Alignment and Comparison of Directed Networks via Transition Couplings of Random Walks

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Abstract

We describe and study a transport based procedure called NetOTC (network optimal transition coupling) for the comparison and alignment of two networks. The networks of interest may be directed or undirected, weighted or unweighted, and may have distinct vertex sets of different sizes. Given two networks and a cost function relating their vertices, NetOTC finds a transition coupling of their associated random walks having minimum expected cost. The minimizing cost quantifies the difference between the networks, while the optimal transport plan itself provides alignments of both the vertices and the edges of the two networks. Coupling of the full random walks, rather than their marginal distributions, ensures that NetOTC captures local and global information about the networks, and preserves edges. NetOTC has no free parameters, and does not rely on randomization. We investigate a number of theoretical properties of NetOTC and present experiments establishing its empirical performance.

Keywords: graph alignment, graph comparison, graph factor, optimal transport

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1 Introduction

Networks have long been used as a means of representing and studying the pairwise interactions between a set of individuals or objects under study. More recently, networks themselves have become objects of study, including exploratory analysis and statistical modeling. When an application of interest involves multiple networks, analysis often begins with the problem of network alignment or comparison, tasks that have been studied in a number of fields. Network alignment compares and finds correspondences among nodes or edges within multiple networks. The aim is to recognize similar substructures, unveiling hidden relationships and functional similarities that exist within different networks. In the simplest version of the network alignment problem, one is given two networks with vertex sets of equal size and seeks to find a bijection between the vertex sets that maximizes the number of aligned edges. Numerous approaches to network alignment have been considered in the literature, e.g. [Kelley et al. (2003); Kuchaiev et al. (2010); Kuchaiev and Przulj (2011); Kalaev et al. (2008); Klau (2009)]. By contrast, the goal of network comparison is more general: given two networks of different size or structure, identify and quantify similarities between them in a rigorous manner. Perhaps the simplest form of comparison is a numerical measure of similarity between networks, which one might hope to have the properties of a metric. Potentially more informative measures of comparison include soft alignment of vertices and edges in the two networks.

Network alignment and comparison arise in a number of disciplines where network models are common. In biology, networks have been used to represent protein-protein interactions and gene regulatory systems. Network alignment has been used to identify interaction structures and topological similarities, facilitating the transfer of biological insights from familiar to unexplored species [Singh et al. (2008); Elmsallati et al. (2016); Ma and Liao (2020)]. In connectomics and neuroimaging, networks are used to model connectivity and interactions of different brain regions. Network alignment and comparison methods have been used to compare the connectomes of healthy and diseased individuals [Zalesky et al. (2010); Milano et al. (2017)] as an initial step in identifying potential indicators of disease, understanding disease origins, and identifying specific locations within the brain that could influence the progression or onset of the disease. Beyond biology and neuroscience, network comparison methods have found applications in economics [Paglione et al. (2010); Engel et al. (2021)], where they have been used to compare trade networks over time, and to identify shifts and trends in economic dynamics. In social science, comparisons of social networks have offered insights into the relationships and interactions between different groups [Jackson et al. (2014); Mislove et al. (2007)].

In this paper, we propose and analyze NetOTC, a procedure for the comparison and soft alignment of two networks. The networks of interest may be directed or undirected, weighted or unweighted, and may have distinct vertex sets of different sizes. NetOTC, which is short for network optimal transition coupling, is based on applying a process-level optimal transport method to the random walks arising from each network. In more detail, the NetOTC procedure takes as input two connected networks $G_1$ and $G_2$ with non-negative edge weights, which may be directed or undirected, and a cost function relating their vertices. Each network gives rise to a stationary random walk on its vertex set whose transition probabilities are determined by normalizing the edge weights at each node. NetOTC proceeds by finding a joint chain on the product of the vertex sets of $G_1$ and $G_2$ that has the following properties: the joint chain is stationary and Markov; the joint chain minimizes the expected value of the cost function at any fixed time point; and the transition distribution from each state $(u, v)$ in the joint chain is obtained by coupling the transition distribution of $u$ in $G_1$ with the transition distribution of $v$ in $G_2$. The latter condition, which gives rise to transition couplings, ensures that the joint chain is a coupling of the initial chains on the individual graphs. More information about process couplings and transition couplings can be found in Section 3.

We note that minimization of the expected cost subject to the constraints given above is carried out analytically, and not through Monte Carlo methods.

As described above, the optimal transport plan arising from NetOTC is a stationary random walk on the product of the given networks that favors low cost pairs of vertices, while maintaining the marginal structure of the random walks on each individual network. The cost function used in NetOTC is specified by the user, and will, in general, be application dependent. Cost functions can be based, for example, on the difference between externally specified vertex attributes, the distance between Euclidean embeddings of the vertices, or the difference between the degrees of the vertices. If the given networks have the same vertex set, a cost function based on vertex identity may be used as well.

The NetOTC procedure has a number of desirable methodological and theoretical properties. On the methodological side, NetOTC applies to directed and undirected networks, and readily handles networks with different sizes and connectivity structures. NetOTC has no free parameters and does not make use of randomization or Monte Carlo techniques. As NetOTC considers process-level couplings of random walks, the optimal transport plan captures global information reflected in the stationary distributions of the random walks, as well as local information that is present in the transition probabilities between vertices. The expected cost of the optimal transport plan provides a numerical measure of the difference between the networks. The distribution of the optimal transport plan
plan at a single time point yields a soft, probabilistic alignment of the vertices in the given networks. Moreover, the distribution of the optimal transport plan at two successive time points yields a soft, probabilistic alignment of the edges of the given networks. To the best of our knowledge, native alignment of edges is unique to NetOTC among existing alignment and comparison methods. Once the vertex cost function has been specified, the exact version of the NetOTC procedure has no free parameters and does not make use of randomization.

On the theoretical side, we establish several key properties of the NetOTC procedure that support its use in comparison and alignment tasks. The edge alignment of NetOTC respects edges, in the sense that vertex pairs in the given networks are aligned with positive probability only if each pair is connected by an edge in its respective network. Although the NetOTC optimal transport plan minimizes the expected cost between vertices at time zero, stationarity ensures that the same is true at any other fixed time, and that the coupled random walk has a low average cost between vertices across time. The NetOTC similarity measure is sensitive to differences in the $k$-step behavior of the random walks on $G_1$ and $G_2$ if these differences affect the cumulative cost. For undirected networks with a common vertex set, the NetOTC similarity is a metric on equivalence classes of networks having identical random walks if the cost $c$ is a metric. For the zero-one cost, the NetOTC similarity is lower bounded by the $\ell_1$-difference of the network degree sequences, and the $\ell_1$-difference of the network weight functions.

In addition, we study the structure of the NetOTC method through network factors. Our definition of factor, which arises naturally when considering functions of Markov chains, differs from other definitions in the network theory literature. Informally, a network $G_2$ is a factor of a network $G_1$ if the vertices of $G_2$ can be associated, via a vertex map $f$, with disjoint sets of vertices in $G_1$ between which aggregate weights can be consistently defined. We show that if $G_2$ is a factor of $G_1$, then the vertex map $f$ yields a deterministic transition coupling of their associated random walks. Under suitable compatibility conditions on the cost function, this coupling will be optimal and will provide a solution to the NetOTC problem. The resulting expected cost, vertex alignment, and edge alignment are fully determined by the structure of $G_1$ and the map $f$. Importantly, the existence and precise nature of the map $f$ need not be known to the NetOTC procedure. These results extend to paired factors: an optimal transition coupling for a pair of networks can be mapped in a deterministic fashion to an optimal transition coupling of their factors when the cost functions for each pair are compatible with the factor maps.

As a complement to the theory, we carry out a number of simulations and numerical experiments to assess the performance of NetOTC and compare it with other optimal transport-based comparison methods in the literature. NetOTC is competitive with other methods on a number of network classification tasks. In an extensive experiment on pairs of isomorphic networks with small to moderate sizes, NetOTC was consistently able to recover the isomorphism using a local (degree-based) cost function, substantially outperforming other methods. When applied to stochastic block models (with equivalent blocks of different sizes) using a degree-based cost function, NetOTC was competitive with other methods in its ability to align vertices in equivalent blocks, and substantially better at aligning edges. We also considered the problem of comparing a network to an exact or approximate factor using a distance-based cost derived from Euclidean vertex embeddings of the given networks. NetOTC outperforms other methods in its ability to align vertices in the parent and factor networks. While the performance gap is modest for exact factors, it increases as one considers approximate factors.

1.1 Outline of the Paper

The next section gives an overview of existing work on optimal transport and related approaches to network comparison and alignment. Section 2 provides background concerning random walks on directed networks, optimal transport for Markov chains, and transition couplings. The NetOTC procedure is described in Section 3, including computation, the optimal transport cost, and vertex and edge alignment. Section 4 is devoted to the formal statement and discussion of the theoretical properties of NetOTC. Proofs are given in Section 5. Section 6 contains a number of simulations and a number of experiments that demonstrate the flexibility and potential utility of NetOTC. Additional details concerning the experiments are given in Appendix A.

2 Related Work

The problems of network alignment and comparison have received a lot of recent attention in the literature. Approaches using optimal transport ideas can be divided into several groups: spectral methods, variants of Gromov-Wasserstein, and methods involving random walks and Markov chains. Other approaches make use of quadratic programming and continuous approximations. This related work is discussed below.

Spectral Methods. One line of work [Dong and Sawin 2020; Maretic et al. 2019, 2020] uses techniques from spectral graph theory to define optimal transport (OT) problems for networks. In particular, this approach associates
to each network a multivariate Gaussian with zero mean and covariance matrix equal to the pseudo-inverse of the graph Laplacian. The Wasserstein distance between Gaussian distributions of the same dimension may be computed analytically in terms of their respective covariance matrices. For networks with different numbers of vertices, [Maretic et al., 2020] and [Dong and Sawin, 2020] propose to optimize this distance over soft many-to-one assignments between vertices in either network. At present, this family of approaches is unable to incorporate available feature information or underlying cost functions, relying only on their intrinsic structure.

**Variants of Gromov-Wasserstein.** Another line of work [Mémoli, 2011; Peyré et al., 2016; Titouan et al., 2019; Vayer et al., 2019; 2020] considers the Gromov-Wasserstein (GW) distance and related extensions. In this work, one tries to couple distributions on the vertices in each network so as to minimize an expected transport cost between vertices while minimizing changes in edges between the two networks. This approach allows one to capture differences in both features and structure between networks. We refer the reader to [Dong and Sawin, 2020] for a discussion on the differences between spectral-based network OT methods and GW distances. A number of variants of the GW distance have been proposed for a variety of tasks including cross-domain alignment (Chen et al., 2020), graph partitioning (Xu et al., 2019a), graph matching (Xu et al., 2019a,b), and node embedding (Xu et al., 2019b). The work [Barbe et al., 2020] proposes to incorporate global structure into the Wasserstein and Fused GW (FGW) distances by applying heat diffusion to the vertex features before computing the cost matrix.

**Methods involving random walks and Markov chains.** It is well-known that a weighted network $G$ with non-negative edge weights can be viewed as a Markov chain $X = \{X_k\}_{k=1}^{\infty}$, and there is previous work that uses this perspective to align or compare networks. The paper [Vishwanathan et al., 2010] studies a flexible family of kernels for comparing two given networks. Given networks $G$ and $H$ with associated transition matrices $P$ and $Q$ the kernels take the form $\kappa(G, H) = \sum_{k \geq 1} \mu_k q^k (P \otimes Q)^k p$, where $p$ and $q$ are starting and stopping distributions, $\mu_k$ are non-negative weights, and $(P \otimes Q)^k$ is the $k$-step transition matrix of the independent coupling of the random walks on $G$ and $H$. The free parameters $p, q, \{\mu_k\}$ are user specified; appropriate choices allow for efficient computation. The kernels $\kappa(G, H)$ are distinct from NetOTC, as they employ only independent couplings, and do not involve the use of optimal transport.

Several recent papers [Chen et al., 2022; 2023] have studied a Markov chain-based distance function for networks that has close connections to the classical Weisfeiler-Lehman (WL) test for graph isomorphism. Given two weighted networks $G$ and $H$ and a fixed time $k \geq 1$, the $k$-step WL-distance $d_{WL}^k(G, H)$ is equal to the minimum expected cost $\min \mathbb{E} c(\tilde{X}_k, \tilde{Y}_k)$ at time $k$, where the minimum is taken over all (possibly time-inhomogeneous) Markovian couplings of $X$ and $Y$. The transition couplings used in the present work have the additional requirement that they must be time-homogeneous and stationary (see Section 3.3. The family $\{d_{WL}^k : k \geq 1\}$ is further investigated in [Brugere et al., 2023], where it is shown (in Proposition 23) that

$$d_{WL}^k(G, H) := \lim_{k \to \infty} d_{WL}^k(G, H) = \sup_k d_{WL}(G, H).$$

Moreover, it is shown in Proposition 5 of [Brugere et al., 2023] that

$$d_{WL}^\infty(G, H) \leq d^\infty_{OTC}(G, H),$$

where $d^\infty_{OTC}$ is the NetOTC distance studied in this paper. Using (1) and (2) one may verify that the $k$-step WL-distance is not in general equal to $d^\infty_{OTC}$. Furthermore, (2) ensures that the NetOTC distance has at least as much discriminatory power as the WL-test in the graph isomorphism detection problem. We refer the reader to [Brugere et al., 2023] for more details.

