A Note on Diffusion State Distance

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Abstract

Diffusion state distance (DSD) is a metric on the vertices of a graph, motivated by bioinformatic modeling. Previous results on the convergence of DSD to a limiting metric relied on the definition being based on symmetric or reversible random walk on the graph. We show that convergence holds even when the DSD is based on general finite irreducible Markov chains. The proofs rely on classical potential theory of Kemeny and Snell.

1 Introduction and Main Results

In 2013, Cao et al. [2] defined a metric (or rather, a sequence of metrics) on the set of vertices of a finite undirected graph, motivated by functionality considerations in protein interaction networks. In this class of metrics, called “diffusion state distance” (DSD), [2] considered a random walk on the vertices of the graph, and assessed the closeness of two states $u$ and $v$ by comparing the expected number of visits to all states (within a given time horizon) when the initial state is $u$ and when the initial state is $v$. (See below for the mathematical details.) The following year, Cao et al. [3] extended the metric to graphs with weighted edges (representing confidence in the presence of the edge), which leads to consideration of Markov chains instead of random walks. The paper [3] also permitted directed edges. Further generalizations were considered in [1], in particular to bipartite graphs (which lead to periodic random walks).

To proceed, we now describe a general framework for random walks and Markov chains on graphs. Let $V$ be a (finite) set of points, representing the vertices or nodes of our network. For each (ordered) pair of vertices $i$ and $j$, let $\beta_{ij}$ be a nonnegative number associated with the directed edge from $i$ to $j$. (In [3], the magnitude of $\beta_{ij}$ corresponds to the degree of certainty that this edge is present. If there is certainly no edge from $i$ to $j$, then $\beta_{ij}$ is zero.) We consider the Markov chain on $V$ with the property that when the chain is at a node $i$, it
chooses its next node with probability proportional to the weights on the edges leading out of $i$. That is, the one-step transition probabilities for the Markov chain are

$$p_{ij} = \frac{\beta_{ij}}{\sum_{k \in V} \beta_{ik}} \quad \text{for } i, j \in V.$$  

(1)

(We assume that there is no $i$ for which the denominator in Equation (1) is 0.) The case of a classical random walk on a directed graph (with no weights) is obtained by requiring each $\beta_{ij}$ to equal 0 or 1, according to whether or not there is an edge from $i$ to $j$. The case of a weighted undirected graph is obtained by requiring $\beta_{ij} = \beta_{ji}$ for every $i$ and $j$ in $V$; this is the case assumed by Chung and Yao [4], which in turn was built upon by [1].

Note that the form of Equation (1) is completely general, since the transition probabilities $p_{ij}$ of any given Markov chain satisfy (1) if we let $\beta_{ij}$ be $p_{ij}$ for every $i$ and $j$ (since $\sum_k p_{ik} = 1$ in any Markov chain).

We shall denote the set of states of the Markov chain by $V = \{1, \ldots, n\}$. We shall write $P$ for the (one-step) transition probability matrix with entries $p_{ij}$. For $l = 0, 1, 2, \ldots$, we write $p_{ij}^{(l)}$ for the $l$-step transition probabilities, which are the entries of the matrix $P^l$. We say that the Markov chain (or $P$) is irreducible if it is possible to get from every state to every other state; that is, for every pair of states $i$ and $j$, there is an $l \geq 0$ such that $p_{ij}^{(l)} > 0$. We say that an irreducible Markov chain (or $P$) is periodic if there is an integer $d \geq 2$ such that $p_{11}^{(l)} = 0$ whenever $l$ is not a multiple of $d$; in this case $d$ is called the period. We say that the chain is aperiodic if it is not periodic.

Throughout this paper, except for the generalizations discussed in Section 3, we shall assume that $P$ is the transition probability matrix of a finite irreducible Markov chain.

1.1 The Aperiodic Case

In this section, we shall assume that $P$ is aperiodic as well as finite and irreducible.

Let $\pi$ be the equilibrium distribution of $P$, i.e. the row vector $(\pi_1, \ldots, \pi_n)$ such that $\pi P = \pi$ and $\sum \pi_i = 1$. (This is written $\pi^T$ in [2] and $\alpha$ in [6].) Under our assumptions, $\pi$ exists and is unique. Moreover, the limit matrix

$$W := \lim_{k \to \infty} P^k$$  

exists, and $W_{ij} = \pi_j$ for all states $i$ and $j$. (This is called $W$ in [2], and $A$ in [6] and [6].) Writing $\mathbf{1}$ to denote the column vector with all entries equal to 1, we have $W = \mathbf{1} \pi$.

