Comparing Graph Transformers via Positional Encodings

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Abstract

The distinguishing power of graph transformers is tied to the choice of positional encoding: features used to augment the base transformer with information about the graph. There are two primary types of positional encoding: absolute positional encodings (APEs) and relative positional encodings (RPEs). APEs assign features to each node and are given as input to the transformer. RPEs instead assign a feature to each pair of nodes, e.g., shortest-path distance, and are used to augment the attention block. A priori, it is unclear which method is better for maximizing the power of the resulting graph transformer. In this paper, we aim to understand the relationship between these different types of positional encodings. Interestingly, we show that graph transformers using APEs and RPEs are equivalent in their ability to distinguish non-isomorphic graphs. In particular, we demonstrate how to interchange APEs and RPEs while maintaining their distinguishing power in terms of graph transformers. However, in the case of graphs with node features, we show that RPEs may have an advantage over APEs. Based on our theoretical results, we provide a study of different APEs and RPEs—including the shortest-path and resistance distance and the recently introduced stable and expressive positional encoding (SPE)—and compare their distinguishing power in terms of graph transformers.

1. Introduction

Graph transformers (GTs) (Dwivedi & Bresson, 2021; Ying et al., 2021) have recently emerged as a competitor to message passing neural networks (MPNNs) (Gilmer et al., 2017) for graph representation learning. While MPNNs only consider the immediate neighbors of a node when updating that node’s feature, GTs consider all nodes in the graph. Accordingly, graph transformers can capture global information of graphs that can potentially be used to address the issue of oversquashing faced by MPNNs. Likewise, the attention mechanism of transformers can address the issue of oversmoothing faced by MPNNs. See (Müller et al., 2024).

However, one caveat in applying transformers to graph data is that transformers are equivariant, meaning they treat nodes symmetrically and cannot distinguish two nodes at different positions in the graph. Accordingly, much of the research on graph transformers has been focused on the design of positional encodings that incorporate information about the graph structure into the input or architecture of transformers. There are currently two major types of positional encodings:

Absolute positional encodings (APEs) encode the graph structure as an embedding of the vertices $\phi: V \rightarrow \mathbb{R}^d$. APEs are either added to or concatenated with the initial vertex features that are the input to the transformer. Typical examples are the Laplacian eigenvectors (Dwivedi & Bresson, 2021) or information about random walks (Rampášek et al., 2022). Recent works have also proposed learnable APEs (Lim et al., 2022; Huang et al., 2024).

Relative positional encodings (RPEs) encode the graph structure as an embedding of pairs of vertices $\psi: V \times V \rightarrow \mathbb{R}^d$. RPEs are incorporated into a GT via a modified attention mechanism. Examples of RPEs include the shortest-path distance (Ying et al., 2021), resistance distance (Zhang et al., 2023), and heat kernels (Choromanski et al., 2022). The adjacency matrix can also serve as an RPE, which will result in an RPE GT with the same distinguishing power as MPNNs (Corollary 4.17).

Although different kinds of APEs and RPEs have been proposed to encode graph structure and enhance the performance of GTs, there is a lack of understanding of how different positional encodings compare—e.g., shortest-path

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vs. resistance distance—for distinguishing non-isomorphic graphs. Only a few works (Zhang et al., 2023) have attempted to compare different RPEs, let alone conduct a systematic study comparing APEs and RPEs. This results in a lack of guidance for the design of positional encodings for GTs: which type of positional encoding—absolute or relative—should be used in practice? Furthermore, this could lead to inefficiency in constructing positional encodings. In some recent works on designing APEs like BasisNet (Lim et al., 2022) and the stable and expressive positional encoding (SPE) (Huang et al., 2024), the authors first construct well-defined RPEs and then use some extra machinery to artificially transform RPEs into APEs. This raises the natural question of whether the transition is worthwhile given the expensive extra computation.

**Our contributions.** We establish a theoretical framework for comparing positional encodings, not only for those in the same category, i.e., absolute or relative, but also across APEs and RPEs. Our main contributions are as follows:

1. In Section 3, we establish that specific types of APE and RPE GTs (cf. Definition 2.2) are equivalent in their ability to distinguish non-isomorphic graphs. In particular, we show how to map APEs to RPEs and vice versa while maintaining their distinguishing power. We empirically validate our theoretical results on several graph classification datasets.

2. We show that RPEs may have an advantage over APEs for distinguishing graphs with node features. In particular, we show that transforming an RPE to an APE results in a GT that is able to distinguish strictly fewer graphs with node features than a GT that uses the RPE directly.

3. The techniques for proving the above results enable us to compare the distinguishing power of different positional encodings. In Section 4, we provide a case study on several popular APEs and RPEs by comparing their distinguishing power. For example, we prove that GTs using SPE (Huang et al., 2024) as an APE are stronger than the GTs using resistance distance as an RPE (Zhang et al., 2023).

4. In the process of establishing our main results, we identify a new variant of the Weisfeiler-Lehman (WL) test (Weisfeiler & Leman, 1968) that we call the RPE-aug WL test that allows us to connect the distinguishing power of RPEs and corresponding GTs. This RPE-aug WL test is interesting in itself as a way to further the theoretical formulation of the representation power of graph learning frameworks. We generalize the equivalence between the WL and 2-WL tests to our RPE-aug WL test and establish the equivalence between the resistance distance and the pseudoinverse of the Laplacian in terms of distinguishing power via the RPE-aug WL test. Furthermore, we identify a class of RPEs resulting in a family of RPE GTs at least as strong as MPNNs.

### 2. Positional Encodings and Graph Transformers

In this section, we introduce some preliminaries on positional encodings and graph transformers, as well as some auxiliary results that will be used to prove our main results.

Let $G = (V, E)$ denote an unweighted graph, which can be either directed or undirected. A **featured graph** $(G, X)$ includes node features $X \in \mathbb{R}^{|V| \times d}$, indicating a $d$-dimensional feature $X(v)$ for each node in $v \in V$. Let $A$ denote the adjacency matrix, $D$ the diagonal matrix of the degrees, and $L = D - A$ the graph Laplacian matrix. To prevent ambiguity when working with multiple graphs, we use $G$ as a subscript in our notations, such as $V_G$ for the vertex set or $X_G$ for the node features of graph $G$.

For two graphs $G$ and $H$, a graph isomorphism is a bijection $\sigma : V_G \rightarrow V_H$ such that $\{u, v\} \in E_G$ if and only if $\{\sigma(u), \sigma(v)\} \in E_H$. Two graphs $G$ and $H$ are isomorphic if there is a graph isomorphism $\sigma : V_G \rightarrow V_H$.

#### 2.1. Positional Encodings

A positional encoding (PE) of a graph is a way of summarizing structural or positional information of the graph. In their most general form, there are two types of positional encodings we consider in this paper:

**Definition 2.1.** (Positional Encodings)

An **absolute positional encoding (APE)** $\phi$ assigns each graph $G$ a map $\phi_G : V_G \rightarrow \mathbb{R}^l$ such that for any two isomorphic graphs $G$ and $H$ and graph isomorphism $\sigma : V_G \rightarrow V_H$, one has that $\phi_G = \phi_H \circ \sigma$.

A **relative positional encoding (RPE)** $\psi$ assigns each graph $G$ a map $\psi_G : V_G \times V_G \rightarrow \mathbb{R}^k$ such that for any two isomorphic graphs $G$ and $H$ and graph isomorphism $\sigma : V_G \rightarrow V_H$, one has that $\psi_G = \psi_H \circ (\sigma \times \sigma)$.

An APE is also naturally expressed as a matrix in $\mathbb{R}^{\lvert V_G \rvert \times l}$ and an RPE as a tensor $\mathbb{R}^{\lvert V_G \rvert \times \lvert V_G \rvert \times k}$.

**Note:** While node features and APEs both assign a vector to each node, we emphasize that the difference between node features and APEs is that APEs are dependent on the topology of a graph, while two isomorphic graphs can have different node features.

One of the simplest APEs is the degree map $\text{deg}$: for any graph $G$, $\text{deg}_G(u)$ is the degree of the vertex $u$. Any graph distance is an RPE, e.g., shortest-path distance (SPD) or resistance distance (RD).

Laplacian eigenvectors are commonly used as APEs (Dwivedi & Bresson, 2021; Kreuzer et al., 2021). However, there is no unique choice of eigenvector for a given eigenspace. Therefore, Laplacian eigenvectors are not a well-defined APE by our definition, as isomorphic graphs...
may have different eigenvector encodings due to the choice of basis. However, the projection matrices onto the eigenspaces are a well-defined RPE (Lim et al., 2022).

2.2. Graph Transformers

A transformer is an architecture $T$ composed of multiheaded attention layers $T = \text{MHA}^{(L)} \circ \cdots \circ \text{MHA}^{(1)}$, where a multiheaded attention layer with heads $1 \leq h \leq H$ is a map $\text{MHA}^{(l)}$ that sends $X^{(l)} \in \mathbb{R}^{n \times d}$ to $\text{MHA}^{(l)}(X^{(l)}) = X^{(l+1)} \in \mathbb{R}^{n \times d}$ as defined below:

$$A^{(l,h)}(X^{(l)}) = \text{softmax} \left( \frac{X^{(l)}W_Q^{(l,h)}(X^{(l)}W_K^{(l,h)})^T}{\sqrt{d_h}} \right)$$

$$Y^{(l)} = X^{(l)} + \left( \sum_{h=1}^{H} A^{(l,h)}(X^{(l)})X^{(l)}W_V^{(l,h)} \right)W_O^{(l)}$$

$$X^{(l+1)} = Y^{(l)} + \sigma \left( Y^{(l)}W_1^{(l)} \right)W_2^{(l)}$$

where $W_O^{(l,h)} \in \mathbb{R}^{d \times d_h}$, $W_V^{(l,h)} \in \mathbb{R}^{d \times d_h}$, $W_O^{(l)} \in \mathbb{R}^{d \times d_h}$, $W_1^{(l)} \in \mathbb{R}^{d_h \times d_h}$, $W_2^{(l)} \in \mathbb{R}^{d_h \times d_h}$ and $\sigma$ is an activation function. Here $Q$, $K$, $V$ refer to “query”, “key” and “value”, respectively, in the terminology of the attention literature (Vaswani et al., 2017), and $d_h$ and $d$ are the dimension of the hidden layer and the dimension of the residual layer, respectively. The activation function $\sigma$ is usually the Gaussian error linear units (GELU) (Hendrycks & Gimpel, 2016).

Fact 1 (Transformers are Permutation Equivariant). Let $T$ be a transformer. Let $X \in \mathbb{R}^{n \times d}$. Let $P \in \mathbb{R}^{n \times n}$ be a permutation matrix. Then $PT(X) = T(PX)$.

When applying a transformer to a graph $G$, the input is a set of node features $X_G \in \mathbb{R}^{|V_G| \times d}$; however, initial node features often do not contain any information about the topology of a graph, so two graphs with the same multiset of features but different topologies will have the same output from a transformer. Graph transformers augment the transformer by incorporating information about the input graph in the form of absolute or relative positional encodings.

Definition 2.2 (Graph Transformers). An APE graph transformer with APE $\phi$ ($\phi$-APE-GT) is a transformer that either: concatenates the node features $X_G \in \mathbb{R}^{|V_G| \times d}$ with the APE $\phi_G \in \mathbb{R}^{|V_G| \times l}$, i.e. $\bar{X}_G = [X_G \ | \phi_G] \in \mathbb{R}^{|V_G| \times (d+l)}$, or adds the node features and APE, i.e. $\bar{X}_G = X_G + \phi_G$, before passing them through a transformer. An RPE graph transformer with RPE $\psi$ ($\psi$-RPE-GT) is a transformer whose attention layer is modified as follows for a graph $G$ with node features $X \in \mathbb{R}^{|V_G| \times d}$:

$$A(X) = f_1(\psi_G) \circ \text{softmax} \left( \frac{XW_Q(XW_K)^T}{\sqrt{d_h}} + f_2(\psi_G) \right)$$

where $f_1, f_2 : \mathbb{R}^k \rightarrow \mathbb{R}$ are functions applied entrywise to the tensor $\psi_G \in \mathbb{R}^{|V_G| \times |V_G| \times k}$.