Lastly, let us mention that there is a constrained optimal transport method called Causal Optimal Transport (COT) that has been used in finance and machine learning [Lassalle, 2013]. By Lemma 3.11 in [Chen et al., 2023], any Markovian coupling is also a bi-causal coupling, and therefore the transition couplings considered in this paper are also bi-causal. However, Theorem 3.12 from [Chen et al., 2023] states that the $k$-step WL distance is equal to the bi-causal transport distance in which the given cost function is evaluated at time $k$. Thus, the relationship between the OTC distance and COT is the same as the relationship between OTC and the WL-distances: they are distinct notions, with $d^\infty_{OTC}$ greater than or equal to bi-causal transport distance at any fixed time.

**Other Methods for Network Alignment and Comparison.** There is also a large body of work devoted to network alignment and comparison that does not use optimal transport methods. The network alignment problem can be generally defined as a quadratic programming problem under discrete and doubly stochastic constraints [Yan et al., 2016; Jiang et al., 2017; Loiola et al., 2007; Cho et al., 2010; Cour et al., 2007]. However, as the optimal network alignment problem is well known to be an NP-hard problem [Garey and Johnson, 1990], it is
computationally challenging to obtain an optimal alignment for networks. For this reason, many authors have proposed approximate solutions for network alignment (Cho et al., 2010; Zhou and De la Torre, 2016; Yu et al., 2018; Enqvist et al., 2009; van Wyk and van Wyk, 2004; Zaslavskiy et al., 2009). Among these approximate methods, most of the successful algorithms start with relaxing the discrete constraints to create a continuous condition. Several authors (Schellewald and Schnörr, 2005; Torr, 2003) relax the discrete conditions to form a positive semi-definite problem. A non-convex quadratic programming problem was adopted in Gold and Rangarajan (1996); Cho et al. (2010); Zhou and De la Torre (2016). In another direction, Leordeanu and Hebert (2005) introduces spectral matching as a simple relaxation, and Cour et al. (2007) strengthens this approach by giving an affine constraint. Also, Jiang et al. (2017) proposes an algorithm that can efficiently solve a general quadratic programming problem with doubly stochastic constraints. Each step of the algorithm is easy to implement and the convergence is guaranteed. Generally, after finding the optimal solution for the relaxed continuous problem, the discrete alignment is attained through a final discretization process (Cho et al., 2010; Leordeanu and Hebert, 2005; Leordeanu et al., 2009). We note that these approaches may find a solution that is locally optimal but not globally optimal.

Another line of research is devoted to the statistical and probabilistic analysis of graph matching when the given graphs are generated at random but are correlated with one another, e.g., each is a random perturbation of a given graph (Ding et al., 2020; Barak et al., 2019; Cullina et al., 2020; Cullina and Kiyavashi, 2017; Feizi et al., 2020; Korula and Lattanzi, 2014; Lyzinski et al., 2014; Yartseva and Grossglauser, 2013). Much of this work investigates various matching procedures under specific random graph models, such as correlated Erdos-Renyi graphs, and is concerned with the information-theoretic threshold for exact recovery, and the time complexity of the matching procedures.

3 Transition Couplings of Random Walks on Networks

This section provides background for the detailed description of the NetOTC procedure. We begin by recalling how a weighted network gives rise to a random walk on its vertex set and reviewing the definition and framework of optimal transport. We then consider transition couplings of random walks, which preserve stationarity and the Markov property. The computation of optimal transition couplings is the basis for the NetOTC procedure, which is described in Section 4 below.

3.1 Random Walks on Directed Networks

Let $G = (U, E, w)$ denote a network with finite vertex set $U$, edge set $E \subseteq U \times U$, and non-negative weight function $w : U \times U \rightarrow \mathbb{R}_+$. An ordered pair $(u, u') \in E$ represents a directed edge from $u$ to $u'$ with weight $w(u, u')$. We assume in what follows that $w(u, u') > 0$ if and only if $(u, u') \in E$. For any vertex $u \in U$, we let $d(u) = \sum_{u' \in U} w(u, u')$ be the weighted out-degree of $u$. An undirected network is represented by a directed network in which $w(u, u') = w(u', u)$ for each $u, u' \in U$. A path in $G$ is an ordered sequence of vertices $u_0, \ldots, u_n \in U$ such that $(u_{i-1}, u_i) \in E$ for each $i = 1, \ldots, n$. A network $G$ is strongly connected if for each ordered pair $(u, v) \in U \times U$ there exists a path $u_0, \ldots, u_n$ in $G$ such that $u_0 = u$ and $u_n = v$. In this case $d(u) > 0$ for each vertex $u \in U$.

To any network $G = (U, E, w)$, one may associate a Markov transition kernel $P(\cdot \mid \cdot)$ with state space $U$ as follows: for each pair of vertices $u$ and $u'$, the probability of transitioning from $u$ to $u'$ is

$$P(u' \mid u) = \frac{w(u, u')}{d(u)}.$$  \hspace{1cm} (3)

Recall that a probability distribution $p$ on $U$ is said to be stationary for $P(\cdot \mid \cdot)$ if $p(u') = \sum_{u \in U} P(u) P(u' \mid u)$ for all $u' \in U$. It follows from the Perron-Frobenius theorem that the transition kernel $P(\cdot \mid \cdot)$ admits at least one stationary distribution $p$. Together, $P$ and $p$ define a stationary Markov chain $X = X_0, X_1, X_2, \cdots \in U$ such that for any $u_0, \ldots, u_n$ in $U$

$$P(X_0 = u_0, \ldots, X_n = u_n) = p(u_0) \prod_{i=0}^{n-1} P(u_{i+1} \mid u_i).$$

The Markov chain $X$ is commonly referred to as a random walk on $G$. When $G$ is strongly connected, the kernel $P(\cdot \mid \cdot)$ admits a unique stationary distribution, and we refer to $X$ as the random walk on $G$. Random walks on networks have been studied extensively in the probability literature, and have found numerous applications in fields ranging from genomics to computer science, including recent work on network embedding (Hamilton, 2020).
Optimal Transport

Let $X$ and $Y$ be random objects taking values in sets $\mathcal{X}$ and $\mathcal{Y}$, respectively. In what follows we are primarily interested in the case that $X$ and $Y$ are processes. A coupling of $X$ and $Y$ is a jointly distributed pair $(\tilde{X}, \tilde{Y})$ of random objects taking values in $\mathcal{X} \times \mathcal{Y}$ with the property that $\tilde{X} \equiv X$ and $\tilde{Y} \equiv Y$. Here $\tilde{X}$ and $\tilde{Y}$ arise from the fact that $X$ and $Y$ are understood and specified through their individual distributions, whereas $\tilde{X}$ and $\tilde{Y}$ are understood and specified as a jointly distributed pair. (In general, $X$ and $Y$ may be defined on different probability spaces, whereas $\tilde{X}$ and $\tilde{Y}$ are necessarily defined on the same probability space.) Couplings have been widely studied in the probability literature, and are the basic objects of interest in optimal transport.

A minimizer of the optimal transport problem is called an optimal coupling of $X, Y$. Let $\Pi(X, Y)$ denote the set of all couplings $(\tilde{X}, \tilde{Y})$ of $X$ and $Y$. Note that $\Pi(X, Y)$ is not empty, as it always contains the independent coupling $(\tilde{X}, \tilde{Y})$ in which $\tilde{X}$ and $\tilde{Y}$ are independent copies of $X$ and $Y$, respectively. Each coupling $(\tilde{X}, \tilde{Y}) \in \Pi(X, Y)$ is associated with a joint distribution $\pi$ on $(\mathcal{X} \times \mathcal{Y}, \mathcal{A} \times \mathcal{B})$ that can be viewed conditionally as a plan for transporting the distribution of $X$ to that of $Y$ and vice versa. Let $c : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}_+$ be a measurable, non-negative cost function relating the elements of $\mathcal{X}$ and $\mathcal{Y}$. The optimal transport problem is to minimize the expected value of the cost function over all couplings of $X$, $Y$, namely

$$\text{minimize } \mathbb{E}c(\tilde{X}, \tilde{Y}) \text{ over } (\tilde{X}, \tilde{Y}) \in \Pi(X, Y).$$

A minimizer of the optimal transport problem is called an optimal coupling of $X$, $Y$, or an optimal transport plan. The theory and applications of optimal transport are active areas of research. See [Peyré and Cuturi, 2019; Villani, 2008] for further reading and more details.

Transition Couplings

Let $G_1 = (U, E_1, w_1)$ and $G_2 = (V, E_2, w_2)$ be weighted directed networks, and let $c : U \times V \to \mathbb{R}_+$ be a cost function relating their vertex sets. As described above, the network $G_1$ is associated with a random walk $X = X_0, X_1, \ldots$ on the vertex set $U$. We may regard the process $X$ as a random element of the set $\mathcal{X} = U^\mathbb{N}$ equipped with the Borel sigma-field arising from the usual product topology on $U^\mathbb{N}$. Similarly, the network $G_2$ is associated with a random walk $Y = Y_0, Y_1, \ldots$ taking values in $\mathcal{Y} = V^\mathbb{N}$. A coupling of the processes $X$ and $Y$ is a joint process $(\tilde{X}, \tilde{Y}) = (\tilde{X}_0, \tilde{Y}_0), (\tilde{X}_1, \tilde{Y}_1), (\tilde{X}_2, \tilde{Y}_2), \ldots$ with values in $U \times V$ such that $\tilde{X} = \tilde{X}_0, \tilde{X}_1, \ldots \equiv X$ and $\tilde{Y} = \tilde{Y}_0, \tilde{Y}_1, \ldots \equiv Y$, where $\equiv$ indicates equality of distribution. In general, a coupling of $X$ and $Y$ need not be stationary, or Markov, an issue that we take up below.

In studying optimal transport of the random walks $X$ and $Y$ we make use of the single letter cost $\tilde{c} : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ defined by $\tilde{c}(x, y) = c(x_0, y_0)$. The standard optimal transport problem with the cost $\tilde{c}$ seeks to minimize $\mathbb{E}c(\tilde{X}_0, \tilde{Y}_0)$ over the family $\Pi(X, Y)$ of all couplings of the Markov chains $X$ and $Y$. However, for most purposes $\Pi(X, Y)$ is too large: in general, it will include couplings that are non-stationary, and not Markov of any order. Without further restrictions, an optimal coupling will minimize the expected cost only at time zero, after which the processes $\tilde{X}$ and $\tilde{Y}$ may evolve independently (and potentially have a large realized cost). Restricting attention to stationary couplings addresses some of these issues (O’Connor et al., 2022). We note that stationary couplings of stationary processes, also known as joinings, have been widely studied in the ergodic theory literature (see De La Rue, 2005; Glasner, 2003; Ornstein, 1973 and the references therein).

When considering random walks $\tilde{X}$ and $Y$ on graphs, which are Markov chains, it is natural to consider couplings $(\tilde{X}, \tilde{Y})$ that are themselves Markov chains, so that the structure of the couplings matches that of the walks. Unfortunately, even the family of stationary first order Markov couplings presents some difficulties: there is no fast method for computing optimal couplings, and the optimal expected cost need not have the properties of a metric even when the cost $c$ does (Ellis, 1976; 1978). For these reasons, we restrict attention to the subfamily of transition couplings, which are defined below.

**Definition 1.** Let $X$ be a stationary Markov chain with values in $U$ and transition kernel $P$, and let $Y$ be a stationary Markov chain with values in $V$ and transition kernel $Q$. A stationary Markov chain $(\tilde{X}, \tilde{Y})$ with values
in $U \times V$ is a transition coupling of $X$ and $Y$ if it is a coupling of $X$ and $Y$ and if it has a transition kernel $R$ such that for every $u_0, u_1 \in U$ and $v_0, v_1 \in V$:

$$\sum_{v \in V} R(u_1, v \mid u_0, v_0) = P(u_1 \mid u_0) \quad \text{and} \quad \sum_{u \in U} R(u, v_1 \mid u_0, v_0) = Q(v_1 \mid v_0).$$

(4)

Let $\Pi_{\text{TC}}(X, Y)$ denote the set of all transition couplings of $X$ and $Y$. When (4) holds, we will also say that $R$ is a transition coupling of $P$ and $Q$.

The transition coupling condition (4) can be stated equivalently as follows: for every state $(v_0, v_1) \in U \times V$ of the joint chain, the distribution $R(\cdot \mid u_0, v_0)$ of the next state is a coupling of the next state distributions $P(\cdot \mid u_0)$ and $Q(\cdot \mid v_0)$ of the individual chains. The set of transition couplings $\Pi_{\text{TC}}(X, Y)$ is non-empty, as the independent coupling of $X$ and $Y$, with transition kernel $R(u', v' \mid u, v) = P(u' \mid u) Q(v' \mid v)$, is a transition coupling.

Couplings have long been employed in the analysis of Markov chains, often to study the rate at which the marginal distribution of a chain started in a particular state converges to the stationary distribution of the chain. In a typical analysis, two versions of a chain are run from different initial conditions until they reach the same state, and if it has a transition kernel $R(\cdot \mid u_0)$, $v_0)$ such that $R(\cdot \mid u_0)$ is a transition coupling of $P$ and $Q$.

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4 NetOTC

In this section, we describe the NetOTC procedure in more detail, including a statement of the NetOTC problem, as well as exact and approximate computational methods for its solution.

