  

6 **Examples of biological networks**

In this section, we will examine the distribution of the DSD distances for some biological networks. The set of graphs analyzed in this section include three graphs of brain data from the Open Connectome Project [25] and two more graphs built from the *S. cerevisiae* PPI network and *S. pombe* PPI network used in [3]. Figure 1 and 2 serves as a visual representation of one of the two brain
Fig. 1. The brain networks: (a), a Cat; (b), a Rhesus Monkey.

data graphs: the graph of a cat and the graph of a Rhesus monkey. The network of the cat brain has 65 nodes and 1139 edges while the network of rhesus monkey brain has 242 nodes and 4090 edges.

Each node in the Rhesus graph represents a region in the cerebral cortex originally analyzed in [18]. Each edge represents axonal connectivity between regions and there is no distinction between strong and weak connections in this graph [18]. The Cat data-set follows a similar pattern where each node represents a region of the brain and each edge represents connections between them. The Cat data-set represents 18 visual regions, 10 auditory regions, 18 somatomotor regions, and 19 frontolimbic regions [23].

For each network above, we calculated all-pair DSD $L_1$-distances. Divide the possible values into many small intervals and compute the number of pairs falling into each interval. The results are shown in Figure 1. The patterns are quite surprising to us.

Both graphs has a small interval consisting of many pairs while other values are more or less uniformly distributed. We think, that phenomenon might be caused by the clustering of a dense core. The two graphs have many branches sticking out. Since we are using $L_1$-distance, it doesn’t matter the directions of these branches sticking out when they are embedded into $\mathbb{R}^n$ using Green’s function.

When we change $L_1$-distance to $L_2$-distance, the pattern should be broken. This is confirmed in Figure 3. The actual distributions are mysterious to us.

References

1. S. Baroni, P. Giannozzi, and A. Testa, Greens-function approach to linear response in solids. Physical Review Letters, 58(18) (1987), 1861-1864.
2. S. Bhamidi, R.W. van der Hofstad, and J.S.H. van Leeuwaarden, Scaling limits for critical inhomogeneous random graphs with finite third moments, Electronic Journal of Probability, 15(54) (2010) 1682-1702.
Fig. 2. The distribution of the DSD $L_1$-distances of brain networks: (a), a Cat; (b): a Rhesus Monkey

Fig. 3. The distribution of the DSD $L_2$-distances of brain networks: (a), a Cat; (b): a Rhesus Monkey
3. M. Cao, H. Zhang, J. Park, N.M. Daniels, M.E. Crovella, L.J. Cowen, and B. Hescott, Going the distance for protein function prediction: a new distance metric for protein interaction networks, PLoS ONE (2013), 8(10):e76339.
4. S.P. Chin, E. Reilly, and L. Lu. Finding structures in large-scale graphs. SPIE Defense, Security, and Sensing. International Society for Optics and Photonics, 2012.
5. F. Chung and S.-T. Yau, Discrete Green’s functions, *J. Combinatorial Theory (A)* 91 (2000), 191-214.
6. F. Chung, *Spectral graph theory*, AMS publications, 1997.
7. F. Chung and L. Lu. Connected components in a random graph with given degree sequences, *Annals of Combinatorics*, 6 (2002), 125–145.
8. F. Chung and L. Lu. The average distances in random graphs with given expected degrees, *Proc. Natl. Acad. Sci.* 99 (2002), 15879–15882.
9. F. Chung and L. Lu, *Complex graphs and networks*, CBMS Regional Conference Series in Mathematics; number 107, (2006), 264+vii pages. ISBN-10: 0-8218-3657-9, ISBN-13: 978-0-8218-3657-6.
10. F. Chung, L. Lu, and V. H. Vu, Eigenvalues of random power law graphs, *Ann. Comb.,* 7 (2003), 21–33.
11. F. Chung, L. Lu, and V. H. Vu, Spectra of random graphs with given expected degrees, *Proc. Natl. Acad. Sci. USA* 100(11) (2003), 6313–6318.
12. F. Chung and M. Radcliffe, On the spectra of general random graphs, *Electron. J. Combin.*, 18(1) (2011), P215.
13. A. Coja-Oghlan, On the Laplacian eigenvalues of $G(n,p)$, *Combin. Probab. Comput.*, 16(6) (2007), 923–946.
14. A. Coja-Oghlan and A. Lanka, The spectral gap of random graphs with given expected degrees, *Electron. J. Combin.*, 16 (2009), R138.
15. E.B. Davies, *Heat Kernels and Spectral Theory*, Vol. 92, Cambridge University Press, 1990.
16. D.G. Duffy, *Green’s Functions with Applications*, CRC Press, 2010.
17. G. Green, *An Essay on the Application of Mathematical Analysis to the Theories of Electricity and Magnetism*, Nottingham, 1828.
18. L. Harriger, M. P. van den Heuvel, and O. Sporns, Rich club organization of macaque cerebral cortex and its role in network communication, PloS one 7.9 (2012): e46497.
19. L. Hedin, New method for calculating the one-particle Green’s function with application to the electron-gas problem, *Physical Review*, 139(3A) (1965) , 796-823.
20. R.W. van der Hofstad, Critical behavior in inhomogeneous random graphs, *Random Structures and Algorithms*, 42(4) (2013), 480-508.
21. M. Krivelevich and B. Sudakov, The largest eigenvalue of sparse random graphs, *Combin. Probab. Comput.*, 12 (2003), 61–72.
22. L. Lu and X. Peng, Spectra of edge-independent random graphs, *Electronic Journal of Combinatorics*, 20 (4), (2013) P27.
23. M.A. de Reus and M.P. van den Heuvel, Rich club organization and intermodule communication in the cat connectome, *The Journal of Neuroscience*, 33.32 (2013): 12929-12939.
24. I. Stakgold and M.J. Holst, *Green’s Functions and Boundary Value Problems*, John Wiley & Sons, 2011.
25. Open Connectome Project, Web. 25 June 2014, [http://www.openconnectomeproject.org](http://www.openconnectomeproject.org).