The original transformer (Vaswani et al., 2017) used sines and cosines as APEs for sequences. Transformers for sequences with RPEs were subsequently proposed by Shaw et al. (2018). The first instance of an APE-GT for graphs was proposed by Dwivedi & Bresson (2021) using the Laplacian eigenvectors. The first instance of an RPE-GT was proposed by Ying et al. (2021) using the shortest-path distance, while the form of RPE-GT we consider was proposed by Zhang et al. (2023). Although other ways of incorporating an RPE into a transformer have been proposed (Mialon et al., 2021; Ma et al., 2023), in this paper, APE-GT and RPE-GT only refer to transformers of the forms in Definition 2.2.

2.3. Properties of RPEs

In this subsection, we describe two special types of RPEs that will be useful later.

Diagonally-Aware RPEs. One benefit of using graph distances as RPEs—compared to e.g., the adjacency matrix—is their distinct diagonal entries are all zeros, in contrast to the positive off-diagonal terms. We characterize this property as “diagonal-awareness”. As we will see throughout the paper, this property is important as it allows various algorithms to distinguish the feature at a node from all other features.

Definition 2.3. An RPE $\psi$ is diagonally-aware if for any two graphs $G$ and $H$ and vertices $v \in V_G$ and $x, y \in V_H$, then $\psi_G(v, u) = \psi_H(x, y)$ only if $x = y$.

Diagonally-awareness is a very mild condition as one can always augment an RPE so that it becomes diagonally-aware:

Definition 2.4. The diagonal augmentation $D^\psi$ of an RPE $\psi$ is defined, for a graph $G$, as the stacking $D^\psi_G := (I_G, \psi_G)$ where $I_G$ is the identity matrix.

For any graph $G$, the diagonal augmentation $D^\psi_G(u, v)$ has a 1 in the first coordinate iff $u = v$ and 0 otherwise. Therefore, $D^\psi$ is diagonally-aware:

Proposition 2.5. Let $\psi$ be an RPE. The diagonal augmentation $D^\psi$ is diagonally-aware.

Asymmetric RPEs. Most popular RPEs for undirected graphs are symmetric. However, for directed graphs, it is natural to consider asymmetric RPEs such as the adjacency matrix, the directed distance matrix, or the Laplacian matrix.

We identify the following special type of (possibly asymmetric) RPEs, which will be useful later:

Definition 2.6 (Pseudo-symmetric RPEs). Let $\psi$ be an RPE valued in $\mathbb{R}^k$ for either directed or undirected graphs. Let $f : \mathbb{R}^k \rightarrow \mathbb{R}^k$ be any injective function such that $f \circ f = 1d$. Then, $\psi$ is $(f)$-pseudo-symmetric if $\psi_G(u, v) = f(\psi_G(v, u))$ for any graph $G$ and any vertices $u, v \in V_G$.
Examples of \( f \) satisfying \( f \circ f = \text{Id} \) include the identify map, the reflection map, and any coordinate switching map. Obviously, any symmetric RPE \( \psi \) is \( \text{Id} \)-pseudo-symmetric. Any skew-symmetric matrix is pseudo-symmetric for \( f(x) = -x \). If we consider complex-valued RPEs, then any Hermitian matrix is pseudo-symmetric for \( f(x) = \pi \), the complex conjugate map.

Although the adjacency or the Laplacian matrix of a directed graph can also serve as RPEs, they are in general not pseudo-symmetric. In order to guarantee pseudo-symmetry, given any RPE \( \psi \), we can define an augmented RPE \( S^\psi := (\psi, \psi^T) \), i.e., for any graph \( G \), \( S^\psi_G := (\psi_G, \psi_G^T) \).

**Lemma 2.7 (Pseudo-symmetric augmentation).** Let \( \psi \) be any RPE. Define \( f : \mathbb{R}^{2k} \to \mathbb{R}^{2k} \) by letting \( (x, y) \mapsto (y, x) \) for any \( x, y \in \mathbb{R}^k \). Then, \( S^\psi \) is \( f \)-pseudo-symmetric.

### 3. Comparison of APE-GT and RPE-GT

In this section, we establish the equivalence of the distinguishing power of APE and RPE GTs for distinguishing graphs without node features. This is done by showing that any RPE can be mapped to an APE without changing its distinguishing power and vice versa. Our strategy is to relate the distinguishing power of APE and RPEs, as well as the maps between the two, to variants of the Weisfeiler-Lehman tests. This approach generalizes the method of Zhang et al. (2023) for studying the expressive power of the Graphormer-GD. Our main results are summarized in Figure 1.

However, for the case of graphs with node features, we prove that our map from RPEs to APEs can result in a strict decrease in the distinguishing power of the corresponding GTs. In this way, our results suggest that (1) the two types of positional encodings are theoretically equivalent for solving graph isomorphism problems but (2) RPE GTs may be better suited for tasks where graph node features are involved.

Our theoretical results are tested empirically in Appendix C.

### 3.1. Distinguishing Power: PEs vs. Graph Transformers

Positional encodings provide a way of distinguishing different, non-isomorphic graphs. In their most basic form, two graphs can be distinguished by a positional encoding if it takes different values on the two graphs. For graphs with node features, a positional encoding can distinguish two graphs if it takes different values on nodes with different features. Specifically, two featured graphs \( (G, X_G) \) and \( (H, X_H) \) are indistinguishable by an APE \( \phi \) if the concatenation of their features with their images by the APE \( \phi \) are the same multiset, i.e., \( \{ (X_G(x), \phi_G(x)) : x \in V_G \} = \{ (X_H(x), \phi_H(x)) : x \in V_H \} \), and \( G \) and \( H \) are indistinguishable by an RPE \( \psi \) if \( \{ (X_G(u), X_G(v), \psi_G(u,v)) : (u, v) \in V_G \times V_G \} = \{ (X_H(x), X_H(y), \psi_H(x,y)) : (x, y) \in V_H \times V_H \} \). Likewise, two graphs are indistinguishable by a graph transformer if their outputs have the same multiset of node features.

Next, we compare the distinguishing power of positional encodings and GTs using these positional encodings.

### APE vs. APE-GT

Interestingly, APE-GTs are only as strong as their initial APEs in distinguishing power. This was previously noted by Müller et al. (2024, Section 2.1), although we include a short proof (which follows from the permutation-equivariance of transformers) in Appendix A.4 for completeness.

**Lemma 3.1 (Equivalence of APEs and APE-GT).** Any two graphs \( (G, X_G) \) and \( (H, X_H) \) are indistinguishable by an APE \( \phi \) iff \( (G, X_G) \) and \( (H, X_H) \) are indistinguishable by all \( \phi \)-APE-GTs.

### RPE vs. RPE-GT

An analogous result does not hold for RPEs and RPE-GTs, as using an RPE in an RPE-GT can increase its distinguishing power; see Appendix A.1 for an example. In fact, one can obtain a stronger notion of distinguishing power of RPEs via a variation of the Weisfeiler-Lehman (WL) graph isomorphism test (Weisfeiler & Leman, 1968). This new notion of indistinguishability for RPEs will be equivalent to the indistinguishability of RPE-GTs.

We first recall the standard WL algorithm, which iteratively assigns colors to the vertices of a graph and utilizes the multisets of node colors to distinguish non-isomorphic graphs. The color updating process is defined explicitly as follows:

**Definition 3.2.** Let \( G \) be a graph. The **Weisfeiler-Lehman (WL) algorithm** assigns a coloring to the vertices \( \chi_G^{(t)} : V_G \to C_t \) for each \( t \geq 0 \) defined by

\[
\chi_G^{(0)}(v) = 1, \quad \chi_G^{(t+1)}(v) = (\chi_G^{(t)}(v), \{ \chi_G^{(t)}(u) : v, u \in E_G \}).
\]

However, to understand the distinguishing power of RPE transformers, we need to consider the following augmented WL test for graphs with node features and RPEs.

**Definition 3.3.** Let \( \psi \) be an RPE. Let \( (G, X_G) \) be a featured graph. The **Weisfeiler-Lehman algorithm augmented with RPE \( \psi \) (RPE-augWL or \( \psi \)-WL)** assigns a coloring to the vertices \( \chi_{\psi G}^{(t)} : V_G \to C_t \) for each \( t \geq 0 \) defined by

\[
\chi_{\psi G}^{(0)}(v) = X_G(v), \quad \chi_{\psi G}^{(t+1)}(v) = (\chi_{\psi G}^{(t)}(v), \{ \chi_{\psi G}^{(t)}(u) : v, u \in E_G \}).
\]

**Note:** For unfeatured graphs, \( \psi \)-WL is defined by setting \( \chi_{\psi G}^{(0)}(v) = 1 \) (where 1 is an arbitrary constant). We adopt this convention for all later constructions.

Note that the RPE-augWL algorithm has a different color updating mechanism from the WL algorithm: RPE-augWL
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Figure 1. Illustration of main results. Arrows denote non-decreasing in distinguishing power. Our main results are the two red arrows on the left. The proofs of the two theorems are illustrated by other parts of the diagram. Our contributions are in bold. The two-head arrow from RPE-2-WL to APEs indicates that the non-decreasing property only holds for unfeatured graphs.

considers all nodes in the update stage, whereas WL considers only neighbors. However, when the RPE is the adjacency matrix $A$, $A$-WL is equivalent to WL (cf. Proposition B.16). Hence, we consider RPE-augWL to be a generalization of the WL algorithm.

The definition of RPE-augWL is inspired by the GD-WL test of Zhang et al. (2023) where the new feature is updated as $\chi^{(t+1)}_{\psi_G} (v) = \{(\chi^{(t)}_{\psi_G}(u), \psi_G (v, u)) : u \in V\}$, where $\psi_G$ is a graph distance. We note that GD-WL is equivalent to our $\psi$-WL; in GD-WL, the previous color of the node can be deduced from the fact that $\psi_G (v, v) = 0$ since $\psi_G$ is a graph distance.

The WL algorithm has a family of higher-order generalizations called the $k$-WL algorithms that assign colors to $k$-tuples of nodes. While Definition 3.3 augments the WL test by using RPEs within the feature updating step, we can also directly use RPEs as the initial colors for 2-WL.

Definition 3.4. Let $\psi$ be an RPE. Let $(G, X)$ be a featured graph. The 2-Weisfeiler-Lehman algorithm with RPE $\psi$ (RPE-2-WL or $\psi$-2-WL) assigns a color to each pair of vertices $\chi^{(t)}_{2, \psi_G} (u, v) : V \times V \to C_t$ for each $t \geq 0$ defined by

$$\chi^{(0)}_{2, \psi_G} (u, v) = (X_G (u), X_G (v), \psi_G (u, v)),$$

$$\chi^{(t+1)}_{2, \psi_G} (u, v) = \{(\chi^{(t)}_{2, \psi_G} (u, v), \chi^{(t)}_{2, \psi_G} (w, v)) : w \in V\}.$$

Because RPEs are dependent on the graph structure and will be the same (up to permutation) for two isomorphic graphs, we can use the RPE-augWL or RPE-2-WL as heuristics to distinguish non-isomorphic graphs. We say two featured graphs $(G, X_G)$ and $(H, X_H)$ are $\psi$-WL indistinguishable if $\chi^{(t)}_{2, \psi_G} (v) = \chi^{(t)}_{2, \psi_H} (v)$ for all $t \geq 0$. We denote this as $\chi_{\psi} (G) = \chi_{\psi} (H)$.

Interestingly, these two WL tests—RPE-augWL and RPE-2-WL—are equivalent for pseudo-symmetric RPEs. See Appendix A.2 for a proof.

Theorem 3.5 (Equivalence of RPE-augWL and RPE-2-WL). Let $\psi$ be a pseudo-symmetric RPE. Then two featured graphs $(G, X_G)$ and $(H, X_H)$ are $\psi$-WL indistinguishable if and only if they are $\psi$-2-WL indistinguishable.

This result generalizes the well-known fact that the WL and 2-WL tests are equivalent; see (Huang & Villar, 2021).

Finally, in contrast to Lemma 3.1, we have the following slight generalization of (Zhang et al., 2023, Theorem 4) who only consider the case where the RPE is a distance function. See Appendix A.6 for a sketch of the proof.