4.1 The NetOTC Problem

Let $G_1$ and $G_2$ be strongly connected networks of interest. Each network gives rise to a unique random walk on its vertex set, whose transition probabilities are determined by their connectivity and edge weights; the stationary distribution of the walk reflects the global structure of the network, while the transition probabilities of the walk reflect the local structure of the network. Let $X$ and $Y$ be the walks associated with $G_1$ and $G_2$, respectively. In the NetOTC problem, we seek to minimize the expected cost $\mathbb{E}C(X_0, Y_0)$ over all transition couplings $(X, Y)$ of $X$ and $Y$. In particular, we wish to identify both the minimizing value

$$\rho(G_1, G_2) = \min_{(X, Y) \in \Pi_{\text{TC}}(X, Y)} \mathbb{E}C(X_0, Y_0),$$

(5)

and an associated optimal transition coupling

$$(X^*, Y^*) \in \arg\min_{(X, Y) \in \Pi_{\text{TC}}(X, Y)} \mathbb{E}C(X_0, Y_0).$$

(6)

An optimal transition coupling is a stationary random walk

$$(X^*, Y^*) = (X_0^*, Y_0^*), (X_1^*, Y_1^*), \ldots$$

on the product $U \times V$ that preserves the marginal behavior of the walks $X$ and $Y$, while favoring pairs $u, v$ with low cost. In particular, $(X^*, Y^*)$ is an optimal coupling of the processes $X$ and $Y$, not just their one-dimensional (stationary) distributions. As such, the optimal transport plan identified by NetOTC captures and links the local and global structure of the given networks.

As noted above, the set $\Pi_{\text{TC}}(X, Y)$ of transition couplings is non-empty. We endow $\Pi_{\text{TC}}(X, Y)$ with the standard topology (inherited as a subset of the weak* topology on the space of finite-valued stochastic processes) under which it is compact and the expected cost function $(X_0, Y_0) \mapsto \mathbb{E}C(X_0, Y_0)$ is continuous. Thus, the minimum in (5) is achieved, and there exists an optimal transition coupling in (6). In general, there may be many solutions to the NetOTC problem. For example, if the cost function is constant, then all transition couplings are optimal.
Workflow 1 Solving the NetOTC Problem

Input: Networks $G_1 = (U, E_1, w_1)$ and $G_2 = (V, E_2, w_2)$. Cost function $c(u, v)$.

Step 1. Compute the transition probabilities $P$ and $Q$ of the random walks associated with $G_1$ and $G_2$ according to (5).

Step 2. Pass $P$ and $Q$ to the procedure of O’Connor et al. (2022), which yields the optimal cost $\rho$, as well as the stationary distribution $\pi$ and transition kernel $R$ of an optimal transition coupling.

Step 3. Calculate vertex alignment as in (7) and edge alignment as in (8).

Output: NetOTC cost $\rho$, Vertex alignment $\pi_v$, Edge alignment $\pi_e$

While the objective function of the NetOTC problem involves only the first time point of the joint process $(X, Y)$, the restriction to transition couplings ensures that the optimal coupling performs well on average over multiple time points (see Proposition 4 below), and that it captures the dynamics of the individual chains. In general, the minimizing value of $E c(\tilde{X}_0, \tilde{Y}_0)$ will (strictly) decrease as one moves from transition couplings to general Markov couplings, from Markov couplings to stationary couplings, and from stationary couplings to general couplings (Ellis, 1976, 1978; Ellis et al., 1980; Ellis, 1980; O’Connor et al., 2022, 2021).

We note that the NetOTC problem is not equivalent to the problem of finding a one-step optimal transition coupling, which is considered in Song et al. (2016) and Zhang (2000). In the latter problem one finds, for every $u \in U$ and $v \in V$, a coupling $\tilde{X}_0, \tilde{Y}_0$ of $X_0 \sim P(x|u)$ and $Y_0 \sim Q(y|v)$ minimizing $E c(\tilde{X}_0, \tilde{Y}_0)$. A one-step optimal transition coupling does not necessarily exhibit good performance over multiple time steps, as it does not account for the global structure of the given networks.

4.2 Cost Functions

In practice, the specification of a cost function depends on the goals of the network alignment or comparison problem. The cost function is typically based on prior information about the vertex sets of the given networks, including vertex features and embeddings, if these are available. If $U = V$ we may use the 0-1 cost $c(u, v) = 1(u \neq v)$. If the vertices of $G_1$ and $G_2$ are associated with features or attributes in a common, discrete set $S$ then one may take $c(u, v) = \rho(\tilde{u}, \tilde{v})$ where $\rho$ is a cost function relating the elements of $S$, and $\tilde{u}, \tilde{v} \in S$ are the features associated with vertices $u$ and $v$, respectively. If $S$ is a finite set, the zero-one cost $c(u, v) = 1(\tilde{u} \neq \tilde{v})$ is often a good choice. If the vertices of $G_1$ and $G_2$ are embedded in a common Euclidean space $\mathbb{R}^d$ via embeddings $h_1 : U \to \mathbb{R}^d$ and $h_2 : V \to \mathbb{R}^d$, then it is natural to use an embedding-based cost such as $c(u, v) = ||h_1(u) - h_2(v)||$ or $c(u, v) = ||h_1(u) - h_2(v)||^2$. In cases where such prior maps are unavailable, one may consider costs defined in terms of intrinsic properties of the networks of interest, or embed the vertices in a Euclidean space a priori using methods such as Laplacian eigenmaps (Belkin and Niyogi, 2003).

A cost function that is applicable in general is the degree-based cost: $c(u, v) = (\deg(u) - \deg(v))^2$. For undirected networks, $\deg(u)$ is sum of weights of all edges adjacent to $u$. For directed networks, one may use in-degree, out-degree, or a combination of these. Unless otherwise specified, we use out-degree in this paper. One may also use the standardized degree $\bar{d}(u) = \deg(u)/\sum_{u' \in U} \deg(u')$ when comparing networks of significantly different sizes. Extending this idea, one may employ cost $c(u, v)$ based on the degree distributions of a fixed local neighborhood of $u$ and $v$.

4.3 Computation of NetOTCs

A workflow for NetOTC is given in Workflow 1. The NetOTC procedure does not rely on randomization, and has no free parameters; its output is fully determined by the given networks and the cost function $c$. Finding an optimal transition coupling (OTC) of the random walks $X$ and $Y$ derived from the given networks is a non-convex, constrained optimization problem that is not amenable to standard optimization routines. Instead, NetOTC uses the method of O’Connor et al. (2022), in which the problem of finding an OTC is reframed as a Markov decision process (MDP) with state space $\mathcal{S} = \mathcal{X} \times \mathcal{Y}$, where the admissible actions in state $s = (x, y)$ correspond to couplings $r_s$ of the transition distributions $P(x, \cdot)$ and $Q(y, \cdot)$. The transition distribution of the MDP in state $s$ with action $r_s$ is simply given by $r_s$, while the reward function of the MDP is simply the negative of the cost function $R(s, r_s) = -c(x, y)$, where $s = (x, y)$. Reformulated in this way, the OTC problem corresponds to finding an optimal policy for the MDP, a problem to which policy iteration (Howard, 1960) may be applied (with standard optimal transport solvers used in the policy update steps). The algorithm requires $O((|U||V|)^3)$ operations per iteration. In practice, it converges after fewer than 5 iterations. O’Connor et al. (2022) also describes a more efficient
algorithm based on entropic regularization and Sinkhorn iterations. When applied to NetOTC, the regularized algorithm requires $O((|U||V|)^2)$ operations per iteration (up to poly-logarithmic factors), which is nearly-linear in the dimension of the couplings under consideration, and in this sense comparable to the state-of-the-art for entropic OT algorithms (Peyré and Cuturi 2019). Pseudocode and more details on the method can be found in Section 4 of O’Connor et al. (2022).

In general, NetOTC problem may have multiple solutions. The NetOTC algorithm is only guaranteed to return a single minimizer, which is not guaranteed to be irreducible. On the other hand, the entropically regularized problem has a unique minimizer, which is aperiodic and irreducible when $X$ and $Y$ are aperiodic and irreducible. The current implementation of NetOTC can handle networks with up to 200 vertices. Research on faster computation of OTCs is currently ongoing.

4.4 NetOTC Deliverables

**Difference measure for networks.** The solution of the NetOTC problem yields the minimizing value $\rho(G_1, G_2)$ of the expected cost, and the associated optimal transition plan $(X^*, Y^*)$. The minimum cost $\rho(G_1, G_2)$ measures the difference between $G_1$ and $G_2$ and can be utilized for network comparison tasks. For undirected networks with the same vertex set, $\rho(\cdot, \cdot)$ is a metric if the cost function is a metric (see Proposition 8).

**Vertex alignment.** The optimal transport plan $(X^*, Y^*)$ itself provides soft, probabilistic alignments of the vertices and edges of $G_1$ and $G_2$ based on the joint distribution of pairs in the coupled chain. The vertex alignment $\pi_v$ produced by NetOTC is derived from the stationary distribution of the optimal transport plan $(X^*, Y^*)$, which is the distribution of the pair $(X^*_0, Y^*_0)$. The vertex alignment is defined by

$$\pi_v(u, v) = \mathbb{P}((X^*_0, Y^*_0) = (u, v)). \quad (7)$$

One may define probabilistic vertex alignments in a similar manner for other OT-based network comparison methods (see Section 6.3 and 6.4).

**Edge alignment.** A unique feature of NetOTC is that the optimal transport plan naturally yields a probabilistic alignment of the edges of the given networks. The edge alignment is obtained from the first two pairs $\{(X^*_0, Y^*_0), (X^*_1, Y^*_1)\}$ of the optimal transport plan. For $u, u' \in U$ and $v, v' \in V$ the edge alignment is defined by

$$\pi_e((u, u'), (v, v')) = \mathbb{P}((X^*_0, Y^*_0) = (u, v), (X^*_1, Y^*_1) = (u', v')). \quad (8)$$

It is straightforward to show (see Proposition 2) that vertex pairs aligned with positive probability must be adjacent in their respective networks. In other words, NetOTC aligns only existing edges; it does not create new ones. By contrast, most alignment methods in the literature have as their primary focus the matching of vertices, with edges functioning primarily as a means of evaluating matchings. Alignments arising in this way can map adjacent vertices in $G_1$ to non-adjacent vertices in $G_2$, or vice versa.

5 Theoretical Properties of NetOTC

In this section, we explore some theoretical properties of NetOTC, beginning with the edge-alignment property and several results concerning the behavior of NetOTC under average cost criteria. For undirected networks with a common vertex set, we establish that the NetOTC cost has the properties of a metric when the cost $\epsilon$ does, and we investigate the sensitivity of NetOTC to local information arising from degree and weight functions. We then define a notion of network factor that captures the idea of one network being “folded” or “compressed” to produce another. Although the literature contains several definitions of network factors or factor networks, the definition given here appears to be new. We establish a close connection between factors and transition couplings, and then we present two results describing the behavior of NetOTC in the presence of this type of network factor structure. All proofs of the results in this section may be found in Section 8.

5.1 NetOTC Edge Alignment

The NetOTC edge alignment function $\pi_e$ respects edges, in the sense that vertex pairs aligned with positive probability must be adjacent in the given networks.

**Proposition 2.** Let $\pi_e$ be the NetOTC edge alignment of networks $G_1 = (U, E_1, w_1)$ and $G_2 = (V, E_2, w_2)$ based on the optimal transport plan $(X^*, Y^*)$. If $\pi_e((u, u'), (v, v')) > 0$ then $(u, u') \in E_1$ and $(v, v') \in E_2$. 

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5.2 NetOTC and Multistep Cost

The NetOTC cost $\rho(G_1, G_2)$ is the expected cost $\mathbb{E}_c(\tilde{X}_0, \tilde{Y}_0)$ at the initial state of the optimal transport plan. Stationarity ensures that the NetOTC problem is equivalent to minimizing the long-term average cost over the set of transition couplings.

Definition 3. For an infinite sequence $x_0, x_1, \ldots$ and integers $0 \leq i \leq j$ let $x_i^j = (x_i, \ldots, x_j)$. For each $k \geq 1$ define the $k$-step average cost $c_k(x_i^{k-1}, y_0^{k-1}) = k^{-1} \sum_{j=0}^{k-1} c(x_j, y_j)$ and the limiting average cost $\bar{c}(x, y) = \limsup_{k \to \infty} c_k(x_0^{k-1}, y_0^{k-1})$.

Proposition 4. Let $G_1$ and $G_2$ be networks with associated random walks $X$ and $Y$. Then

$$\rho(G_1, G_2) = \min_{(\tilde{X}, \tilde{Y}) \in \Pi_{TC}(X,Y)} \mathbb{E}_{\tilde{c}}(\tilde{X}, \tilde{Y}),$$

and the optimal transport plans minimizing $\mathbb{E}_{\tilde{c}}(\tilde{X}, \tilde{Y})$ coincide with those minimizing $\mathbb{E}_c(\tilde{X}_0, \tilde{Y}_0)$.

The long-term behavior of the random walks $X$ and $Y$ encodes information about the global structure of the networks $G_1$ and $G_2$, respectively. The next result shows that NetOTC also captures local information arising from the finite time behavior of the walks $X$ and $Y$. For example, if $G_1$ and $G_2$ are distinguishable based on optimal transport of their $k$-step random walks, then they are distinguishable by NetOTC.

Proposition 5. Let $G_1$ and $G_2$ be networks with associated random walks $X$ and $Y$. For each $k \geq 1$

$$\rho(G_1, G_2) \geq \min \mathbb{E}_{\bar{c}}(\tilde{X}_0^{k-1}, \tilde{Y}_0^{k-1}),$$

where the minimum is over the family of all couplings of $X_0^{k-1}$ and $Y_0^{k-1}$.

5.3 Undirected Networks with a Common Vertex Set

In this section, we consider undirected networks $G_1 = (U, E_1, w_1)$ and $G_2 = (U, E_2, w_2)$ with the same vertex set, but potentially different edge sets and weight functions. We assume throughout that the networks are connected. We begin by defining a natural equivalence relation on such networks.

