Graph Similarity and Homomorphism Densities

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Abstract

We introduce the tree distance, a new distance measure on graphs. The tree distance can be computed in polynomial time with standard methods from convex optimization. It is based on the notion of fractional isomorphism, a characterization based on a natural system of linear equations whose integer solutions correspond to graph isomorphism. By results of Tinhofer (1986, 1991) and Dvořák (2010), two graphs $G$ and $H$ are fractionally isomorphic if and only if, for every tree $T$, the number of homomorphisms from $T$ to $G$ equals the corresponding number from $T$ to $H$, which means that the tree distance of $G$ and $H$ is zero. Our main result is that this correspondence between the equivalence relations “fractional isomorphism” and “equal tree homomorphism densities” can be extended to a correspondence between the associated distance measures. Our result is inspired by a similar result due to Lovász and Szegedy (2006) and Borgs, Chayes, Lovász, Sós, and Vesztergombi (2008) that connects the cut distance of graphs to their homomorphism densities (over all graphs), which is a fundamental theorem in the theory of graph limits. We also introduce the path distance of graphs and take the corresponding result of Dell, Grohe, and Rattan (2018) for exact path homomorphism counts to an approximate level. Our results answer an open question of Grohe (2020) and help to build a theoretical understanding of vector embeddings of graphs.

The distance measures we define turn out to be closely related to the cut distance. We establish our main results by generalizing our definitions to graphons, which are limit objects of sequences of graphs, as this allows us to apply techniques from functional analysis. We prove the fairly general statement that, for every “reasonably” defined graphon pseudometric, an exact correspondence to homomorphism densities can be turned into an approximate one. We also provide an example of a distance measure that violates this reasonableness condition. This incidentally answers an open question of Grebík and Rocha (2021).

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1 Introduction

Vector representations of graphs allow to apply standard machine learning techniques to graphs, and a variety of methods to generate such embeddings has been studied in the machine learning literature. However, from a theoretical point of view, these embeddings have not received much attention and are not well understood. Some machine learning methods only implicitly operate on such vector representations as they only access the inner products of these vectors. These methods are known as kernel methods and most graph kernels are based on counting occurrences of certain substructures, e.g., walks or trees. See [14] for a recent survey on vector embeddings.

Many kinds of substructure counts in a graph such as graph motifs are actually just homomorphism counts “in disguise”, and hence, homomorphisms provide a formal and flexible framework for counting all kinds of substructures in graphs [4]: a homomorphism from a graph $F$ to a graph $G$ is a mapping from the vertices of $F$ to the vertices of $G$ such that every edge of $F$ is mapped to an edge of $G$. A theorem of Lovász from 1967 [17], which states that two graphs $G$ and $H$ are isomorphic if and only if, for every graph $F$, the number $\text{hom}(F, G)$
of homomorphisms from $F$ to $G$ equals the corresponding number $\text{hom}(F,H)$ from $F$ to $H$, led to the development of the theory of graph limits \cite{2 19}, where one considers convergent sequences of graphs and their limit objects, graphons. In terms of the homomorphism vector $\text{Hom}(G) := (\text{hom}(F,G))_{F \in \mathcal{F}}$ of a graph $G$, the result of Lovász states that graphs are mapped to the same vector if and only if they are isomorphic.

Computing an entry of $\text{Hom}(G)$ is $\#P$-complete and recent results have mostly focused on restrictions $\text{Hom}_F(G) := (\text{hom}(F,G))_{F \in \mathcal{F}}$ of these vectors to classes $\mathcal{F}$ for which computing these entries is actually tractable. Under a natural assumption from parameterized complexity theory, this is the case for precisely the classes $\mathcal{F}$ of bounded tree width \cite{5}. This has led to various surprisingly clean results, e.g., for trees and, more general, graphs of bounded treewidth \cite{9}, cycles and paths \cite{3}, planar graphs \cite{21}, and, most recently, graphs of bounded tree-depth \cite{13}. These results only show what it means for graphs to be mapped to the same homomorphism vector; they do not say anything about the similarity of two graphs if the homomorphism vectors are not exactly the same but close. Grohe formulated the vague hypothesis that, for suitable classes $\mathcal{F}$, the embedding $\text{Hom}_F$ combined with a suitable inner product on the latent space induces a natural similarity measure on graphs \cite{14}. This is supported by initial experiments, which show that homomorphism vectors in combination with support vector machines perform well on standard graph classification. Our results further support this hypothesis from a theoretical standpoint by showing that tree homomorphism counts provide a robust similarity measure.

For the class $\mathcal{T}$ of trees and two graphs $G$ and $H$, we have $\text{Hom}_T(G) = \text{Hom}_T(H)$ if and only if $G$ and $H$ are not distinguished by color refinement (also known as the 1-dimensional Weisfeiler-Leman algorithm) \cite{9}, a popular heuristic for graph isomorphism. Another characterization of this equivalence due to Tinhofer is that of fractional isomorphism \cite{26}, \cite{27}. Let $A \in \mathbb{R}^{V(G) \times V(G)}$ and $B \in \mathbb{R}^{V(H) \times V(H)}$ be the adjacency matrices of $G$ and $H$, respectively, and consider the following system $F_{\text{iso}}(G,H)$ of linear equations:

$$F_{\text{iso}}(G,H) : \begin{cases} AX = XB \\ X1_{V(H)} = 1_{V(G)} \\ 1_{V(G)}^T X = 1_{V(H)}^T \\ \end{cases}$$

Here, $X$ denotes a $(V(G) \times V(H))$-matrix of variables, and $1_U$ denotes the all-1 vector over the index set $U$. The non-negative integer solutions to $F_{\text{iso}}(G,H)$ are precisely the permutation matrices that describe isomorphisms between $G$ and $H$. The non-negative real solutions are called fractional isomorphisms of $G$ and $H$. Tinhofer proved that $G$ and $H$ are not distinguished by the color refinement algorithm if and only if there is a fractional isomorphism of $G$ and $H$. Grohe proposed to define a similarity measure based on this characterization \cite{14}: For a matrix norm $\|\cdot\|$ that is invariant under permutations of the rows and columns, consider

$$\text{dist}_{\|\cdot\|}(G,H) := \min_{X \in [0,1]^{V(G) \times V(H)}, \text{ doubly stochastic}} \|AX - XB\|.$$ 

Most graph distance measures based on matrix norms are highly intractable as the problem of their computation is related to notoriously hard maximum quadratic assignment problem \cite{22}. This hardness, which stems from the minimization over the set of all permutation matrices, motivated Grohe to propose $\text{dist}_{\|\cdot\|}$, where the set of all permutation matrices is relaxed to the the convex set of doubly stochastic matrices, yielding a convex optimization problem. With the results of Tinhofer and Dvořák, we know that the graphs of distance zero w.r.t. $\text{dist}_{\|\cdot\|}$ are precisely those that cannot be distinguished by tree homomorphism counts.
So far, the only known connection between a graph distance measure based on matrix norms and graph homomorphisms is between the cut distance and normalized homomorphism numbers (called homomorphism densities) \[2\]. Grohe asks whether a similar correspondence between \(\|\cdot\|\) and restricted homomorphism vectors can be established, and we give a positive answer to this question. We introduce the tree distance \(\delta^T\) of graphs, which is a normalized variant of \(\|\cdot\|\) and show the following theorem, which is stated here only informally. We also introduce the path distance \(\delta^P\) of graphs and prove the analogous theorem to Theorem 1 for \(\delta^P\) and normalized path homomorphism counts.

\[\textbf{Theorem 1 (Informal Theorem 6 and Theorem 7).}\] Two graphs \(G\) and \(H\) are similar w.r.t. \(\delta^T\) if and only if the homomorphism densities \(t(T,G)\) and \(t(T,H)\) are close for trees \(T\).

In the theory of graph limits, graphons serve as limit objects for sequences of graphs. By defining distance measures on the more general graphons, we are able to use techniques from functional analysis to show that any “reasonably” defined pseudometric on graphons satisfying an exact correspondence to homomorphism densities also has to satisfy an approximate one. As an application, we get that both the tree and the path distance satisfy this correspondence to tree and path homomorphism densities, respectively. For the case of trees, we rely on a generalization of the notion of fractional isomorphism to graphons by Grebík and Rocha \[12\]. For the case of paths, we prove this generalization of the result of Dell, Grohe, and Rattan \[6\] by ourselves.

This paper is organized as follows. In the preliminaries, Section 2, we collect the definitions of graphs, the space \(L_2[0,1]\), graphons, and the cut distance. In Section 3, we define the tree distance and the path distance for graphs and formally state Theorem 1 and its path counterpart. In Section 4, we state and prove the theorems that allow us to show these correspondences for graphon pseudometrics. Section 5 provides the first application of these tools for the tree distance: we first state the needed result of fractional isomorphism of graphons due to Grebík and Rocha and then use this to define the tree distance of graphons. These definitions and results specialize to the ones presented in Section 3 for graphs. The treatment of the path distance for graphons is similar to the one of the tree distance, except for the fact that we prove a characterization of graphons with the same path homomorphism densities ourselves, and can be found in Section 6. In Section 7, we define another distance measure on graphs based on the invariant computed by the color refinement algorithm and show that it only satisfies one direction of the approximate correspondence to tree homomorphism densities. Our counterexample incidentally answers an open question of Grebík and Rocha \[12\]. Section 8 poses some interesting open questions that come up during the study of these distance measures. All missing proofs are collected in Appendix A together with a compilation of results on operators, graphons, and Markov operators used in these proofs.

2 Preliminaries

2.1 Graphs

By the term graph, we refer to a simple, undirected, and finite graph. For a graph \(G\), we denote its vertex set by \(V(G)\) and its edge set by \(E(G)\), and we let \(v(G) := |V(G)|\) and \(e(G) := |E(G)|\). We usually view the adjacency matrix \(A\) of a graph \(G\) as a matrix \(A \in \mathbb{R}^{V(G) \times V(G)}\), i.e., it is indexed by the vertices of \(G\). Sometimes, we assume without loss of generality that the vertex set of a graph is \([n] := \{1, \ldots, n\}\), where \(n \in \mathbb{N}\) is a natural number. A homomorphism from a graph \(F\) to a graph \(G\) is a mapping \(\varphi: V(F) \to V(G)\) such that \(\varphi(u)\varphi(v) \in E(G)\)
for every \( uv \in E(F) \). We denote the number of homomorphisms from \( F \) to \( G \) by \( \text{hom}(F,G) \). The homomorphism density from \( F \) to \( G \) is given by \( \text{t}(F,G) := \text{hom}(F,G)/\alpha(G)^{\varepsilon(F)} \).

A weighted graph \( G = (V,a,B) \) consists of a vertex set \( V \), a positive real vector \( a = (a_v)_{v \in V} \in \mathbb{R}^V \) of vertex weights and a real symmetric matrix \( B = (b_{uv}) \in [0,1]^{V \times V} \) of edge weights; that is, we restrict ourselves to edge weights from \([0,1]\]. We write \( \nu(G) = |V| \), \( V(G) = V \), \( \alpha_i(G) = a_i \), \( \alpha_G = \sum_{v \in V(G)} a_v \alpha_v(G) \) and \( \beta_{uv}(G) = b_{uv} \). A weighted graph is called normalized if \( \alpha_G = 1 \). For a simple graph \( F \) and a weighted graph \( G \), we define the homomorphism number

\[
\text{hom}(F,G) = \sum_{\varphi : V(F) \to V(G)} \prod_{uv \in E(F)} a_{\varphi(u)}(G) \prod_{uv \in E(F)} b_{\varphi(u)\varphi(v)}(G)
\]

and the homomorphism density \( \text{t}(F,G) = \text{hom}(F,G)/\alpha_G^{\varepsilon(F)} \). When viewing a graph as a weighted graph in the obvious way, these notions coincide with the ones for graphs.

### 2.2 The Space \( L_2[0,1] \) and Graphons

A detailed introduction to functional analysis can be found in [7]; here, we only repeat some notions we use throughout the main body of the paper. Let \( L_2[0,1] \) denote the space of \( \mathbb{R} \)-valued \( 2 \)-integrable functions on \([0,1]\) (modulo equality almost anywhere). We could consider consider an arbitrary standard Borel space instead, but for the sake of convenience, we stick to \([0,1]\) with the Lebesgue measure just as [19]. The space \( L_2[0,1] \) is a Hilbert space with the inner product defined by \( \langle f,g \rangle := \int_{[0,1]} f(x)g(x) \, dx \) for functions \( f,g \in L_2[0,1] \). Let \( T : L_2[0,1] \to L_2[0,1] \) be a bounded linear operator, or operator for short. We write \( \|T\|_{2 \to 2} \) for its operator norm, i.e., \( \|T\|_{2 \to 2} = \sup_{\|g\|_2 \leq 1} \|Tg\|_2 \). The Hilbert adjoint of \( T \) is the unique operator \( T^* : L_2[0,1] \to L_2[0,1] \) such that \( \langle Tf,g \rangle = \langle f,T^*g \rangle \) for all \( f,g \in L_2[0,1] \), and \( T \) is called self-adjoint if \( T^* = T \).

Let \( W \) denote the set of all bounded symmetric measurable functions \( W : [0,1]^2 \to \mathbb{R} \), called kernels. Let \( W_0 \subseteq W \) denote all such \( W \) that satisfy \( 0 \leq W \leq 1 \); such a \( W \) is called a graphon. Every kernel \( W \in W \) defines a self-adjoint operator \( T_W : L_2[0,1] \to L_2[0,1] \) by setting \( (T_Wf)(x) = \int_{[0,1]} W(x,y)f(y) \, dy \) for every \( x \in [0,1] \), which then is a Hilbert-Schmidt operator, and in particular, compact [19].

A kernel \( W \in W \) is called a step function if there is a partition \( S_1 \cup \cdots \cup S_k \) of \([0,1]\) such that \( W \) is constant on \( S_i \times S_j \) for all \( i,j \in [k] \). For a weighted graph \( H \) on \([n]\), one can define a step function \( W_H \in W \) by splitting \([0,1]\) into \( n \) intervals \( I_1, \ldots, I_n \), where \( I_i \) has length \( \lambda(I_i) = \alpha_i(H)/\alpha(H) \) for every \( i \in [n] \), and letting \( W_H(x,y) := \beta_{ij}(H) \) for all \( x \in I_i, y \in I_j \) and \( i,j \in [n] \). Of course, \( W_H \) depends on the labeling of the vertices of \( H \). Note that \( W_H \) is a graphon, and in particular, \( W_G \) is a graphon for every graph \( G \).

### 2.3 The Cut Distance

See [19] for a thorough introduction to the cut distance. The usual definition of the cut distance involves the blow-up \( G(k) \) of a graph \( G \) by \( k \geq 0 \), where every vertex of \( G \) is replaced by \( k \) identical copies, to get graphs on the same number of vertices. Going this route is rather cumbersome, and we directly define the cut distance for weighted graphs via fractional overlays; this definition also applies to graphs in the straightforward way. A fractional overlay of weighted graphs \( G \) and \( H \) is a matrix \( X \in \mathbb{R}^{V(G) \times V(H)} \) such that \( X_{uv} \geq 0 \) for all \( u \in V(G), v \in V(H) \), \( \sum_{v \in V(H)} X_{uv} = \alpha_u(G)/\alpha_G \) for every \( u \in V(G) \), and \( \sum_{u \in V(G)} X_{uv} = \alpha_v(H)/\alpha_H \) for every \( v \in V(H) \). Let \( X(G,H) \) denote the set of all fractional overlays of \( G \) and \( H \). Note that, for graphs \( G \) and \( H \), the second and third condition just
say that the row and column sums of $X$ are $1/\nu(G)$ and $1/\nu(H)$, respectively. For weighted graphs $G$ and $H$ and a fractional overlay $X \in X(G, H)$, let

$$d_\square(G, H, X) := \max_{Q, R \subseteq V(G) \times V(H)} \left| \sum_{i \in Q, j \in R} X_{ij} X_{ju} (\beta_{ij}(G) - \beta_{uv}(H)) \right|.$$ 

Then, define the cut distance $\delta_\square(G, H) := \min_{X \in X(G, H)} d_\square(G, H, X)$.

Defining the cut distance of graphons is actually much simpler. Define the cut norm on the linear space $W$ of kernels by $\|W\|_\square := \sup_{S, T \subseteq [0, 1]} \left| \int_{S \times T} W(x, y) \, dx \, dy \right|$ for $W \in W$; here, as in the whole of the paper, we tacitly assume sets (and functions) we take an infimum or supremum over to be measurable. Let $S_{[0, 1]}$ denote the group of all invertible measure-preserving maps $\varphi : [0, 1] \to [0, 1]$. For a kernel $W \in W$ and a $\varphi \in S_{[0, 1]}$, let $W^\varphi$ be the kernel defined by $W^\varphi(x, y) := W(\varphi(x), \varphi(y))$. For kernels $U, W \in W$, define their cut distance by setting $\delta_\square(U, W) := \inf_{\varphi \in S_{[0, 1]}} \|U - W^\varphi\|_\square$. This coincides with the previous definition when viewing weighted graphs as graphons [19, Lemma 8.9]. We can also express $\delta_\square(U, W)$ via the kernel operator as $\delta_\square(U, W) = \sup_{f, g : [0, 1] \to [0, 1]} \|f, T_0U - W\|_\square$ [19, Lemma 8.10].

The definition of the cut distance is quite robust. For example, allowing $f$ and $g$ in the previous definition to be complex-valued or choosing a different operator norm does not make a difference in most cases [15, Appendix E].