Lemma 3.6 (Equivalence of RPE-augWL and RPE-GT). Let $\psi$ be a diagonally-aware RPE. Let $(G, X_G)$ and $(H, X_H)$ be featured graphs. Then $(G, X_G)$ and $(H, X_H)$ are indistinguishable by the $\psi$-WL test if $(G, X_G)$ and $(H, X_H)$ are indistinguishable by all $\psi$-RPE-GTs.

3.2 Main Results: APE vs RPE Transformers

In this section, we show that any APE can be turned into an RPE without changing its distinguishing power in terms of transformers and vice versa.

Mapping APEs to RPEs. Let $S$ be any set, and let $\text{Mul}_2 (S)$ denote the collection of all 2-element multi-
subsets of $S$. For a map $f : S \to \mathbb{R}^d$, define the map $h_f : \text{Mul}_2(S) \to \mathbb{R}^d$ as $h_f(\langle x, y \rangle) = f(x) + f(y)$. The map $h_f$ is a special case of the DeepSets network (Zaheer et al., 2017) as it operates on multisets. Accordingly, we refer to $h_f$ as a DeepSet network in this paper.

We propose the following way of mapping APEs to RPEs: given a function $f$ and an APE $\phi$, we define the RPE $\psi_f$ for a graph $G$ as $\psi_f(\langle u, v \rangle) := h_f(\langle \phi_G(u), \phi_G(v) \rangle)$. Our key observation is that given an APE $\phi$, there exists a universal function $f$ whose induced RPE $\psi_f$ distinguishes the same pairs of graphs as $\phi$ (Lemma 3.7). The main Theorem 3.8 will then follow. Proofs of these results can be found in Appendix A.7.

**Lemma 3.7.** Let $\phi$ be an APE. Then there is a function $f$ such that any two featured graphs $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\phi$ iff $(G, X_G)$ and $(H, X_H)$ cannot be distinguished by the $\psi_f$-2-WL test.

**Theorem 3.8.** For any APE $\phi$, there exists a function $f$ such that any two graphs $(G, X_G)$ and $(H, X_H)$ are indistinguishable by all $\psi_f$-APE-GTs iff they are indistinguishable by all $\psi_f$-RPE-GTs.

**Mapping RPEs to APEs.** In the other direction, we can transform an RPE $\psi$ to an APE $\phi$ by passing $\psi$ through a 2-equivariant graph network (2-EGN) $g$. (See (Maron et al., 2019b) or Appendix A.3 for a definition of 2-EGN.) As 2-EGNs are permutation equivariant, the output $\phi$ will be a well-defined APE in the sense of Definition 2.1. This is the approach taken by Lim et al. (2022) to compute an APE from the eigenspaces of the graph Laplacian. It turns out that mapping RPEs to APEs using 2-EGNs can preserve their ability to distinguish non-featured graphs; however, mapping an RPE to an APE may decrease its ability to distinguish featured graphs. Proofs of the following theorems and example can be found in Appendix A.8.

**Lemma 3.9.** Let $\psi$ be a diagonally-aware RPE.

For any 2-EGN $g$, if $(G, X_G)$ and $(H, X_H)$ are indistinguishable by the $\psi$-2-WL test then $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\phi^g$.

Moreover, for any finite set of unfeatured graphs $G$, there is a 2-EGN $g$ such that if $G, H \in G$ are indistinguishable by $\phi^g$, then $G$ and $H$ are indistinguishable by the $\psi$-2-WL test.

**Theorem 3.10.** Let $\psi$ be a diagonally-aware RPE.

For any 2-EGN $g$, if $(G, X_G)$ and $(H, X_H)$ are indistinguishable by all $\psi$-RPE-GTs, then $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\phi^g$.

Moreover, for any finite set of unfeatured graphs $G$, there is a 2-EGN $g$ such that if $G, H \in G$ are indistinguishable by all $\phi^g$-APE-GTs, then $G$ and $H$ are indistinguishable by all $\psi$-RPE-GTs.

**Example 1.** There exists an RPE $\psi$ and featured graphs $(G, X_G)$ and $(H, X_H)$ that are distinguishable by $\psi$-2-WL but are indistinguishable by $\phi^g$ for any 2-EGN $g$.

**Remark 3.11.** Even in the case of unfeatured graphs, there is still a slight asymmetry in the statements of the results for APEs (Theorem 3.8) and RPEs (Theorem 3.10), as the result for APEs does not have the restriction on “a finite set” of graphs. This restriction arises because there is no known universal 2-EGN equal in power to the RPE-2-WL test. This is in part due to the fact that known 2-EGNs would need an unbounded hidden dimension and number of layers to distinguish all pairs of graphs (Maron et al., 2019a).

**More expressive RPE to APE maps.** Theorem 3.10 shows that RPEs can be transformed into equally-powerful (for unfeatured graphs) APEs using 2-EGNs. However, it is worth noting that RPEs can be turned into APEs that are even more powerful than the original RPE using $k$-EGNs for $k > 2$ (Maron et al., 2019a). In the extreme case of $k \in \Omega(n)$, $k$-EGNs can distinguish all pairs of non-isomorphic graphs with $n$ vertices. Such techniques for constructing APEs from RPEs have been previously explored in the literature (Huang et al., 2024); for example, Expressive BasisNet (Lim et al., 2022). However, the downside to these techniques is that their computational cost increases with their expressive power; $k$-EGNs take $\Theta(n^k)$ time as they operate on tensors of size $\Theta(n^k)$. In practice, techniques that map RPEs to APEs typically only use 2-EGNs because of the computational cost of higher $k$-EGNs.

**Restrictions and Implications.** Our main findings (Theorems 3.8 and 3.10) show that APE-GTs and RPE-GTs have comparable distinguishing capabilities for unfeatured graphs. However, in practice, learning the DeepSet (to serve as $f$) in Theorem 3.8 or the 2-EGN (to serve as $g$) in Theorem 3.10 may not always yield the desired maps. Hence, it remains an interesting open question to figure out whether it is theoretically easier to learn the DeepSet or the 2-EGN. For example, one would benefit in designing architectures from understanding which method requires a lower dimension for hidden layers.

Finally, we would like to point out that converting RPEs to APEs to fit a specific graph transformer architecture is not recommended, as shown by Example 1. See also discussion in Remark 4.5 and Appendix A.3 for some empirical validation of this point.

**4. Comparing Graph Transformers with Different Positional Encodings**

In this section, we compare the distinguishing power of graph transformers with different (absolute or relative) positional encodings. The main results are summarized in
Comparing Graph Transformers via Positional Encodings

**Figure 2. Hierarchy of PEs.** The arrows indicate that the corresponding positional encoding is less strong than the one it points to in terms of distinguishing power. The two-head arrow indicates that the non-decreasing property only holds for unfeatured graphs. The dotted arrow between SPD and RD refers to some partial evidence (cf. Theorem B.18) that RD is stronger than SPD in some respects; however, it is an open question how the two compare as RPEs.

Figure 2. Intuitively, by Theorem 3.8, APE-GTs can be turned into RPE-GTs preserving the distinguishing power. This enables us to compare APE-GTs with RPE-GTs. When comparing two RPE-GTs, by Lemma 3.6 we simply need to compare the corresponding RPEs via the RPE-augWL test. For two RPEs $\psi_1$ and $\psi_2$, we say that $\psi_1$-WL is at least as strong as $\psi_2$-WL if for any two featured graphs $(G, X_G)$ and $(H, X_H)$ such that $\chi_{\psi_1}(G) = \chi_{\psi_1}(H)$, then we have $\chi_{\psi_2}(G) = \chi_{\psi_2}(H)$. Moreover, we say that $\psi_1$-WL and $\psi_2$-WL are equally strong if for any two featured graphs $(G, X_G)$ and $(H, X_H)$, we have that $\chi_{\psi_1}(G) = \chi_{\psi_1}(H)$ iff $\chi_{\psi_2}(G) = \chi_{\psi_2}(H)$.

Some highlights of this section include a comparison of SPE-APE-GTs with RD-RPE-GTs (Theorem 4.4), identification of a class of RPEs whose corresponding RPE-GTs are at least as strong as MPNNs (Proposition 4.10 and Corollary 4.17), and suggesting new RPEs for directed graphs (Proposition 4.12).

### 4.1. Resistance Distance, Spectral Kernels, and SPE

Many popular APEs (such as BasisNet (Lim et al., 2022) and SPE (Huang et al., 2024))) and RPEs (such as RD (Zhang et al., 2023))) are defined using the spectrum of the Laplacian $L$. While BasisNet and SPE have been shown to be equivalent (Huang et al., 2024, Proposition 3.2), it is unclear how either of these compares to RD in terms of transformers. More generally, it is unknown how much information RD-WL carries about the spectrum of $L$.

In this section, we establish that SPE-APE-GTs are stronger than resistance distance RPE-GTs (Theorem 4.4). As one step to prove this, we show that two graphs are indistinguishable by RD-WL iff they are indistinguishable by $L^\dagger$-WL where $L^\dagger$ is the pseudoinverse of $L$ (Corollary 4.3). This result gives a partial answer to the question of how much information RD-WL carries about the Laplacian spectrum. This is weaker than saying that RD-WL indistinguishable graphs have the same $L^\dagger$ up to permutation, but it does show that $L^\dagger$ of these graphs are indistinguishable when combined with RPE-augWL (and thus RPE-GTs).

In fact, our result about RD-WL is a corollary to a stronger result about the equivalence of RPE-augWL tests with spectral distance and spectral kernel as RPEs.

**Definition 4.1.** Let $L = \sum_{i=2}^{n} \lambda_i z_i z_i^T$ be the spectral decomposition, where $\{\lambda_2, \ldots, \lambda_n\}$ are the non-zero eigenvalues and $\{z_2, \ldots, z_n\}$ is an orthonormal basis of eigenvectors. Let $f : \mathbb{R}^+ \to \mathbb{R}^+$ be a function. The **spectral kernel** (Hammond et al., 2011) corresponding to $f$ is the matrix $K_G^f = \sum_{i=2}^{n} f(\lambda_i) z_i z_i^T$. The **spectral distance** corresponding to $f$ is defined

$$d_G^f(u, v) := \sqrt{K_G^f(u, u) + K_G^f(v, v) - 2 K_G^f(u, v)}.$$

**Example 2.** The diffusion distance (at time $t$) (Coifman & Lafon, 2006) is the spectral distance $D^f$ for the function $f(x) = e^{-tx}$. The **heat kernel** is the corresponding spectral kernel denoted by $H(t) = \sum_{i=2}^{n} e^{-\lambda_i t} z_i z_i^T$, which has been proposed as an RPE by Choromanski et al. (2022).

**Note:** Although eigenvectors are not unique due to the choice of bases for eigenspaces, the spectral kernel and spectral distance are unique up to graph isomorphism and so are well-defined RPEs.

Let $D^f$ denote the RPE assigning the matrix of spectral distance $d_G^f$ to a graph $G$ and let $K^f$ denote the RPE assigning the matrix of spectral kernel $K_G^f$.

**Theorem 4.2.** Let $f : \mathbb{R}^+ \to \mathbb{R}^+$. $D^f$-WL is at least as strong as $K^f$-WL. $K^f$-WL with diagonal augmentation is at least as strong as $D^f$-WL.

Theorem 4.2 is the result of the fact that the spectral distance and kernel are the distance and Gram matrix, respectively, of a point cloud in $\mathbb{R}^d$. A variant of the WL-algorithm for general distance matrices of point clouds was studied...
by delle Rose et al. (2023) as a heuristic for determining if two point clouds are isometric, so our proof may have implications for these algorithms as well. A proof of this theorem can be found in Appendix B.2.

The resistance distance (RD) is the squared spectral distance of the function \( f(x) = x^{-1} \), and the pseudoinverse of the Laplacian \( L^\dagger \) is the corresponding spectral kernel, so Theorem 4.2 applies to RD and \( L^\dagger \). Interestingly, RD has additional properties that allow us to drop the assumption of diagonal augmentation. A proof of the following theorem can be found in Appendix B.2.

**Corollary 4.3.** RD-WL and \( L^\dagger\)-WL are equally strong.

Finally, as an immediate consequence of Corollary 4.3 (combined with Theorem 3.10), we compare RD-RPE-GT, with existing APE-GPTs using the so-called Stable and Expressive Positional Encodings (SPE) (Huang et al., 2024). A proof of this theorem can be found in Appendix B.3.