Definition 6. Undirected networks $G_1$ and $G_2$ are equivalent, denoted by $G_1 \sim G_2$, if they have the same vertex set $U$, the same edge set $E$, and there exists a constant $C > 0$ such that $w_1(u, u') = C w_2(u, u')$ for every $u, u' \in U$.

The following result relates the equivalence of networks to their random walks.

Proposition 7. Connected undirected networks $G_1$ and $G_2$ are equivalent if and only if their respective random walks are identical.

Whatever the underlying cost $c$, the cost $\rho(G_1, G_2)$ and optimal transport plan arising from NetOTC depends only on the equivalence classes of the networks $G_1$ and $G_2$. In particular, NetOTC is invariant under (positive) scaling of weight functions. When the underlying cost $c$ is a metric on $U$, the NetOTC cost is a metric on these equivalence classes.

Proposition 8. If the cost function $c : U \times U \to \mathbb{R}_+$ satisfies the properties of a metric on $U$, then $\rho$ is a metric on the equivalence classes of undirected networks with vertex set contained in $U$ defined by $\sim$.

We now investigate the sensitivity of NetOTC to differences between the degree and weight functions of the given networks.

Definition 9. The degree function of an undirected network $G = (U, E, w)$ is given by $d(u) = \sum_{u' \in U} w(u, u')$ for $u \in U$. Let $D = \sum_{u \in U} d(u)$ denote the total degree of $G$.

The next proposition strengthens the general result of Proposition 8.

Proposition 10. Let $G_1$ and $G_2$ be undirected networks with the same vertex set. Let $d_1(u)$ and $d_2(u)$ be the degree functions of $G_1$ and $G_2$, respectively, and assume that each network has a total degree of $D$. Then under the zero-one cost $c(u, u') = 1(u \neq u')$,

$$\rho(G_1, G_2) \geq \frac{1}{\alpha} \sum_{u \in V} |d_1(u) - d_2(u)|$$
The factor map $G$ ensures that the partitioning of the vertices is consistent with the transition probabilities of the random walk on $G$.

In this case, we will say that $G$ ensures that the partitioning of the vertices is consistent with the transition probabilities of the random walk on $G$.

Consider the networks $G_1$ and $G_2$ drawn in Figure 1 with vertices embedded in $\mathbb{R}^2$. $G_2$ is a factor of $G_1$ with respect to the map $f$ that takes $(-1,1)$ and $(-1,-1)$ to $(-1,0)$, $(0,0)$ to $(0,0)$, and $(1,0)$ and $(1,-1)$ to $(1,0)$.

The definition of factor arises naturally from the random walk perspective. If $G_1$ and $G_2$ have associated random walks $X$ and $Y$, and $G_2$ is a factor of $G_1$ under the map $f$, then the process $f(X) := f(X_0), f(X_1), \ldots$ is equal in distribution to $Y$, see Theorem 16 below for more details. Factors have been well studied in ergodic theory and symbolic dynamics. The existence of a factor map (in the sense above) ensures that $Y$ is a stationary coding of $X$, which is a special case of a factor relationship in ergodic theory. Moreover, if $G_2$ is a factor of $G_1$, then the subshift of finite type (SFT) consisting of all bi-infinite walks on $G_2$ is a topological factor of the SFT associated with $G_1$ given by a 1-block code, see [Lind and Marcus, 1995] for detailed definitions. Our definition of factor has points of contact with compressed representations of weighted networks, explored in [Toivonen et al., 2011], but in general the relationship need not hold for compressed representations.

The definition of factor formalizes the idea that $G_2$ (the factor) is a collapsed or compressed version of $G_1$ (the extension). The factor map $f$ associates the vertices in $G_2$ with a partition of the vertices in $G_1$. Condition (9) ensures that the partitioning of the vertices is consistent with the transition probabilities of the random walk on $G_1$.

**5.4 Deterministic Transition Couplings and Factor Maps**

The graph theory and network literature contain several definitions of “network factor” and “factor network”. A network factor of $G$ is often defined to be any spanning subnetwork of $G$, while the term factor network is used in the context of message passing algorithms and error-correcting codes to refer to a bipartite network that captures the factorization of a function or a probability distribution. Here we define a notion of network factor that appears to be the context of message passing algorithms and error-correcting codes to refer to a bipartite network that captures the factorization of a function or a probability distribution. Here we define a notion of network factor that appears to be

\[ \rho(G_1, G_2) \geq \frac{1}{|U|} \sum_{u, u' \in U} |w_1(u, u') - w_2(u, u')| \]

**Remark 11.** Proposition 7 can be readily extended to cases where $G_1$ and $G_2$ have different total degrees $D_1$ and $D_2$, respectively. Nevertheless, when comparing two undirected networks using NetOTC, we may assume that they share equal total degrees. As indicated in Proposition 7 for a connected undirected network $G_2 = (U, E_2, w_2)$ with total degree $D_2$, an equivalent graph $G'_2 = \left( U, E_2, \frac{D_2}{w_2} \right)$ with total degree $D_1$ can be constructed.

Figure 1: An example of two networks related by a factor map. Here $G_2$ is a factor of $G_1$ via the map that collapses vertices along vertical lines.
If \( P \) and \( Q \) are the transition kernels for \( G_1 \) and \( G_2 \), then Condition (9) is equivalent to the statement that for all \( v, v' \in V \) and \( u \in f^{-1}(v) \),
\[
\sum_{w' \in f^{-1}(w')} P(w' \mid u) = Q(w' \mid v).
\] (10)

This is also equivalent to the condition \( P( f(X_1) = v' \mid X_0 = u) = P(Y_1 = v' \mid Y_0 = v) \), where \( X \) and \( Y \) are the random walks associated with \( G_1 \) and \( G_2 \). Since \( P \) and \( Q \) are irreducible, Condition (9) implies that the (unique) stationary distributions \( p \) on \( G_1 \) and \( q \) on \( G_2 \) are such that for all \( v \in V \),
\[
\sum_{w \in f^{-1}(v)} p(u) = q(v),
\] (11)
which is equivalent to \( f(X_0) \xrightarrow{d} Y_0 \). The factor relationship can also be expressed in matrix form. If \( f \) is a factor map from \( G_1 \) to \( G_2 \), then (9) is equivalent to the condition \( PF = FQ \) where \( F \in \mathbb{R}^{U \times V} \) is defined by \( F(u, v) = 1 \) if \( f(u) = v \) and \( F(u, v) = 0 \) otherwise. Furthermore, equation (11) is equivalent to \( pF = q \).

The next proposition establishes a close connection between transition couplings and factor maps. Let \( G_1 \) and \( G_2 \) be strongly connected, weighted directed networks with associated Markov chains \( X \) and \( Y \). Note that any stationary Markov coupling \((\tilde{X}, \tilde{Y})\) of \( X \) and \( Y \) corresponds to a weighted, directed network \( H \) with vertex set \( W \subset U \times V \). Let \( \pi_U : U \times V \to U \) and \( \pi_V : U \times V \to V \) be the standard projections onto the first and second coordinates, respectively.

**Proposition 14.** If \((\tilde{X}, \tilde{Y})\) is a stationary Markov coupling corresponding to a strongly connected network \( H \) with vertex set \( W \), then \((\tilde{X}, \tilde{Y})\) is a transition coupling of \( X \) and \( Y \) if and only if the restriction of \( \pi_U \) to \( W \) is a factor map from \( H \) to \( G_1 \) and the restriction of \( \pi_V \) to \( W \) is a factor map from \( H \) to \( G_2 \).

We next investigate connections between factors and deterministic transition couplings.

**Definition 15.** Suppose \( G_1 = (U, E_1, v_1) \) and \( G_2 = (V, E_2, v_2) \) are two strongly connected, weighted, directed networks with associated Markov chains \( X \) and \( Y \), respectively. A transition coupling \((X, Y)\) is said to be deterministic from \( X \) to \( Y \) if for each \( u \in U \) there exists \( v \in V \) such that \( P(Y_0 = v \mid X_0 = u) = 1 \).

In optimal transport theory, deterministic couplings are associated with the so-called Monge problem, see Villani [2008] for more context and discussion. A deterministic coupling \((\tilde{X}, \tilde{Y})\) of \( X \) and \( Y \) is associated with a map \( f : U \to V \), where \( f(u) \) is the (necessarily unique) element \( v \in V \) for which \( P(Y_0 = v \mid X_0 = u) = 1 \). In particular, \((\tilde{X}, \tilde{Y}) \xrightarrow{d} (X, f(X))\). Moreover, as \( G_2 \) is strongly connected, \( P(Y_0 = v) > 0 \) for each \( v \in V \), and the edge-alignment property (Proposition 2) ensures that \( f \) is a surjective graph homomorphism from \( G_1 \) to \( G_2 \).

**Theorem 16.** Suppose \( G_1 \) and \( G_2 \) are strongly connected, weighted directed networks with associated random walks \( X \) and \( Y \), respectively.

1. If \( G_2 \) is a factor of \( G_1 \) with factor map \( f \), then \( Y \xrightarrow{d} f(X) \), and \((X, f(X))\) is a deterministic transition coupling from \( X \) to \( Y \).
2. If \((\tilde{X}, \tilde{Y})\) is a deterministic transition coupling from \( X \) to \( Y \), then the induced map \( f : U \to V \) is a factor map from \( G_1 \) to \( G_2 \).

When \( G_2 \) is a factor of \( G_1 \) under \( f \), Theorem 16 ensures that \((X, f(X))\) is a transition coupling of their random walks. If the cost function \( c \) is such that \( c(u, v) \) is minimized by \( v = f(u) \) then, as the next result shows, this coupling is also optimal, and there is a deterministic solution to the NetOTC problem.

**Definition 17.** Let \( f \) be a factor map from \( G_1 \) to \( G_2 \). A cost function \( c \) is compatible with \( f \) if \( c(u, f(u)) \leq c(u, v) \) for each \( u \in U \) and \( v \in V \).

One may verify that the cost compatibility condition is satisfied in Example 13 under an Euclidean metric cost.

**Corollary 18.** Suppose \( G_1 \) and \( G_2 \) are strongly connected, weighted directed networks and \( f \) is a factor map from \( G_1 \) to \( G_2 \). If \( c \) is compatible with \( f \) then \((X, f(X))\) is an OTC of \( X \) and \( Y \).

An example illustrating Corollary 18 is given in Figure 2. Corollary 18 provides some insight into the structure of the NetOTC problem. If \( G_1 \) and \( G_2 \) are related by a factor map \( f : U \to V \), then \( G_2 \) is essentially a compressed version of the network \( G_1 \). Corollary 18 ensures that an optimal coupling of the random walks on \( G_1 \) and \( G_2 \) is obtained by running the random walk on \( G_1 \) and mapping every state \( u \in U \) in this chain to the corresponding
Let Theorem 19.

The latter include network classification, network isomorphism, alignment of stochastic block models, and network factors. Complete experimental details may be found in Appendix A. In the example and experiments, we larger graphs \( G \) the smaller factor graphs, and Theorem 19 guarantees that the result would be consistent with the alignment of the point of view, if one has access to factor graphs \( f \) reference to, and requires no knowledge of, the factor maps \( f \) of the NetOTC procedure, in the sense that the operation of NetOTC on the extensions obtained in this way. Thus NetOTC respects factor structure whenever factor structure is present: the NetOTC optimal transport plan for the factors \( H \) of \( G \) that an optimal transport plan for the extensions \( c \) obtained in this way. The next result provides further information about how NetOTC behaves in the presence of factor conditions described in Corollary 18, the NetOTC problem aligns vertices according to the factor map relating the two networks. In this example, \( G_2 \) is a factor of \( G_1 \). Figure 2c illustrates the NetOTC vertex alignment, which is supported on pairs of the form \((u, f(u))\).

Figure 2: An illustration of the relationship between factors and the NetOTC problem. Under the conditions described in Corollary 18, the NetOTC problem aligns vertices according to the factor map relating the two networks. In this example, \( G_2 \) is a factor of \( G_1 \). Figure 2c illustrates the NetOTC vertex alignment, which is supported on pairs of the form \((u, f(u))\).

state \( f(u) \in V \). In practice, the conclusion of Corollary 18 approximately holds when the factor condition (9) approximately holds; the results of experiments involving exact and approximate factors are given in Section 6.5. In such situations, NetOTC can be used to identify (approximate) factor maps between \( G_1 \) and \( G_2 \).

Under the conditions of Corollary 18 the NetOTC cost and associated vertex and edge alignments will have a special form. In particular, the NetOTC cost will satisfy \( \rho(G_1, G_2) = \sum_{u \in U} c(u, f(u))p(u) \) where \( p \) is the stationary distribution of the random walk on \( G_1 \). Furthermore, \( \pi_v(u, v) = \mathbb{I}(f(u) = v) \) and \( \pi_v((u, u'), (v, v')) = \mathbb{I}((f(u), f(u')) = (v, v')) \). Note that, while the deterministic coupling appears as a solution of the NetOTC problem, the NetOTC algorithm itself makes no reference to, and does not require prior information about, the factor map \( f \). The next result provides further information about how NetOTC behaves in the presence of factor maps.

**Theorem 19.** Let \( G_1, G_2, H_1, \) and \( H_2 \) be networks with vertex sets \( U, V, A, \) and \( B, \) and associated Markov chains \( X, Y, W, \) and \( Z, \) respectively. Suppose that \( f : U \to A \) and \( g : V \to B \) are factor maps from \( G_1 \) to \( H_1 \) and \( G_2 \) to \( H_2 \), and that there are cost functions \( c_{ext} : U \times V \to \mathbb{R}_+ \) and \( c : A \times B \to \mathbb{R}_+ \) such that \( c_{ext}(u, v) = c(f(u), g(v)) \).