For a graph $F$ and a kernel $W \in W$, define the homomorphism density

$$t(F, W) := \int_{[0, 1]} W(x, x) \prod_{xy \in E(F)} dx_1 \cdots dx_n,$$

which coincides with the previous definition when viewing weighted graphs as graphons [19, Equation (7.2)]. Lemma 2 and Lemma 3 state the connection between the cut distance and homomorphism densities: Informally, the Lemma 2 states that graphons that are close in the cut distance have similar homomorphism densities, while Lemma 3 states that graphs that have similar homomorphism densities are close in the cut distance. We refer to such statements as a counting lemma and an inverse counting lemma, respectively.

**Lemma 2 (Counting Lemma 20).** Let $F$ be a simple graph, and let $U, W \in W_0$ be graphons. Then, $|t(F, U) - t(F, W)| \leq e(F) \cdot \delta_\square(U, W)$.

**Lemma 3 (Inverse Counting Lemma 3, 19).** Let $k > 0$, let $U, W \in W_0$ be graphons, and assume that, for every graph $F$ on $k$ vertices, we have $|t(F, U) - t(F, W)| \leq 2^{-k^2}$. Then, $\delta_\square(U, W) \leq 50/\sqrt{\log k}$.

In particular, graphons $U$ and $W$ have cut distance zero if and only if, for every graph $F$, we have $t(F, U) = t(F, W)$. Call a sequence $(W_n)_{n \in \mathbb{N}}$ of graphons convergent if, for every graph $F$, the sequence $(t(F, W_n))_{n \in \mathbb{N}}$ is Cauchy. The two theorems above yield that $(W_n)_{n \in \mathbb{N}}$ is convergent if and only if $(W_n)_{n \in \mathbb{N}}$ is Cauchy in $\delta_\square$. Let $W_0$ be obtained from $W_0$ by identifying graphons with cut distance zero; such graphons are called weakly isomorphic.

One of the main results from graph limit theory is the compactness of the space $(\mathcal{W}_0, \delta_\square)$.

**Theorem 4 (19).** The space $(\mathcal{W}_0, \delta_\square)$ is compact.

### 3 Similarity Measures of Graphs

In this section, we define the tree and path distances of graphs and formally state the correspondences to tree and path homomorphism densities, respectively. All presented results are specializations of the results for graphons proven in Section 5 and Section 6.
3.1 The Tree Distance of Graphs

Recall that two graphs $G$ and $H$ have the same tree homomorphism counts if and only if the system $F_{\text{iso}}(G, H)$ of linear equations has a non-negative solution. Based on this, Grohe proposed $\text{dist}_T$ as a similarity measure of graphs. This is nearly what we define as the tree distance of graphs. What is missing is, first, a more general definition for graphs with different numbers of vertices and, second, an appropriate choice of a matrix norm with an appropriate normalization factor; analogously to the cut distance, we normalize the tree distance to values in $[0, 1]$. As in the definition of the cut distance in the preliminaries, we handle graphs on different numbers of vertices by considering fractional overlays instead of blow-ups (and doubly stochastic matrices). Recall that a fractional overlay of graphs $G$ and $H$ is a matrix $X \in \mathbb{R}^{(V(G) \times V(H))}$ such that $X_{uv} \geq 0$ for all $u \in V(G)$, $v \in V(H)$, $\sum_{v \in V(H)} X_{uv} = 1/\nu(G)$ for every $u \in V(G)$, and $\sum_{u \in V(G)} X_{uv} = 1/\nu(H)$ for every $v \in V(H)$. If $\nu(G) = \nu(H)$, then the difference between a fractional overlay and a doubly stochastic matrix is just a factor of $\nu(G)$. Also recall that $\mathcal{X}(G, H)$ denotes the set of all fractional overlays of $G$ and $H$.

We consider two matrix norms for the tree distance: First, just like in the definition of the cut distance, we use the cut norm for matrices, introduced by Frieze and Kannan [11], defined as $\|A\| := \max_{X\subseteq[m],T\subseteq[n]} |\sum_{i,j \in T} A_{ij}|$ for $A \in \mathbb{R}^{m \times n}$. Second, we also consider the more standard spectral norm $\|A\|_2 := \sup_{x \in \mathbb{R}^n, \|x\|_2 \leq 1} \|Ax\|_2$ of a matrix $A \in \mathbb{R}^{m \times n}$. From a computational point of view, the Frobenius norm might also be appealing, but this would lead to a different topology, cf. [15 Appendix E].

**Definition 5 (Tree Distance of Graphs).** Let $G$ and $H$ be graphs with adjacency matrices $A \in \mathbb{R}^{V(G) \times V(G)}$ and $B \in \mathbb{R}^{V(H) \times V(H)}$, respectively. Then, define

$$
\delta_T^\square(G, H) := \inf_{X \in \mathcal{X}(G, H)} \frac{1}{\nu(G) \cdot \nu(H)} \|\nu(H) \cdot AX - \nu(G) \cdot XB\|_2 \\
\delta_T^2(G, H) := \inf_{X \in \mathcal{X}(G, H)} \frac{1}{\sqrt{\nu(G) \cdot \nu(H)}} \|\nu(H) \cdot AX - \nu(G) \cdot XB\|_2.
$$

Note that the spectral norm requires an adapted normalization factor in Definition 5. The advantage of $\delta_T^\square$ is the close connection to the cut distance, which also utilizes the cut norm. However, the crucial advantage of the spectral norm is that minimization of the spectral norm of a matrix is a standard application of interior-point methods in convex optimization. In particular, an $\varepsilon$-solution to $\delta_T^\square$ can be computed in polynomial time [23 Section 6.3.3]. For $\delta_T^2$, it is not clear whether this is possible.

From the results of Section 5 we get that $\delta_T^\square$ and $\delta_T^2$ are pseudometrics (Lemma 16) and that two graphs have distance zero if and only if their tree homomorphism densities are the same (Lemma 18). Moreover, we have $\delta_T^2 \leq \delta_\square$ (Lemma 19), and these pseudometrics are invariant under blow-ups. Finally, we get the following counting lemma (Corollary 20) and inverse counting lemma (Corollary 21).

**Theorem 6 (Counting Lemma for $\delta_T$, Graphs).** Let $\delta_T \in \{\delta_T^\square, \delta_T^2\}$. For every tree $T$ and every $\varepsilon > 0$, there is an $\eta > 0$ such that, for all graphs $G$ and $H$, if $\delta_T(G, H) \leq \eta$, then $|t(T, G) - t(T, H)| \leq \varepsilon$.

**Theorem 7 (Inverse Counting Lemma for $\delta_T$, Graphs).** Let $\delta_T \in \{\delta_T^\square, \delta_T^2\}$. For every $\varepsilon > 0$, there are $k > 0$ and $\eta > 0$ such that, for all graphs $G$ and $H$, if $|t(T, G) - t(T, H)| \leq \eta$ for every tree $T$ on at most $k$ vertices, then $\delta_T(G, H) \leq \varepsilon$. 
3.2 The Path Distance of Graphs

Dell, Grohe, and Rattan proved that two graphs $G$ and $H$ have the same path homomorphism counts if and only if the system $F_{iso}(G, H)$ of linear equations has a real solution. This transfers to the definition of the path distance, i.e., we define the path distance analogously to the tree distance but relax the non-negativity condition of fractional overlays. For graphs $G$ and $H$, we call a matrix $X \in \mathbb{R}^{V(G) \times V(H)}$ a signed fractional overlay of $G$ and $H$ if $\|Xy\|_2 \leq \|y\|_2/\sqrt{v(H)}$ for every $y \in \mathbb{R}^{V(H)}$, $\sum_{v \in V(H)} X_{uv} = 1/v(G)$ for every $u \in V(G)$, and $\sum_{u \in V(G)} X_{uv} = 1/v(H)$ for every $v \in V(H)$. Let $\mathcal{S}(G, H)$ denote the set of all signed fractional overlays of $G$ and $H$. The first condition requires that $X$ is a contraction (up to a scaling factor) in the spectral norm; we need this to guarantee that our definition of the path distance actually yields a pseudometric. This restriction to the spectral norm stems from the fact that the proof of Dell, Grohe, and Rattan [6] (and our generalization thereof to graphons) only guarantees that the constructed solution is a contraction in the spectral norm, cf. Section 3 for the details.

Definition 8 (Path Distance of Graphs). Let $G$ and $H$ be graphs with adjacency matrices $A \in \mathbb{R}^{V(G) \times V(G)}$ and $B \in \mathbb{R}^{V(H) \times V(H)}$, respectively. Then, define

$$\delta^2_\square(G, H) := \inf_{X \in \mathcal{S}(G, H)} \frac{1}{\sqrt{v(G)v(H)}} \|v(H) \cdot AX - v(G) \cdot XB\|_2.$$ 

From Section 3, we get that $\delta^2_\square$ is a pseudometric (Lemma 25) that is invariant under blow-ups and that has as graphs of distance zero precisely those with the same path homomorphism densities. Moreover, we get the following (quantitative) counting lemma (Corollary 27) and inverse counting lemma (Corollary 30).

Theorem 9 (Counting Lemma for $\delta^2_\square$, Graphs). Let $P$ be a path, and let $G$ and $H$ be graphs. Then, $|t(P, G) - t(P, H)| \leq \epsilon(P) \cdot \delta^2_\square(G, H)$.

Theorem 10 (Inverse Counting Lemma for $\delta^2_\square$, Graphs). For every $\epsilon > 0$, there are $k > 0$ and $\eta > 0$ such that, for all graphs $G$ and $H$, if $|t(P, G) - t(P, H)| \leq \eta$ for every path $P$ on at most $k$ vertices, then $\delta^2_\square(G, H) \leq \epsilon$.

4 Graphon Pseudometrics and Homomorphism Densities

In this section, we provide the main tools we need to prove the correspondences between the tree and path distances and tree and path homomorphism densities, respectively. Consider a pseudometric $\delta$ on graphons. We say that $\delta$ is compatible with $\delta_\square$ if, for every sequence of graphons $(U_n)_n$, $U_n \in \mathcal{W}_0$, and every graphon $\bar{U} \in \mathcal{W}_0$, $\delta_\square(U_n, \bar{U}) \xrightarrow{n \to \infty} 0$ implies $\delta(U_n, \bar{U}) \xrightarrow{n \to \infty} 0$. For example, this is the case if $\delta \leq \delta_\square$, i.e., graphons only get closer if we consider $\delta$ instead of $\delta_\square$. We anticipate that the pseudometrics we are interested in, the tree distance and the path distance, are compatible with $\delta_\square$.

Together, the next two theorems state that every pseudometric that is compatible with $\delta_\square$ and whose graphons of distance zero can be characterized by homomorphism densities from a class of graphs $\mathcal{F}$ already has to satisfy both a counting lemma and an inverse counting lemma for this class $\mathcal{F}$. The proof of these theorems is a simple compactness argument, utilizing the compactness of the graphon space, Theorem 4 and the counting lemma for $\delta_\square$, Lemma 2. Therefore, it is absolutely crucial that we consider a pseudometric defined on graphons as the limit of a sequence of graphs may not be a graph.
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**Theorem 11** (Counting Lemma for $F$). Let $F$ be a class of graphs, and let $\delta^F$ be a pseudometric on graphons such that (1) $\delta^F$ is compatible with $\delta_C$ and (2), for all graphons $U, W \in \mathcal{W}_0$, $\delta^F(U, W) = 0$ implies $t(F, U) = t(F, W)$ for every graph $F \in F$. Then, for every graph $F \in F$ and every $\varepsilon > 0$, there is an $\eta > 0$ such that, for all graphons $U, W \in \mathcal{W}_0$, if $\delta^F(U, W) \leq \eta$, then $|t(F, U) - t(F, W)| \leq \varepsilon$.

**Proof of Theorem 11.** We proceed by contradiction and assume that the statement does not hold. Then, there is a graph $F \in F$ and an $\varepsilon > 0$ such that, for every $\eta > 0$, there are graphons $U, W \in \mathcal{W}_0$ such that $\delta^F(U, W) \leq \eta$ and $|t(F, U) - t(F, W)| > \varepsilon$.

Let $k > 0$. Then, by choosing $\eta = \frac{1}{k}$, we get that there are graphons $U_k, W_k \in \mathcal{W}_0$ such that $\delta^F(U_k, W_k) \leq \frac{1}{k}$ and $|t(F, U_k) - t(F, W_k)| > \varepsilon$. By the compactness theorem, Theorem 4, we get that the sequence $(U_k)_k$ has a convergent subsequence $(U_{k_i})_i$ converging to a graphon $\tilde{U}$ in the metric $\delta_C$. By another application of that theorem, we get that $(W_{k_i})_i$ has a convergent subsequence $(W_{k_i})_i$ converging to a graphon $\tilde{W}$ in the metric $\delta_C$. Then, $(U_{k_i})_i$ and $(W_{k_i})_i$ are sequences converging to $\tilde{U}$ and $\tilde{W}$ in the metric $\delta_C$, respectively.

Now, for every $i > 0$, we have

$$\delta^F(\tilde{U}, \tilde{W}) \leq \delta^F(U_{k_i}, \tilde{U}) + \delta^F(U_{k_i}, W_{k_i}) + \delta^F(W_{k_i}, \tilde{W}).$$

By assumption, we have $\delta^F(U_{k_i}, W_{k_i}) \leq \frac{1}{k}$, which means that $\delta^F(U_{k_i}, W_{k_i}) \xrightarrow{i \to \infty} 0$. Since $\delta_C(U_{k_i}, \tilde{U}) \xrightarrow{i \to \infty} 0$ and $\delta_C(W_{k_i}, \tilde{W}) \xrightarrow{i \to \infty} 0$, the first assumption about $\delta^F$ yields that we also have $\delta^F(U_{k_i}, \tilde{U}) \xrightarrow{i \to \infty} 0$ and $\delta^F(W_{k_i}, \tilde{W}) \xrightarrow{i \to \infty} 0$. Hence, we must have $\delta^F(\tilde{U}, \tilde{W}) = 0$.

Since $\delta^F(\tilde{U}, W) = 0$, we have $t(F, \tilde{U}) = t(F, \tilde{W})$ by the second assumption about $\delta^F$. By the Counting Lemma, Lemma 2, we get that $|t(F, U_{k_i}) - t(F, \tilde{U})| \xrightarrow{i \to \infty} 0$ and $|t(F, \tilde{W}) - t(F, W_{k_i})| \xrightarrow{i \to \infty} 0$. Now, for every $i > 0$, we have

$$|t(F, U_{k_i}) - t(F, W_{k_i})| \leq |t(F, U_{k_i}) - t(F, \tilde{U})| + |t(F, \tilde{U}) - t(F, \tilde{W})| + |t(F, \tilde{W}) - t(F, W_{k_i})|$$

Hence, $|t(F, U_{k_i}) - t(F, W_{k_i})| \xrightarrow{i \to \infty} 0$. This contradicts the fact that $|t(F, U_{k_i}) - t(F, W_{k_i})| > \varepsilon$ for every $i$.

Just as the proof of Theorem 11, the proof of Theorem 12 only relies on the compactness of the graphon space and the counting lemma for $\delta_C$, and not on a counting lemma for a specific class of graphs or the inverse counting lemma for $\delta_C$.

**Theorem 12** (Inverse Counting Lemma for $F$). Let $F$ be a class of graphs, and let $\delta^F$ be a pseudometric on graphons such that (1) $\delta^F$ is compatible with $\delta_C$ and (2), for all graphons $U, W \in \mathcal{W}_0$, $t(F, U) = t(F, W)$ for every graph $F \in F$ implies $\delta^F(U, W) = 0$. Then, for every $\varepsilon > 0$, there are $k > 0$ and $\eta > 0$ such that, for all graphons $U, W \in \mathcal{W}_0$, if $|t(F, U) - t(F, W)| \leq \eta$ for every graph $F \in F$ on at most $k$ vertices, then $\delta^F(U, W) \leq \varepsilon$.

**Proof.** We proceed by contradiction and assume that the statement does not hold. Then, there is an $\varepsilon > 0$ such that, for every $k > 0$ and every $\eta > 0$, there are graphons $U, W \in \mathcal{W}_0$ such that $|t(F, U) - t(F, W)| \leq \eta$ for every graph $F \in F$ on at most $k$ vertices but $\delta^F(U, W) > \varepsilon$.