For states $u$ and $v$ and any integer $k \geq 0$, we follow [2] and define

$$H^{(k)}(u, v) = \sum_{l=0}^{k} p_{uv}^{(l)}.$$
Thus $He^{(k)}(u, v)$ is the expected number of visits to $v$ within the first $k$ steps of the chain, given that the chain starts at $u$. (This is called $N_{uv}^{(k)}$ in [6], and $M_u[Y_v^{(k+1)}]$ in [5].)

**Proposition 1** For an aperiodic finite irreducible Markov chain:

(a) The matrix $Z$ defined by

$$Z = \sum_{k=0}^{\infty} (P - W)^k$$

exists and equals $(I - P + W)^{-1}$. (Note: [2] writes $D$ for $P - W$).

(b) For all states $u$, $v$, and $w$, we have

$$\lim_{k \to \infty} He^{(k)}(u, w) - He^{(k)}(v, w)$$

exists and equals $Z_{uw} - Z_{vw}$.

**Remark 2** Part (b) agrees with Lemma 3 of [2], since $Z_{uw} - Z_{vw} = (b_i^T - b_i^v)Z b_w$ (where $b_i$ is the column vector having $i$th entry equal to 1 and all other entries equal to 0.)

We now define the diffusion state distance metrics. For states $u$ and $v$ and integers $k \geq 0$, let

$$DSD^{(k)}(u, v) = \sum_{w=1}^{n} |He^{(k)}(u, w) - He^{(k)}(v, w)|.$$

(3)

Lemma 1 of [2] shows that $DSD^{(k)}$ is a metric for aperiodic irreducible random walks; see Section 3 below for discussion and generalization. We also write

$$DSD^{(\infty)}(u, v) = \lim_{k \to \infty} DSD^{(k)}(u, v)$$

(4)

if this limit exists.

**Corollary 3** Consider an aperiodic finite irreducible Markov chain. Then the limit [7] exists, and

$$DSD^{(\infty)}(u, v) = \sum_{w} |Z_{uw} - Z_{vw}|.$$

(5)

Moreover, $DSD^{(\infty)}$ is a metric.

Corollary 3 was proven in [2] for undirected unweighted graphs ($\beta_{ij} = \beta_{ji} \in \{0, 1\}$), and in [1] for graphs with symmetric weights ($\beta_{ij} = \beta_{ji}$). (Observe that the Green’s function matrix $G$ in [1] is precisely our $Z$.) Both proofs rely on the diagonalization of the matrix $P$, which holds because the symmetry of weights implies that $P$ can be expressed as a self-adjoint operator (equivalently, that
the Markov chain is reversible). In contrast, the proofs in the present paper rely on the classical potential theory for general finite (and countable) Markov chains in [5] and/or [6].

We remark that [1] also considers the \( DSD^k \) metric for \( q \geq 1 \), defined by replacing the \( l_1 \) norm on the right hand side of Equation (3) by the \( l_q \) norm, i.e.

\[
DSD^k_q(u, v) = \left( \sum_{w=1}^{n} |He^k(u, w) - He^k(v, w)|^q \right)^{1/q}.
\]

The extension of Corollary 3 and Equation (4) to \( DSD^k \) is immediate.

### 1.2 The Periodic Case

In this section, we shall consider the case that \( P \) is periodic as well as finite and irreducible. An important example is the case of a random walk on a bipartite graph. This example was considered in [1].

As explained in Chapter 5.1 of [5], the relevant theory for aperiodic Markov chains extends to the periodic case with some modifications. There is a unique equilibrium probability distribution \( \pi \) such that \( \pi P = \pi \). We still define the matrix \( W \) by \( W_{ij} = \pi_j \). However, the limit of Equation (2) does not exist in the usual sense, but the equation is correct for the Cesaro limit. Moreover, the matrix \( I - P + W \) is invertible, and Proposition 1(a) holds if we interpret the infinite sum defining \( Z \) to be the Cesaro sum.