1. If \( (\tilde{X}, \tilde{Y}) \) is an optimal transition coupling of \( X \) and \( Y \) with respect to \( c_{ext} \), then \( (f(\tilde{X}), g(\tilde{Y})) \) is an optimal transition coupling of \( W \) and \( Z \) with respect to \( c \).

2. If \( (\tilde{W}, \tilde{Z}) \) is an optimal transition coupling of \( W \) and \( Z \) with respect to \( c \), then there exists an optimal transition coupling \( (\tilde{X}, \tilde{Y}) \) of \( X \) and \( Y \) with respect to \( c_{ext} \) such that \( (f(\tilde{X}), g(\tilde{Y})) \preceq (\tilde{W}, \tilde{Z}) \).

A simple illustration of Theorem 19 is given in Figure 3. For compatible cost functions, the theorem ensures that an optimal transport plan for the extensions \( G_1 \) and \( G_2 \) can be transferred through the maps \( f \) and \( g \) to an optimal transport plan for the factors \( H_1 \) and \( H_2 \); moreover, every optimal transport plan for the factors can be obtained in this way. Thus NetOTC respects factor structure whenever factor structure is present: the NetOTC alignment of the extensions is consistent with the NetOTC alignment of the factors. This is a fundamental property of the NetOTC procedure, in the sense that the operation of NetOTC on the extensions \( G_1 \) and \( G_2 \) makes no reference to, and requires no knowledge of, the factor maps \( f \) and \( g \) or the factors \( H_1 \) and \( H_2 \). From a practical point of view, if one has access to factor graphs \( H_1 \) and \( H_2 \), then one could save computational expense by aligning the smaller factor graphs, and Theorem 19 guarantees that the result would be consistent with the alignment of the larger graphs \( G_1 \) and \( G_2 \).

### 6 Example and Experiments

In this section, we illustrate the properties of NetOTC through an example and several numerical experiments. The latter include network classification, network isomorphism, alignment of stochastic block models, and network factors. Complete experimental details may be found in Appendix A. In the example and experiments, we
compare NetOTC to several existing, optimal transport-based approaches to network alignment: marginal optimal transport (OT), Gromov-Wasserstein (GW) [Peyré et al., 2016], Fused Gromov-Wasserstein (FGW) [Titouan et al., 2019; Vayer et al., 2020], and Coordinated Optimal Transport (COPT) [Dong and Sawin, 2020]. Here marginal optimal transport refers to the optimal coupling of the stationary distributions of the random walks on the given networks. When applying the FGW method, following Titouan et al. (2019); Vayer et al. (2020), we use a uniform distribution on the vertices of each network. Code for reproducing the example and experiments may be found at https://github.com/austinyi/NetOTC.

6.1 Edge Awareness Example

We begin with a toy example to demonstrate the edge preservation property of NetOTC (see Proposition 2): network $G_1$ is an octagon network, network $G_2$ is a copy of $G_1$ with one edge on the right removed, and network $G_3$ is topologically identical to $G_2$, but its vertices are located in the left half plane. See Figure 4 below.

Figure 4: Three networks in which all vertices are located on the unit circle in $\mathbb{R}^2$. $G_1$ is an octagon network. $G_2$ is obtained by removing an edge $G_1$. In $G_3$, the vertices are uniformly distributed in the left semicircle.

Table I shows the ratio of the costs obtained when comparing different pairs of networks under a cost function.
equal to the squared Euclidean distance between vertex positions. We considered the methods NetOTC, OT, and FGW, as they allow the use of the Euclidean cost function. The ratio of the cost between \( G_2 \) and \( G_1 \) and the cost between \( G_2 \) and \( G_3 \) varies greatly between the methods. Observe that NetOTC is the only method with a ratio that exceeds 1, that is, NetOTC finds \( G_2 \) to be closer to \( G_1 \) than \( G_1 \). This example illustrates that NetOTC is sensitive to topological differences between the given networks, and in particular that topological similarity can dominate differences in the vertex costs.

| Algorithm | \( G_2 \) vs. \( G_1 \) | \( G_2 \) vs. \( G_3 \) | Ratio |
|-----------|----------------|----------------|-------|
| NetOTC    | 0.5714         | 0.4464         | 1.28  |
| OT        | 0.2857         | 0.4464         | 0.64  |
| FGW       | 0.0313         | 0.2725         | 0.11  |

Table 1: Comparison of OT-based costs between networks in Figure 4.

### 6.2 Network Classification

In our next experiment, we examine the utility of NetOTC for network classification tasks. We consider a selection of benchmark network datasets from Kersting et al. (2016). Each dataset contains a collection of networks with discrete vertex attributes and class labels. We considered the datasets AIDS (Riesen and Bunke 2008), BZR (Sutherland et al. 2003), Cuneiform (Kriege et al. 2018), MCF-7 (Yan et al. 2008), MOLT-4 (Yan et al. 2008), MUTAG (Debnath et al. 1991), and Yeast (Yan et al. 2008). For each dataset, we employed an attribute-based cost function, where \( c(u, v) = 0 \) if vertices \( u \) and \( v \) have the same attribute and \( c(u, v) = 1 \) otherwise. For each OT-based comparison method, we constructed a 5-nearest neighbor classifier using a random training set containing 80% of the available networks and used this classifier to predict the labels of the remaining networks.

Table 2 shows the average classification accuracy over 5 random samplings of the training and test sets for each comparison method. As the table demonstrates, NetOTC is competitive with other network OT based methods on several cases, without the need for tuning or specification of free parameters.

| Algorithm | AIDS       | BZR       | Cuneiform | MCF-7      | MOLT-4     | MUTAG      | Yeast       |
|-----------|------------|-----------|-----------|------------|------------|------------|-------------|
| NetOTC    | 88.0 ± 4.9 | 84.8 ± 6.6| 73.2 ± 7.8| 92.8 ± 4.2 | 92.0 ± 2.0 | 85.4 ± 7.1 | 90.8 ± 6.4  |
| OT        | 84.4 ± 6.1 | 76.4 ± 4.6| 71.3 ± 7.7| 93.6 ± 3.3 | 92.0 ± 2.0 | 63.2 ± 7.3 | 91.2 ± 7.0  |
| GW        | 98.8 ± 1.8 | 78.0 ± 8.5| 12.8 ± 4.6| 93.6 ± 3.3 | 91.6 ± 2.6 | 81.6 ± 7.0 | 91.6 ± 6.2  |
| FGW       | 99.2 ± 1.1 | 80.0 ± 7.1| 74.8 ± 3.6| 92.8 ± 4.2 | 91.6 ± 2.6 | 84.3 ± 8.6 | 89.2 ± 6.6  |
| COPT      | 98.0 ± 1.4 | 73.6 ± 7.9| 16.6 ± 3.1| 92.4 ± 4.8 | 91.6 ± 2.6 | 80.0 ± 5.6 | 90.4 ± 6.7  |

Table 2: 5-nearest neighbor classification accuracies for networks with discrete vertex attributes. Average accuracies observed over 5 random samplings of the training and test sets are reported along with their standard deviation.

### 6.3 Network Isomorphism

Two undirected, unweighted networks \( G_1 = (U, E_1) \) and \( G_2 = (V, E_2) \) are isomorphic if there is a bijection \( \phi : U \to V \) of their vertex sets that preserves edges in the sense that \((u, u') \in E_1 \) if and only if \((\phi(u), \phi(u')) \in E_2 \). Determining when two networks are isomorphic, and if so identifying an isomorphism, are important problems in network theory that have received much attention in the literature (McKay and Piperno 2014, Cordella et al. 2004). In general, it is challenging to find isomorphisms in an efficient fashion (Babai 2015).

To evaluate the ability of the alignment methods under study to successfully identify network isomorphisms, we carried out the following experiment. Given a network \( G_1 \), we create an isomorphic copy \( G_2 \) by applying a permutation \( \phi \) to its vertices. We then applied NetOTC, FGW, GW, and OT to \( G_1 \) and \( G_2 \) with a degree-based cost function. From each method we obtained a soft vertex alignment \( \pi_v : U \times V \to [0, 1] \) of the given networks, and from \( \pi_v \) we derived a hard vertex alignment \( \psi(u) = \arg \max_{v \in V} \pi_v(u, v) \). If the hard alignment \( \psi \) is identical to the isomorphism \( \phi \), the algorithm has successfully identified the isomorphism map. See Appendix A.2 for more details. Figure 5 shows an example of isomorphic “lollipop” networks (another example is shown in Appendix A.2 Figure 5). NetOTC correctly finds the isomorphism map between two isomorphic networks, but the other methods
do not. Note that the cost function used by each method to align the vertices depends only on their degree, and that the majority of the vertices in the lollipop network have degree 2. This example demonstrates that, while the objective function of the NetOTC problem is univariate (it depends only on the cost between vertices at time zero), both the NetOTC distance and optimal transition coupling depend critically on the topological properties of the given networks.

Further experiments demonstrate the ability of NetOTC to recover isomorphisms in different classes of networks: random (Erdos-Renyi) networks, stochastic block models (SBMs), networks with a random weighted (0,1,2) adjacency matrix, and random lollipop networks. Table 3 shows the average performance of each method for 300 random networks of each class. See Appendix 2 for further details of the network generation process. NetOTC exhibits perfect performance for networks with random adjacency matrices and all types of SBMs, with very high accuracy in Erdos-Renyi and random lollipop networks. On all classes but the random adjacency matrix, the competing methods perform markedly worse. The poor performance of OT demonstrates the substantial performance gains obtained from coupling the full random walks on $G_1$ and $G_2$, rather than their stationary distributions.
Table 3: Isomorphism map identification success rate (%). We generate 300 random networks in each class. For each random network, we permute its vertices and apply the algorithms to the two isomorphic networks. We report the percentage of times the output alignment of an algorithm yields an isomorphism of the given graphs.

| Model                  | NetOTC | FGW  | GW   | OT   |
|------------------------|--------|------|------|------|
| Erdos-Renyi \(n \in \{6, \ldots, 15\}, p = 1/3\) | 96.73  | 71.50| 54.67| 2.80 |
| Erdos-Renyi \(n \in \{6, \ldots, 15\}, p = 2/3\) | 94.86  | 57.19| 48.63| 8.56 |
| Erdos-Renyi \(n \in \{16, \ldots, 25\}, p = 1/4\) | 99.64  | 88.45| 69.68| 0.00 |
| Erdos-Renyi \(n \in \{16, \ldots, 25\}, p = 3/4\) | 100.00 | 71.33| 50.00| 0.00 |
| SBM \((7, 7, 7, 7)\) | 100.00 | 84.62| 54.85| 0.00 |
| SBM \((10, 8, 6)\) | 100.00 | 78.33| 58.67| 0.00 |
| SBM \((7, 7, 7)\) | 100.00 | 71.28| 41.89| 0.00 |
| Random weighted adjacency matrix \(\{0, 1, 2\}\) | 100.00 | 96.67| 96.33| 5.67 |
| Random Lollipop network | 98.00 | 13.67| 6.00 | 0.00 |

Figure 6: The adjacency matrices of random networks \(G_1\) and \(G_2\) drawn from SBMs. Block structure arises from different connection probabilities within the blocks. Networks \(G_1\) and \(G_2\) are designed to have the same block structure with a different number of vertices.

6.4 Block Alignment in Stochastic Block Models

Stochastic block models ([Holland et al.](1983)) (SBMs) are frequently used to model random networks with community structure. SBMs have found application in a variety of network problems, including community detection and network clustering, see for example [Abbe (2018); Lee and Wilkinson (2019); Abbe and Sandon (2015)]. In an SBM, each vertex is assigned (deterministically or at random) to one of a small number of groups, also known as blocks. Once group assignment is complete, edges are placed between pairs of vertices independently, with the probability of an edge being present depending on the group assignments of its endpoints. In most cases, edge probabilities are higher within groups than between groups, so that the vertices in a group constitute, informally at least, a community.

We wished to assess the ability of OT-based comparison methods to align the vertices and edges of stochastically equivalent blocks in SBMs of different sizes. To this end, we generated 10 realizations \(G_1, G_2\) of SBMs with 4 blocks. In each case, the network \(G_1\) had 12 vertices per block, and \(G_2\) had 8 vertices per block. For each network, the within block connection probabilities were 1, 0.8, 0.6, and 0.4, while the between block connection probability was equal to 0.1. The adjacency matrix of a typical realization of \(G_1\) and \(G_2\) is depicted in Figure 6. Note that the networks \(G_1\) and \(G_2\) are undirected and unweighted.

We applied the five comparison methods under study to each of the 10 realizations of \(G_1\) and \(G_2\) using the standardized degree-based cost function. Each method returns a vertex alignment \(\pi_v : U \times V \rightarrow \mathbb{R}_+\) associated with the respective optimal transport plans. Vertex alignment accuracy was assessed by summing \(\pi_v\) over vertex pairs in corresponding blocks, i.e., blocks with the same connection probability.
As described above, the NetOTC optimal transport plan also provides a native edge alignment \( \pi_e : U^2 \times V^2 \to \mathbb{R}_+ \). For other methods, we formed an edge alignment by setting \( \pi_e((u, u'), (v, v')) = \pi(u, v) \pi(u', v') \). Edge alignment accuracy was evaluated by summing the alignment probabilities of all pairs of edges connecting stochastically equivalent blocks, i.e., summing all \( \pi_e((u, u'), (v, v')) \) where \( u \) and \( v \), and \( u' \) and \( v' \) are from blocks with equal connection probabilities.