Let $k > 0$. Then, by choosing $\eta = \frac{1}{k}$, we get that there are graphons $U_k, W_k \in \mathcal{W}_0$ such that $|t(F, U_k) - t(F, W_k)| \leq \frac{1}{k}$ for every graph $F \in F$ on at most $k$ vertices and $\delta^F(U_k, W_k) > \varepsilon$. By the compactness theorem, Theorem 4, we get that the sequence $(U_k)_k$ has a convergent subsequence $(U_{k_i})_i$ converging to a graphon $\tilde{U}$ in the metric $\delta_C$. By another application of that theorem, we get that $(W_{k_i})_i$ has a convergent subsequence
\[(W_t), \text{ converging to a graphon } \widehat{W} \text{ in the metric } \delta_\square. \text{ Then, } (U_t), \text{ and } (W_t), \text{ are sequences converging to } \widehat{U} \text{ and } \widehat{W} \text{ in the metric } \delta_\square, \text{ respectively.} \]

Let \( F \in \mathcal{F} \) be a graph. Now, for every \( i > 0, \) we have

\[
|t(F, \widehat{U}) - t(F, \widehat{W})| \leq |t(F, \widehat{U}) - t(F, U_t)| + |t(F, U_t) - t(F, W_t)| + |t(F, W_t) - t(F, \widehat{W})|
\]

By the counting lemma for \( \delta_\square, \) Lemma \[2\] we get that \( |t(F, \widehat{U}) - t(F, U_t)| \xrightarrow{i \to \infty} 0 \) and \( |t(F, W_t) - t(F, \widehat{W})| \xrightarrow{i \to \infty} 0. \) Moreover, by assumption, we have \( |t(F, U_t) - t(F, W_t)| \leq \frac{1}{i} \) for large enough \( i, \) which means that also \( |t(F, U_t) - t(F, W_t)| \xrightarrow{i \to \infty} 0. \) Hence, we must have \( t(F, \widehat{U}) = t(F, \widehat{W}). \)

As we have \( t(F, \widehat{U}) = t(F, \widehat{W}) \) for every graph \( F \in \mathcal{F}, \) the second assumption about \( \delta^F \) yields that \( \delta^F(\widehat{U}, \widehat{W}) = 0. \) Since \( \delta_\square(U_t, \widehat{U}) \xrightarrow{i \to \infty} 0 \) and \( \delta_\square(W_t, \widehat{W}) \xrightarrow{i \to \infty} 0, \) we also have \( \delta^F(U_t, \widehat{U}) \xrightarrow{i \to \infty} 0 \) and \( \delta^F(W_t, \widehat{W}) \xrightarrow{i \to \infty} 0 \) by the first assumption about \( \delta^F. \) Now, for every \( i > 0, \) we have

\[
\delta^F(U_t, W_t) \leq \delta^F(U_t, \widehat{U}) + \delta^F(\widehat{U}, \widehat{W}) + \delta^F(\widehat{W}, W_t).
\]

Hence, \( \delta^F(U_t, W_t) \xrightarrow{i \to \infty} 0. \) This contradicts the fact that \( \delta^F(U_t, W_t) > \varepsilon \) for every \( i. \)

5 Homomorphisms from Trees

In this section, we define the tree distance of graphons. To use the results from Section \[4\] we prove that the graphons of distance zero are precisely those with the same tree homomorphism densities (Lemma \[18\]) and that the tree distance is compatible with the cut distance (Lemma \[19\]). As for graphs, we define two variants of the tree distance, which yield the same topology (Lemma \[17\]): one using the analogue of the cut norm and one using the analogue of the spectral norm.

5.1 Fractional Isomorphism of Graphons

Recall that two graphs \( G \) and \( H \) with adjacency matrices \( A \in \mathbb{R}^{V(G) \times V(G)} \) and \( B \in \mathbb{R}^{V(H) \times V(H)}, \) respectively, are called fractionally isomorphic if there is a doubly stochastic matrix \( X \in \mathbb{R}^{V(G) \times V(H)} \) such that \( AX = XB. \) Grebík and Rocha proved Theorem \[13\] which generalizes this to graphons \[12\]: doubly stochastic matrices become Markov operators \[10\]. An operator \( S: L_2[0,1] \to L_2[0,1] \) is called a Markov operator if \( S \geq 0, \) i.e., \( f \geq 0 \) implies \( S(f) \geq 0, S(1) = 1, \) and \( S^*(1) = 1, \) where \( 1 \) is the all-one function on \([0,1].\) We denote the set of all Markov operators \( S: L_2[0,1] \to L_2[0,1] \) by \( \mathcal{M}. \)

\[\text{Theorem 13 \[12\], Part of Theorem 1.2. Let } U, W \in \mathcal{W}_0 \text{ be graphons. There is a Markov operator } S: L_2[0,1] \to L_2[0,1] \text{ such that } T_U \circ S = S \circ T_W \text{ if and only if } t(T, U) = t(T, W) \text{ for every tree } T.\]

5.2 The Tree Distance

Recall that, for graphons \( U, W \in \mathcal{W}_0, \) the cut distance of \( U \) and \( W \) can be written as \( \delta_\square(U, W) = \inf_{\phi \in \phi_{[0,1]} \setminus \{0,1\}} \sup_{f: [0,1] \to [0,1]} |f| T_U - W \circ g|, \) \( g \). We obtain the tree distance of \( U \) and \( W \) by relaxing measure-preserving maps to Markov operators.
Graph Similarity and Homomorphism Densities

Definition 14 (Tree Distance). Let $U, W \in \mathcal{W}_0$ be graphons. Then, define

$$
\delta^T(U, W) := \inf_{S \in \mathcal{M}} \sup_{f, g : [0, 1] \to [0, 1]} |\langle f, (T_U \circ S - S \circ T_W)g \rangle| \quad \text{and}
$$

$$
\delta_{2 \to 2}^T(U, W) := \inf_{S \in \mathcal{M}} \|T_U \circ S - S \circ T_W\|_{2 \to 2}.
$$

As the notation $\delta^T_{2 \to 2}$ indicates, the definition of $\delta^T$ is based (although not explicitly) on the cut norm, while $\delta_{2 \to 2}^T$ is defined via the operator norm $\|\cdot\|_{2 \to 2}$, which corresponds to the spectral norm for matrices. One can verify that these definitions specialize to the ones for graphs from Section 3.1. The proof can be found in Appendix A.4.

Lemma 15. Let $G$ and $H$ be graphs. Then, $\delta^T_G(G, H) = \delta^T_{2 \to 2}(W_G, W_H)$ and $\delta^T_H(G, H) = \delta_{2 \to 2}^T(W_G, W_H)$.

We verify that the tree distance actually is a pseudometric. To prove the triangle inequality for $\delta^T$ and $\delta_{2 \to 2}^T$, we use that a Markov operator is a contraction on $L_\infty[0, 1]$ and $L_2[0, 1]$, respectively [10, Theorem 13.2 b)]. The proof can be found in Appendix A.5.

Lemma 16. $\delta^T$ and $\delta_{2 \to 2}^T$ are pseudometrics on $\mathcal{W}_0$.

The Riesz-Thorin Interpolation Theorem (see, e.g., [11, Theorem 1.1.1]) allows to prove that both variants of the tree distance define the same topology. The proof of Lemma 17 can be found in Appendix A.6.

Lemma 17. Let $U, W \in \mathcal{W}_0$ be graphons. Then, $\delta^T(U, W) \leq \delta_{2 \to 2}(U, W) \leq 4\delta^T(U, W)^{1/2}$.

To be able to apply the results from Section 4 we need that the tree distance of two graphons is zero if and only if their tree homomorphism densities are the same. Let $U, W \in \mathcal{W}_0$ be graphons. From the respective definitions, it is not immediately clear that $\delta^T(U, W) = 0$ or $\delta_{2 \to 2}(U, W) = 0$ implies $t(T, U) = t(T, W)$ for every tree $T$ since the infimum over all Markov operators might not be attained. Here, we can use a continuity argument as the set of Markov operators is compact in the weak operator topology [10, Theorem 13.8]. However, we have to take a detour via a third variant of the tree distance where compactness in the weak operator topology suffices. All the details can be found in Appendix A.6.

Lemma 18. Let $U, W \in \mathcal{W}_0$ be graphons. Then, $\delta^T(U, W) = 0$ if and only if $t(T, U) = t(T, W)$ for every tree $T$.

The Koopman operator $T_\varphi : f \mapsto f \circ \varphi$ of a measure-preserving map $\varphi : [0, 1] \to [0, 1]$ is a Markov operator [11, Example 13.1, 3)]. Hence, the tree distance can be seen as the relaxation of the cut distance obtained by relaxing measure-preserving maps to Markov operators. In particular, this means that the tree distance is compatible with the cut distance. The proof of Lemma 19 can be found in Appendix A.7.

Lemma 19. Let $U, W \in \mathcal{W}_0$ be graphons. Then, $\delta^T(U, W) \leq \delta_C(U, W)$.

With Lemma 18 and Lemma 19 we can apply the theorems of Section 4 and get both a counting lemma and an inverse counting lemma for the tree distance.

Corollary 20 (Counting Lemma for $\delta^T$). Let $\delta^T \in \{\delta^T_1, \delta^T_{2 \to 2}\}$. For every tree $T$ and every $\varepsilon > 0$, there is an $\eta > 0$ such that, for all graphons $U, W \in \mathcal{W}_0$, if $\delta^T(U, W) \leq \eta$, then $|t(T, U) - t(T, W)| \leq \varepsilon$.

Corollary 21 (Inverse Counting Lemma for $\delta^T$). Let $\delta^T \in \{\delta^T_1, \delta^T_{2 \to 2}\}$. For every $\varepsilon > 0$, there are $k > 0$ and $\eta > 0$ such that, for all graphons $U, W \in \mathcal{W}_0$, if $|t(T, U) - t(T, W)| \leq \eta$ for every tree $T$ on $k$ vertices, then $\delta^T(U, W) \leq \varepsilon$. 
6 Homomorphisms from Paths

In this section, we define the path distance of graphons. We prove a quantitative counting lemma for it (Corollary 27) and only rely on the results from Section 4 to obtain an inverse counting lemma. To this end, we prove that the graphons of distance zero are precisely those with the same path homomorphism densities (Lemma 28) and that the path distance is compatible with the cut distance (Lemma 29). Since there is no existing characterization of graphons with the same path homomorphism densities that we can rely on, we first generalize the result of Dell, Grohe, and Rattan to graphons (Theorem 22).

6.1 Path Densities and Graphons

Dell, Grohe, and Rattan have shown the surprising fact that $G$ and $H$ have the same path homomorphism counts if and only if the system $F_{iso}(G, H)$ has a real solution $\theta$. We need a generalization of their characterization to graphons in order to define the path distance of graphons and apply the results from Section 4. If two graphons $U, W \in \mathcal{W}_0$ have the same path homomorphism densities, the proof of Theorem 22 yields an operator $S: L_2[0,1] \to L_2[0,1]$ such that $S(1) = 1$ and $S^*(1) = 1$, which generalizes the result of [6] in a straightforward fashion. An important detail is that the proof also yields that $S$ is an $L_2$-contraction; this guarantees that the path distance satisfies the triangle inequality, i.e., that it is a pseudometric in the first place. For the sake of brevity, we call an operator $S: L_2[0,1] \to L_2[0,1]$ a signed Markov operator if $S$ is an $L_2$-contraction, i.e., $\|Sf\|_2 \leq \|f\|_2$ for every $f \in L_2[0,1]$, $S(1) = 1$, and $S^*(1) = 1$. Let $\mathcal{S}$ denote the set of all signed Markov operators. It is easy to see that $\mathcal{S}$ is closed under composition and Hilbert adjoints.

Theorem 22. Let $U, W \in \mathcal{W}_0$. There is a signed Markov operator $S: L_2[0,1] \to L_2[0,1]$ such that $T_U \circ S = S \circ T_W$ if and only if $t(P, U) = t(P, W)$ for every path $P$.

Homomorphism densities from paths can be expressed in terms of operator powers. For $\ell \geq 0$, let $P_\ell$ denote the path of length $\ell$. Then, for a graphon $U$, we have

$$t(P_\ell, U) = \int_{[0,1]^{\ell+1}} \prod_{i \in [\ell]} U(x_i, x_{i+1}) \prod_{i \in [\ell+1]} dx_i = \langle 1, T_U^\ell 1 \rangle$$

for every $\ell \geq 0$. The proof of Theorem 22 utilizes the Spectral Theorem for compact operators on Hilbert spaces to express $1$ as a sum of orthogonal eigenfunctions. For a kernel $K \in \mathcal{W}$, $T_W: L_2[0,1] \to L_2[0,1]$ is a Hilbert-Schmidt operator and, hence, compact [19]. Since $L_2[0,1]$ is separable and $T_W$ is compact and self-adjoint, the Spectral Theorem yields that there is a countably infinite orthonormal basis $\{f^i\}$ of $L_2[0,1]$ consisting of eigenfunctions of $T_W$ with the corresponding multiset of eigenvalues $\{\lambda_i\} \subseteq \mathbb{R}$ such that $\lambda_n \xrightarrow{n \to \infty} 0$ (see, e.g., [8]). If graphons $U$ and $W$ have the same path homomorphism densities, an interpolation argument yields that the lengths of the eigenvectors in the decomposition of $1$ and their eigenvalues have to be the same. Then, one can define the operator $S$ from these eigenfunctions of $U$ and $W$. The detailed proof can be found in Appendix A.8.

6.2 The Path Distance

We define the path distance of graphons can analogously to the tree distance. However, as the proof of Theorem 22 does not yield that the resulting operator is an $L_\infty$-contraction, we are limited in our choice of norms.
Graph Similarity and Homomorphism Densities

Definition 23 (Path Distance). Let $U, W \in W_0$ be graphons. Then, define

$$\delta_{2-2}(U, W) := \inf_{S \in S} \| T_U \circ S - S \circ T_W \|_{2-2}.$$  

One can verify that this definition specializes to the one for graphs from Section 3.2. The proof can be found in Appendix A.4.

Lemma 24. Let $G$ and $H$ be graphs. Then, $\delta_{2}^G(G, H) = \delta_{2-2}(W_G, W_H)$.

The proof that $\delta_{2-2}$ is a pseudometric can be found in Appendix A.5.

Lemma 25. $\delta_{2-2}$ is a pseudometric on $W_0$.

To apply the theorems of Section 4, we need that two graphons have distance zero in the path distance if and only if their path homomorphism densities are the same and that $\delta_{2-2}$ is compatible with $\delta_\square$. For the former, we deviate from the way we proceeded for the tree distance as we actually can prove a quantitative counting lemma.

Theorem 26 (Counting Lemma for Paths). Let $P$ be a path, and let $U, W \in W_0$ be graphons. Then, for every operator $S$: $L_2[0,1] \rightarrow L_2[0,1]$ with $S(1) = 1$ and $S^*(1) = 1$,

$$|t(P, U) - t(P, W)| \leq e(P) \cdot \sup_{f,g: [0,1] \rightarrow [0,1]} |\langle f, (T_U \circ S - S \circ T_W)g \rangle|.$$  

Proof. Let $\ell \in \mathbb{N}$ and $S \in S$. Then,

$$|t(P, U) - t(P, W)| = |\langle 1, T_U^\ell(S(1)) \rangle - \langle (S^*1), T_W^\ell(1) \rangle|$$

$$= \left| \sum_{i \in [\ell]} (\langle 1, (T_U^{\ell-i} \circ S \circ T_W^{-1})1 \rangle - \langle 1, (T_U^{\ell-i} \circ S \circ T_W^{-1})1 \rangle) \right|$$

$$= \left| \sum_{i \in [\ell]} (T_U^{\ell-i}1, (T_U \circ S - S \circ T_W)(T_W^{i-1}1)) \right|$$

$$\leq \ell \cdot \sup_{f,g: [0,1] \rightarrow [0,1]} |\langle f, (T_U \circ S - S \circ T_W)g \rangle|.$$  

\hfill ▶

Theorem 26 suggests that, for graphons $U, W \in W_0$, one should define

$$\delta_2^U(U, W) := \inf_{S \in S} \sup_{f,g: [0,1] \rightarrow [0,1]} |\langle f, (T_U \circ S - S \circ T_W)g \rangle|.$$  

Then, we have $|t(P, U) - t(P, W)| \leq e(P) \cdot \delta_2^U(U, W)$ for every path $P$. However, as mentioned before, we cannot verify that $\delta_2^U$ is a pseudometric as the operator $S$ might not be an $L_\infty$-contraction.

Corollary 27 (Counting Lemma for $\delta_{2-2}^U$). Let $P$ be a path, and let $U, W \in W_0$ be graphons. Then, $|t(P, U) - t(P, W)| \leq e(P) \cdot \delta_{2-2}^U(U, W)$.

Proof. By the Cauchy-Schwarz inequality, we have

$$\sup_{f,g: [0,1] \rightarrow [0,1]} |\langle f, (T_U \circ S - S \circ T_W)g \rangle| \leq \sup_{f,g: [0,1] \rightarrow [0,1]} \|f\|_2 \|\langle (T_U \circ S - S \circ T_W)g \rangle\|_2$$

$$\leq \sup_{g: [0,1] \rightarrow [0,1]} \|T_U \circ S - S \circ T_W\|_{2-2} \|g\|_2$$

$$\leq \|T_U \circ S - S \circ T_W\|_{2-2}$$

for every operator $S$: $L_2[0,1] \rightarrow L_2[0,1]$. Hence, the statement follows from Theorem 26.  

\hfill ▶
With this explicit counting lemma, we obtain that two graphons have distance zero in the path distance if and only if their path homomorphism densities are the same.

**Lemma 28.** Let $U, W \in \mathcal{W}_0$ be graphons. Then, $\delta_{2-\varepsilon}^p(U, W) = 0$ if and only if $t(P, U) = t(P, W)$ for every path $P$.

**Proof.** If $\delta_{2-\varepsilon}^p(U, W) = 0$, then Corollary 27 yields that $t(P, U) = t(P, W)$ for every path $P$. On the other hand, if $t(P, U) = t(P, W)$ for every path $P$, then there is a signed Markov operator $S \in S$ with $T_U \circ S = S \circ T_W$ by Theorem 22. Then, $\delta_{2-\varepsilon}^p(U, W) = 0$ follows immediately from the definition.

By definition, the path distance is bounded from above by the tree distance (with the appropriate norm), which means that it also is compatible with the cut distance.

**Lemma 29.** Let $U, W \in \mathcal{W}_0$ be graphons. Then, $\delta_{2-\varepsilon}^p(U, W) \leq \delta_{2-\varepsilon}^c(U, W)$.

With these lemmas, we can apply Theorem 12 and obtain the following inverse counting lemma for the path distance.

**Corollary 30 (Inverse Counting Lemma for $\delta_{2-\varepsilon}^p$).** For every $\varepsilon > 0$, there are $k > 0$ and $\eta > 0$ such that, for all graphons $U, W \in \mathcal{W}_0$, if $|t(P, U) - t(P, W)| \leq \eta$ for every path $P$ on at most $k$ vertices, then $\delta_{2-\varepsilon}^p(U, W) \leq \varepsilon$.