**Theorem 4.4.** For unfeatured graphs, diagonally augmented SPE-APE-GT is at least as strong as RD-RPE-GT.

**Remark 4.5.** In Appendices C.1 and C.2, we empirically validate this theorem by showing that SPE-APE-GTs perform similarly to RD-RPE-GTs on some unfeatured graph classification/isomorphism tasks. However, when node features are involved, the theorem may not hold since the 2-EGN involved in the construction of SPE-APE-GT may have weaker distinguishing power than the RD-RPE-GT (cf. Example 1). In Appendix C.3, we empirically observe that for graph regression tasks when node features are involved, using RD-RPE-GT can indeed give us an edge in performance over SPE-APE-GT.

### 4.2. Resistance Distance and Cut Edges.

The first proposed RPE for graph transformers was the shortest-path distance (SPD) (Ying et al., 2021). Later, Zhang et al. (2023) proposed to use the stack of RD and SPD as an RPE. It is natural to wonder how RD-WL compares with SPD-WL. While this remains an open question, we prove that RD-WL is at least as strong as SPD-WL in at least one regard.

Zhang et al. (2023) showed that SPD-WL could distinguish cut edges but not cut vertices in unfeatured graphs. Furthermore, the authors showed that RD-WL could distinguish cut vertices. However, it was not known whether or not RD-WL could distinguish cut edges in a graph. We answer this open question in the affirmative: RD-WL can distinguish cut edges in a graph. See Theorem B.18 for a precise theorem statement and proof.

However, our experiments on the BREC dataset (Wang & Zhang, 2024) suggest (but do not prove) that RD-WL may not be strictly stronger than SPD-WL, as there are pairs of graphs in this dataset that an SPD-RPE-GT was able to learn to distinguish, while we were unsuccessful in training a RD-RPE-GT to distinguish these graphs. See Appendix C.2 for details.

### 4.3. Powers of Matrices and Spectral Kernels

Another common type of RPE is the stack of powers of some matrix associated with the graph; for example, GRIT (Ma et al., 2023) uses a stack of powers of the random-walk adjacency matrix of a graph called the relative random-walk positional encoding (RRWP). In this section, we show that using stacks of various matrices as an RPE is at least as strong as any spectral kernel RPEs for any \( f : \mathbb{R}^+ \rightarrow \mathbb{R}^+ \). Proofs for this section can be found in Appendix B.4.

We first prove that using sufficiently many powers of the Laplacian is at least as strong as any spectral kernel.

**Theorem 4.6.** \((I, L, \ldots, L^{2n-1})\)-WL is at least as strong as \( K_f\)-WL on graphs with at most \( n \) nodes.

**Remark 4.7.** While it may seem excessive to consider \( 2n \) powers of \( L \) to match the power of a single spectral kernel, this is not computationally more expensive than computing the spectral kernel in the first place, which requires adding \( n \) matrices \( f(\lambda_i)z_iz_i^T \) of size \( n^2 \), which takes \( O(n^3) \) time.

A variant of RRWP that uses stacks powers of the symmetrically-normalized adjacency matrix \( \tilde{A} = D^{-1/2}AD^{-1/2} \) is at least as strong as spectral kernels using the symmetrically-normalized Laplacian \( \tilde{K}_f \) (see Appendix B.4 for definition).

**Theorem 4.8.** \((I, \tilde{A}, \ldots, \tilde{A}^{2n-1})\)-WL is at least as strong as \( \tilde{K}_f\)-WL on graphs with at most \( n \) nodes.

Finally, we show that stacked heat kernels \( H^{(1)} \) (cf. Example 2) are also at least as strong as any spectral kernel.

**Theorem 4.9.** \((I, H^{(1)}, \ldots, H^{(2n-1)})\)-WL is at least as strong as \( K_f\)-WL on graphs with at most \( n \) nodes.

### 4.4. RPEs: Common Matrices for Graphs

There are multiple common matrices used to characterize graphs, such as the adjacency matrix, Laplacian matrix and their normalized versions. We will examine their corresponding RPEs and compare their distinguishing power.

#### Undirected graphs

For undirected graphs, we show that various common matrices lead to equivalent RPEs.

Let \( \tilde{A} = D^{-1}A \). Let \( \tilde{L} = I - \tilde{A} \) and \( \tilde{L} = I - A \) denote the symmetrically-normalized and the random-walk graph Laplacians, respectively. These, along with \( A \), \( L \) and \( \tilde{A} \), give rise to six RPEs and hence five corresponding RPE-augWL tests. The following result suggests that in practice, perhaps there is no need to use more than one such type of information with RPE-GTs and one can interchangeably use any of the matrix as RPE.
**Proposition 4.10.** $A, 	ilde{A}, 	ilde{A}, L, 	ilde{L}$ and $L$ induce equivalent RPE-augWL tests. In particular, all of these RPE-augWL tests are equally strong as the WL test.

**Directed graphs.** Directed graphs are sometimes turned into a magnetic graph to obtain a Hermitian matrix called the magnetic Laplacian (Fanuel et al., 2018). Let $G$ be a directed graph with adjacency matrix $A$. Let $A^* := (A + A^T)/2$ and let $D^*$ denote the corresponding degree matrix. Then, given a parameter $\alpha$, the magnetic Laplacian is defined as

$$L^\alpha := D^\alpha - T^\alpha \circ A^*,$$

where $T_{ij}^\alpha = \exp(\nu \cdot 2\pi\alpha \cdot \text{sgn}(A_{ji} - A_{ij}))$ and $\nu$ is the imaginary unit. As mentioned in Section 2, $L^\alpha$ can serve as a pseudo-symmetric RPE. In fact, $L^\alpha$ can be obtained via the pseudo-symmetric augmentation $(A, A^T)$ of $A$ (cf. Lemma 2.7) as well as an extra augmentation via $D^*$:

**Lemma 4.11.** $L^\alpha = f^\alpha((D^*, A, A^T))$ where $f^\alpha : \mathbb{R} \rightarrow \mathbb{R}$ is applied to each channel $n \times n \times \cdot$ such that

$$f^\alpha(x, y, z) := x - \exp(\nu \cdot 2\pi\alpha \cdot \text{sgn}(z - y)) \cdot \frac{y + z}{2}.$$

In this way, we obtain an RPE $(D^*, A, A^T)$ more general than the magnetic Laplacian matrix. Hence, instead of using magnetic Laplacian as positional encoding, one should consider using $(D^*, A, A^T)$-RPE-GT.

**Proposition 4.12.** The $(D^*, A, A^T)$-WL test is at least as strong as the $L^\alpha$-WL test for any $\alpha$.

**4.5. RPEs: Combinatorial-Awareness and WL**

It is an interesting question what information about a graph a transformer can extract from a positional encoding. In Definition 2.2, the learnable functions in an RPE-GT $f_i$ are applied elementwise to the RPEs. Moreover, the functions are also applied elementwise to the attention scores. In other words, given an RPE $\psi$, even though the graph structure can be obtained indirectly through more complicated operations on $\psi$, such hidden information may not be accessible to the transformer because of the limited set of operations it can perform on the RPE. For example, while a graph can be reconstructed from its resistance distance matrix, an RPE-GT may not have access to the edges of a graph as it cannot perform the necessary operations to reconstruct the graph.

One basic piece of information a GT may want to access through an RPE is—of course—the adjacency matrix. We identify a desirable type of RPE where a GT will have this information.

**Definition 4.13.** An RPE $\psi$ is **combinatorially-aware** if for any two graphs $G$ and $H$ and vertices $u, v \in V_G$ and $x, y \in V_H$, then $\psi_G(u, v) = \psi_H(x, y)$ iff one of the following conditions hold: (i) $(u, v) \in E_G$ and $(x, y) \in E_H$ (ii) $(u, v) \notin E_G$ and $(x, y) \notin E_H$.

As it turns out, elementwise operations are insufficient for reconstructing the graph structure from the resistance distance, as evidenced by the following example.

**Example 3.** The shortest-path distance (SPD) is combinatorially-aware as SPD$(u, v) = 1$ iff $(u, v) \in E$. The resistance distance is, however, not combinatorially-aware. See Appendix B.7 for a counterexample.

As in the case of diagonal-awareness, given any RPE, one can always augment it to be combinatorially-aware.

**Definition 4.14 (Combinatorial Augmentation).** Let $\psi$ be any RPE. We define its **combinatorial augmentation** $C^\psi$ as follows: for any graph $G$, $C^\psi_G(u, v) := (A_G(u, v), \psi_G(u, v))$ for any $u, v \in V$, where $A_G$ denotes the adjacency matrix of $G$.

This in fact provides an equivalent characterization of combinatorially-aware RPEs.

**Proposition 4.15.** An RPE $\psi$ is combinatorially-aware if for any $G$, the following condition holds for all $u, v, x, y \in V_G$:

$$\psi_G(u, v) = \psi_G(x, y) \iff C^\psi_G(u, v) = C^\psi_G(x, y).$$

The reason combinatorially-aware RPEs are important is because RPE-augWL with combinatorially-aware RPEs are at least as strong as the WL test (Weisfeiler & Leman, 1968). A proof of this theorem can be found in Appendix B.6.

**Theorem 4.16.** Let $\psi$ be a combinatorially-aware RPE. Then, $\psi$-WL is at least as strong as WL.

Theorem 4.16 is of interest because the WL test is equally strong at distinguishing graphs as message passing graph neural networks (MPNNs) (Xu et al., 2018).

**Corollary 4.17.** Let $\psi$ be a combinatorially-aware RPE. Then $\psi$-RPE-GTs are at least as strong as MPNNs.

**5. Conclusion and Open Questions**

We have established a framework for comparing different types of positional encodings. Future work can continue this line of work of comparing different specific positional encodings, e.g. shortest-path vs. resistance distance or resistance distance vs. SPE. Furthermore, our theoretical results provide some suggestions for designing new positional encodings, e.g., one may not want to convert RPEs into APEs as done in the literature. Finally, it would be interesting to shift the focus of research on positional encodings for graph transformers from coarse-grained distinguishing-power results (what pairs of graphs can GTs distinguish) to more fine-grained results on expressive power, for example, approximation results (Azizian & Lelarge, 2021) or results using RPE-augWL-inspired distances to study graph transformers (Chen et al., 2022; 2023; Böker et al., 2024).
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Impact Statement

This paper presents work whose goal is to advance the field of Machine Learning. There are many potential societal consequences of potentially more effective graph learning models due to our work, none of which we feel must be specifically highlighted here.

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A. Details from Section 3

A.1. Example of RPE vs RPE-augWL

By induction, Item 1 implies that First assume that χ now inductively suppose this is true for some value t. By item 3, there is a bijection σ that assigns each graph its adjacency matrix. Both graphs have 4 vertices and 4 edges, so their adjacency matrices A_G and A_H are indistinguishable. However, after one iteration of A-WL, all vertices of G will have the same color, while the degree 1 vertex in H will have a different color from all vertices in G. Therefore, G and H are distinguishable by A-WL.

A.2. Equivalence of RPE-augWL and RPE-2-WL: Proof of Theorem 3.5

Our proof of Theorem 3.5 is based on the following lemma.

Lemma A.1. Let ψ be a pseudo-symmetric RPE. Let (G, X_G) and (H, X_H) be featured graphs. Let u, v ∈ V_G and x, y ∈ V_H. Then χ_{2,ψ_G}^{(t)}(u, v) = χ_{2,ψ_H}^{(t)}(x, y) iff ψ_G(u, v) = ψ_H(x, y), χ_{ψ_G}^{(t)}(u) = χ_{ψ_H}^{(t)}(x), and χ_{ψ_G}^{(t)}(v) = χ_{ψ_H}^{(t)}(y).

Proof of Lemma A.1. We prove this by induction on t. For t = 0, this follows directly from definition as χ_{ψ_G}^{(0)}(v) = X_G(v) and χ_{2,ψ_G}^{(0)}(u, v) = (X_G(u), X_G(v), ψ_G(u, v)).

Now inductively suppose this is true for some value t; we will show this is true for t + 1.