Figure 7 shows the vertex and edge alignment accuracies for each of the methods tested. As background, we note that random guessing yields an accuracy of 25% for vertex alignment and 6.25% for edge alignment. For vertex alignment, NetOTC, GW, and FGW exhibit similar performance (substantially better than random guessing) while OT and COPT do worse. As indicated by the error bars in Figure 7, the vertex alignment accuracy of NetOTC has a lower variance than the accuracies of OT, GW, and FGW. As expected, NetOTC outperforms other methods from the standpoint of edge alignment.

Figure 7: SBM alignment accuracies. Average accuracies observed over 10 random pairs of SBMs are reported along with their standard deviation. The horizontal dashed line in each plot indicates the accuracy of random guessing.

6.5 Network Factors

Lastly, we considered the task of aligning corresponding vertices when the network \( G_2 \) is a factor of \( G_1 \) and the cost is compatible with the factor map (see Section 5.4). We construct networks \( G_1 \) and \( G_2 \) via vertex embeddings in \( \mathbb{R}^5 \) as follows. The network \( G_2 \) has 6 vertices, each associated with a feature vector generated from a 5-dimensional normal distribution with mean zero and variance \( \sigma^2 I \). The network \( G_1 \) has 30 vertices, each associated with a feature vector sampled from a 6-component Gaussian mixture model. The means of the 6 components correspond to the feature vectors associated with the 6 vertices of \( G_2 \), while the variances are \( I_5 \). Here, the factor map \( f \) is determined by the component from which the feature vector was sampled. Next, we randomly set the edge weights of network \( G_2 \) to an integer between 1 and 10. Then, the edge weights of network \( G_1 \) are randomly determined so that equation (9) holds, and therefore \( G_2 \) is a factor of \( G_1 \). The networks considered are undirected, in order to enable comparison with other methods. See Table 5 of Appendix A.4 for results on directed networks; there was no significant difference in the performance of NetOTC between directed and undirected networks. The experiment was repeated in a setting where \( G_2 \) is an approximate factor of \( G_1 \), that is, when the factor condition only holds approximately. See Appendix A.4 for explanations of how we generated an approximate factor.

NetOTC, FGW, and OT were applied to the generated networks \( G_1 \) and \( G_2 \) using an embedding-based cost equal to the squared Euclidean distances between the vectors associated with the vertices. Table 4 reports the vertex alignment accuracy of each method for different values of the variance \( \sigma^2 \). Vertex alignment accuracy was assessed by summing the mass of the optimal coupling on factor pairs of the form \( (u, f(u)) \). NetOTC outperforms the other methods, with the performance gap growing as \( \sigma \) decreases. For an exact factor with compatible cost, which occurs when \( \sigma = 2.5 \), NetOTC returns a perfect alignment, as guaranteed by Corollary 18. Results from other cases demonstrate that the performance of NetOTC is robust when the factor and cost conditions hold only approximately. It is also noteworthy that FGW and OT yield nearly identical alignment accuracy in all cases.
When we presented simulations and numerical experiments showing that NetOTC is competitive with, and sometimes better than, previous methods. NetOTC identifies an optimal coupling between two networks. Given two networks, $\mathcal{G}_1$ and $\mathcal{G}_2$, with node-related cost functions, NetOTC identifies an optimal coupling that respects edges: edges are aligned with edges in the same position in the two networks. The cost resulting from the optimal coupling serves as a numerical measure of the dissimilarity between the networks.

### 8 Proofs

In this paper we have introduced the NetOTC method for comparison and alignment of weighted networks. This new approach is based on constrained optimal transport of the random walks (Markov chains) associated with each network. Given two networks and a vertex-related cost function, NetOTC identifies an optimal coupling for the random walks, rather than stationary or other node-level distributions. We established several theoretical properties of NetOTC that support its use, including metric properties of the minimizing cost as well as its connection to other node-level distributions.

#### 8.1 Result for NetOTC Edge Preservation

**Proposition 2.** Let $\pi_e$ be the NetOTC edge alignment of networks $G_1 = (U, E_1, w_1)$ and $G_2 = (V, E_2, w_2)$ based on the optimal transport plan $\langle X^*, Y^* \rangle$. If $\pi_e((u, u'), (v, v')) > 0$ then $(u, u') \in E_1$ and $(v, v') \in E_2$.

| $\sigma$ | Exact factor | Approximate factor |
|----------|--------------|-------------------|
|         | NetOTC | FGW | OT | NetOTC | FGW | OT |
| 2.5     | 100.00 ± 0.00 | 98.17 ± 3.95 | 98.38 ± 3.40 | 98.57 ± 0.20 | 98.07 ± 4.55 | 98.32 ± 3.96 |
| 2.0     | 99.95 ± 0.46 | 96.57 ± 5.22 | 96.75 ± 5.08 | 98.09 ± 1.64 | 95.83 ± 5.35 | 96.00 ± 5.11 |
| 1.5     | 97.45 ± 5.10 | 90.20 ± 8.24 | 90.57 ± 8.18 | 96.43 ± 4.40 | 91.23 ± 7.85 | 91.65 ± 7.72 |
| 1.0     | 81.60 ± 13.88 | 73.23 ± 12.08 | 73.85 ± 12.05 | 79.44 ± 12.14 | 72.00 ± 11.74 | 72.00 ± 12.06 |

Table 4: Undirected networks: alignment accuracies of network factors. Average accuracies observed over 100 random network factors are reported along with their standard deviation.

### 7 Conclusion

In this paper we have introduced the NetOTC method for comparison and alignment of weighted networks. This new approach is based on constrained optimal transport of the random walks (Markov chains) associated with each network. Given two networks and a vertex-related cost function, NetOTC identifies an optimal coupling between their associated random walks that minimizes the expected cost at time zero. NetOTC applies to both directed and undirected networks, as well as networks with different numbers of nodes. Once edge weights and node-cost functions are specified, NetOTC has no free parameters and involves no randomization. The expected cost resulting from the optimal coupling serves as a numerical measure of the dissimilarity between the networks. In addition, the optimal transport plan itself offers interpretable, probabilistic alignments of both vertices and edges between the two networks.

We have demonstrated that NetOTC effectively incorporates global and local structure by focusing on coupling the full random walks, rather than stationary or other node-level distributions. We established several theoretical properties of NetOTC that support its use, including metric properties of the minimizing cost as well as its connection with short- and long-run average cost. A key feature of NetOTC is that it respects edges: edges are aligned with positive probability only if they are present in the given networks. In addition, we introduced a new notion of factor for weighted networks and established a close connection between factors and NetOTC. Complementing the theory, we presented simulations and numerical experiments showing that NetOTC is competitive with, and sometimes superior to, other optimal transport-based network comparison methods in the literature. In particular, NetOTC showed promise in identifying isomorphic networks using a local (degree-based) cost function.
Throughout this section, we will make use of the well-known fact that the stationary distribution of a simple random walk is identical.

**Proposition 7.** Connected undirected networks $G_1$ and $G_2$ are equivalent if and only if their respective random walks are identical.

---

**8.2 Properties of $\rho(G_1, G_2)$**

**Proposition 4.** Let $G_1$ and $G_2$ be networks with associated random walks $X$ and $Y$. Then

$$\rho(G_1, G_2) = \min_{(\bar{X}, \bar{Y}) \in \Pi_{TC}(X, Y)} \mathbb{E}c(\bar{X}, \bar{Y}),$$

and the optimal transport plans minimizing $\mathbb{E}c(\bar{X}, \bar{Y})$ coincide with those minimizing $\mathbb{E}c(X_0, \bar{Y}_0)$.

**Proof.** Let $(\bar{X}, \bar{Y})$ be a transition coupling of $X$ and $Y$. As $(\bar{X}, \bar{Y})$ is stationary, the ergodic theorem (Theorem C.1 of Levin and Peres (2017)) ensures that the limit

$$\bar{c}(\bar{X}, \bar{Y}) := \lim_k c_k(\bar{X}_0^{k-1}, \bar{Y}_0^{k-1})$$

exists almost surely and that $\mathbb{E}\bar{c}(\bar{X}, \bar{Y}) = \mathbb{E}c(\bar{X}, \bar{Y})$. It then follows from the definition of $\bar{c}$ that

$$\mathbb{E}c(\bar{X}, \bar{Y}) = \mathbb{E}\bar{c}(\bar{X}, \bar{Y}) = \mathbb{E}c(\bar{X}, \bar{Y}).$$

Taking minima over the set of all transition couplings of $X$ and $Y$ yields the result. 

**Proposition 5.** Let $G_1$ and $G_2$ be networks with associated random walks $X$ and $Y$. For each $k \geq 1$

$$\rho(G_1, G_2) \geq \min_k \mathbb{E}c_k(\bar{X}_0^{k-1}, \bar{Y}_0^{k-1}),$$

where the minimum is over the family of all couplings of $X_0^{k-1}$ and $Y_0^{k-1}$.

**Proof.** Every transition coupling of $X$ and $Y$ is also a joining of $X$ and $Y$ and therefore, as noted in (12), $\rho(G_1, G_2) \geq S_c(X, Y)$. Let $(\bar{X}, \bar{Y})$ be any joining of $X$ and $Y$. Stationarity of $(\bar{X}, \bar{Y})$ implies that

$$\mathbb{E}c(\bar{X}_0, \bar{Y}_0) = \mathbb{E}c_k(\bar{X}_0^{k-1}, \bar{Y}_0^{k-1})$$

and therefore $S_c(X, Y) = S_{c_k}(X, Y)$. Moreover, $(\bar{X}_0^{k-1}, \bar{Y}_0^{k-1})$ is also a coupling of $X_0^{k-1}$ and $Y_0^{k}$ so

$$S_{c_k}(X, Y) \geq \min_{(\bar{X}_0^{k-1}, \bar{Y}_0^{k-1}) \in \Pi(X_0^{k-1}, Y_0^{k-1})} \mathbb{E}c_k(\bar{X}_0^{k-1}, \bar{Y}_0^{k-1}).$$

Combining these inequalities gives the result. 

---

**8.3 Results for Undirected Networks with a Common Vertex Set**

Here we consider undirected networks on a common vertex set. We assume that the networks are connected. Throughout this section, we will make use of the well-known fact that the stationary distribution of a simple random walk $X = X_0, X_1, \ldots$ on a connected undirected network $G = (U, E, w)$ satisfies $p(u) = d(u)/D$, where $d(u)$ is the weighted degree of $u$ and $D$ is the sum of all the weights in the network.

**Proposition 7.** Connected undirected networks $G_1$ and $G_2$ are equivalent if and only if their respective random walks are identical.
Applying Proposition 5 yields the bound for $q$.

Proof. The random walks $0$—$1$ cost associated stationary Markov chains. As it defines a distance on stationary processes $S$ stationary for the transition coupling satisfying $\rho$. It suffices to show that $\rho$ transition coupling cost satisfies the triangle inequality for Markov chains when the cost $\rho$ and clearly $\rho(u, v) \geq 0$ is achieved by $\lambda$ satisfying $\lambda(u, v) = p(u)\|v = u\|$ which is stationary for the transition coupling satisfying $R(u', v' | u, v) = \begin{cases} P(u' | u)P(v' | v) & u = v, \\ P(u' | u) & otherwise \end{cases}$.

Now suppose that $G \sim G_2$. By Proposition 2 P and $Q$ are necessarily distinct, and consequently so are their associated stationary Markov chains. As it defines a distance on stationary processes $S_c(X, Y) > 0$ and applying Proposition 2, we conclude that $\rho(G_1, G_2) > 0$ as well.

Proposition 8. If the cost function $c : U \times U \rightarrow \mathbb{R}_+$ satisfies the properties of a metric on $U$, then $\rho$ is a metric on the equivalence classes of undirected networks with vertex set contained in $U$ defined by $\sim$.

Proof. The symmetry of $\rho$ is clear. It is established in Proposition 25 of O’Connor et al. (2022) that the optimal transition coupling cost satisfies the triangle inequality for Markov chains when the cost $c$ does, and therefore $\rho$ satisfies the triangle inequality. Thus it suffices to show that $\rho(G_1, G_2) = 0$ if and only if $G_1 \sim G_2$. Let $G_1$ and $G_2$ be networks satisfying $G \sim G_2$ with associated transition matrices $P$ and $Q$. By Proposition 7, $P$ and $Q$ are equal and clearly $\rho(G_1, G_2) = 0$ since $(\lambda, c) = 0$ is achieved by $\lambda$ satisfying $\lambda(u, v) = p(u)\|v = u\|$. We conclude that $\rho(G_1, G_2) > 0$ as well.