### 7 The Color Distance

**Color Refinement**, also known as the *1-dimensional Weisfeiler-Leman algorithm*, is a heuristic graph isomorphism test. It computes a coloring of the vertices of a graph in a sequence of refinement rounds; we say that color refinement *distinguishes* two graphs if the computed color patterns differ. Formally, for a graph $G$, we let $C^G_i(u) = 1$ for every $u \in V(G)$ and $C^G_{i+1}(u) = \{C^G_i(v) \mid wv \in E(G)\}$ for every $i \geq 0$. Let $C^G_{\infty} = C^G_i$ for the smallest $i$ such that $C^G_i(u) = C^G_i(v) \iff C^G_i+1(u) = C^G_i+1(v)$ for all $u, v \in G$ (“$C_i$ is stable”). Then, color refinement distinguishes two graphs $G$ and $H$ if there is an $i \geq 0$ such that $\{C^G_i(v) \mid v \in V(G)\} \neq \{C^H_i(v) \mid v \in V(H)\}$. It is well-known that the partition $\{C^{-1}_i(i) \mid i \in C_{\infty}(V(G))\}$ is the coarsest equitable partition of $V(G)$, where a partition $\Pi$ of $V(G)$ is called equitable if for all $P, q \in \Pi$ and $u, v \in P$, the vertices $u$ and $v$ have the same number of neighbors in $Q$.

For a graph $G$, we can define a weighted graph $G/C_{\infty}^G$ by letting $V(G/C_{\infty}^G) := \{C^{-1}_i(i) \mid i \in C_{\infty}(V(G))\}$, $\alpha_{G/C_{\infty}^G}(C) := |C|$ for $C \in V(G/C_{\infty}^G)$, and $\beta_{G/C_{\infty}^G}(G) := M^G_{D^G/d^G}$ for all $C, D \in V(G/C_{\infty}^G)$, where $M^G_{D^G/d^G}$ is the number of neighbors a vertex from $C$ has in $D$, which is the same for all vertices in $C$ as the partition induced by the colors of $C^G_{\infty}$ is equitable. Note that we have $|C|M^G_{C^G_D} = |D|M^G_{C^G_C}$ as both products describe the number of edges between $C$ and $D$, i.e., $G/C_{\infty}^G$ is well-defined. Usually, when talking about the invariant $T^C_2$ computed by color refinement (see, e.g., 16), one does not normalize $M^G_{D^G}$ by $|D|$. However, by doing so, we do not only get a weighted graph (with symmetric edge weights), but the graphs $G$ and $G/C_{\infty}^G$ actually have the same tree homomorphism counts. Grebik and Rocha already introduced the graphon analogue $U/C(U)$ of $G/C_{\infty}^G$ and proved the same fact for it 12 Corollary 4.3; hence, we omit the proof.

**Lemma 31.** Let $T$ be a tree, and let $G$ be a graph. Then, $\text{hom}(T, G) = \text{hom}(T, G/C_{\infty}^G)$.

By the result of Dvořák 19, $G/C_{\infty}^G$ and $H/C_{\infty}^H$ are isomorphic if and only if $G$ and $H$ have the same tree homomorphism counts. Hence, it is tempting to define a tree distance-like similarity measure on graphs by simply considering the cut distance of $G/C_{\infty}^G$ and $H/C_{\infty}^H$. 
For graphs $G$ and $H$, we call $\delta^T_G(G, H) := \delta_G(G/C^G_{\infty}, H/C^H_{\infty})$ the color distance of $G$ and $H$. As the cut distance $\delta^T_G$ is a pseudometric on graphs, so is $\delta^T_{C^G_{\infty}}$. For $\delta^T_{C^G_{\infty}}$, we immediately obtain a quantitative counting lemma from Lemma 2 and Lemma 31.

**Corollary 32** (Counting Lemma for $\delta^T_{C^G_{\infty}}$). Let $T$ be a tree, and let $G$ and $H$ be graphs. Then, $|t(T, G) - t(T, H)| \leq |E(T)| \cdot \delta^T_{C^G_{\infty}}(G, H)$.

Clearly, $\delta^T_G$ and $\delta^T_{C^G_{\infty}}$ have the same graphs of distance zero. Moreover, one can easily verify that the tree distance is bounded from above by the color distance.

**Lemma 33.** Let $G$ and $H$ be graphs. Then, $\delta^T_G(G, H) \leq \delta^T_{C^G_{\infty}}(G, H)$.

**Proof.** We have $\delta^T_G(G, H) = \delta^T_G(G/C^G_{\infty}, H/C^H_{\infty}) \leq \delta_G(G/C^G_{\infty}, H/C^H_{\infty}) = \delta^T_{C^G_{\infty}}(G, H)$ by Lemma 31 and Lemma 19.

Now, the obvious question is whether these pseudometrics are the same or, at least, define the same topology. But it is not hard to find a counterexample; the color distance sees differences between graphs that the tree distance and tree homomorphisms do not see. In particular, an inverse counting lemma cannot hold for the color distance. See Figure 1 and for the moment, assume that we can construct a sequence $(G_n)_n$ of graphs such that $G_n/C^G_{\infty}$ is as depicted. It is easy to verify that $\delta_{C^G_{\infty}}(G_n/C^G_{\infty}, K_3) \xrightarrow{n \to \infty} 0$, and thus, both $\delta^T_{C^G_{\infty}}(G_n, K_3) \xrightarrow{n \to \infty} 0$ and $|t(T, G_n) - t(T, K_3)| \xrightarrow{n \to \infty} 0$ for every tree $T$. But, $\delta^T_{C^G_{\infty}}(G_n, K_3) \geq \frac{1}{3} - \frac{1}{3} - \frac{2}{3}$ for every $n$ since $G_n/C^G_{\infty}$ has a vertex without a loop.

The existence of graphs $G_n$ such that $G_n/C^G_{\infty}$ is as depicted in Figure 1 follows easily from inversion results for the color refinement invariant $I^G_{C^G_{\infty}}$. Otto first proved that $I^G_{C^G_{\infty}}$ admits polynomial time inversion on structures [22], and Kiefer, Schweitzer, and Selman gave a simple construction to show that $I^G_{C^G_{\infty}}$ admits linear-time inversion on the class of graphs [16]. Basically, we partition $3n$ vertices into three sets of size $n$ and add edges between these partitions such that they induce $n$, $(n-1)$-, and $(n-2)$-regular bipartite graphs.

The example in Figure 1 actually answers an open question of Grebík and Rocha [12] Question 3.1. They ask whether the set $\{W/C(W) \mid W \in \mathcal{W}_0\}$ is closed in $\mathcal{W}_0$: it is not. With a more refined argument, we can actually show that $\{W_{G/C^G_{\infty}} \mid G \text{ graph}\}$ is already dense in $\mathcal{W}_0$. By properly rounding the weights of a given weighted graph, we can turn the inversion result of [16] into a statement about approximate inversion. The proof of Theorem 34 can be found in Appendix A.9.

**Theorem 34.** Let $H$ be a weighted graph. For every $n \geq 2 \cdot \nu(H)$, there is a graph $G$ on $n^2$ vertices such that $\delta_{C^G_{\infty}}(G/C^G_{\infty}, H) \leq 3 \cdot \nu(H)/n + \frac{1}{2} \cdot (\nu(H)/n)^2$.

In Theorem 34, the size of the resulting graph depends on how close we want it to be to the input graph. A simple consequence of the compactness of the graphon space is that, for $\varepsilon > 0$, we can approximate any graphon with an error of $\varepsilon$ in $\delta_G$ by a graph on $N(\varepsilon)$.
vertices, where $N(\varepsilon)$ is independent of the graphon \cite{19} Corollary 9.25. With Theorem 34 this implies that the same is possible with the weighted graphs $G/C^G\infty$. This also means that the closure of the set $\{W_{G/C^G}\mid G \text{ graph}\}$ is already $\tilde{W}_0$.

8 Conclusions

We have introduced similarity measures for graphs that can be formulated as convex optimization problems and shown surprising correspondences to tree and path homomorphism densities. This takes previous results on the “expressiveness” of homomorphism counts from an exact to an approximate level. Moreover, it helps to give a theoretical understanding of kernel methods in machine learning, which are often based on counting certain substructures in graphs. Proving the correspondences to homomorphism densities was made possible by introducing our similarity measures for the more general case of graphons, where tools from functional analysis let us prove the general statement that every “reasonably defined” pseudometric has to satisfy a correspondence to homomorphism densities.

Various open questions remain. The compactness argument used in Section 4 only yields non-quantitative statements. Hence, we do not know how close the graphs have to be in the pseudometric for their homomorphism densities to be close and vice versa. Only for paths we were able to prove a quantitative counting lemma, which uses the same factor $e(F)$ as the counting lemma for general graphs. It seems conceivable that a quantitative counting lemma for trees that uses the same factor $e(T)$ also holds. As the proof of the quantitative inverse counting lemma is quite involved \cite{3,19}, proving such statements for trees and paths should not be easy.

More in reach seems to be the question of how the tree distance generalizes to the class $T_k$ of graphs of treewidth at most $k$. Homomorphism counts from graphs in $T_k$ can also be characterized in terms of linear equations in the case of graphs \cite{9} (see also \cite{6}). How does such a characterization for graphons look like? And how does one define a distance measure from this?

Another open question concerns further characterizations of fractional isomorphism, e.g., the color refinement algorithm, which gives a characterization based on equitable partitions. Can one prove a correspondence between the tree distance and, say, $\varepsilon$-equitable partitions? It is not hard to come up with a definition for such partitions; the hard part is to prove that graphs that are similar in the tree distance possess such a partition.

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Appendix

This appendix contains the proofs omitted from the main body of the paper and collects some results used in these proofs. We start with some additions to the preliminaries.

For $1 \leq p < \infty$, let $L_p[0,1]$ denote the space of $\mathbb{R}$-valued $p$-integrable functions on $[0,1]$ (modulo equality almost anywhere). Likewise, $L_\infty[0,1]$ denotes the space of essentially bounded $\mathbb{R}$-valued functions on $[0,1]$ (modulo equality almost anywhere). Unless explicitly stated otherwise, the functions that we consider are $\mathbb{R}$-valued. Let $1 \leq p < q \leq \infty$. By Hölder’s inequality, we have $\|f\|_p \leq \|f\|_q$ for every function $f \in L_q[0,1]$ since $[0,1]$ has measure one. In particular, we have $L_q[0,1] \subseteq L_p[0,1]$. Among these spaces, $L_2[0,1]$ plays a special role as it is a Hilbert space as mentioned in the preliminaries. For an operator $T$: $L_p[0,1] \rightarrow L_q[0,1]$, where $1 \leq p, q \leq \infty$, let $\|T\|_{p\rightarrow q}$ denote its operator norm, i.e., $\|T\|_{p\rightarrow q} = \sup_{\|g\|_p \leq 1} \|Tg\|_q$, and let $\|T\|_{\infty,p\rightarrow q}$ be the operator norm when viewing $T$ as an operator on the complex $L_p[0,1]$, i.e., $\|T\|_{\infty,p\rightarrow q} = \sup_{\|g\|_p \leq 1, g \in [0,1]} \|Tg\|_q$.

For $p \in [1, \infty]$, an operator $S$: $L_p[0,1] \rightarrow L_p[0,1]$ is called a Markov operator if $S \geq 0$ (“$S$ is positive”), i.e., $S(f) \geq 0$ implies $S(1) = 1$, and $\int_{[0,1]} (Sf)(x) \, dx = \int_{[0,1]} f(x) \, dx$ for every $f \in L_p[0,1]$. Here, $1$ is the one-function on $[0,1]$. For $L_2[0,1]$, the third condition can be reformulated as $S^*(1) = 1$, where $S^*$ is the Hilbert adjoint of $S$. Unless explicitly stated otherwise, we work with Markov operators $S$: $L_2[0,1] \rightarrow L_2[0,1]$ and denote the set of all such operators by $\mathcal{M}$. By Theorem 45 it does not really matter which space $L_p[0,1]$ one considers Markov operators on. Also note that the results on Markov operators in Appendix A.3 are originally stated for complex $L_p[0,1]$ spaces. Since we work with graphons, which are $\mathbb{R}$-valued, and Markov operators map $\mathbb{R}$-valued functions to $\mathbb{R}$-valued functions, cf. Lemma 12 this does not make a different for us.

Recall that every kernel $W \in \mathcal{W}$ defines an operator $T_W$ by setting $(T_Wf)(x) = \int_{[0,1]} W(x,y)f(y) \, dy$ for every $x \in [0,1]$. Unless specified otherwise, we view it as an operator $T_W$: $L_2[0,1] \rightarrow L_2[0,1]$. Then it is a Hilbert-Schmidt operator, and in particular, compact [19]. The definition of $T_W$ also allows to view it as an operator $T_W: L_1[0,1] \rightarrow L_\infty[0,1]$, and hence, by the aforementioned inclusions of $L_p$ spaces, we can view $T_W$ as an operator $T_W: L_p[0,1] \rightarrow L_q[0,1]$ for all $1 \leq p, q \leq \infty$.

A.1 Operators

- **Lemma 35** ([25, Theorem 12.7]). Let $T$ be a bounded linear operator on a Hilbert space $\mathcal{H} \neq \{0\}$. If $(Tg, g) = 0$ for every $g \in \mathcal{H}$, then $T = 0$.

- **Theorem 36** (Riesz-Thorin Interpolation Theorem, e.g., [1, Theorem 1.1.1]). In the following, all $L_p[0,1]$ spaces are complex. Assume that $p_0 \neq p_1$, $q_0 \neq q_1$, $T$: $L_{p_0}(X,S,\mu) \rightarrow L_{q_0}(Y,T,\nu)$ with norm $\|T\|_{p_0\rightarrow q_0}$, and $T$: $L_{p_1}(X,S,\mu) \rightarrow L_{q_1}(Y,T,\nu)$ with norm $\|T\|_{p_1\rightarrow q_1}$. Then, $T$: $L_p(X,S,\mu) \rightarrow L_q(Y,T,\nu)$ with norm $\|T\|_{p\rightarrow q} \leq \|T\|_{p_0\rightarrow q_0}$,$\|T\|_{p_1\rightarrow q_1}^\theta$, provided that $0 < \theta < 1$ and $\frac{1}{p} = \frac{1-\theta}{p_0} + \frac{\theta}{p_1}$, $\frac{1}{q} = \frac{1-\theta}{q_0} + \frac{\theta}{q_1}$.

A.2 Graphons

- **Lemma 37** ([19, Equation (7.2)]). Let $F$ be a graph and $H$ be a weighted graph. Then, $t(F,H) = t(F,W_H)$.

- **Lemma 38** ([19, Lemma 8.9]). Let $G$ and $H$ be weighted graphs. Then, $\delta_\Delta(G,H) = \delta_\Delta(W_G,W_H)$. 
Then, the restriction mapping 

\[ \Phi_p: M(X; Y) \to M_p(X; Y), \]

\[ \Phi_p(S) := S|_{L_p} \]

is a bijection satisfying \( \Phi_p(S') = (\Phi_p(S))' \) for every \( S \in M(X; Y) \). Finally, for \( 1 \leq p < \infty \), the mapping \( \Phi_p \) is a homeomorphism for the weak as well as the strong operators topologies.

By Theorem 45, the weak operator topology on the set of Markov operators does not change when one considers Markov operators as mappings \( L_p[0, 1] \to L_p[0, 1] \) for different \( p \in [1, \infty) \).

\[ \text{Theorem 46 ([10] Theorem 13.8]).} \quad \text{The set of Markov operators is compact with respect to the weak operator topology.} \]
A.4 Proof of Lemma 15 and Lemma 24 (Definitions Coincide)

We first prove Lemma 15, i.e., that the definitions of the tree distance for graphs coincide with the ones for graphons. In this subsection, we fix two graphs $G$ and $H$, where we w.l.o.g. assume that $V(G) = \{1, \ldots, n\} \times \{1, \ldots, m\}$. Let $I_1, \ldots, I_n$ and $J_1, \ldots, J_m$ be the partitions of $[0, 1]$ into the steps of $W_G$ and $W_H$, respectively, such that $I_i$ and $J_j$ correspond to vertex $i \in V(G)$ and $j \in V(H)$, respectively. Let $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{m \times m}$ be the adjacency matrices of $G$ and $H$, respectively. For a matrix $X \in \mathbb{R}^{n \times m}$, let the kernel $W_X$ be given by setting $W_X(x, y) := nm \cdot X_{ij}$ for all $x \in I_i$, $y \in J_j$, $i \in [n]$, $j \in [m]$. Then, let $T_X := T_{W_X}$ be the operator defined by $W_X$, i.e.,

$$(T_X f)(x) = \int_{[0, 1]} W_X(x, y) f(y) \, dy$$

for every $x \in [0, 1]$.

**Lemma 47.** For a fractional overlay $X \in \mathbb{R}^{n \times m}$, the operator $T_X$ is a Markov operator with Hilbert adjoint $T_X^* = T_{X^*}$.