First assume that χ_{2,ψ_G}^{(t+1)}(u, v) = χ_{2,ψ_H}^{(t+1)}(x, y). Then, it follows from the definition that

1. χ_{2,ψ_G}^{(t)}(u, v) = χ_{2,ψ_H}^{(t)}(x, y).
2. \{χ_{2,ψ_G}^{(t)}(u, w) : w ∈ V_G\} = \{χ_{2,ψ_H}^{(t)}(x, z) : z ∈ V_H\};
3. \{χ_{2,ψ_G}^{(t)}(w, v) : w ∈ V_G\} = \{χ_{2,ψ_H}^{(t)}(z, y) : z ∈ V_H\}.

By induction, Item 1 implies that

4. ψ_G(u, v) = ψ_H(x, y), and by pseudo-symmetry, ψ_G(v, u) = ψ_H(y, x);
5. χ_{ψ_G}^{(t)}(u) = χ_{ψ_H}^{(t)}(x) and χ_{ψ_G}^{(t)}(v) = χ_{ψ_H}^{(t)}(y);

By item 2, there is a bijection σ : V_G → V_H such that χ_2^{(t)}(u, w) = χ_2^{(t)}(x, σ(w)). The inductive hypothesis implies that ψ_G(u, w) = ψ_H(x, σ(w)) and χ_ψ^{(t)}(w) = χ_ψ^{(t)}(σ(w)). Therefore, the ψ-WL colors of u and x at t + 1 are the same as

χ_ψ^{(t+1)}(u) = (χ_ψ^{(t)}(u), \{ (χ_ψ^{(t)}(w), ψ_G(u, w)) : w ∈ V_G \})
= (χ_ψ^{(t)}(x), \{ (χ_ψ^{(t)}(z), ψ_H(x, z)) : z ∈ V_H \}) = χ_ψ^{(t+1)}(x).

By item 3, there is a bijection σ' : V_G → V_H such that χ_2^{(t)}(w, v) = χ_2^{(t)}(σ'(w), y). The inductive hypothesis implies that ψ_G(w, v) = ψ_H(σ'(w), y) and χ_ψ^{(t)}(w) = χ_ψ^{(t)}(σ'(w)). By pseudo-symmetry, one also has that ψ_G(v, w) =
We show that $\chi_{WL, \psi}$ and $\chi_{RPE-augWL}$ are the same as

$\chi_{WL, \psi}(v) = \chi_{RPE-augWL}(v)$, for all $v \in V_G$, i.e., every vertex $v$ is the same in both graphs.

Conversely, assume that $\chi_{WL, \psi}(u, v) = \chi_{RPE-augWL}(u, v) = \chi_{WL, \psi}(x, y)$. By definition of $\psi$-WL, we have that $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(x)$ and $\chi_{WL, \psi}(v) = \chi_{WL, \psi}(y)$. Hence, by induction, we have that $\chi_{WL, \psi}(u, v) = \chi_{WL, \psi}(x, y)$. Therefore, for any $u, v \in V_G$, $\chi_{WL, \psi}(u, v)$ is $\psi$-WL indistinguishable if and only if $\chi_{WL, \psi}(x, y)$ is $\psi$-WL indistinguishable.

Theorem 3.5 (Equivalence of RPE-augWL and RPE-2-WL). Let $\psi$ be a pseudo-symmetric RPE. Then two features graphs $(G, X_G)$ and $(H, X_H)$ are $\psi$-WL indistinguishable if and only if they are $\psi$-2-WL indistinguishable.

Proof of Theorem 3.5. For the forward direction, we will show that for all $t \geq 0$, if $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(v)$, then $\chi_{WL, \psi}(u, v) = \chi_{WL, \psi}(x, y)$.

We first prove the base case of $t = 0$. As $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(v)$, there is a bijection $\sigma : V_G \rightarrow V_H$ such that $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(\sigma(u))$. Moreover, by the definition of $\chi_{WL, \psi}(u)$, for each $u \in V_G$, there is a bijection $\sigma_u : V_G \rightarrow V_H$ such that $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(\sigma_u(u))$. Therefore, we can define a bijection $\Phi : V_G \rightarrow V_H$ defined $\Phi(u) = \sigma(u)$.

We now prove that for each $t \geq 1$, if $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(v)$, then $\chi_{WL, \psi}(u, v) = \chi_{WL, \psi}(x, y)$. Assume that both graphs are assigned $k^{t+1}$ colors by $\chi_{WL, \psi}$. More specifically, assume there are partitions $V_G = \bigcup_{i=1}^{k^{t+1}} V_{G,i}$ and $V_H = \bigcup_{i=1}^{k^{t+1}} V_{H,i}$ such that

1. $|V_{G,i}| = |V_{H,i}|$;
2. for any $u \in V_{G,i}$ and $v \in V_{H,i}$, $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(v)$ if $i = j$;
3. for any $u \in V_{G,i}$ and $x \in V_{H,i}$, $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(x)$.

We can define analogous partitions for $\chi_{WL, \psi}$.

These partitions induce a partition on the set of pairs of vertices $V_G \times V_G = \bigcup_{1 \leq i \leq k^{t+1}} \bigcup_{1 \leq j \leq k^{t+1}} V_{G,i} \times V_{G,j}$ and $V_H \times V_H = \bigcup_{1 \leq i \leq k^{t+1}} \bigcup_{1 \leq j \leq k^{t+1}} V_{H,i} \times V_{H,j}$, see Figure 4 for an illustration of the decomposition.

We show that $\chi_{WL, \psi}$ has the same multiset of colors on $V_{G,i} \times V_{G,j}$ and $V_{H,i} \times V_{H,j}$. By the definition of the partitions, there exists a bijection $\sigma_{i,j} : V_{G,i} \rightarrow V_{H,j}$ such that $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(\sigma_{i,j}(u))$ for any $u \in V_{G,i}$. By definition of $\psi$-WL, we have that $\chi_{WL, \psi}(u) = \chi_{WL, \psi}(\sigma_{i,j}(u))$ for any $u \in V_{G,i}$. Furthermore, for any $u \in V_{G,i}$,
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![Figure 4. Decomposition of $V_G \times V_G$.](image)

Now for each $1 \leq j \leq k^{(t)}$, consider the sub-multiset $\{ (\chi_{\psi_G}^{(t)}(w), \psi_G(u, w)) : w \in V_{G,j}^{(t)} \}$ of $\{ (\chi_{\psi_G}^{(t)}(w), \psi_G(u, w)) : w \in V_G \}$, then we have that

$$\{ (\chi_{\psi_G}^{(t)}(w), \psi_G(u, w)) : w \in V_{G,j}^{(t)} \} = \{ (\chi_{\psi_H}^{(t)}(z), \psi_H(\sigma_i^{(t+1)}(u), z)) : z \in V_{H,j}^{(t)} \}.$$ 

This is because when $j \neq b$, one has that $\chi_{\psi_G}^{(t)}(w) \neq \chi_{\psi_H}^{(t)}(z)$ for $w \in V_{G,j}^{(t)}$ and $z \in V_{H,b}^{(t)}$. Therefore,

$$\{ (\psi_G(u, w), \chi_{\psi_G}^{(t)}(u), \chi_{\psi_G}^{(t)}(w)) : w \in V_{G,j}^{(t)} \} = \{ (\psi_H(\sigma_i^{(t+1)}(u), z), \chi_{\psi_H}^{(t)}(\sigma_i^{(t+1)}(u)), \chi_{\psi_H}^{(t)}(z)) : z \in V_{H,j}^{(t)} \}.$$ 

Therefore, by Lemma A.1, one has that

$$\{ \chi_{\psi_G}^{(t)}(u, w) : w \in V_{G,j}^{(t)} \} = \{ \chi_{\psi_H}^{(t)}(\sigma_i^{(t+1)}(u), z) : z \in V_{H,j}^{(t)} \}.$$ 

Since $\sigma_i^{(t+1)}$ is bijective, we conclude that

$$\{ \chi_{\psi_G}^{(t)}(u, v) : u \in V_{G,j}^{(t+1)}, v \in V_{G,j}^{(t)} \} = \{ \chi_{\psi_H}^{(t)}(x, y) : x \in V_{H,i}^{(t+1)}, y \in V_{H,j}^{(t)} \}.$$ 

Taking the multiset union over $1 \leq i \leq k^{(t+1)}$ and $1 \leq j \leq k^{(t)}$, this implies that $\{ \chi_{\psi_G}^{(t)}(u, v) : u, v \in V_G \} = \{ \chi_{\psi_H}^{(t)}(x, y) : x, y \in V_H \}$. Conversely, we will show that for $t \geq 0$, if $\{ \chi_{\psi_G}^{(t)}(u, v) : u, v \in V_G \} = \{ \chi_{\psi_H}^{(t)}(x, y) : x, y \in V_H \}$, then $\{ \chi_{\psi_G}^{(t)}(u) : u \in V_G \} = \{ \chi_{\psi_H}^{(t)}(x) : x \in V_H \}$. For the base case of $t = 0$, we have that $\{ (X_G(u), X_G(v)) : u, v \in V_G \} = \{ (X_H(x), X_H(y), \psi_H(x, y)) : x, y \in V_H \}$. Therefore, $\{ (X_G(u), X_G(v)) : u, v \in V_G \} = \{ (X_H(x), X_H(y)) : x, y \in V_H \}$ and hence $\{ X_G(u) : u \in V_G \} = \{ X_H(x) : x \in V_H \}$. Now we apply the following fact:

**Fact 3.** Let $A$ and $B$ be two finite multisets. If $A^2 = B^2$, then $A = B$.

Then, we have that $\{ X_G^{(0)}(u) : u \in V_G \} = \{ X_H^{(0)}(x) : x \in V_H \}$. Now assume that for $k \geq 1$, we have that

$$\{ \chi_{\psi_G}^{(t)}(u, v) : u, v \in V_G \} = \{ \chi_{\psi_H}^{(t)}(x, y) : x, y \in V_H \}.$$ 

Lemma A.1 implies that

$$\{ (\psi_G(u, v), \chi_{\psi_G}^{(t)}(u), \chi_{\psi_G}^{(t)}(v)) : u, v \in V_G \} = \{ (\psi_H(x), \chi_{\psi_H}^{(t)}(x), \chi_{\psi_H}^{(t)}(y)) : x, y \in V_H \}.$$ 

Dropping the $\phi$ term, one has that

$$\{ (X_G(u), X_G(v)) : u, v \in V_G \} = \{ (X_H(x), X_H(y)) : x, y \in V_H \}.$$
This implies that the following Cartesian products are equal:
\[ \ell \{ \chi_{\psi_G}^{(t)}(u) : u \in V_G \}^2 = \ell \{ \chi_{\psi_H}^{(t)}(x) : x \in V_H \}^2. \]

Then, by Fact 3 again, we have that
\[ \ell \{ \chi_{\psi_G}^{(t)}(u) : u \in V_G \} = \ell \{ \chi_{\psi_H}^{(t)}(x) : x \in V_H \}. \]

This means that \( G \) and \( H \) are indistinguishable by \( \psi \)-WL.

We now end this proof by proving Fact 3.

Proof of Fact 3. We let \( C := A \cup B \) denote the set of all distinct elements in \( A \) and \( B \). Let \( C = \{ c_1, \ldots, c_n \} \) and assume that \( A \) contains \( r_i^A \) many \( c_i \) and \( B \) contains \( r_i^B \) many \( c_i \) for each \( i = 1, \ldots, n \). Then, \( A^2 \) contains \( r_i^A r_j^A \) many \( (c_i, c_j) \) and \( B^2 \) contains \( r_i^B r_j^B \) many \( (c_i, c_j) \). Therefore, \( A^2 = B^2 \) implies that \( r_i^A r_j^A = r_i^B r_j^B \) for all \( i, j = 1, \ldots, n \). For each \( i = 1, \ldots, n \), we let \( j = i \) and hence \( (r_i^A)^2 = (r_i^B)^2 \). Since we are dealing with nonnegative integers, we must have that \( r_i^A = r_i^B \). Therefore, \( A = B \).

A.3. RPE-2-WL vs 2-EGN

Equivariant or invariant graph networks (EGNs and IGNs) (Maron et al., 2019b) are another important type of graph neural networks. These models will be important when trying to understand the distinguishing power of positional encodings later.