For now, consider the general case that \( P \) is finite and irreducible (not necessarily periodic). For 0 \( \leq \alpha < 1 \), let \( P_\alpha = \alpha I + (1 - \alpha)P \) be the “lazy Markov chain”, which moves according to \( P \) except that with probability \( \alpha \) it decides to stay wherever it is for one time unit. Observe that \( \pi = \pi P_\alpha \), so the equilibrium distribution is independent of \( \alpha \), as is the matrix \( W \). Let \( Z_\alpha = (I - P_\alpha + W)^{-1} \).

Since this is well-defined, we can use Equation (5) as our definition of \( DSD^{(\infty)} \) for our periodic chain \( P \), even though the limit of Proposition 1 may not exist except in the Cesaro sense. The following result shows that this definition is consistent with the usual definition. Observe that if 0 \( < \alpha < 1 \), then \( P_\alpha \) is aperiodic (and irreducible), and so the results of Section 1.1 apply.

**Proposition 4** Assume that \( P \) is finite and irreducible.

(a) For every \( \alpha \in [0, 1) \), we have \( Z_\alpha = (1 - \alpha)^{-1}(Z_0 - \alpha W) \).

(b) Let \( DSD^{(\infty;\alpha)} \) be the \( DSD^{(\infty)} \) metric of the Markov chain \( P_\alpha \). Then for all states \( u \) and \( v \),

\[
DSD^{(\infty;\alpha)}(u, v) = (1 - \alpha)^{-1}DSD^{(\infty;0)}(u, v).
\]

In particular, part (b) generalizes Theorem 1 of [1] to general Markov chains. It shows that for periodic chains, the formal definition of Equation (5) is consistent by continuity with the (more directly motivated) definition (4) for aperiodic chains, i.e.

\[
\lim_{\alpha \to 0} DSD^{(\infty;\alpha)}(u, v) = DSD^{(\infty;0)}(u, v) \quad \text{for all } u, v.
\]
2 Proofs of Results

Proof of Proposition 1 (a) This is direct from Propositions 9-75 and 9-76(4) of [6], or Theorem 4.3.1 of [5].

(b) This follows from Corollary 4.3.5 of [5]. Alternatively, here is a proof using the theory for denumerable chains (see discussion at the beginning of Section 3 below). Definition 9-24 of [6] defines the matrix $C$ by

$$C_{ij} = \lim_{k \to \infty} (N^{(k)}_{jj} - N^{(k)}_{ij}) = \lim_{k \to \infty} (He^{(k)}(j, j) - He^{(k)}(i, j))$$

whenever this limit exists. Proposition 9-77 of [6] shows that $C$ exists for aperiodic finite irreducible chains and that

$$C_{ij} = Z_{jj} - Z_{ij}.$$ 

It follows that

$$\lim_{k \to \infty} He^{(k)}(u, w) - He^{(k)}(v, w) = C_{vw} - C_{uw} = (Z_{ww} - Z_{uw}) - (Z_{ww} - Z_{uw}) = Z_{uw} - Z_{vw}.$$ 

□

Proof of Corollary 3 The second sentence of the corollary follows immediately from Proposition 1. To show the final sentence, observe that Equation (5) says that $DSD^{(\infty)}(u, v)$ is the $l_1$ distance between rows $u$ and $v$ of the matrix $Z$. Since $Z$ is invertible (by Proposition 1(a)), it must have distinct rows. It follows immediately that $DSD^{(\infty)}$ is a metric. □

Proof of Proposition 4 By Theorem 5.1.3 of [5], we have $Z\hat{I} = \hat{I}$ and $\pi Z = \pi$, where $Z$ denotes either $Z_{\alpha}$ or $Z_0$. Therefore

$$ZW = Z\hat{I}\pi = \hat{I}\pi = W \quad \text{and} \quad (6)$$

$$WZ = \hat{I}\pi Z = \hat{I}\pi = W. \quad (7)$$

Therefore we have

$$I = Z_{\alpha}(I - P_{\alpha} + W) = Z_{\alpha} ((1 - \alpha)(I - P + W) + \alpha W) = (1 - \alpha)Z_{\alpha}Z_0^{-1} + \alpha Z_{\alpha}W \quad \text{by Eq. (6)},$$

which yields

$$Z_0 = (1 - \alpha)Z_{\alpha} + \alpha WZ_0 = (1 - \alpha)Z_{\alpha} + \alpha W \quad \text{by Eq. (7)}.$$

1To explain the notation of [6] in this proposition: $E$ is the matrix of all 1’s, and $Z_{dg}$ is the diagonal matrix obtained from $Z$ by making all off-diagonal entries 0.
Part (a) follows immediately.