**Proof.** For $x \in I_i$, we have

$$(T_X 1)(x) = \int_{[0, 1]} W_X(x, y) \, dy = \sum_{j \in [m]} \int_{J_j} nm \cdot X_{ij} \, dy = \sum_{j \in [m]} n \cdot X_{ij} = 1.$$ 

For $f, g \in L_2[0, 1]$, we have

$$\langle T_X f, g \rangle = \int_{[0, 1]} \int_{[0, 1]} W_X(x, y) f(y) g(x) \, dy \, dx = \int_{[0, 1]} \int_{[0, 1]} W_{X^*}(y, x) f(y) g(x) \, dx \, dy = \int_{[0, 1]} f(y) \int_{[0, 1]} W_{X^*}(y, x) g(x) \, dx \, dy = \langle f, T_{X^*} g \rangle,$$

where we, of course, used the Theorem of Fubini. Hence, $T_{X^*}$ is the Hilbert adjoint of $T_X$, and since $X$ is arbitrary, we also have $T_{X^*}(1) = 1$. Therefore, $T_X$ is a Markov operator. ◊

Let $S: L_2[0, 1] \to L_2[0, 1]$ be an operator. For $i \in [n]$, $j \in [m]$, we define

$$(X_S)_{ij} := \int_{I_i} S(\mathbb{1}_{J_j})(x) \, dx.$$ 

**Lemma 48.** For a Markov operator $S: L_2[0, 1] \to L_2[0, 1]$, the matrix $X_S$ is a fractional overlay of $G$ and $H$.

**Proof.** We have $X_S \in \mathbb{R}^{n \times m}$ with non-negative entries. For $i \in [n]$, the linearity of $S$ yields

$$\sum_{j \in [m]} (X_S)_{ij} = \sum_{j \in [m]} \int_{I_i} S(\mathbb{1}_{J_j})(x) \, dx = \int_{I_i} S(\mathbb{1})(x) \, dx = \int_{I_i} 1 \, dx = \frac{1}{n}.$$ 

For $j \in [m]$, we get

$$\sum_{i \in [n]} (X_S)_{ij} = \sum_{i \in [n]} \int_{J_j} S(\mathbb{1}_{J_i})(x) \, dx = \int_{[0, 1]} S(\mathbb{1}_{J_j})(x) \, dx = \int_{[0, 1]} \mathbb{1}_{J_j}(x) \, dx = \frac{1}{m}. \quad \square$$
Proof of Lemma 15 First Equality. First, we prove that $\delta^T_{\mathbb{F}}(G, H) \geq \delta^T_{\mathbb{F}}(W_G, W_H)$. Let $X \in \mathbb{R}^{n \times m}$ be a fractional overlay of $G$ and $H$. By Lemma 17, the operator $T_X$ is a Markov operator. For a measurable function $f: [0, 1] \to [0, 1]$, let $u^f \in \mathbb{R}^n$ be the vector with $u^f_i = n \cdot \int_{I_i} f(x) \, dx$ for every $i \in [n]$, and let $v^f \in \mathbb{R}^m$ be the vector with $v^f_j = m \cdot \int_{J_j} f(x) \, dx$ for every $j \in [m]$. For $x \in I_i$ and a measurable function $g: [0, 1] \to [0, 1]$, we have

$$((T_{W_G} \circ T_X)g)(x) = \int_{[0, 1]} W_G(x, y) \left( \int_{[0, 1]} W_X(y, z) g(z) \, dz \right) \, dy$$

$$= \sum_{k \in [n]} \int_{I_k} A_{ik} \left( \sum_{j \in [m]} \int_{J_j} n \cdot X_{kj} g(z) \, dz \right) \, dy$$

$$= \sum_{k \in [n]} A_{ik} \int_{I_k} \left( \sum_{j \in [m]} n \cdot X_{kj} v^g_j \right) \, dy$$

$$= (AXv^g)_i.$$ 

Hence, we get

$$(f, (T_{W_G} \circ T_X)g) = \int_{[0, 1]} f(x)((T_{W_G} \circ T_X)g)(x) \, dx$$

$$= \sum_{i \in [n]} \int_{I_i} f(x)(AXv^g)_i \, dx$$

$$= \frac{1}{n} \cdot \sum_{i \in [n]} (AXv^g)_i u^f_i$$

$$= \frac{1}{nm} \cdot u^T (n \cdot AX)v^g$$

for all measurable $f, g: [0, 1] \to [0, 1]$. In a similar fashion, one can verify that, for $x \in I_i$ and a measurable function $g: [0, 1] \to [0, 1]$, we have

$$((T_X \circ T_{W_H})g)(x) = \left( \frac{n}{m} \cdot XBv^g \right)_i$$

and, thus,

$$(f, (T_{W_G} \circ T_X)g) = \frac{1}{nm} \cdot u^T (n \cdot XB)v^g$$

for all measurable $f, g: [0, 1] \to [0, 1]$. Combining this yields

$$\delta^T_{\mathbb{F}}(W_G, W_H) = \inf_{S \in \mathcal{M}} \sup_{f, g: [0, 1] \to [0, 1]} |(f, (T_{W_G} \circ S \circ T_{W_H})g)|$$

$$\leq \inf_{X \in \mathcal{X}(G, H)} \sup_{f, g: [0, 1] \to [0, 1]} |(f, (T_{W_G} \circ T_X \circ T_{W_H})g)|$$

$$= \inf_{X \in \mathcal{X}(G, H)} \frac{1}{nm} \sup_{f, g: [0, 1] \to [0, 1]} |u^T (n \cdot AX - n \cdot XB)v^g|$$

$$= \inf_{X \in \mathcal{X}(G, H)} \frac{1}{nm} \|m \cdot AX - n \cdot XB\|$$

$$= \delta^T_{\mathbb{F}}(G, H)$$

since the maximum is attained at 0-1-vectors.
To prove that $\delta_T(G, H) \leq \delta_T(W_G, W_H)$, let $S : L_2[0, 1] \to L_2[0, 1]$ be a Markov operator. By Lemma 48, $X_S \in \mathbb{R}^{n \times m}$ is a fractional overlay of $G$ and $H$. For a set $P \subseteq [n]$, let $\mathbb{1}_P := \sum_{i \in P} \mathbb{1}_{I_i}$ and, for a set $Q \subseteq [m]$, let $\mathbb{1}_Q := \sum_{j \in Q} \mathbb{1}_{J_j}$. Then, for $x \in I_i$, the linearity of $S$ yields

\[
((T_W \circ S) \mathbb{1}_Q^T)(x) = \int_{[0,1]} W_G(x, y)(S \mathbb{1}_Q^T)(y) \, dy = \sum_{j \in Q} \int_{[0,1]} W_G(x, y)(\mathbb{1}_J_j)(y) \, dy
\]

\[
= \sum_{j \in Q} \sum_{k \in [n]} \int_{I_k} A_{ik}(\mathbb{1}_J_j)(y) \, dy
\]

\[
= \sum_{j \in Q} \sum_{k \in [n]} A_{ik}(X_S)_{kj}
\]

and, thus,

\[
\langle \mathbb{1}_P, (T_W \circ S) \mathbb{1}_Q^T \rangle = \int_{[0,1]} \mathbb{1}_P(x)((T_W \circ S) \mathbb{1}_Q^T)(x) \, dx = \sum_{i \in [n]} \int_{I_i} \mathbb{1}_P(x)\left(\sum_{j \in Q} (AX_S)_{ij}\right) \, dx
\]

\[
= \sum_{i \in [n]} \sum_{j \in Q} (AX_S)_{ij} \int_{I_i} \mathbb{1}_P(x) \, dx
\]

\[
= \frac{1}{nm} \sum_{i \in P, j \in Q} (m \cdot AX_S)_{ij}.
\]

In a similar fashion, one can show that, for a set $Q \subseteq [m]$ and $x \in [0, 1]$, we have

\[
((S \circ T_W) \mathbb{1}_Q^T)(x) = \sum_{k \in [m]} \left(\sum_{j \in T} \frac{1}{m} B_{kj}\right) S(\mathbb{1}_J_k)(x)
\]

and, thus,

\[
\langle \mathbb{1}_P, (S \circ T_W) \mathbb{1}_Q^T \rangle = \frac{1}{nm} \sum_{i \in P, j \in Q} (n \cdot XSB)_{ij}.
\]

Combining this yields

\[
\delta_T(G, H) = \inf_{X \in X(G, H)} \frac{1}{nm} \|m \cdot AX - n \cdot XB\|\]

\[
\leq \inf_{S \in M} \frac{1}{nm} \|m \cdot AXS - n \cdot XSB\|\]

\[
= \inf_{S \in M} \sup_{P \subseteq [n], Q \subseteq [m]} |\langle \mathbb{1}_P, (T_W \circ S - S \circ T_W) \mathbb{1}_Q^T \rangle|
\]

\[
\leq \delta_T(W_G, W_H).
\]

Proving the second equality is similar, although a bit more complicated due to the non-linearity of the square function. Here, we have to apply the Cauchy-Schwarz inequality at certain points.
Proof of Lemma 15 \[ \text{Second Equality.} \] First, we prove that \( \delta^T_{2} (G, H) \geq \delta^T_{2} (W_G, W_H) \). Let \( X \in \mathbb{R}^{n \times m} \) be a fractional overlay of \( G \) and \( H \). By Lemma 14, the operator \( T_X \) is a Markov operator. For \( g : [0, 1] \to \mathbb{R} \) with \( \| g \|_2 \leq 1 \), let \( v^g \in \mathbb{R}^m \) be given by \( v_j^g := \sqrt{m} \cdot \int_{I_j} g(x) \, dx \) for every \( j \in [m] \). Then,

\[
\| v^g \|_2^2 = \sum_{j \in [m]} m \cdot \left( \int_{I_j} g(x) \, dx \right)^2 \leq \sum_{j \in [m]} m \cdot \frac{1}{m} \cdot \int_{I_j} g(x)^2 \, dx \quad \text{(Cauchy-Schwarz)}
\]

that is, \( \| v^g \|_2 \leq \| g \|_2 \leq 1 \). For \( x \in I_i \), we have

\[
((T_{W_G} \circ T_X) g)(x) = \int_{[0,1]} W_G(x, y) \left( \int_{[0,1]} W_X(y, z) g(z) \, dz \right) dy
\]

\[
= \sum_{k \in [n]} \int_{I_k} A_{ik} \left( \sum_{j \in [m]} \int_{I_j} n m \cdot X_{kj} g(z) \, dz \right) dy
\]

\[
= \sum_{k \in [n]} A_{ik} \int_{I_k} \left( \sum_{j \in [m]} n \cdot m \cdot X_{kj} v_j^g \right) dy
\]

\[
= \frac{1}{\sqrt{m}} (m \cdot AXv^g)_i.
\]

In a similar fashion, one can verify that, for \( x \in I_i \), we have

\[
((T_X \circ T_{W_H}) g)(x) = \frac{1}{\sqrt{m}} (n \cdot XBv^g)_i
\]

and, thus,

\[
\| (T_{W_G} \circ T_X - T_X \circ T_{W_H}) g \|_2^2 = \int_{[0,1]} ((T_{W_G} \circ T_X - T_X \circ T_{W_H}) g(x))^2 \, dx
\]

\[
= \sum_{k \in [n]} \int_{I_k} \left( \frac{1}{\sqrt{m}} (m \cdot AX - n \cdot XB)v^g \right)_i^2 \, dx
\]

\[
= \sum_{k \in [n]} \left( \frac{1}{\sqrt{mnm}} (m \cdot AX - n \cdot XB)v^g \right)_i^2
\]

\[
= \| \frac{1}{\sqrt{nm}} (m \cdot AX - n \cdot XB)v^g \|_2^2.
\]

Hence,

\[
\delta^T_{2} (W_G, W_H) = \inf_{S \in \mathcal{M}} \sup_{\| g \|_2 \leq 1} \| (T_{W_G} \circ S - S \circ T_{W_H}) g \|_2
\]

\[
\leq \inf_{X \in \mathcal{X}(G, H)} \sup_{\| g \|_2 \leq 1} \| (T_{W_G} \circ T_X - T_X \circ T_{W_H}) g \|_2
\]

\[
= \inf_{X \in \mathcal{X}(G, H)} \sup_{\| g \|_2 \leq 1} \| \frac{1}{\sqrt{nm}} (m \cdot AX - n \cdot XB)v^g \|_2
\]

\[
\leq \inf_{X \in \mathcal{X}(G, H)} \sup_{v \in \mathbb{R}^m} \| \frac{1}{\sqrt{nm}} (m \cdot AX - n \cdot XB)v \|_2
\]

\[
= \delta^T_{2} (G, H).
\]
To prove that $\delta^T_2(G,H) \leq \delta^T_2(W_G,W_H)$, let $S: L_2[0,1] \to L_2[0,1]$ be a Markov operator. By Lemma [43], $X_S \in \mathbb{R}^{n \times m}$ is a fractional overlay of $G$ and $H$. For $v \in \mathbb{R}^m$, let $g_v := \sum_{j \in [m]} \sqrt{m} \cdot v_j \mathbb{1}_{J_j}$. Then,

$$
\|g_v\|^2_2 = \int_{[0,1]} g_v(x)^2 \, dx = \sum_{j \in [m]} B_v \|v_j\|^2_{J_j} = \sum_{j \in [m]} v_j^2 = \|v\|^2_2,
$$

that is, $\|g_v\|_2 = \|v\|_2 \leq 1$. Then, for $x \in I_i$, the linearity of $S$ yields

$$
((T_{W_G} \circ S)g_v)(x) = \int_{[0,1]} W_G(x,y)(Sg_v)(y) \, dy
= \sqrt{m} \sum_{j \in [m]} v_j \int_{[0,1]} W_G(x,y)(S\mathbb{1}_{J_j})(y) \, dy
= \sqrt{m} \sum_{j \in [m]} v_j \sum_{k \in [n]} A_{ik}(S\mathbb{1}_{J_j})(y) \, dy
= \sqrt{m} \sum_{j \in [m]} v_j \sum_{k \in [n]} A_{ik}(X_S)_{kj}
= \frac{1}{\sqrt{m}}(m \cdot X_Sv)_i.
$$

In a similar fashion, one can show that, for $x \in [0,1]$, we have $((S \circ T_{W_H})g_v)(x) = \frac{1}{\sqrt{m}} \sum_{k \in [m]} (Bv)_k S(\mathbb{1}_{J_k})(x)$. In the following, let $a_i := \frac{1}{\sqrt{m}}(m \cdot AX_Sv)_i$ and $b_i := \frac{1}{\sqrt{m}}(m \cdot X_SBv)_i$ for $i \in [n]$. Moreover, let $b(x) := \frac{1}{\sqrt{m}} \sum_{k \in [m]} (Bv)_k S(\mathbb{1}_{J_k})(x)$ for $x \in [0,1]$. Then,

$$
\|(T_{W_G} \circ S - S \circ T_{W_H})g_v\|^2_2 = \int_{[0,1]} \left( ((T_{W_G} \circ S - S \circ T_{W_H})g_v)(x) \right)^2 \, dx
= \sum_{i \in [n]} \left( \int_{I_i} (a_i - b(x))^2 \, dx \right)
= \sum_{i \in [n]} \left( \int_{I_i} a_i^2 \, dx - \int_{I_i} 2a_i b(x) \, dx + \int_{I_i} b(x)^2 \, dx \right)
= \sum_{i \in [n]} \left( \frac{a_i^2}{n} - 2 \frac{a_i b_i}{\sqrt{m} \sqrt{m}} + \int_{I_i} b(x)^2 \, dx \right)
\geq \sum_{i \in [n]} \left( \frac{a_i^2}{n} - 2 \frac{a_i b_i}{\sqrt{m} \sqrt{m}} + n \left( \int_{I_i} b(x) \, dx \right)^2 \right)
\quad \text{(C.-S.)}
= \sum_{i \in [n]} \left( \frac{a_i^2}{n} - 2 \frac{a_i b_i}{\sqrt{m} \sqrt{m}} + \frac{b_i^2}{m} \right)
= \sum_{i \in [n]} \left( \frac{1}{\sqrt{mn}}(m \cdot AX_Sv)_i - \frac{1}{\sqrt{mn}}(n \cdot X_SBv)_i \right)^2
= \| \frac{1}{\sqrt{mn}}(m \cdot AX_S - n \cdot X_SB)v\|^2_2.
$$
Combining this yields

\[ \delta_2^T(G, H) = \inf_{X \in \mathcal{X}(G, H)} \sup_{v \in \mathbb{R}^m, \|v\|_2 \leq 1} \left\| \frac{1}{\sqrt{nm}} (m \cdot AX - n \cdot XB)v \right\|_2 \]

\[ \leq \inf_{S \in \mathcal{M}} \sup_{v \in \mathbb{R}^m, \|v\|_2 \leq 1} \left\| \frac{1}{\sqrt{nm}} (m \cdot AX_S - n \cdot XB_S)v \right\|_2 \]

\[ \leq \inf_{S \in \mathcal{M}} \sup_{\|g\|_2 \leq 1} \left\| (TW_G \circ S - S \circ TW_H)g \right\|_2 \]

\[ \leq \delta_{2 \rightarrow 2}(W_G, W_H). \]

For the path distance, we have to verify that a signed fractional overlay can be turned into a signed Markov operator (Lemma 49) and vice versa (Lemma 50). Then, the proof of Lemma 24 is essentially analogous to the one of the second equality of Lemma 15, which is why we omit it.

\[ \Box \]

**Lemma 49.** For a signed fractional overlay \( X \in \mathbb{R}^{n \times m} \), the operator \( T_X \) is a signed Markov operator with Hilbert adjoint \( T_X^* = T_X \).