Definition A.2 (EGNs). A \( k \)th order Equivariant Graph Network (\( k \)-EGN) is a function \( F : \mathbb{R}^{n^k \times d_0} \to \mathbb{R}^{n^s \times d_e} \) for \( s \leq k \) of the form
\[
F = h \circ m \circ L^{(T)} \circ \sigma \circ \cdots \circ \sigma \circ L^{(1)}
\]
where \( h \) and \( L^{(t)} : \mathbb{R}^{n^{k-t} \times d_{t-1}} \to \mathbb{R}^{n^{k-t} \times d_t} \) are equivariant linear layers for each \( t = 1, \ldots, T \) such that \( k_t \leq k \), \( k_0 = k \) and \( k_T = s \). \( \sigma \) is an activation function, and \( m \) is a pointwise MLP. When \( s = 0 \), the resulting \( k \)-EGN is also called a \( k \)th order Invariant Graph Network (\( k \)-IGN).

Note: Some implementations of 2-IGNs and 2-EGNs (e.g. (Maron et al., 2019b)) stack the adjacency matrix to the input \( W \). In this paper, unless otherwise stated, the adjacency matrix is not stacked to the input.

EGNs are permutation equivariant in the sense that permutation of the order of input tensors will result in a corresponding permutation of the order of output tensors. Likewise, IGNs are permutation invariant as any permutation of the input tensors results in the same output.

We are interested in 2-EGNs and 2-IGNs since they are closely related to the 2-WL graph isomorphism test. Let \( \psi \) be an RPE valued in \( \mathbb{R}^k \) and let \( g : \mathbb{R}^{n^k \times k} \to \mathbb{R}^{n^s \times l} \) be any 2-EGN. Recall that for any graph \( G \) with \( n \) vertices, the RPE \( \psi_G \) can be represented as a tensor in \( \mathbb{R}^{n^2 \times k} \). If \( X_G \in \mathbb{R}^{n \times l} \) are node features for \( G \), let \( \text{row}(X_G) \) and \( \text{col}(X_G) \in \mathbb{R}^{n^2 \times l} \) be the tensors where each row or column respectively are the node feature \( X_G \), e.g. \( \text{row}(X_G)[i, : ;] = X_G \) and \( \text{col}(X_G)[: ; j] = X_G \) for all \( 1 \leq i, j \leq n \).

We now show that 2-EGNs with the input \( [\psi_G, \text{row}(X_G), \text{col}(X_G)] \in \mathbb{R}^{n^2 \times (k+2l)} \) have the same distinguishing powers as the \( \psi \)-2-WL test.

Proposition A.3 (Equivalence of RPE-2-WL and 2-EGN). Let \( \psi \) be a diagonally-aware RPE valued in \( \mathbb{R}^k \). Let \( \mathcal{G} \) be any finite set of featured graphs. Then there exists a 2-EGN \( g : \mathbb{R}^{n^2 \times k} \to \mathbb{R}^{n^s \times l} \) such that any \((G, X_G), (H, X_H) \in \mathcal{G} \) can be distinguished by \( g \) with the input \([\psi_G, \text{row}(X), \text{col}(X)] \) iff \( G \) and \( H \) can be distinguished by the \( \psi \)-2-WL test.

This result is a generalization of existing results showing that 2-IGNs of the form \( g : \mathbb{R}^{n^2 \times k} \to \mathbb{R}^m \) are equivalent to the 2-WL test (Maron et al., 2019a; Chen et al., 2020).

Proof of Proposition A.3. We will prove the forward and backward direction of this statement separately in the following lemmas. However, we emphasize that only Lemma A.5 needs the assumption of diagonal-awareness. Moreover, we
emphasize that the “proofs” of both of these lemmas are just slightly adapting existing results connecting 2-IGNs to the 2-WL test.

**Lemma A.4** (2-EGNs are stronger than RPE-2-WL). Let \( \psi \) be an RPE valued in \( \mathbb{R}^k \). Let \( G \) be a finite set of graphs. Then, there exists a 2-EGN \( g : \mathbb{R}^{n^2 \times (k+2)} \rightarrow \mathbb{R}^{n \times m} \) such that if any \((G, X_G), (H, X_H) \in G\) can be distinguished by \( \psi \)-2-WL test then \( \|g(\rho_G, \text{row}(X_G), \text{col}(X_G))(u) : u \in V_G \| \neq \|g(\rho_H, \text{row}(X_H), \text{col}(X_H))(v) : v \in V_H \| \).

**Proof.** This follows from the proof by Maron et al. (2019a, Theorem 1) showing that there exists a 2-EGN that can distinguish any two graphs from a finite set of graphs as well as the classical 2-WL algorithm. (While their statement of Theorem 1 is only for two graphs, their proof explains why this can be generalized to a finite set of graphs.) This lemma shows how this result can be generalized to the RPE-2-WL test.

Their proof is broken into two steps. First, the authors show that given a tensor \( W \in \mathbb{R}^{n^2 \times (k+1)} \) of a diagonal feature matrix stacked with the adjacency matrix, there is a 2-equivariant linear layer \( f : \mathbb{R}^{n^2 \times (k+1)} \rightarrow \mathbb{R}^{n^2 \times 4 \times (k+2)} \) such that, for each pair \((u, v)\), the vector \( f(W)[u, v, \cdot] \) corresponds to the isomorphism type of \((u, v)\), which is the initial color of \((u, v)\) in the 2-WL test. Second, they show that there is a \( d \) layers 2-EGN \( f = L^{(d)} \circ \sigma \circ \cdots \circ \sigma \circ L^{(1)} : \mathbb{R}^{n^2 \times k} \rightarrow \mathbb{R}^{n^2 \times l} \) that can implement \( d \) iterations of the 2-WL algorithm; that is to say, \( f(A_G)(u, v) = f(A_H)(u, v) \) iff \( \chi^{(d)}(u, v) = \chi^{(d)}(x, y) \). Finally, they show that there exists an MLP \( m \), together with a final layer \( h \) of summing over all entries, such that \( g = h \circ m \circ f \) implements the 2-WL test, i.e. \( g(A_G) = g(A_H) \) iff \( \chi(G) = \chi(H) \).

The difference between the 2-WL test and the RPE-2-WL test lies in the initialization step. In the classical 2-WL test, a pair \((u, v)\) is colored with its isomorphism type, while in the RPE-2-WL test, the initial color is \((X_G(u), X_G(v), \psi_G(u, v))\). If the input to the 2-EGN is the RPE matrix concatenated with the node features (i.e. the initial coloring), we can skip the initialization step and just perform the update steps of the RPE-2-WL through a 2-EGN \( f = L^{(d)} \circ \sigma \circ \cdots \circ \sigma \circ L^{(1)} : \mathbb{R}^{n^2 \times k} \rightarrow \mathbb{R}^{n^2 \times l} \). Finally, instead of taking the sum of all entries, we can apply the operation of row sum (which is equivalent) to the output of \( f \) to obtain our target 2-EGN \( g : \mathbb{R}^{n^2 \times k} \rightarrow \mathbb{R}^{n \times l} \).

**Lemma A.5** (RPE-2-WL is stronger than 2-EGNs). Let \( \psi \) be a diagonally-aware RPE. Let \((G, X_G)\) and \((H, X_H)\) be graphs. If \( G \) and \( H \) cannot be distinguished by \( \psi \)-2-WL, then \((G, X_G)\) and \((H, X_H)\) cannot be distinguished by any 2-EGN with input \([\psi, \text{row}(X), \text{col}(X)]\).

**Proof.** This follows directly from the proof showing that if two graphs cannot be distinguished by the 2-WL, they cannot be distinguished by 2-EGNs (Chen et al., 2020, Lemma 4.2). The only reason we cannot apply this proof directly is that it relies on the fact that the initial colors to the 2-WL—and therefore all subsequent colors—are diagonally-aware (Chen et al., 2020, Lemma D.1), which is not necessarily the case for the initial colors of RPE-2-WL for general RPEs. However, if the RPE is diagonally-aware, then our lemma can be proven following the proof of Chen et al. (2020, Lemma 4.2).

**Importance of diagonal-awareness.** In the proof of Proposition A.3 (specifically in Lemma A.5), we show that RPE-2-WL is at least as strong as 2-EGNs if the RPE is diagonally-aware. We emphasize that if we drop the assumption of diagonal-awareness, the lemma does not hold. Therefore, 2-EGN can be strictly stronger than the RPE-2-WL test for non-diagonally-aware RPEs, as shown by the following simple example.

Consider the two graphs on two vertices \( G \) and \( H \) where \( G \) has an edge and \( H \) does not. (In this example, the graphs have no node features.) Consider the (artificial) RPE \( \psi \) that assigns

\[
\psi_G = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \psi_H = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.
\]

Note that \( \psi \) is not diagonally-aware, as the values 0 and 1 appear on both the diagonal and off-diagonal elements.

The \( \psi \)-2-WL colorings for \( t = 0 \) are

\[
\chi_{2,\psi}^{(0)}(G) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \chi_{2,\psi}^{(0)}(H) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.
\]
A similar argument shows that $A.4$. Equivalence of APEs and APE-GTs: Proof of Lemma 3.1

Proof. We will denote the input at the $l$-th layer of the RPE-GT for graph $G$ as $X_G^{(l)}(u) \in \mathbb{R}^{|V_G| \times \ell}$, and for each node $u \in V_G$, its feature is denoted by $X_G^{(l)}(u)$. Note $X_G^{(l)}(u) = X_G(u)$. We adopt similar notations for $H$.

For the forward direction, it suffices to show that if $G$ and $H$ are indistinguishable by the $\psi$-WL test, they are indistinguishable by any $\psi$-RPE-GT. We will prove the stronger statement that if the multiset of colors $\{\chi_{\psi_G}^{(t)}(u) : v \in V_G\} = \{\chi_{\psi_H}^{(t)}(x) : x \in V_H\}$.
The key observation is that the only part of the transformer architecture that is not applied separately to the node features \(X^{(t)}(u)\) is the multiplication by the attention matrix \(A^{(t,h)}(X^{(t)}(u))\), meaning for all other parts of the transformer, if the inputs \(X^{(t)}(u) = X^{(t)}(v)\) are equal, then the outputs at \(u\) and \(v\) are equal.

For the base case of \(t = 0\), the statement holds as the initial node features equals the \(\psi\)-WL colors for \(t = 0\), i.e. \(\{\chi^{(0)}_{\psi_G}(v) : v \in V_G\} = \{X^{(0)}_{\psi_G}(v) : v \in V_G\}\).

Now suppose the theorem inductively holds for some \(t\). Assume that \(\{\chi^{(t+1)}_{\psi_G}(u) : v \in V_G\} = \{\chi^{(t+1)}_{\psi_H}(x) : x \in V_H\}\) and let \(\sigma^{(t+1)} : V_G \rightarrow V_H\) denote any bijection such that \(\chi^{(t+1)}_{\psi_G}(u) = \chi^{(t+1)}_{\psi_H}(\sigma^{(t+1)}(u))\) for any \(u \in V_G\). By the definition of \(\chi_{\psi}\) and the inductive hypothesis, we have that \(\{\chi^{(t+1)}_{\psi_G}(u) : v \in V_G\} = \{\chi^{(t+1)}_{\psi_H}(x) : x \in V_H\}\) and \(X^{(t)}_G(u) = X^{(t)}_H(\sigma^{(t+1)}(u))\) for all \(u \in V_G\).

Now for any \(v \in V_G\) and \(y \in V_H\) such that \(X^{(t)}_G(v) = X^{(t)}_H(y)\), we have that

\[
X^{(t)}_G(u)W_Q(X^{(t)}_G(v)W_K)^T = X^{(t)}_H(\sigma^{(t+1)}(u))W_Q(X^{(t)}_H(y)W_K)^T
\]

for any matrices \(W_Q\) and \(W_K\).