Next, recall the observation and notation of Remark 2 above. By this and Equation (5), we see that part (b) will follow if we can prove that \( \gamma Z_\alpha = (1 - \alpha)^{-1} \gamma Z_0 \), where \( \gamma = b_y^T - b_e^T \). But this is a direct consequence of part (a) and the fact that \( \gamma W = \gamma 1 \pi = 0 \). □

3 Some Generalizations

Since much of the potential theory for finite Markov chains in [5] also extends to countable chains [6], it is of theoretical interest to consider whether DSD theory extends to chains with countably many states. Our proof of Proposition 1 using results of [6] shows that this proposition extends to Markov chains that are strong ergodic (i.e., chains that are positive recurrent and have the property that for all states \( i \) and \( j \), the expected square of the time to reach \( j \) when starting from \( i \) is finite); in [6], see Section 9.5, p. 274, as well as Definition 9-71. However it is less clear whether Corollary 3 holds in this case, since even the convergence of the infinite sum is not obvious.

Finally, we show that \( DSD^{(k)} \) is a metric for every finite or countable Markov chain except for some very special cases. For one counterexample, consider the irreducible Markov chain with states \( V = \{1, 2, 3, 4\} \) such that \( p_{12} = p_{13} = 0.5 \), \( p_{24} = p_{34} = p_{41} = 1 \), and \( p_{ij} = 0 \) otherwise. It is not hard to check that \( H_{e^{(2)}}(1, i) = H_{e^{(2)}}(4, i) \) for every \( i \), and so \( DSD^{(2)} \) is not a metric. Note that this chain has period 3. The next result shows that all counterexamples have features in common with this example.

**Proposition 5** Let \( P \) be the matrix of a (finite or countable) Markov chain, and let \( k \) be a finite nonnegative integer. Assume that there do not exist two distinct states \( i \) and \( j \) such that \( p_{ii}^{(k+1)} = p_{jj}^{(k+1)} = 1 \) and \( p_{ij}^{(t)} > 0 \) for some \( t \). Then \( DSD^{(k)} \) is a metric.

In particular, if \( P \) is aperiodic or if the period of \( P \) does not divide \( k + 1 \), then \( DSD^{(k)} \) is a metric. But the condition \( p_{ii}^{(k+1)} = 1 \) is much more restrictive than requiring the period to divide \( k + 1 \). Also note that Proposition 5 does not assume that \( P \) is irreducible.

The following proof is essentially a streamlined generalization of the proof of Lemma 1 in [2].

**Proof of Proposition 5** Write \( N^{(t)} = 1 + P + \cdots + P^t \) for \( t = 0, 1, \ldots \). Since \( DSD^{(k)}(u, v) \) is the the \( l_1 \) distance between rows \( u \) and \( v \) of the (possibly infinite) matrix \( N^{(k)} \), it suffices to show that all rows of \( N^{(k)} \) are distinct.

Assume that \( u \) and \( v \) are distinct states such that rows \( u \) and \( v \) of \( N^{(k)} \) are the same. For vectors \( b \) as defined in Remark 2, let \( \gamma = b_y^T - b_e^T \). Then \( \gamma N^{(k)} = 0 \). Hence \( \gamma N^{(k)} P = 0 \). From the definition, we have \( N^{(k)} P + I = N^{(k)} + P^{k+1} \), and hence it follows that

\[
\gamma = \gamma P^{k+1}.
\]
Multiplying this equation on the right by $b_u$ gives the equation $1 = (P^{k+1})_{uu} - (P^{k+1})_{vu}$. This can only happen if $(P^{k+1})_{uu} - (P^{k+1})_{vu} = 1$. Similarly, we deduce $(P^{k+1})_{vv} = 1$. Finally, since $N_{uu}^{(k)} = N_{vv}^{(k)}$ and $N_{uv}^{(k)} \geq I_{uv} = 1$, there must be a $t \leq k$ such that $(P^t)_{uv} > 0$. This contradicts the hypothesis of the proposition, and thus the proof is complete. □

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