**Proof.** We verify that \( T_X \) is an \( L_2 \)-contraction; the remaining part of the proof is the same as the proof of Lemma 47. For an \( f \in L_2[0, 1] \), we have

\[ \|T_Xf\|^2 = \sum_{i \in [n]} \left( \sum_{j \in [m]} \int_{J_j} nm \cdot X_{ij} \cdot f(y) \, dy \right)^2 \]

\[ = nm^2 \cdot \sum_{i \in [n]} \left( \sum_{j \in [m]} X_{ij} \cdot \int_{J_j} f(y) \, dy \right)^2 \]

\[ \leq nm^2 \cdot \frac{1}{nm} \cdot \sum_{j \in [m]} \left( \int_{J_j} f(y) \, dy \right)^2 \quad (\|Xv\|_2^2 \leq \frac{1}{nm} \|v\|_2^2 \text{ for every } v \in \mathbb{R}^m) \]

\[ \leq nm^2 \cdot \frac{1}{nm} \cdot \sum_{j \in [m]} \frac{1}{m} \int_{J_j} f(y)^2 \, dy \quad \text{(Cauchy-Schwarz)} \]

\[ = \|f\|^2. \]

\[ \Box \]

**Lemma 50.** For a signed Markov operator \( S : L_2[0, 1] \to L_2[0, 1] \), the matrix \( X_S \) is a signed fractional overlay of \( G \) and \( H \).

**Proof.** We have \( X_S \in \mathbb{R}^{n \times m} \) and verify that \( \|X_Sv\|_2 \leq \|v\|_2 / \sqrt{nm} \) for every \( v \in \mathbb{R}^m \). The
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remaining part of the proof is the same as the proof of Lemma 18. For \( v \in \mathbb{R}^m \), we have

\[
\|X_{uv}\|^2 = \sum_{i \in [n]} \left( \sum_{j \in [m]} v_j \cdot \int_{I_i} S(\mathbb{1}_{I_j})(x) \, dx \right)^2
\]

\[
= \sum_{i \in [n]} \left( \int_{I_i} S(\mathbb{1}_{I_j})(x) \, dx \right)^2
\]

\[
\leq \sum_{i \in [n]} \frac{1}{n} \int_{I_i} S(\mathbb{1}_{I_j})(x)^2 \, dx
\]

(Cauchy-Schwarz)

\[
\leq \frac{1}{n} \int_{[0,1]} \left( \sum_{j \in [m]} v_j \cdot \mathbb{1}_{I_j}(x) \right)^2 \, dx
\]

\[
\leq \frac{1}{nm} \left\| v \right\|^2.
\]

A.5 Proof of Lemma 16 and Lemma 25 (Pseudometrics)

Proof of Lemma 16. First, let \( U \in \mathcal{W}_0 \) be a graphon. Since the identity operator is a Markov operator, we immediately get \( \delta^T_2(U, U) = \delta^T_2(U, U) = 0 \). Second, let \( U, W \in \mathcal{W}_0 \) be graphons. Then, \((T_U \circ S - S \circ T_W)^* = S^* \circ T_U - T_W \circ S^*\) since \(T_U\) and \(T_W\) are self-adjoint. Moreover, \(S^*\) is a Markov operator by Lemma 43. Thus

\[
\delta^T_2(U, W) = \inf_{S \in \mathcal{M}_{f,g}^{[0,1]}} \sup_{[0,1]} |\langle f, (T_U \circ S - S \circ T_W)g \rangle|
\]

\[
= \inf_{S \in \mathcal{M}_{f,g}^{[0,1]}} \sup_{[0,1]} \left| \langle (S^* \circ T_U - T_W \circ S^*)f, g \rangle \right|
\]

\[
= \inf_{S \in \mathcal{M}_{f,g}^{[0,1]}} \sup_{[0,1]} \left| \langle g, (T_W \circ S^* - S^* \circ T_U) f \rangle \right| \quad \text{(Linearity and symmetry)}
\]

\[
= \inf_{S \in \mathcal{M}_{f,g}^{[0,1]}} \sup_{[0,1]} \left| \langle g, (T_W \circ S - S \circ T_U) f \rangle \right| \quad \text{\((S^*\text{ is Markov and }S^{**} = S)\)}
\]

\[
= \delta^T_2(W, U).
\]

For \(\delta^T_2\), proving symmetry is analogous as the operator norm is invariant under Hilbert adjoints.

Let \( U, V, W \in \mathcal{W}_0 \) be graphons. For all Markov operators \( S_1, S_2 : L^2(0,1) \rightarrow L^2(0,1) \), their composition \(S_1 \circ S_2\) is also a Markov operator by Lemma 15 and

\[
\delta^T_2(U, W) = \inf_{S \in \mathcal{M}_{f,g}^{[0,1]}} \sup_{[0,1]} |\langle f, (T_U \circ S - S \circ T_W)g \rangle|
\]

\[
\leq \sup_{f,g : [0,1] \rightarrow [0,1]} |\langle f, (T_U \circ S_1 \circ S_2 - S_1 \circ S_2 \circ T_W)g \rangle|
\]

\[
= \sup_{f,g : [0,1] \rightarrow [0,1]} \left| \langle f, ((T_U \circ S_1 \circ T_V \circ S_2 + S_1 \circ (T_V \circ S_2 - S_2 \circ T_W))g) \right|\]

\[
\leq \sup_{f,g : [0,1] \rightarrow [0,1]} |\langle f, ((T_U \circ S_1 - S_1 \circ T_V) \circ S_2)g \rangle|
\]

\[
+ \sup_{f,g : [0,1] \rightarrow [0,1]} |\langle f, (S_1 \circ (T_V \circ S_2 - S_2 \circ T_W))g \rangle|.
\]
For measurable functions $f, g : [0, 1] \to [0, 1]$, we have that $S_1^* f$ and $S_2 g$ again are measurable functions $[0, 1] \to [0, 1]$ by Lemma [43] (in the case of $S_1^*$) and Lemma [44]. Thus,\
\[
\begin{align*}
\sup_{f, g : [0, 1] \to [0, 1]} |(f, (T_U \circ S_1 - S_1 \circ T_V) \circ S_2)g)| \\
\leq \sup_{f, g : [0, 1] \to [0, 1]} |(f, (T_U \circ S_1 - S_1 \circ T_V)g)| \\
\end{align*}
\]
and\
\[
\begin{align*}
\sup_{f, g : [0, 1] \to [0, 1]} |(f, (S_1 \circ (T_V \circ S_2 - S_2 \circ T_W))g)| \\
= \sup_{f, g : [0, 1] \to [0, 1]} |(S_1^* f, (T_V \circ S_2 - S_2 \circ T_W)g)| \\
\leq \sup_{f, g : [0, 1] \to [0, 1]} |(f, (T_V \circ S_2 - S_2 \circ T_W)g)|
\end{align*}
\]
Hence, $\delta^P_{1,2}(U, W) \leq \delta^P_{1,2}(U, V) + \delta^P_{1,2}(V, W)$. For $\delta^P_{2,2}$, the proof is analogous using the sub-multiplicativity of the operator norm and Lemma [44] the fact that a Markov operator is a contraction, cf. also the proof of Lemma [25]. ▶

**Proof of Lemma [25]** First, for a graphon $U \in W_0$, we immediately get $\delta^P_{2,2}(U, U) = 0$ since the identity operator is a signed Markov operator. Second, let $U, W \in W_0$ be graphons. Then, $(T_U \circ S - S \circ T_W)^* = S^* \circ T_U - T_W \circ S^*$ since $T_U$ and $T_W$ are self adjoint. The operator norm is invariant under taking the Hilbert adjoint, and we get\
\[
\begin{align*}
\delta^P_{2,2}(U, W) &= \inf_{S \in S} \|T_U \circ S - S \circ T_W\|_{2 \to 2} \\
&= \inf_{S \in S} \|S^* \circ T_U - T_W \circ S^*\|_{2 \to 2} \\
&= \inf_{S \in S} \|T_W \circ S - S \circ T_U\|_{2 \to 2} \\
&= \inf_{S \in S} \|T_W \circ S - S \circ T_U\|_{2 \to 2} \\
&= \delta^P_{2,2}(W, U). \\
\end{align*}
\]
Third, let $U, V, W \in W_0$ be graphons. For all signed Markov operators $S_1, S_2 : L_2[0, 1] \to L_2[0, 1]$, their composition $S_1 \circ S_2$ is also a signed Markov operator, and we get\
\[
\begin{align*}
\delta^P_{2,2}(U, W) &= \inf_{S \in S^M} \|T_U \circ S - S \circ T_W\|_{2 \to 2} \\
&\leq \|T_U \circ S_1 \circ S_2 - S_1 \circ T_V \circ S_2 + S_1 \circ T_V \circ S_2 - S_1 \circ S_2 \circ T_W\|_{2 \to 2} \\
&= \|T_U \circ S_1 - S_1 \circ T_V \circ S_2 + S_1 \circ T_V \circ S_2 - S_1 \circ S_2 \circ T_W\|_{2 \to 2} \\
&\leq \|T_U \circ S_1 - S_1 \circ T_V \circ S_2\|_{2 \to 2} + \|S_1 \circ T_V \circ S_2 - S_2 \circ T_W\|_2 \quad (\text{sub-mult.}) \\
&\leq \|T_U \circ S_1 - S_1 \circ T_V\|_{2 \to 2} + \|T_V \circ S_2 - S_2 \circ T_W\|_2. \\
\end{align*}
\]
Thus, $\delta^P_{2,2}(U, W) \leq \delta^P_{2,2}(U, V) + \delta^P_{2,2}(V, W)$. ▶

**A.6 Proof of Lemma [17] and Lemma [18] (Tree Distance Zero)**

Lemma [17] is a special case of the following Lemma [51]. Note that a Markov operator $S : L_2[0, 1] \to L_2[0, 1]$ uniquely extends to a Markov operator $S_1 : L_1[0, 1] \to L_1[0, 1]$, which
restricts to a Markov operator \( S_p : L_p[0, 1] \rightarrow L_p[0, 1] \) for any \( 1 \leq p \leq \infty \), cf. Theorem 45. For graphons \( U, W \in \mathcal{W}_0 \), we can view \( T_U \) and \( T_W \) as operator \( T_U, T_W : L_1[0, 1] \rightarrow L_\infty[0, 1] \). Hence, we can view \( T_U \circ S - S \circ T_W \) as an operator \( L_1[0, 1] \rightarrow L_\infty[0, 1] \), and letting \( \delta_{T,U}^{\ast,q}(U, W) := \inf_{\delta \in \mathcal{M}} \| T_U \circ S - S \circ T_W \|_{p \rightarrow q} \) and \( \delta_{S,T}^{\ast,q}(U, W) := \inf_{\delta \in \mathcal{M}} \| T_U \circ S - S \circ T_W \|_{C_p \rightarrow \infty} \) for all \( U, W \in \mathcal{W}_0 \) is well-defined for all \( 1 \leq p, q \leq \infty \); the Riesz-Thorin Interpolation Theorem makes the detour via complex \( L_p[0, 1] \) spaces necessary. For the proof of Lemma 18, another variant of the tree distance is helpful, and we let

\[
\delta_{T,U}^{T,2}(U, W) := \inf_{\delta \in \mathcal{M}} \sup_{\| f \|_2 \leq 1, \| g \|_2 \leq 1} |(f, (T_U \circ S - S \circ T_W)g)|
\]

for all \( U, W \in \mathcal{W}_0 \). As with the cut distance, one can prove that these variants of the tree distance yield the same topology, cf. [19] Lemma 8.11, and \([15] \) E.2 and E.3, and in particular, Lemma 10.

**Lemma 51.** We have

1. \( \delta_{T,\infty}^{T,1} \leq \delta_{T,\infty}^{T,2} \leq \delta_{T,2}^{T,2} \leq \delta_{T,2}^{T,1} \leq \sqrt{2}(\delta_{T,\infty}^{T,1})^{1/2} \),
2. \( \delta_{T,\infty}^{T,\infty} \leq 2\delta_{T,\infty}^{T,1} \),
3. \( \delta_{T,\infty}^{T,1} \leq 4\delta_{T,1}^{T} \), and
4. \( \delta_{T,2}^{T,2} \leq \delta_{T,2}^{T,2} \leq 2\delta_{T,2}^{T,2} \).

**Proof of Lemma 51** Let \( U, W \in \mathcal{W}_0 \) be graphons.

1. For a measurable function \( f : [0, 1] \rightarrow [0, 1] \), we have \( \| f \|_2 \leq \| f \|_\infty \leq 1 \) and trivially get \( \delta_{T,\infty}^{T,2}(U, W) \leq \delta_{T,2}^{T,2}(U, W) \). Furthermore, for an operator \( T : L_2[0, 1] \rightarrow L_2[0, 1] \), we have

\[
\sup_{\| f \|_2 \leq 1, \| g \|_2 \leq 1} |(f, Tg)| \leq \sup_{\| f \|_2 \leq 1, \| g \|_2 \leq 1} \| f \|_2 \| Tg \|_2 \leq \sup_{\| g \|_2 \leq 1} \| Tg \|_2 \leq \| T \|_2 \rightarrow 2 \leq \| T \|_{C,2} \rightarrow 2
\]

by the Cauchy-Schwarz inequality, which that \( \delta_{T,2}^{T,2}(U, W) \leq \delta_{T,2}^{T,2}(U, W) \leq \delta_{T,2}^{T,2}(U, W) \). The last inequality is a consequence of the Riesz-Thorin Interpolation Theorem. Let \( S : L_2[0, 1] \rightarrow L_2[0, 1] \) be a Markov operator, and let \( S_1 \) be its unique extension to a Markov operator \( S_1 : L_1[0, 1] \rightarrow L_1[0, 1] \), cf. Theorem 45. Let \( p = q = 2 \), \( p_0 = 1 \), \( q_0 = \infty \), \( p_1 = \infty \), \( q_1 = 1 \), and \( \theta = 1/2 \). Then,

\[
\frac{1}{p} = \frac{1 - \theta}{p_0} + \frac{\theta}{p_1} \quad \text{and} \quad \frac{1}{q} = \frac{1 - \theta}{q_0} + \frac{\theta}{q_1},
\]

that is, the Riesz-Thorin Interpolation Theorem, Theorem 46 is applicable, and we get

\[
\| T_U \circ S_1 - S_1 \circ T_W \|_{C,2 \rightarrow 2} \leq \| T_U \circ S_1 - S_1 \circ T_W \|_{C,1 \rightarrow \infty}^{1/2}\| T_U \circ S_1 - S_1 \circ T_W \|_{C,\infty \rightarrow 1}^{1/2}.
\]

As

\[
\| T_U \circ S_1 - S_1 \circ T_W \|_{C,\infty \rightarrow 1} \leq \| T_U \circ S_1 \|_{C,1 \rightarrow \infty} + \| S_1 \circ T_W \|_{C,1 \rightarrow \infty}
\]

\[
\leq \| T_U \|_{C,1 \rightarrow \infty} \| S_1 \|_{C,1 \rightarrow \infty} + \| S_1 \circ T_W \|_{C,\infty \rightarrow \infty} \| T_W \|_{C,1 \rightarrow \infty} \quad \text{(sub-multiplicativity)}
\]

\[
\leq \| T_U \|_{C,1 \rightarrow \infty} + \| T_W \|_{C,1 \rightarrow \infty} \quad \text{(Lemma 44)}
\]

\[
\leq 2,
\]

\( (U, W \text{ graphons}) \)

we get \( \| T_U \circ S_1 - S_1 \circ T_W \|_{C,2 \rightarrow 2} \leq \sqrt{2}\| T_U \circ S_1 - S_1 \circ T_W \|_{C,\infty \rightarrow 1} \) and, hence,

\[
\| T_U \circ S - S \circ T_W \|_{C,2 \rightarrow 2} \leq \sqrt{2}\| T_U \circ S - S \circ T_W \|_{C,\infty \rightarrow 1}.
\]
This means that \( \delta_{C, \infty \to 1}^T(U, W) \leq \sqrt{2}\delta_{C, \infty \to 1}^T(U, W)^{1/2} \).

2: Let \( S : L_2[0, 1] \rightarrow L_2[0, 1] \) be a Markov operator. Then,
\[
\|T_U \circ S \circ T_W\|_{C, \infty \to 1} = \sup_{g : [0, 1] \to C, \|g\|_{\infty \to 1} \leq 1} \|(T_U \circ S \circ T_W)(\text{Re} g + i \text{Im} g)\|_1 \\
= \sup_{g : [0, 1] \to C, \|g\|_{\infty \to 1} \leq 1} \|(T_U \circ S \circ T_W)(\text{Re} g) + i(T_U \circ S \circ T_W)(\text{Im} g)\|_1 \\
\leq \sup_{g : [0, 1] \to C, \|g\|_{\infty \to 1} \leq 1} \|(T_U \circ S \circ T_W)(\text{Re} g)\|_1 + \|(T_U \circ S \circ T_W)(\text{Im} g)\|_1 \\
\leq 2 \cdot \sup_{g : [0, 1] \to \mathbb{R}, \|g\|_{\infty \to 1} \leq 1} \|(T_U \circ S \circ T_W)g\|_1, \quad (\|\text{Re} g\|_{\infty \to 1}, \|\text{Im} g\|_{\infty \to 1} \leq \|g\|_{\infty \to 1})
\]
which yields \( \delta_{C, \infty \to 1}^T(U, W) \leq 2\delta_{C, \infty \to 1}^T(U, W) \).