Now, for any \(u \in V_G\), \(\chi^{(t+1)}_{\psi_G}(u) = \chi^{(t+1)}_{\psi_H}(\sigma^{(t+1)}(u))\) implies that

\[
\{ (\chi^{(t)}_{\psi_G}(v), \psi_G(u, v)) : v \in V_G \} = \{ (\chi^{(t)}_{\psi_H}(y), \psi_H(\sigma^{(t+1)}(u), y)) : y \in V_H \}.
\]

Hence,

\[
\{ (X^{(t)}_G(v), \psi_G(u, v)) : v \in V_G \} = \{ (X^{(t)}_H(y), \psi_H(\sigma^{(t+1)}(u), y)) : y \in V_H \}.
\]

Note that for any given value \(a\),

\[
\{\psi_G(u, v) : v \in V_G, X^{(t)}_G(v) = a\} = \{\psi_H(\sigma^{(t+1)}(u), y) : y \in V_H, X^{(t)}_H(y) = a\}.
\]

Then, we have that

\[
[A^{(t,h)}(X^{(t)}_G)X^{(t)}_G](u) = \sum_v A^{(t,h)}(X^{(t)}_G)(u, v)X^{(t)}_G(v) \]

\[
= \sum_v f_1(\psi_G(u, v))\text{softmax}(X^{(t)}_G(u)W_Q(X^{(t)}_G(\cdot)W_K)^T / \sqrt{d_h} + f_2(\psi_G(u, \cdot))(v)X^{(t)}_G(v) \]

\[
= \sum_y f_1(\psi_H(\sigma^{(t+1)}(u), y))\text{softmax}(X^{(t)}_H(\sigma^{(t+1)}(u))W_Q(X^{(t)}_H(\cdot)W_K)^T / \sqrt{d_h} + f_2(\psi_H(\sigma^{(t+1)}(u), \cdot))(y)X^{(t)}_H(y) \]

\[
= [A^{(t,h)}(X^{(t)}_H)X^{(t)}_H](\sigma^{(t+1)}(u)).
\]

Here the third equation follows from Equation (1) and Equation (2).

It is then easy to check that \(X^{(t+1)}_G(u) = X^{(t+1)}_H(\sigma^{(t+1)}(u))\) for any \(u \in V_G\) and this concludes the proof.

For the other direction, the proof follows from the one of Zhang et al. (2023, Theorem 4): More precisely, Zhang et al. (2023) are dealing with the case when the RPE \(\psi\) is taking value from a finite set \(D\) for graphs with bounded sizes. Furthermore, their RPE \(\psi\) is a distance (or a stack of distance functions) so that \(\psi_G(u, v) = 0\) iff \(u = v \in V_G\) for any graph \(G\). In this way, elements in \(D\) can be written as \(0 = r_0 < r_1 < \cdots < r_H\). Note that, for one step of \(\psi\)-WL, the second argument can be decomposed by

\[
\{ (\chi^{(t)}_{\psi_G}(u), \psi_G(v, u)) : u \in V_G \} = \bigcup_{r_i} \{ (\chi^{(t)}_{\psi_G}(u), r_i) : \psi_G(v, u) = r_i, u \in V_G \}.
\]
Then, Zhang et al. (2023) explicitly constructed $H + 1$ different RPE attention heads $A_{RPE}^h$ which can simulate $\left\{(\chi_{G}^{(t)}(u), r_{h}) : \psi_{G}(v, u) = r_{h}, u \in V_{G}\right\}$ in an injective manner for each $h = 0, \ldots, H$. In this way, they argue that by concatenating these heads, one can simulate their GD-WL test where each step is updated by $\tilde{x}_{\psi_{G}}^{(t+1)}(v) = \left\{ \left(\tilde{x}_{\psi_{G}}^{(t)}(u), \psi_{G}(v, u) \right) : u \in V_{G}\right\}$. But as mentioned already in Section 3.1, this GD-WL test is equivalent to the $\psi$-WL test when $\psi$ is a graph distance (or a stack of graph distances), so their one layer RPE transformer can simulate one step of $\psi$-WL in an injective manner.

Recall that GD-WL is equivalent to $\psi$-WL due to the fact that $\psi$ takes value 0 on diagonal entries and $\psi$ takes non-zero values on off-diagonal entries. This is the reason why one can drop the first argument in $(\chi_{G}^{(t)}(v), \left\{(\chi_{G}^{(t)}(u), \psi_{G}(v, u)) : u \in V\right\})$ without losing distinguishing power. Hence, the same argument in the proof of (Zhang et al., 2023, Theorem 4) can be applied to the setting of diagonally-aware RPEs due to the following simple result.

**Lemma A.6.** When $\psi$ is a diagonally-aware RPE, then $\psi$-WL is equivalent to the following variant of $\psi$-WL:

$$\tilde{x}_{\psi_{G}}^{(0)}(v) = X_G(v),$$

$$\tilde{x}_{\psi_{G}}^{(t+1)}(v) = \left\{ \left(\tilde{x}_{\psi_{G}}^{(t)}(u), \psi_{G}(v, u) \right) : u \in V\right\}.$$  

Now, to prove our theorem, we simply let $D := \left\{ \psi_G(v, u) : u, v \in V_G \right\} \cup \left\{ \psi_H(x, y) : x, y \in V_H \right\}$ and apply the same argument as in the proof of (Zhang et al., 2023, Theorem 4) to conclude the proof. 

### A.7. Mapping APEs to RPEs: Proof of Lemma 3.7 and Theorem 3.8

We first recall a key lemma from Xu et al. (2018). For any set $S$, we let $\text{Mul}(S)$ denote the collection of all finite multi-subsets of $S$ and recall that $\text{Mul}_2(S)$ denotes the collection of all multi-subsets of size 2 in $S$.

**Lemma A.7** (Xu et al., 2018, Lemma 5). If $S$ is countable, then there exists a function $f : S \to \mathbb{R}$ such that the map $h_f : \text{Mul}(S) \to \mathbb{R}$ defined by sending $h_f(X) = \sum_{x \in X} f(x)$ is injective.

As a direct consequence, we immediately have the following corollary.

**Corollary A.8.** If $S$ is countable, then there exists a function $f : S \to \mathbb{R}$ such that the map $h_f : \text{Mul}_2(S) \to \mathbb{R}$ defined by sending $h_f(\{x, y\}) = f(x) + f(y)$ is injective.

**Lemma 3.7.** Let $\phi$ be an APE. Then there is a function $f$ such that any two featured graphs $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\phi$ iff $(G, X_G)$ and $(H, X_H)$ cannot be distinguished by the $\psi_f$-2-WL test.

**Proof.** Let $S = \bigcup_{G \in \mathbb{G}} \text{im} \phi_G$, where $\mathbb{G}$ is the set of all finite graphs. We first note that $S$ is countable as the set of all finite graphs is countable. Let $f$ be any function such that $h_f$ that is injective on $S$; such a function must exist by Corollary A.8 as $S$ is countable. Assume that $G$ and $H$ are indistinguishable by the $\psi_f$-2-WL test. This, in particular, implies that the multisets of initial colors are the same:

$$\left\{(X_G(u), X_G(v), \psi_f^{(v)}(v, w)) : u, v \in V_G\right\} = \left\{(X_H(x), X_H(y), \psi_f^{(x)}(x, y)) : x, y \in V_H\right\}.$$  

By the definition of $\psi_f$ and the fact that $h_f$ is injective, one has that

$$\left\{(X_G(u), X_G(v), \phi_G(u), \phi_G(v)) : u, v \in V_G\right\} = \left\{(X_H(x), X_H(y), \phi_H(x), \phi_H(y)) : x, y \in V_H\right\}.$$  

Hence, the following two Cartesian products of multisets are equal:

$$\left\{(X_G(u), \phi_G(u)) : u \in V_G\right\}^2 = \left\{(X_H(x), \phi_H(x)) : x \in V_H\right\}^2.$$  

By Fact 3, we have that $\left\{(X_G(u), \phi_G(u)) : u \in V_G\right\} = \left\{(X_H(x), \phi_H(x)) : x \in V_H\right\}$.

Conversely, assume that $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\phi$. Then $\left\{(X_G(u), \phi_G(u)) : u \in V_G\right\} = \left\{(X_H(x), \phi_H(x)) : x \in V_H\right\}$. Let $\sigma : V_G \to V_H$ be a bijection such that $\phi_G(v) = \phi_H(\sigma(v))$ and $X_G(v) = X_H(\sigma(v))$ for all $v \in V_G$. We will prove that $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\psi_f$-WL for any function $f$. In fact, we will prove the stronger statement that $\chi_{\psi_G}^{(t)}(v) = \chi_{\psi_H}^{(t)}(\sigma(v))$ for all $t \geq 0$. This is stronger than proving they are $\psi_f$-WL indistinguishable as we use the same bijection for all iterations $t$. 

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We prove this by induction on the iteration $t$. For $t = 0$, this is true as the initial $\psi^0$-WL colors $\chi^{(t)}_{\psi_G}(v)$ are just the node features $X_G(v)$, which are implied by the definition of indistinguishability by an APE. Now suppose this is true for some iteration $t$; we will show it is true for $t + 1$. Let $v \in V_G$. The inductive hypothesis implies that the first element of the colors are equal $\chi^{(t)}_{\psi_G}(v) = \chi^{(t)}_{\psi_H}(\sigma(v))$. Moreover, if we consider the second element of the colors, we find that

$$
\langle \chi^{(t)}_{\psi_G}(w), \psi^f_G(w, v, w) \rangle : w \in V_G \rangle = \langle \chi^{(t)}_{\psi_H}(w), \psi^f_H(\sigma(w), \sigma(v)) : w \in V_G \rangle
$$

(definition of $\psi^f_G$)

$$
= \langle \chi^{(t)}_{\psi_G}(w), \sigma(w) + f(\sigma(w)) : w \in V_G \rangle
$$

(definition of $\sigma$)

$$
= \langle \chi^{(t)}_{\psi_H}(w), \sigma(w) + f(\sigma(w)) : w \in V_G \rangle
$$

(inductive hypothesis)

$$
= \langle \chi^{(t)}_{\psi_H}(w), \psi^f_H(\sigma(w), \sigma(v)) : w \in V_G \rangle
$$

(definition of $\psi^f_H$)

$$
= \langle \chi^{(t+1)}_{\psi_H}(w), \psi^f_H(\sigma(v), w) : w \in V_H \rangle
$$

($\sigma$ is a bijection)

Therefore, $\chi^{(t+1)}_{\psi_H}(v) = \chi^{(t+1)}_{\psi_H}(\sigma(v))$ as claimed.

**Theorem 3.8.** For any APE $\phi$, there exists a function $f$ such that any two graphs $(G, X_G)$ and $(H, X_H)$ are indistinguishable by all $\phi$-APE-GTs iff they are indistinguishable by all $\psi^f$-RPE-GTs.

**Proof.** By Lemma 3.1, two graphs $(G, X_G)$ and $(H, X_H)$ are indistinguishable by all APE transformers with APE $\phi$ iff they are indistinguishable by $\phi$. By Lemma 3.7, this is equivalent to being indistinguishable by $\psi^f$-2-WL. Hence, by Lemma 3.6, this is equivalent to being indistinguishable by any RPE transformer with RPE $\psi^f$. \qed

**A.8. Mapping RPE to APE: Proof of Theorem 3.10**

**Lemma 3.9.** Let $\psi$ be a diagonally-aware RPE.

For any 2-EGN $g$, if $(G, X_G)$ and $(H, X_H)$ are indistinguishable by the $\psi$-2-WL test then $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\phi^0$.

Moreover, for any finite set of unfeatured graphs $\mathcal{G}$, there is a 2-EGN $g$ such that if $G, H \in \mathcal{G}$ are indistinguishable by $\phi^0$, then $G$ and $H$ are indistinguishable by the $\psi$-2-WL test.

**Proof.** Let $(G, X_G)$ and $(H, X_H)$ be featured graphs that are indistinguishable by $\psi$-2-WL. By Lemma A.5, this means that for any 2-EGN $g$ of the appropriate dimension, $g([\psi_G, \text{row}(X_G), \text{col}(X_G)]) = g([\psi_H, \text{row}(X_G), \text{col}(X_G)])$. In particular, for any 2-EGN $h$ of appropriate dimension, there is a 2-EGN $g_h$ such that $g_h([\psi_G, X_G, X^2_G]) = [h(\psi_G), X^2_G]$; the 2-EGN $g_h$ runs $h$ on the first columns of $[\psi_G, \text{row}(X_G), \text{col}(X_G)]$ and then copies the mean of the rows of $\text{row}(X_G)$ on the remaining columns. The output of $g_h$ is exactly the APE $\psi^0_G$ concatenated to the node features $X_G$.