Proposition 10. Let $G_1$ and $G_2$ be undirected networks with the same vertex set. Let $d_1(u)$ and $d_2(u)$ be the degree functions of $G_1$ and $G_2$, respectively, and assume that each network has a total degree of $D$. Then under the zero-one cost $c(u, u') = \mathbb{I}(u \neq u')$,

\begin{align*}
\rho(G_1, G_2) &\geq \frac{1}{2D} \sum_{u \in U} |d_1(u) - d_2(u)| \\
\rho(G_1, G_2) &\geq \frac{1}{2D} \sum_{u, u' \in U} |w_1(u, u') - w_2(u, u')|
\end{align*}

Proof. The random walks $X$ and $Y$ associated with $G_1$ and $G_2$ have stationary distributions $p(u) = d_1(u)/D$ and $q(u) = d_2(u)/D$. Using the well-known connection between total variation distance and optimal transport under the $0$—$1$ cost (see, e.g., Equation 6.11 of Villani (2008)), we have

\begin{align*}
\min_{(\hat{X}_0, \hat{Y}_0) \in \Pi(X_0, Y_0)} \mathbb{E}c(\hat{X}_0, \hat{Y}_0) &= \min_{(\hat{X}_0, \hat{Y}_0) \in \Pi(X_0, Y_0)} \mathbb{E}1(\hat{X}_0 \neq \hat{Y}_0) \\
&= \frac{1}{2} \sum_{u \in U} |p(u) - q(u)| = \frac{1}{2D} \sum_{u \in U} |d_1(u) - d_2(u)|.
\end{align*}

Applying Proposition 5 yields the bound for $k = 1$. To obtain the bound for $k = 2$, let $\delta_2((u, u'), (v, v')) = \mathbb{I}((u, u') \neq (v, v'))$ and note that

\begin{align*}
\delta_2((u, u'), (v, v')) &\leq \mathbb{I}(u \neq v) + \mathbb{I}(u' \neq v') = 2c_2((u, u'), (v, v')).
\end{align*}

By Proposition 5

\begin{align*}
\rho(G_1, G_2) &\geq \min_{(\hat{X}_0, \hat{Y}_0) \in \Pi(X_0, Y_0)} \mathbb{E}c_2(\hat{X}_0, \hat{Y}_0) \geq \frac{1}{2} \min_{(\hat{X}_0, \hat{Y}_0) \in \Pi(X_0, Y_0)} \mathbb{E}\delta_2(\hat{X}_0, \hat{Y}_0).
\end{align*}
Then using the connection between the transport cost with respect to $\delta_2$ and the total variation distance once again, we obtain

$$
\rho(G_1, G_2) \geq \frac{1}{4} \sum_{u, u' \in U} |\mathbb{P}(X_0^1 = (u, u')) - \mathbb{P}(Y_0^1 = (u, u'))|
$$

$$
= \frac{1}{4} \sum_{u, u' \in U} |p(u)\mathbb{P}(X_1 = u'|X_0 = u) - q(u)\mathbb{P}(Y_1 = u'|Y_0 = u)|
$$

$$
= \frac{1}{4} \sum_{u, u' \in U} \left| \frac{d_1(u)}{D} w_1(u, u') - \frac{d_2(u)}{D} w_2(u, u') \right|
$$

$$
= \frac{1}{4D} \sum_{u, u' \in U} |w_1(u, u') - w_2(u, u')|.
$$

\[ \square \]

8.4 Results Concerning Network Factors

In this section, we prove the results about factor maps, including Theorems [16] and [19].

**Proposition 14.** If $(\tilde{X}, \tilde{Y})$ is a stationary Markov coupling corresponding to a strongly connected network $H$ with vertex set $W$, then $(\tilde{X}, \tilde{Y})$ is a transition coupling of $X$ and $Y$ if and only if the restriction of $\pi_V$ to $W$ is a factor map from $H$ to $G_1$ and the restriction of $\pi_V$ to $W$ is a factor map from $H$ to $G_2$.

**Proof.** In this setting, the conditions in Definition [1] for $(\tilde{X}, \tilde{Y})$ to be a transition coupling are precisely equivalent to Condition [9] for the restrictions of $\pi_U$ and $\pi_V$ to $W$. \[ \square \]

**Theorem 16.** Suppose $G_1$ and $G_2$ are strongly connected, weighted directed networks with associated random walks $X$ and $Y$, respectively.

1. If $G_2$ is a factor of $G_1$ with factor map $f$, then $Y \overset{d}{=} f(X)$, and $(X, f(X))$ is a deterministic transition coupling from $X$ to $Y$.

2. If $(\tilde{X}, \tilde{Y})$ is a deterministic transition coupling from $X$ to $Y$, then the induced map $f : U \to V$ is a factor map from $G_1$ to $G_2$.

**Proof.** To prove 1., let $f$ be a factor map from $G_1$ to $G_2$. We first show $Y \overset{d}{=} f(X)$. In order to simplify notation, we will let $f(X_0^{n-1}) = f(X_0), \ldots, f(X_{n-1})$. Let us prove by induction that for any $v_0^n \in V$, we have

$$
\mathbb{P}(f(X_0^n) = v_0^n) = \mathbb{P}(Y_0^n = v_0^n).
$$

The base case ($n = 0$) is immediate from Equation [11]. For the inductive step, we suppose it is true for some $n \geq 0$. Let $v_0^{n+1} \in V$. Then we have

$$
\mathbb{P}(f(X_0^n) = v_0^{n+1}) = \sum_{u_0^{n+1} \in f^{-1}(v_0^{n+1})} \mathbb{P}(X_0^{n+1} = u_0^{n+1})
$$

$$
= \sum_{u_0^{n+1} \in f^{-1}(v_0^{n+1})} \mathbb{P}(X_0^n = u_0^n) \cdot \mathbb{P}(X_{n+1} = u_{n+1} \mid X_0^n = u_0^n)
$$

$$
= \sum_{u_0^n \in f^{-1}(v_0^n)} \mathbb{P}(X_0^n = u_0^n) \cdot \sum_{u_{n+1} \in f^{-1}(v_{n+1})} \mathbb{P}(u_{n+1} \mid u_n)
$$

$$
= Q(v_{n+1} \mid v_n) \cdot \sum_{u_0^n \in f^{-1}(v_0^n)} \mathbb{P}(X_0^n = u_0^n)
$$

$$
= \mathbb{P}(Y_{n+1} = v_{n+1} \mid Y_n = v_n) \cdot \mathbb{P}(Y_0^n = v_0^n)
$$

$$
= \mathbb{P}(Y_0^{n+1} = v_0^{n+1}),
$$

where we have used Equation [10] and the inductive hypothesis.
Next, we show that \((X, f(X))\) is a transition coupling of \(X\) and \(Y\). We begin by verifying that \((X, f(X))\) is Markov. Fixing \((u, v) \in U \times V\) and \(n \geq 1\), we have
\[
P((X_n, f(X_n)) = (u, v) | \{(X_i, f(X_i))\}_{i<n}) = P(X_n = u)\{X_{i<n}\}(f(u) = v) = P(X_n = u)\{X_{n-1}\}(f(u) = v) = P((X_n, f(X_n)) = (u, v) | X_{n-1}) = P((X_n, f(X_n)) = (u, v) | (X_{n-1}, f(X_{n-1}))),
\]
so the process \((X, f(X))\) is Markov.

This Markov chain clearly has a \(U\) marginal that is equal in distribution to \(X\) and the \(V\) marginal is equal in distribution to \(Y\) as we proved above. Thus the joint process is a coupling of \(X\) and \(Y\). So it suffices to check the transition coupling condition. Let \(R \in [0, 1]^{U \times |V|} \times [0, 1]^{U \times |V|}\) denote the transition matrix satisfying
\[
R(u', v' | u, v) = \begin{cases} 
P(u'|u)\mathbb{I}(f(u') = v') & f(u) = v \\
P(u'|u)Q(v'|v) & \text{otherwise} \end{cases}.
\]

Let \(p\) be the stationary distribution of \(X\). Then \(\lambda(u, v) = p(u)I(f(u) = v)\) is equal in distribution to \((X_0, f(X_0))\). Observe that for all \((u', v') \in U \times V\), we have
\[
\sum_{(u, v) \in U \times V} \lambda(u, v)R(u', v' | u, v) = \sum_{(u, v) \in U \times V} p(u)\mathbb{I}(f(u) = v)P(u'|u)\mathbb{I}(f(u') = v')
\]
\[
= \mathbb{I}(f(u') = v') \sum_{v' \in V} \sum_{u \in f^{-1}(v)} p(u)P(u'|u) = \mathbb{I}(f(u') = v') \sum_{u \in U} p(u)P(u'|u)
\]
\[
= p(u')\mathbb{I}(f(u') = v')
\]
\[
= \lambda(u', v'),
\]
and therefore \(\lambda\) is stationary for \(R\). So lastly, we only need to show that \(R \in \Pi_{TC}(P, Q)\). For pairs \((u, v) \in U \times V\) with \(f(u) \neq v\), we see that \(R(\cdot | u, v)\) is the independent coupling of \(P(\cdot | u)\) and \(Q(\cdot | v)\), which clearly satisfies the transition coupling condition. Thus we need only check the transition coupling condition for pairs \((u, v)\) satisfying \(f(u) = v\). Let \(u, u' \in U\) and \(v, v' \in V\) and suppose that \(f(u) = v\). Then
\[
\sum_{v' \in V} R(u', v' | u, v) = \sum_{v' \in V} P(u'|u)\mathbb{I}(f(u') = v') = P(u'|u).
\]

Now checking the other half of the transition coupling condition, let \(u \in U\) and \(v, v' \in V\) be such that \(f(u) = v\). Then by Equation (10), we have
\[
\sum_{u' \in U} R(u', v' | u, v) = \sum_{u' \in U} P(u'|u)\mathbb{I}(f(u') = v') = \sum_{u' \in f^{-1}(v')} P(u'|u) = Q(v'|v).
\]

Thus \((X, f(X))\) is a transition coupling of \(X\) and \(Y\). It is forward-deterministic by construction.

Now we prove 2. To that end, suppose \((\hat{X}, \hat{Y})\) is a forward-deterministic coupling of \(X\) and \(Y\), and let \(f : U \to V\) be the induced map. For notation, let \(R\) be the transition matrix associated to the joint Markov chain \((\hat{X}, \hat{Y})\). To verify that \(f\) is a factor map, let \(v, v' \in V\) and \(u \in f^{-1}(v)\). Since \((\hat{X}, \hat{Y})\) is forward deterministic, for every \(u' \in f^{-1}(v')\) we have that \(P(u'|u) = R((u', v') | (u, v))\). Then, also using the transition coupling property of \(R\), we see that
\[
\sum_{u' \in f^{-1}(v')} P(u' | u) = \sum_{u' \in f^{-1}(v')} R((u', v') | (u, v)) = \sum_{u' \in U} R((u', v') | (u, v)) = Q(v', v).
\]

\[\square\]

**Corollary 18.** Suppose \(G_1\) and \(G_2\) are strongly connected, weighted directed networks and \(f\) is a factor map from \(G_1\) to \(G_2\). If \(c\) is compatible with \(f\) then \((X, f(X))\) is an OTC of \(X\) and \(Y\).
Proof. By part 1. of Theorem\[16\], we have that \((X, f(X))\) is a transition coupling of \(X\) and \(Y\). Let \((\tilde{X}, \tilde{Y})\) be any transition coupling of \(X\) and \(\tilde{Y}\). Then,
\[
\mathbb{E}c(\tilde{X}_0, \tilde{Y}_0) \geq \mathbb{E}c(\tilde{X}_0, f(\tilde{X}_0)) = \mathbb{E}c(X_0, f(X_0)).
\]
Taking an infimum over all transition couplings \((\tilde{X}, \tilde{Y})\) of \(X\) and \(Y\), we conclude that \((X, f(X))\) is an optimal transition coupling of \(X\) and \(Y\), as desired. \(\square\)

In the following proof of our two-factor result (Theorem\[19\]), we will use the notion of relatively independent couplings. Suppose \(X, Y\), and \(Z\) are random variables and there are maps \(f\) and \(g\) such that \(f(X) \overset{d}{=} Z\) and \(g(Y) \overset{d}{=} Z\). The main property that we need is that there exists a coupling \((\tilde{X}, \tilde{Y})\) of \(X\) and \(Y\) such that \(f(\tilde{X}) = g(\tilde{Y})\) almost surely. The existence of such a coupling is usually demonstrated by constructing the relatively independent coupling of \(X\) and \(Y\) over \(Z\), which is defined by the property that
\[
\mathbb{P}(\tilde{X} \in A, \tilde{Y} \in B) = \mathbb{E}[\mathbb{P}(X \in A \mid Z) \cdot \mathbb{P}(Y \in B \mid Z)],
\]
where the expectation is taken with respect to \(Z\). In words, the relatively independent coupling makes \(\tilde{X}\) and \(\tilde{Y}\) conditionally independent given \(Z\). This construction is useful in optimal transport for proving the triangle inequality. In the context of ergodic theory, when the random variables are replaced by stationary processes, it is called the relatively independent joining of \(X\) and \(Y\) (De La Rue\[2005\]). We note if the stationary processes are the random walks on some strongly connected networks and the maps \(f\) and \(g\) are factor maps in the sense of Section\[5.4\] then the relatively independent joinings are in fact transition couplings.

**Proposition 20.** Suppose \(G_1 = (U, E_1, w_1), G_2 = (V, E_2, w_2), \) and \(G_3 = (W, E_3, w_3)\) are strongly connected weighted directed networks with associated random walks \(X, Y, \) and \(Z\). Further suppose that there are factor maps \(f : U \to W\) from \(G_1\) to \(G_3\) and \(g : V \to W\) from \(G_2\) to \(G_3\). Then there is a transition coupling \((\tilde{X}, \tilde{Y})\) of \(X\) and \(Y\) such that \(f(\tilde{X}) = g(\tilde{Y})\) holds almost surely.