3: Let \( S : L_2[0, 1] \rightarrow L_2[0, 1] \) be a Markov operator. The one-dimensional cut norm coincides with the \( L_1 \)-norm \[15, \text{Remark 4.4}, \] i.e., for a function \( g \in L_1[0, 1] \), we have
\[
\|g\|_1 = \sup_{\|f\|_{\infty \to 1} \leq 1} \int_{[0, 1]} f(x)g(x) \, dx, \text{ and get}
\]
\[
\sup_{g : [0, 1] \to \mathbb{R}, \|g\|_{\infty \to 1} \leq 1} \|(T_U \circ S \circ T_W)g\|_1 \\
= \sup_{f, g : [0, 1] \to [-1, 1]} |\langle f, (T_U \circ S \circ T_W)g \rangle| \\
= \sup_{f, f', g' : [0, 1] \to [0, 1]} |\langle f - f', (T_U \circ S \circ T_W)(g - g') \rangle| \\
\leq 4 \cdot \sup_{f, g : [0, 1] \to [0, 1]} |\langle f, (T_U \circ S \circ T_W)g \rangle| \\
\]
since, for \( T := T_U \circ S \circ T_W \),
\[
\langle f - f', T(g - g') \rangle = \langle f, Tg \rangle - \langle f', Tg \rangle - \langle f, Tg' \rangle + \langle f', Tg' \rangle.
\]
Hence, \( \delta_{\infty \to 1}^T(U, W) \leq 4\delta_{C, \infty \to 1}^T(U, W) \).

4: The first inequality is trivial. To prove the second, let \( S \in \mathcal{M} \) be a Markov operator and \( g : [0, 1] \rightarrow C \) be a function in \( L_2[0, 1] \) with \( \|g\|_2 \leq 1 \). Then, \( \text{Re} g, \text{Im} g \in L_2[0, 1] \) with \( \|\text{Re} g\|_2, \|\text{Im} g\|_2 \leq 1 \). Moreover,
\[
\|(T_U \circ S \circ T_W)g\|_2 = \|(T_U \circ S \circ T_W)(\text{Re} g + i \text{Im} g)\|_2 \\
\leq \|(T_U \circ S \circ T_W)(\text{Re} g)\|_2 + \|(T_U \circ S \circ T_W)(\text{Im} g)\|_2 \\
= \|(T_U \circ S \circ T_W)(\text{Re} g)\|_2 + \|(T_U \circ S \circ T_W)(\text{Im} g)\|_2.
\]
and, hence,
\[
\|T_U \circ S \circ T_W\|_{C, 2 \to 2} = \sup_{g : [0, 1] \to C, \|g\|_{2 \to 1} \leq 1} \|(T_U \circ S \circ T_W)g\|_2 \\
\leq 2 \sup_{g : [0, 1] \to \mathbb{R}, \|g\|_2 \leq 1} \|(T_U \circ S \circ T_W)g\|_2 \\
= 2 \|T_U \circ S \circ T_W\|_{2 \to 2}.
\]
Recall that the set of Markov operators is compact in the weak operator topology, cf. Theorem 46. This is the reason why we consider $\delta^T_{\square,2}$ instead of $\delta^T_{\rightarrow,2}$ in the following lemma; for it, compactness in the weak operator topology suffices to prove that the infimum in its definition is attained.

\textbf{Lemma 52.} The infimum in the definition of $\delta^T_{\square,2}$ is attained.

\textbf{Proof of Lemma 52.} Let $U, W \in \mathcal{W}_0$ be graphons. As the set $\mathcal{M}$ is compact in the weak operator topology by Theorem 46, it suffices to prove that the function $h$ defined by

$$h(S) = \sup_{\|f\|_2 \leq 1, \|g\|_2 \leq 1} |\langle f, (T_U \circ S)g \rangle - \langle f, (S \circ T_W)g \rangle|$$

is lower semi-continuous. To this end, let $\{S_i\}_{i \in I}$ be a net of Markov operators converging to a Markov operator $S^* \in \mathcal{M}$ in the weak operator topology, i.e., we have $\langle f, S_i g \rangle \to \langle f, S^* g \rangle$ for all $f, g \in L_2[0, 1]$. We have to show that $\lim\inf_i h(S_i) \geq h(S^*)$. Let $f, g \in L_2[0, 1]$ with $\|f\|_2, \|g\|_2 \leq 1$. We have

$$\langle f, (T_U \circ S_i)g \rangle = \langle T_U f, S_i g \rangle \to \langle T_U f, S^* g \rangle = \langle f, (T_U \circ S^*)g \rangle,$$

where we used that $T_U$ is self-adjoint, and

$$\langle f, (S_i \circ T_W)g \rangle = \langle f, S_i (T_W g) \rangle \to \langle f, S^* (T_W g) \rangle = \langle f, (S^* \circ T_W)g \rangle.$$

Together, this yields

$$|\langle f, (T_U \circ S_i)g \rangle - \langle f, (S_i \circ T_W)g \rangle| \to |\langle f, (T_U \circ S^*)g \rangle - \langle f, (S^* \circ T_W)g \rangle|,$$

which gives us

$$\lim\inf_i h(S_i) \geq \lim\inf_i |\langle f, (T_U \circ S_i)g \rangle - \langle f, (S_i \circ T_W)g \rangle|$$

$$= |\langle f, (T_U \circ S^*)g \rangle - \langle f, (S^* \circ T_W)g \rangle|.$$ 

Since this holds for all $f, g \in L_2[0, 1]$ with $\|f\|_2, \|g\|_2 \leq 1$, we get $\lim\inf_i h(S_i) \geq h(S^*)$ by definition of the supremum. \hfill\(\blacktriangleleft\)

With Lemma 51 and Lemma 52 proving Lemma 18 is easy.

\textbf{Proof of Lemma 18.} Let $U, W \in \mathcal{W}_0$ be graphons. If $t(T, U) = t(T, W)$ for every tree $T$, then, by Theorem 13 there is a Markov operator $S \in \mathcal{M}$ such that $T_U \circ S = S \circ T_W$, which directly yields $\delta^T_{\square,2}(U, W) = 0$ by the definition of $\delta^T_{\square,2}$.

For the other direction, assume that $\delta^T_{\square,2}(U, W) = 0$. Then, by Lemma 51 we have $\delta^T_{\rightarrow,2}(U, W) = 0$. By Lemma 52 there is a Markov operator $S \in \mathcal{M}$ such that $\langle f, (T_U \circ S)g \rangle = \langle f, (S \circ T_W)g \rangle$ for all $f, g \in L_2[0, 1]$ with $\|f\|_2, \|g\|_2 \leq 1$. Since this, in particular, holds for $f = g$ and, since we can just normalize an arbitrary $g \in L_2[0, 1]$, linearity of the operators and the inner product yields $\langle g, (T_U \circ S)g \rangle = \langle g, (S \circ T_W)g \rangle$ for every $g \in L_2[0, 1]$. Hence, Lemma 35 yields $T_U \circ S = S \circ T_W$, and by Theorem 13 we have $t(T, U) = t(T, W)$ for every tree $T$. \hfill\(\blacktriangleleft\)
A.7 Proof of Lemma 19 ($\delta_d^T \leq \delta_d$)

Proof of Lemma 19 Let $U, W \in \mathcal{W}_0$ be graphons, and let $\varphi \in S_{[0,1]}$ be an invertible measure-preserving map. The Koopman operator $T_\varphi$ of $\varphi$ is a Markov operator, and we observe that

$$T_U \circ T_\varphi - T_\varphi \circ T_W = (T_U \circ T_\varphi - T_\varphi \circ T_W) \circ T_{\varphi^{-1}} \circ T_\varphi$$

$$= (T_U - T_\varphi \circ T_W \circ T_{\varphi^{-1}}) \circ T_\varphi$$

$$= (T_U - T_{W \circ \varphi}) \circ T_\varphi$$

$$= T_{U - W \circ \varphi} \circ T_\varphi.$$

Then, we get

$$\sup_{f,g: [0,1] \to [0,1]} |(f, (T_U \circ T_\varphi - T_\varphi \circ T_W)g)|$$

$$= \sup_{f,g: [0,1] \to [0,1]} |(f, T_{U - W \circ \varphi}g)|.$$  

(\varphi \text{ measure preserving})

Thus,

$$\delta^T_d(U, W) = \inf_{S \in \mathcal{M}} \sup_{f,g: [0,1] \to [0,1]} |(f, (T_U \circ S - S \circ T_W)g)|$$

$$\leq \inf_{\varphi \in S_{[0,1]}} \sup_{f,g: [0,1] \to [0,1]} |(f, (T_U \circ T_\varphi - T_\varphi \circ T_W)g)|$$

$$= \inf_{\varphi \in S_{[0,1]}} \sup_{f,g: [0,1] \to [0,1]} |(f, T_{U - W \circ \varphi}g)|$$

$$= \delta_d(U, W).$$

\hfill \Box

A.8 Proof of Theorem 22 (Path Densities)

The following lemma presents a generalization of the interpolation technique of Dell, Grohe, and Rattan [10, Lemma 10] from finite sums to convergent series and is needed for the proof of Theorem 22.

\textbf{Lemma 53 ([19, Proposition A.21]).} Let $a_i, b_i, c_i, d_i$ be sequences of non-zero real numbers such that $b_i \neq b_j$ and $d_i \neq d_j$ for $i \neq j$. Assume that there is a $k_0 \geq 0$ such that, for every $k \geq k_0$, the sums $\sum_{i=1}^{\infty} a_i b_i^k$ and $\sum_{i=1}^{\infty} c_i d_i^k$ are convergent and equal. Then, there is a permutation $\pi: \mathbb{N} \to \mathbb{N}$ such that $a_i = c_{\pi(i)}$ and $b_i = d_{\pi(i)}$ for every $i \geq 0$.

Note that, if $k_0 = 0$, we can also allow the number zero to appear in the sequences $b_i$ and $d_i$; equality of the two series for $k = 0$ directly implies that the coefficients of the zeros are the same.

\textbf{Proof of Theorem 22} First, assume that there is some operator $S: L_2[0,1] \to L_2[0,1]$ with $S1 = 1$ and $S^*1 = 1$ such that $T_U \circ S = S \circ T_W$. Then, induction yields $T_U^\ell \circ S = S \circ T_W^\ell$ for every $\ell \geq 0$. Hence,

$$(1, T_U^\ell 1) = (1, (T_U^\ell \circ S)1) = (1, (S \circ T_W^\ell)1) = (S^*1, T_W^\ell 1) = (1, T_W^\ell 1).$$
Graph Similarity and Homomorphism Densities

For the backward direction, assume that $t(P_i, U) = t(P_i, W)$ for every $\ell \geq 0$. Let $\{f_i\}_{i \in \mathbb{N}}$ and $\{\lambda_i\}_{i \in \mathbb{N}}$ be the orthonormal basis of the $L_2[0, 1]$ consisting of eigenfunctions of $T_U$ and the corresponding sequence of real eigenvalues obtained from the Spectral Theorem for $T_U$. By definition of an orthonormal basis, we have $1 = \sum_{i \in \mathbb{N}} (1, f_i)^2 f_i$. We call an eigenvalue $\lambda$ from $(\lambda_i)_{i \in \mathbb{N}}$ useful if the finite sum $\sum_{i \in \mathbb{N}, \lambda_i = \lambda}(1, f_i)^2 f_i$ is non-zero, i.e., one of the eigenfunctions corresponding to $\lambda$ is not orthogonal to 1. Let $\{\lambda_i\}_{i \geq 0} \subseteq \{\lambda_1, \lambda_2, \ldots\}$ be the set of these (pairwise distinct) useful eigenvalues and let $f_i := \sum_{j \in \mathbb{N}, \lambda_j = \lambda_i}(1, f_j)^2 f_j$ for $i \geq 0$. Then, $1 = \sum_{i \geq 0} f_i$, where $f_i$ is an eigenfunction of $T_U$ with eigenvalue $\lambda_i$, and the set $\{f_i\}_{i \geq 0}$ of these eigenfunctions is orthogonal. Note that the set $\{\lambda_i\}_{i \geq 0}$ may be finite; in terms of notation, we do not treat this case differently. In the same way, apply the Spectral Theorem to $T_W$ to obtain another orthonormal basis and sequence of eigenvalues and define the useful eigenvalues $\{\mu_i\}_{i \geq 0}$ and the functions $\{g_i\}_{i \geq 0}$ analogously.

Then, since we have $T_U(f_i) = \lambda_i f_i$ for every $i \geq 0$, we get

$$\langle 1, T_U^\ell 1 \rangle = \langle 1, T_U^\ell \left(\sum_{i \geq 0} f_i\right) \rangle = \langle 1, \sum_{i \geq 0} \lambda_i^\ell f_i \rangle = \sum_{i \geq 0} \lambda_i^\ell f_i$$

for every $\ell \geq 0$. Analogously, we get $\langle 1, T_W^\ell 1 \rangle = \sum_{i \geq 0} \|g_i\|_2^\ell \mu_i$, and the assumption can be formulated as $\sum_{i \geq 0} \|f_i\|_2^\ell \lambda_i = \sum_{i \geq 0} \|g_i\|_2^\ell \mu_i$ for every $\ell \geq 0$.

We argue that Lemma 53 is applicable. If both sets $\{\lambda_i\}_{i \geq 0}$ and $\{\mu_i\}_{i \geq 0}$ are infinite, this is clear. If both sets are finite, the lemma also applies as we can simply append a sequence like $(2^{-i})_{i \geq i_0}$ for some $i_0 \geq 0$ to both sequences. We argue that the remaining case, where one of the sets is finite while the other one is infinite, cannot occur. To this end, assume without loss of generality that $\{\lambda_i\}_{i \geq 0}$ is the finite set $\{\lambda_0, \ldots, \lambda_n\}$. Then, the assumption reads as $\sum_{i=0}^n \|f_i\|_2^\ell \lambda_i = \sum_{i=0}^\infty \|g_i\|_2^\ell \mu_i$ for every $\ell \geq 0$, which implies that

$$\sum_{i=0}^n \|f_i\|_2^\ell \lambda_i + \sum_{i=0}^\infty \|g_i\|_2^\ell \mu_i = \sum_{i=0}^\infty 2\|g_i\|_2^\ell \mu_i$$

for every $\ell \geq 0$. By combining the finite sum and the infinite series on the left-hand side, we are again in the situation of Lemma 53 where the sequences $a_i$ and $b_i$ for the left-hand side have finitely many elements of the form $\|f_i\|_2^\ell$ and $\lambda_i$, finitely many elements of the form $\|g_i\|_2^\ell$ and $\lambda_i = \mu_j$, and infinitely many elements of the form $\|g_i\|_2^\ell$ and $\mu_i$, respectively. In contrast, the elements of the sequences $c_i$ and $d_i$ for the right-hand side are of the form $2\|g_i\|_2^\ell$ and $\mu_i$, respectively. Hence, the resulting bijection has to map one of the infinitely many pairs of elements of the form $\|g_i\|_2^\ell$ and $\mu_i$ to a pair $2\|g_j\|_2^\ell$ and $\mu_j$. Then, $i = j$ since the $\{\mu_i\}_{i \geq 0}$ are pairwise distinct and the lemma guarantees that $\mu_i = \mu_j$. But, we have $\|g_i\|_2^\ell \neq 2\|g_j\|_2^\ell$, which contradicts the lemma.

Now, Lemma 53 yields a permutation $\pi : \mathbb{N} \to \mathbb{N}$ such that $\lambda_i = \mu_{\pi(i)}$ and $\|f_i\|_2^\ell = \|g_{\pi(i)}\|_2^\ell$ for every $i \geq 0$. By relabeling, we can assume $\lambda_i = \mu_i$ and $\|f_i\|_2 = \|g_i\|_2$ for every $i \geq 0$. 


Note that, as the convergence in an orthonormal basis is unconditional by definition, this does not change the fact that we have \(1 = \sum_{i \geq 0} g_i\). For a function \(f \in L_2[0, 1]\), define

\[
Sf := \sum_{i \geq 0} \left\langle f, \frac{g_i}{\|g_i\|_2} \right\rangle \frac{f_i}{\|f_i\|_2}.
\]

This actually defines a mapping \(L_2[0, 1] \rightarrow L_2[0, 1]\): As \(\{f_i/\|f_i\|_2\}_{i \geq 0}\) is orthonormal, the Riesz-Fischer Theorem yields that the sum converges to a function in \(L_2[0, 1]\) if and only if we have \(\sum_{i \geq 0} |\langle f, g_i/\|g_i\|_2 \rangle|^2 < \infty\). This however, follows immediately from Bessel’s inequality as the set \(\{g_i/\|g_i\|_2\}_{i \geq 0}\) is also orthonormal, i.e., we have \(\sum_{i \geq 0} |\langle f, g_i/\|g_i\|_2 \rangle|^2 \leq \|f\|_2^2 < \infty\). The linearity of the inner product in its first argument yields that \(S\) is linear. A closer analysis yields that

\[
\|Sf\|_2^2 = \langle Sf, Sf \rangle
\]

\[
= \left\langle \sum_{i \geq 0} \langle f, \frac{g_i}{\|g_i\|_2} \rangle \frac{f_i}{\|f_i\|_2}, Sf \right\rangle
\]

\[
= \sum_{i \geq 0} \langle f, \frac{g_i}{\|g_i\|_2} \rangle \langle \frac{f_i}{\|f_i\|_2}, Sf \rangle
\]

\[
= \sum_{i \geq 0} \langle f, \frac{g_i}{\|g_i\|_2} \rangle \sum_{j \geq 0} \langle f, \frac{g_j}{\|g_j\|_2} \rangle \langle \frac{f_j}{\|f_j\|_2}, \frac{f_i}{\|f_i\|_2} \rangle
\]

\[
= \sum_{i \geq 0} \left| \left\langle f, \frac{g_i}{\|g_i\|_2} \right\rangle \right|^2
\]

\[
\leq \|f\|_2^2 \quad \text{(Bessel’s inequality)}
\]

for every \(f \in L_2[0, 1]\), i.e., \(\|Sf\|_2 \leq \|f\|_2\). Hence, \(S : L_2[0, 1] \rightarrow L_2[0, 1]\) is not only a bounded linear operator but also a contraction. Moreover, we have

\[
S1 = \sum_{i \geq 0} \langle 1, \frac{g_i}{\|g_i\|_2} \rangle \frac{f_i}{\|f_i\|_2}
\]

\[
= \sum_{i \geq 0} \langle 1, g_i \rangle \frac{f_i}{\|g_i\|_2} \quad \text{(\(\|f_i\|_2 = \|g_i\|_2\) for every \(i \geq 0\))}
\]

\[
= \sum_{i \geq 0} \frac{g_i}{\|g_i\|_2} f_i \quad \text{\((g_i)_{i \geq 0}\) orthogonal, \(\langle \cdot, \cdot \rangle\) continuous and linear)}
\]

\[
= \sum_{i \geq 0} f_i
\]

\[
= 1.
\]

It is easy to verify that the Hilbert adjoint \(S^*\) of \(S\) is given by

\[
S^*f = \sum_{i \geq 0} \langle f, \frac{f_i}{\|f_i\|_2} \rangle \frac{g_i}{\|g_i\|_2}
\]

for every \(f \in L_2[0, 1]\), and hence, by symmetry, we also have \(S^*1 = 1\). Therefore, \(S\) is a
signed Markov operator. It remains to prove that $T_U \circ S = S \circ T_W$. We have

$$(T_U \circ S)f = T_U \left( \sum_{i \geq 0} \langle f, \frac{g_i}{\|g_i\|_2} \rangle \frac{f_i}{\|f_i\|_2} \right)$$

$$= \sum_{i \geq 0} \langle f, \frac{g_i}{\|g_i\|_2} \rangle T_U(f_i) \frac{f_i}{\|f_i\|_2}$$

$$= \sum_{i \geq 0} \langle f, \frac{g_i}{\|g_i\|_2} \rangle \lambda_i f_i \frac{f_i}{\|f_i\|_2}$$

$$= \sum_{i \geq 0} \langle f, \frac{\mu_i g_i}{\|g_i\|_2} \rangle \frac{f_i}{\|f_i\|_2}$$

$$= \sum_{i \geq 0} \langle T_W f, \frac{g_i}{\|g_i\|_2} \rangle \frac{f_i}{\|f_i\|_2}$$

$$= (S \circ T_W)f$$

for every $f \in L_2[0,1]$. □

### A.9 Proof of Theorem 34 (Approximate Inversion)

Let us state the inversion result that Theorem 34 is based on.

**Theorem 54** ([16, Corollary 4]). $T_G^2$ admits linear time inversion on the class of graphs.

They show that, given $\tilde{s} \in \mathbb{N}^m$ and $M \in \mathbb{N}^{m \times m}$ such that

1. $M_{ii} < s_i$ for every $i \in [m]$, 3. $M_{ij} \leq s_j$ for all $i, j \in [m]$, and
2. $M_{ii} \cdot s_i$ is even for every $i \in [m]$, 4. $M_{ij} \cdot s_i = M_{ji} \cdot s_j$ for all $i, j \in [m]$.

one can construct a graph $G$ in linear time where $V(G)$ can be partitioned into sets $C_1, \ldots, C_m$ of sizes $s_1, \ldots, s_m$, respectively, such that $G[C_i]$ is a $M_{ii}$-regular graph for every $i \in [m]$ and $G[C_i \cup C_j]$ is a $(M_{ij}, M_{ji})$-biregular graph for all $i, j \in [m]$. That is, these conditions, which are clearly necessary, are also sufficient for such a graph to exist.

For a graph $G$ constructed from $\tilde{s} \in \mathbb{N}^m$ and $M \in \mathbb{N}^{m \times m}$ via the criteria of Theorem 54, the weighted graph $G/C_\tilde{s}^G$ might not be isomorphic to $G_{s,M} := ([m], (s_i/\sum s_j)_{ij}, (M_{ij}/s_j)_{ij})$ as color refinement might compute a coarser partition than $C_1, \ldots, C_m$. The proof of Theorem 54 proceeds in three steps: First, we round the vertex weights of the given weighted graph $H$. Ideally, one would like to use the (scaled) identity matrix as a fractional overlay for this. However, due to the rounded vertex weights, we have to settle for a fractional overlay that is close to the identity matrix, cf. Lemma 55.

**Lemma 55.** Let $\tilde{\alpha} \in \mathbb{R}^m_+ \cap (\mathbb{N}^m \setminus \mathbb{N}^N)$ such that $\sum_{i \in [m]} \alpha_i = 1$. For every $n \geq 1$, there is an $\tilde{s} \in \mathbb{N}^m$ such that $\sum_{i \in [m]} s_i = n$ and $|\tilde{s}_i - \alpha_i| < \frac{1}{n}$ for every $i \in [m]$.

**Proof.** Clearly, the bound $|\frac{s_i}{n} - \alpha_i| < \frac{1}{n}$ can be satisfied by setting $s_i := \lfloor n \cdot \alpha_i \rfloor$ or $s_i := \lceil n \cdot \alpha_i \rceil$ for every $i \in [m]$. However, to also satisfy $\sum_{i \in [m]} s_i = n$, one has to choose correctly between these two alternatives. For $j = 1, \ldots, m$, we proceed as follows: If $\sum_{i \in [j]} \left(\frac{2s_i}{n} - \frac{n \cdot \alpha_i}{n}\right) > 0$, then...
then we set $s_j := [n \cdot \alpha_i]$. Otherwise, we set $s_j := [n \cdot \alpha_i]$. A simple inductive argument yields that, for every $j \in [m]$, the invariant $\sum_{i \in [j]} \left( \frac{\alpha_i}{n} - \frac{\alpha_i}{m} \right) < \frac{1}{n}$ is satisfied. In particular, we have $\sum_{i \in [m]} \left( \frac{\alpha_i}{n} - \frac{\alpha_i}{m} \right) < \frac{1}{n}$. Since $\sum_{i \in [m]} \alpha_i = 1$, we get $\sum_{i \in [m]} \left( \frac{\alpha_i}{n} - \frac{\alpha_i}{m} \right) < \frac{1}{n}$, and by multiplying with $n$, also $|\sum_{i \in [m]} s_i - n| < 1$. Since $s_i \in \mathbb{N}$ for every $i \in [m]$, this implies $\sum_{i \in [m]} s_i = n$.

\textbf{Lemma 56.} Let $\bar{s} \in \mathbb{R}^m_{\geq 0}$ and $\bar{t} \in \mathbb{R}^n_{\geq 0}$ such that $\sum_{j=1}^m s_j = \sum_{i=1}^n t_i$. Then, there is an $X \in \mathbb{R}^{m \times n}_{\geq 0}$ such that

1. $\sum_{j=1}^m X_{ij} = s_i$ for every $i \in [m]$,
2. $\sum_{i=1}^n X_{ij} = t_j$ for every $j \in [n]$, and
3. $X_{ii} = \min\{s_i, t_i\}$ for every $i \in [\min\{m, n\}]$.

\textbf{Proof.} We prove the statement by induction on the total number of non-zero entries of $\bar{s}$ and $\bar{t}$. If $\bar{s}$ and $\bar{t}$ are all-zero vectors, then the desired $X$ is obtained by choosing the all-zero matrix. Now, assume that $\bar{s}$ or $\bar{t}$ has a non-zero entry. Then, since $\sum_{j=1}^m s_j = \sum_{i=1}^n t_i$, both $\bar{s}$ and $\bar{t}$ have a non-zero entry. Since we can just transpose $X$ and swap the roles of $\bar{s}$ and $\bar{t}$, we may assume $m \geq n$ without loss of generality.

Case 1: There is no $k \in [n]$ such that $s_k > 0$ and $t_k > 0$.
Let $k \in [m]$ such that $s_k > 0$ and let $\ell \in [n]$ such that $t_\ell > 0$. Consider

$$s'_j := \begin{cases} s_j & \text{if } j \neq k, \\ s_k - \min\{s_k, t_\ell\} & \text{if } j = k, \end{cases} \quad \text{and} \quad t'_j := \begin{cases} t_\ell & \text{if } i = \ell, \\ t_j - \min\{s_k, t_\ell\} & \text{if } i = j. \end{cases}$$

Then, $\sum_{j=1}^m s'_j = \sum_{j=1}^m t'_j$ and, since $s'_j = 0$ or $t'_j = 0$, in total $s'$ and $t'$ have one less non-zero entry than $\bar{s}$ and $\bar{t}$. The induction hypothesis yields an $X' \in \mathbb{R}^{m \times n}_{\geq 0}$ such that

1. $\sum_{j=1}^m X'_{ij} = s'_i$ for every $i \in [m]$,
2. $\sum_{i=1}^n X'_{ij} = t'_j$ for every $j \in [n]$, and
3. $X'_{ij} = \min\{s'_j, t'_j\}$ for every $j \in [n]$.

Since $s'_k = 0$ or $t'_k = 0$, we have $X'_{kk} = 0$. Let $X$ be the matrix obtained from $X'$ by replacing $X'_{kk}$ with $\min\{s_k, t_\ell\}$. By the case assumption, we have $k \neq \ell$ and also $s'_j = 0$ or $t'_j = 0$ for every $j \in [n]$. Thus, $X_{ij} = X'_{ij} = \min\{s'_j, t'_j\} = 0 = \min\{s_j, t_j\}$ for every $j \in [n]$. Hence, $X$ has the desired properties.

Case 2: There is an $k \in [n]$ such that $s_k > 0$ and $t_k > 0$.
We proceed as in the first case, where we choose $\ell := k$. Then, for the constructed $X$, we have $X_{kk} = \min\{s_k, t_k\}$ and $X_{jj} = X'_{jj} = \min\{s'_j, t'_j\} = \min\{s_j, t_j\}$ for every $j \in [n] \setminus \{k\}$.

\textbf{Proof of Theorem 33} Let $n \geq 2 \cdot \nu(H)$. Assume w.l.o.g. that $H$ is normalized. As a first step, we round the vertex weights of $H$. By Lemma 55, we can choose $\bar{s} \in \mathbb{R}^V(H)$ such that $\sum_{u \in V(H)} s_u = n$ and $|\frac{n \cdot s_u}{n} - \alpha_u(H)| < \frac{1}{n}$ for every $u \in V(H)$. Then, we also have

$$|\frac{n \cdot s_u}{n} - \alpha_u(H)| < \frac{1}{n}$$

for every $u \in V(H)$. In the following, $n \cdot s_u$ is the size of the color class we construct for the vertex $u$. This blow-up of every color class by $n$ is crucial in the next step. Note that it is perfectly fine if we have $s_u = 0$ for some $u \in V(H)$ in the following; we just choose the corresponding values of $M$ as 0.

As a second step, we round the edge weights of non-loops of $H$. For $u, v \in V(H)$ with $u \neq v$, we have to choose $M_{uv} \in \{0, \ldots, n \cdot s_v\}$ and $M_{vu} \in \{0, \ldots, n \cdot s_u\}$ such that $M_{uv} \cdot n \cdot s_u = M_{vu} \cdot n \cdot s_v$. Note that $M_{uv} \cdot n \cdot s_u = M_{vu} \cdot n \cdot s_v$ is a common multiple of $n \cdot s_u$ and $n \cdot s_u$, i.e., we have $M_{uv} \cdot n \cdot s_u = M_{vu} \cdot n \cdot s_v = k \cdot \text{lcm}(n \cdot s_u, n \cdot s_v)$ for some
As \( \sum_{v \in V(H)} n \cdot s_v = n^2 \) vertices with the corresponding partition \((C_u)_{u \in V(H)}\). Note that, since all row sums of \(M\) are pairwise distinct, vertices in different sets of the partition have different degrees, i.e., there is no coarser stable coloring than the one induced by \(\bar{s}\) and \(M\) and not to some coarser partition, we tweak the diagonal entries \(M_{uu}\) a bit. The matrix \(M\) is of dimension \(v(H) \times v(H)\), i.e., we can obtain pairwise distinct row sums by choosing a value that is close to the value \(M_{uu}\) chosen above. More precisely, as \(n \geq 2 \cdot v(H)\), we always have at least \(v(H) - 1\) valid choices that deviate from the above choice of \(M_{uu}\) by at most \(2(v(H) - 1)\). Hence, we can choose \(M_{uu} \in \{0, \ldots, n \cdot s_u - 1\}\) such that \(M_{uu} \cdot n \cdot s_u\) is even, and all row sums of \(M\) are pairwise distinct.

By the criteria of [13], cf. Theorem 54, we obtain a graph \(G\) for \((n \cdot s_u)_{u \in V(H)}\) and \(M\) such that \(\sum_{v \in V(H)} n \cdot s_v = n^2\) vertices with the corresponding partition \((C_u)_{u \in V(H)}\). Note that, since all row sums of \(M\) are pairwise distinct, vertices in different sets of the partition have different degrees, i.e., there is no coarser stable coloring than the one induced by \((C_u)_{u \in V(H)}\). Hence, \(G/C_{\infty}^G\) is isomorphic to the weighted graph \(G_{\bar{s},\bar{M}}\).

It remains to prove that \(G/C_{\infty}^G\) and \(H\) are actually close in the cut distance. As \((\frac{n \cdot s_u}{n})_{u \in V(H)} = (\frac{s_u}{n})_{u \in V(H)}\) and \((\alpha_u(H))_{u \in V(H)}\) sum to 1, Lemma 56 yields a matrix \(X \in \mathbb{R}_{\geq 0}^{V(H) \times V(H)}\) with

1. \(\sum_{u \in V(H)} X_{uv} = \frac{s_u}{n}\) for every \(u \in V(H)\),
2. \(\sum_{v \in V(H)} X_{uv} = \alpha_u(H)\) for every \(v \in V(H)\), and
3. \(X_{uv} = \min\{\frac{s_u}{n}, \alpha_v(H)\}\) for every \(u \in V(H)\).

We have

\[
\delta_{\square}(G/C_{\infty}^G, H) = \max_{X} \delta_{\square}(G_{\bar{s},\bar{M}}, H, X)
\leq d_{\square}(G_{\bar{s},\bar{M}}, H, X)
= \max_{Q, R \subseteq V(H)} \left| \sum_{\substack{i \in Q, j \in R}} X_{iu}X_{jv} (\frac{M_{ij}}{n \cdot s_j} - \beta_{uv}(H)) \right|
\leq \sum_{i,j,u,v \in V(H)} \left| X_{iu}X_{jv} (\frac{M_{ij}}{n \cdot s_j} - \beta_{uv}(H)) \right|
= \sum_{i,j \in V(H)} X_{ii}X_{jj} \left| \frac{M_{ij}}{n \cdot s_j} - \beta_{ij}(H) \right| + \sum_{i,j,u,v \in V(H), i \neq u \text{ or } j \neq v} X_{iu}X_{jv} \left| \frac{M_{ij}}{n \cdot s_j} - \beta_{uv}(H) \right|.
\]
For the first of these two sums, we get

\[ \sum_{i,j \in V(H)} X_{ij} \left( \frac{M_{ij}}{n} - \beta_{ij}(H) \right) \leq \sum_{i,j \in V(H)} \alpha_i(H) \alpha_j(H) \cdot \frac{2\nu(H)}{n} \]
\[ = \frac{2\nu(H)}{n} \cdot \sum_{i \in V(H)} \left( \alpha_i(H) \cdot \sum_{j \in V(H)} \alpha_j(H) \right) \]
\[ = \frac{2\nu(H)}{n} \cdot \sum_{i \in V(H)} \alpha_i(H) \cdot \sum_{j \in V(H)} \alpha_j(H) \]

For the second sum, we note that, for \( u \in V(H) \), we have

\[ \sum_{v \in V(H), v \neq u} X_{uv} + \sum_{v \in V(H), v \neq u} X_{vu} = \sum_{v \in V(H)} X_{uv} + \sum_{v \in V(H)} X_{vu} - 2 \cdot X_{uu} \]
\[ = \frac{s_u}{n} + \alpha_u(H) - 2 \cdot \min\{\frac{s_u}{n}, \alpha_u(H)\} \]
\[ < \frac{1}{n} \]

and, hence,

\[ \sum_{u,v \in V(H), u \neq v} X_{uv} = \frac{1}{2} \cdot \sum_{u \in V(H)} \left( \sum_{v \in V(H), v \neq u} X_{uv} + \sum_{v \in V(H), v \neq u} X_{vu} \right) \leq \frac{1}{2} \cdot \sum_{u \in V(H)} \frac{1}{n} = \frac{\nu(H)}{2n} \]

Then, for the second sum, we get

\[ \sum_{i,j,u,v \in V(H), i \neq u \text{ or } j \neq v} X_{iu} X_{jv} \left( \frac{M_{ij}}{n} - \beta_{uv}(H) \right) \leq \sum_{i,j,u,v \in V(H), i \neq u \text{ or } j \neq v} X_{iu} X_{jv} \]
\[ = \sum_{i,j,u,v \in V(H), i \neq u \text{ or } j \neq v} X_{iu} X_{jv} \]
\[ = (\sum_{i,u \in V(H), i \neq u} X_{iu})^2 + 2 \cdot \left( \sum_{i \in V(H)} X_{ii} \right) \cdot \left( \sum_{j,v \in V(H), j \neq v} X_{jv} \right) \]
\[ \leq \left( \frac{\nu(H)}{2n} \right)^2 + 2 \cdot \left( \sum_{i \in V(H)} \alpha_i(H) \cdot \frac{\nu(H)}{2n} \right) \]
\[ = \frac{1}{4} \cdot \left( \frac{\nu(H)}{n} \right)^2 + \frac{\nu(H)}{2n} \]

Summing up these two bounds, we get an overall upper bound of

\[ 3 \cdot \frac{\nu(H)}{n} + \frac{1}{4} \cdot \left( \frac{\nu(H)}{n} \right)^2. \]