Proof. Define the coupling \((\tilde{X}, \tilde{Y})\) to be the Markov chain with stationary distribution \(r\) and transition kernel \(R\) given as follows. For \(w \in W\) with \(\mathbb{P}(Z_0 = w) > 0\) and \((u, v) \in U \times V\) such that \(f(u) = g(v) = w\), let
\[
r(u, v) = \frac{p(u) \cdot q(v)}{\mathbb{P}(Z_0 = w)},
\]
and otherwise let \(r(u, v) = 0\). Furthermore, for \((w, w') \in E_3\) and \((u, v), (u', v') \in U \times V\) such that \(f(u) = g(v) = w\) and \(f(u') = g(v') = w'\), let
\[
R((u', v') \mid (u, v)) = \frac{p(u' \mid u) \cdot Q(u' \mid v)}{\mathbb{P}(Z_0 = w' \mid Z_0 = w)}.
\]
If \(f(u) = g(v) = w\) while \((u', v')\) does not satisfy \(f(u') = g(v') = w'\), then let \(R((u', v') \mid (u, v)) = 0\). Finally, if \(f(u) = g(v) = w\) does not hold, then let \(R((u', v') \mid (u, v)) = p(u' \mid u) \cdot Q(v' \mid v')\). Using this definition, one may immediately verify Condition\[1\], and thus \((\tilde{X}, \tilde{Y})\) is a transition coupling of \(X\) and \(Y\). Furthermore, by construction we have \(f(\tilde{X}) = g(\tilde{Y})\) almost surely. \(\square\)

With this result in hand, we may now proceed to our second main result concerning factors.

**Theorem 19.** Let \(G_1, G_2, H_1, \) and \(H_2\) be networks with vertex sets \(U, V, A, \) and \(B\), and associated Markov chains \(X, Y, W, \) and \(Z, \) respectively. Suppose that \(f : U \to A\) and \(g : V \to B\) are factor maps from \(G_1\) to \(H_1\) and \(G_2\) to \(H_2\), and that there are cost functions \(c_{ext} : U \times V \to \mathbb{R}_+\) and \(c : A \times B \to \mathbb{R}_+\) such that \(c_{ext}(u, v) = c(f(u), g(v))\).

1. If \((\tilde{X}, \tilde{Y})\) is an optimal transition coupling of \(X\) and \(Y\) with respect to \(c_{ext}\), then \((f(\tilde{X}), g(\tilde{Y}))\) is an optimal transition coupling of \(W\) and \(Z\) with respect to \(c\).

2. If \((\tilde{W}, \tilde{Z})\) is an optimal transition coupling of \(W\) and \(Z\) with respect to \(c\), then there exists an optimal transition coupling \((\tilde{X}, \tilde{Y})\) of \(X\) and \(Y\) with respect to \(c_{ext}\) such that \((f(\tilde{X}), f(\tilde{Y})) \overset{d}{=} (\tilde{W}, \tilde{Z})\).

Proof. Let \((\tilde{X}, \tilde{Y})\) be a transition coupling of \(X\) and \(Y\). Since \(f\) and \(g\) are factor maps, we see that \((f(\tilde{X}), g(\tilde{Y}))\) is a transition coupling of \(W\) and \(Z\). Then by the compatibility condition on the cost function we have
\[
\mathbb{E}(\tilde{X}, \tilde{Y}) = \mathbb{E}(f(\tilde{X}), f(\tilde{Y})).
\]
To ease the notational burden of the following argument, we do not distinguish between different couplings of the same random variables. In particular, the notation $\tilde{X}$ may represent formally distinct random variables (defined on different probability spaces) from one instance to the next, although it always denotes a random variable that is equal in distribution to $X$.

Now let $(\tilde{W}, \tilde{Z})$ be a transition coupling of $W$ and $Z$. We claim that there exists a transition coupling $(\tilde{X}, \tilde{Y})$ such that $(f(\tilde{X}), g(\tilde{Y})) \triangleq (\tilde{W}, \tilde{Z})$. To exhibit the desired transition coupling, we repeatedly use Proposition 20. Let $(X, W, Z)$ denote the relatively independent joining of $(X, f(X))$ and $(\tilde{W}, \tilde{Z})$ over $W$ (with the factor maps given by the natural projections of $(X, f(X))$ onto $f(X)$ and of $(\tilde{W}, \tilde{Z})$ onto $\tilde{W}$, respectively). Similarly, let $(\tilde{W}, \tilde{Z}, Y)$ be the relatively independent joining of $(\tilde{W}, \tilde{Z})$ and $(g(Y), Y)$ over $Z$. Now let $(X, \tilde{Y}, W, \tilde{Z})$ be the relatively independent joining of $(X, \tilde{Y}, W, \tilde{Z})$ and $(\tilde{W}, \tilde{Z}, Y)$ over $W$. Then the projection of $(X, \tilde{Y}, W, \tilde{Z})$ onto the first two coordinates gives a transition coupling of $X$ and $Y$ with the property that $(f(\tilde{X}), g(\tilde{Y})) \triangleq (\tilde{W}, \tilde{Z})$. We have thus established that every transition coupling $(\tilde{W}, \tilde{Z})$ of $W$ and $Z$ can be written as $(f(\tilde{X}), g(\tilde{Y}))$ for some transition coupling $(\tilde{X}, \tilde{Y})$ of $X$ and $Y$.

The two conclusions of the theorem are immediate consequences of (13) and the result of the previous paragraph.

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Appendix A  Experimental Details

In this appendix, we provide further details for the experiments discussed in Section 6. We refer to ExactOTC as the exact implementation of NetOTC, while EntropicOTC specifically represents the regularized version of the NetOTC algorithm.

A.1 Network Classification

In order to compute approximate solutions to the NetOTC problem, we used the EntropicOTC algorithm with \( L = 10, T = 50, \xi = 100, \) and 50 Sinkhorn iterations. The FGW cost was computed with a default parameter choice of \( \alpha = 0.5. \) The experiment was run on Matlab and a 24-core node in a university-owned computing cluster.

A.2 Network Isomorphism

The classes of networks we dealt with in this experiment are as follows. We give details on how we generated the random networks.

- SBM: A description of an SBM is provided in Section 6.4. The given set informs the number of vertices in each block. For example, SBM (7, 7, 7, 7) indicates an SBM having 4 blocks with 7 vertices in each block. SBM (10, 8, 6) has 3 blocks, and each block has 10, 8, and 6 vertices. The connection probabilities within the block were fixed to 0.7, and the probabilities between blocks were 0.1.

- Erdos-Renyi network: Erdos-Renyi network is a random network in which every pair of vertices is connected with an independent probability \( p \) by an unweighted edge. Remark that the Erdos-Renyi network is equivalent to an SBM with a single block. For each network generation, the number of vertices was randomly determined from the given set. The connection probability \( p \) was fixed as given in each class.

- Random weighted adjacency matrix: Each element of the adjacency matrix is randomly sampled from the given set. For example, random weighted adjacency matrix \( \{0, 1, 2\} \) indicates a network that its adjacency matrix elements are all sampled from the set \( \{0, 1, 2\} \). In order to restrict the network to an undirected network, we only sample the upper triangular matrix and the lower triangular matrix is symmetrically filled. Note that the number of vertices is randomly determined between 6 and 20.

- Random Lollipop network: An example of a lollipop network is presented in Figure 5. A lollipop consists of a candy part and a stick part. The number of vertices in the candy part is randomly chosen between 7 and 15. The number of vertices in the stick part is also determined between 7 and 15. We also add edges inside the candy to vary the lollipop. With a probability of 0.5, we connect an edge between pair of vertices in the candy.

We discuss how we establish if the algorithm successfully identified the isomorphism map. For given two isomorphic networks \( G_1 = (U, E_1, w_1) \) and \( G_2 = (V, E_2, w_2) \), each algorithm returns an vertex alignment \( \pi_v : (U, V) \rightarrow [0, 1] \). Define a hard alignment function \( \psi(\cdot) = \arg\max_{v \in V} \pi(\cdot, v) \), where \( \psi : U \rightarrow V \) returns the most aligned vertex in \( G_2 \) for each vertex in \( G_1 \). If \( \psi \) satisfies the following conditions, the algorithm correctly detects the isomorphism.

1. \( \psi \) is bijective.
2. For every \((u_1, u_2) \in E_1\), \((\psi(u_1), \psi(u_2)) \in E_2\) and \(w_2(\psi(u_1), \psi(u_2)) = w_1(u_1, u_2)\).
3. For every \((v_1, v_2) \in E_2\), \((\psi^{-1}(v_1), \psi^{-1}(v_2)) \in E_1\) and \(w_1(\psi^{-1}(v_1), \psi^{-1}(v_2)) = w_2(v_1, v_2)\).

Figure 5 shows an additional example of detecting network isomorphism. As in Figure 5 NetOTC successfully detects isomorphism, while OT and FGW do not.

The ExactOTC algorithm was utilized to solve the NetOTC problem, and a fixed \( \alpha = 0.5 \) was used for FGW. Note that the algorithms were applied only to the connected network among the generated networks. 95.48% of the generated networks were connected on average. The experiment was developed in Matlab and run on a 24-core node in a university-owned computing cluster.

A.3 Stochastic Block Model Alignment

Cross validation was performed for FGW (to select \( \alpha \in \{0, 0.1, \ldots, 1\} \)) by randomly generating 10 pairs of SBM networks and computing alignments of vertices and edges. Parameters that yielded the highest average alignment accuracy were selected, where separate parameters were chosen for optimizing vertex and edge alignment.
Figure 8: Alignment of two isomorphic wheel networks obtained by NetOTC, OT, and FGW. To make the task challenging, two edges were removed.

0.1 and 1 were selected for vertex and edge alignment, respectively. We note that this implies GW and FGW were equivalent for edge alignment in our experiment. The ExactOTC algorithm was used to compute solutions to the NetOTC problem. The experiment was developed and run in Matlab on a personal machine.

A.4 Network Factors

Network $G_2$ has $b$ vertices embedded in $\mathbb{R}^5$ where the vertices are sampled from $\mathcal{N}_5(0, \sigma^2 I_5)$. We denote the vertices of $G_2$ as $V_1, \ldots, V_b$. Then, we sample $m$ points from $\mathcal{N}_5(V_i, I_5)$ for each $i = 1, \ldots, b$ and the points will be the vertices of $G_1$. The total number of vertices of $G_1$ is $bm$. We set $b = 6$ and $m = 5$ in this experiment. We used $\alpha = 0.5$ as a default trade-off parameter when applying FGW. We note that the choice of $\alpha \in \{0, 0.1, \ldots, 1\}$ doesn’t affect the alignment result much.

This experiment was conducted not only in exact factor situations but also when we have approximate factors. We call it an approximate factor when Definition 12 approximately holds as follows. For every $v, v' \in V$ and a given error rate $\epsilon > 0$,

$$\sum_{u' \in f^{-1}(v')} w_1(u, u') \in \left[ (1 - \epsilon) \frac{d_1(u)}{d_2(v)} w_2(v, v'), (1 + \epsilon) \frac{d_1(u)}{d_2(v)} w_2(v, v') \right], \quad \forall u \in f^{-1}(v),$$

and

$$\sum_{v \in f^{-1}(v)} \sum_{u' \in f^{-1}(v')} w_1(u, u') = \sum_{u \in f^{-1}(v)} \frac{d_1(u)}{d_2(v)} w_2(v, v').$$
| Exact factor | Approximate factor |
|--------------|--------------------|
| NetOTC       | NetOTC             |
| $\sigma = 2.5$ | 100.00 ± 0.00     | 97.94 ± 0.26       |
| $\sigma = 2.0$ | 99.91 ± 0.65     | 97.57 ± 1.03       |
| $\sigma = 1.5$ | 97.46 ± 4.84     | 95.87 ± 3.37       |
| $\sigma = 1.0$ | 84.09 ± 11.02    | 84.06 ± 11.07      |

Table 5: Directed networks: alignment accuracies of network factors. Average accuracies observed over 100 random network factors are reported along with their standard deviation.

| AIDS | BZR | Cuneiform | MCF-7 | MOLT-4 | MUTAG | Yeast |
|------|-----|-----------|-------|--------|-------|-------|
| # of Vertices | 13.25 | 34.65 | 20.2 | 26.65 | 26.7 | 17.9 | 20.43 |
| ExactOTC | 4.35 | 37.83 | 10.52 | 22.78 | 24.47 | 9.12 | 10.82 |
| EntropicOTC | 0.43 | 5.57 | 1.04 | 2.91 | 3.07 | 0.77 | 1.12 |

Table 6: Average Runtimes for datasets investigated in Section 6.2 (sec). We also report the average number of vertices for the randomly selected 20 pairs of graphs.

| SBM-48-32 | SBM-96-64 | SBM-128-96 |
|-----------|-----------|------------|
| ExactOTC  | 41.92     | 334.53     |
| EntropicOTC | 6.26     | 156.58     |

Table 7: Runtimes for pairs of SBM (sec). SBM-\(a\text{-}b\) denotes a comparison of two SBMs with a total of \(a\) vertices and \(b\) vertices.

In particular, we allowed 5% error ($\epsilon = 0.05$) for the second condition in this experiment.

Table 5 reports the vertex alignment accuracy of NetOTC for directed networks at various variance settings. We may check that the performances are similar to applying NetOTC to undirected factor network pairs. Similar to the Stochastic Block Model Alignment experiment, the ExactOTC algorithm was used to obtain solutions to the NetOTC problem and was run in Matlab on a personal machine.

### A.5 Runtime Analysis of NetOTC

We report the runtime of NetOTC for the experiments discussed in Sections 6.2 and 6.4. The runtime metrics are presented for both ExactOTC and EntropicOTC, employing our Matlab implementation of these methods. First, we randomly selected 20 pairs of graphs from each of the seven datasets used in Section 6.2. The average computation time for each pair is detailed in Table 6. Next, we investigated the computation time for comparing two stochastic block models (SBMs). Following the procedure detailed in Section 6.4, we generated SBMs with 4 blocks. The within-block connection probabilities were set to 1, 0.8, 0.6, and 0.4, while the between-block connection probability was fixed at 0.1. The runtime results for comparing these SBMs are presented in Table 7.