For the backward direction of the case of graphs without node features, this follows directly from Lemma A.4. \qed

**Theorem 3.10.** Let $\psi$ be a diagonally-aware RPE.

For any 2-EGN $g$, if $(G, X_G)$ and $(H, X_H)$ are indistinguishable by all $\psi$-REPE-GTs, then $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\phi^0$.

Moreover, for any finite set of unfeatured graphs $\mathcal{G}$, there is a 2-EGN $g$ such that if $G, H \in \mathcal{G}$ are indistinguishable by all $\phi^0$-APE-GTs, then $G$ and $H$ are indistinguishable by all $\psi$-RPE-GTs.

**Proof.** By Lemma 3.6 and Theorem 3.5, $G$ and $H$ are indistinguishable by an RPE transformer with RPE $\psi$ iff $G$ and $H$ are indistinguishable by the $\psi$-2-WL test. By Lemma 3.9, this is equivalent to $G$ and $H$ being indistinguishable by $\phi^0$. By Lemma 3.1, this is equivalent to $G$ and $H$ being indistinguishable by any APE transformer with APE $\phi^0$. \qed

We now show that RPEs are strictly stronger than APEs derived from RPEs for graphs with node features.

**Example 1.** There exists an RPE $\psi$ and featured graphs $(G, X_G)$ and $(H, X_H)$ that are distinguishable by $\psi$-2-WL but are indistinguishable by $\phi^0$ for any 2-EGN $g$. 

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We first prove these graphs are distinguishable by \( G \) will assign the same value to each node in \( \phi \), we see that \( G \) has a node of color \( (1, (2, 1), (3, 0), (4, 1)) \); however, \( H \) has no node of that color, as the only node with feature 1 has color \( (1, (3, 1), (2, 0), (4, 1)) \).

We next prove that are indistinguishable by the APE \( \phi \). We first prove these graphs are distinguishable by \( \psi \) will assign the same value to each node in \( \phi \). For any graph \( G \), there is a graph isomorphism \( \sigma : V_G \rightarrow V_H \) such that \( \sigma(u) = v \); likewise for any two nodes \( x, y \in V_H \) or nodes \( u \in V_G \) and \( x \in V_H \). Therefore, as \( (G, X_G) \) and \( (H, X_H) \) have the same multiset of node features and \( \phi \) has uniform entries, they cannot be distinguished by \( \phi \).

\[ \text{Proof.} \] The graph \( G \) and \( H \) are both the cycle graph on 4-vertices \( C_4 \). The RPE \( \psi \) is the adjacency matrix. The node features are \( X_G = \{1, 2, 3, 4\} \) and \( X_H = \{1, 3, 2, 4\} \). See Figure 5.

We first prove these graphs are distinguishable by \( \psi \)-WL. If we consider the first \( \psi \)-WL colors \( \chi^{(1)} \), we see that \( G \) has a node of color \( (1, (2, 1), (3, 0), (4, 1)) \); however, \( H \) has no node of that color, as the only node with feature 1 has color \( (1, (3, 1), (2, 0), (4, 1)) \).

We next prove that are indistinguishable by the APE \( \phi \) for any 2-EGN \( g \). The first thing to observe is that the APE \( \phi \) will assign the same value to each node in \( G \) and \( H \); this follows from the definition of APE and the fact that for any two nodes \( u, v \in V_G \), there is a graph isomorphism \( \sigma : V_G \rightarrow V_H \) such that \( \sigma(u) = v \); likewise for any two nodes \( x, y \in V_H \) or nodes \( u \in V_G \) and \( x \in V_H \). Therefore, as \( (G, X_G) \) and \( (H, X_H) \) have the same multiset of node features and \( \phi \) has uniform entries, they cannot be distinguished by \( \phi \).

\[ \text{B. Details from Section 4} \]

\[ \text{B.1. A Lemma for RPE-augWL Composition.} \]

In this section, we will repeatedly use the following useful property of composing the RPE-augWL test. Let \( \psi \) be an RPE valued in \( \mathbb{R}^d \), and let \( f : \mathbb{R}^d \rightarrow \mathbb{R} \) be a function. Consider the composition \( f \circ \psi \) defined by \( (f \circ \psi)_G(u, v) := f(\psi_G(u, v)) \) for any graph \( G \). One naturally wonders about the distinguishing power of \( \psi \)-WL versus \( f \circ \psi \)-WL. In fact, \( \psi \)-WL will always be at least as strong as \( f \circ \psi \)-WL, and under mild conditions on the input, there will exist a function \( f \) such that \( \psi \)-WL and \( f \circ \psi \)-WL are equally strong.

**Proposition B.1.** Let \( \psi \) be an RPE. Let \( G \) and \( H \) be graphs. Let \( u \in V_G \) and \( v \in V_H \).

1. If \( \chi^{(t)}_{\psi_G}(u) = \chi^{(t)}_{\psi_H}(v) \), then for any function \( f : \mathbb{R}^d \rightarrow \mathbb{R} \), \( \chi^{(t)}_{f \circ \psi_G}(u) = \chi^{(t)}_{f \circ \psi_H}(v) \). In particular, \( \psi \)-WL is as strong as \( f \circ \psi \)-WL.

2. For any set \( \Omega \subset \mathbb{R}^d \) and any function \( f : \mathbb{R}^d \rightarrow \mathbb{R} \) injective on \( \Omega \), if \( \text{im } \psi_G \cup \text{im } \psi_H \subset \Omega \) and \( \chi^{(t)}_{\psi_G}(u) \neq \chi^{(t)}_{\psi_H}(v) \), then \( \chi^{(t)}_{f \circ \psi_G}(u) \neq \chi^{(t)}_{f \circ \psi_H}(v) \). In particular, \( f \circ \psi \)-WL is as strong as \( \psi \)-WL.

**Proof.** For item 1, it follows from (Zhu et al., 2023, Theorem 3).

For item 2, we choose the function \( f \) to be any function that is injective on \( \Omega \); such a function exists as \( \Omega \) are finite. The lemma follows by induction of the iteration \( t \).

**Remark B.2.** It is quite common that RPEs will be drawn from a finite set \( \Omega \subset \mathbb{R}^d \). In particular, if we consider any RPE defined on unweighted graphs with \( n \) vertices that is purely a function of its topology, e.g., the shortest-path distance or Laplacian eigenspace projection, then because there are only finitely many unweighted graphs on \( n \) vertices, then the image of the PE in \( \mathbb{R}^d \) will be finite.
B.2. Proof of Theorem 4.2 and Corollary 4.3

Euclidean Distance and Gram Matrices. Let $P = \{p_1, \ldots, p_n\} \subset \mathbb{R}^d$ be a point cloud. The Gram matrix of $P$ is denoted $G_P \in \mathbb{R}^{n \times n}$ where $(G_P)_{ij} = p_i^T p_j$. The distance matrix of $P$ is denoted $D_P \in \mathbb{R}^{n \times n}$ where $(D_P)_{ij} = \|p_i - p_j\|$. A point cloud $P$ is centered if $\sum_{i=1}^n p_i = 0$.

**Theorem B.3.** Assume that for any graph $G$, there is an embedding of the nodes $P_G : V \rightarrow \mathbb{R}^d$ such that $\text{im} P_G$ is centered. Let $\psi_d$ and $\psi_g$ be RPEs that are the distance and Gram matrix of the point set in $P_G$, respectively. Then, $\psi_d$-WL is at least as strong as are as $\psi_g$-WL. Conversely, $\psi_g$-WL with diagonal augmentation is at least as strong as $\psi_d$.

The proof is based on the following key lemma. We define the squared distance matrix of $P$ to be the matrix $D_P^2 \in \mathbb{R}^{n \times n}$ where $(D_P^2)_{ij} = \|p_i - p_j\|^2$.

**Lemma B.4.** Let $\psi_d$ and $\psi_g$ be RPEs such that, for any graph $G$, $\psi_{d,G}$ and $\psi_{g,G}$ are the squared distance and Gram matrix of a centered point set $P_G \subset \mathbb{R}^d$. Then $\psi_d$-WL is at least as strong as are as $\psi_g$-WL. Conversely, $\psi_g$-WL with diagonal augmentation is at least as strong as $\psi_d$.

**Proof of Theorem B.3 assuming Lemma B.4.** As the square root function is injective, then by Proposition B.1, $G$ and $H$ are indistinguishable by $\psi_d$-WL if and only if $D_P^2$ and $D_Q^2$ are indistinguishable by $\psi_g$-WL.

Now we proceed to prove Lemma B.4.

**Lemma B.5.** Let $P = \{p_1, \ldots, p_n\} \subset \mathbb{R}^d$ be a centered point cloud. For any $1 \leq k \leq n$, $(G_P)_{ii} = \frac{1}{k} \sum_{i=1}^n (D_P^2)_{ik} - \frac{1}{2n^2} \sum_{i=1}^n \sum_{j=1}^n (D_P^2)_{ij}$.

**Proof.** Observe that $(D_P^2)_{ij} = p_i^T p_i + p_j^T p_j - 2p_i^T p_j$. Therefore, the first term simplifies to

$$
\frac{1}{n} \sum_{i=1}^n (D_P^2)_{ik} = p_k^T p_k + \frac{1}{n} \sum_{i=1}^n p_i^T p_i - \frac{2}{n} \sum_{i=1}^n p_i^T p_i = p_k^T p_k + \frac{1}{n} \sum_{i=1}^n p_i^T p_i.
$$

(as $\sum_{i=1}^n p_i = 0$)

The second term simplifies to:

$$
\frac{1}{2n^2} \sum_{i=1}^n \sum_{j=1}^n (D_P^2)_{ij} = \frac{1}{2n^2} \sum_{i=1}^n \sum_{j=1}^n \left( p_i^T p_i + p_j^T p_j - 2p_i^T p_j \right)
$$

$$
= \frac{1}{2n^2} \sum_{i=1}^n \left( np_i^T p_i + \sum_{j=1}^n p_j^T p_j - \sum_{j=1}^n 2p_i^T p_j \right)
$$

$$
= \frac{1}{2n^2} \sum_{i=1}^n \left( np_i^T p_i + \sum_{j=1}^n p_j^T p_j \right)
$$

(as $\sum_{i=1}^n p_i = 0$)

$$
= \frac{1}{2n^2} \sum_{i=1}^n 2np_i^T p_i
$$

$$
= \frac{1}{n} \sum_{i=1}^n p_i^T p_i.
$$

Therefore,

$$
\frac{1}{n} \sum_{i=1}^n (D_P^2)_{ik} - \frac{1}{2n^2} \sum_{i=1}^n \sum_{j=1}^n (D_P^2)_{ij} = p_k^T p_k + \frac{1}{n} \sum_{i=1}^n p_i^T p_i - \frac{1}{n} \sum_{i=1}^n p_i^T p_i = p_k^T p_k = (G_P)_{kk}.
$$
Lemma B.6. Let $\psi_d$ and $\psi_g$ be RPEs such that, for any graph $G$, $\psi_{d,G}$ and $\psi_{g,G}$ are the squared distance and Gram matrix of a centered point set $P_G \subset \mathbb{R}^d$. Let $(G, X_G)$ and $(H, X_H)$ be featured graphs. If $\chi_{\psi_{d,G}}^{(2)}(u) = \chi_{\psi_{d,H}}^{(2)}(x)$, then $(G_{P_G})_{uu} = (G_{P_H})_{xx}$.

Proof. We will prove this using Lemma B.5. First, the fact that $\chi_{\psi_{d,G}}^{(1)}(u) = \chi_{\psi_{d,H}}^{(1)}(x)$ implies $\{ (D_{P_G})_{uv} : v \in V_G \} = \{ (D_{P_H})_{xy} : y \in V_H \}$, which in particular implies that $\frac{1}{n} \sum_{v \in V_G} (D_{P_G})_{uv} = \frac{1}{n} \sum_{y \in V_H} (D_{P_H})_{xy}$. Second, as $\chi_{\psi_{d,G}}^{(2)}(u) = \chi_{\psi_{d,H}}^{(2)}(x)$, then as the second coordinate of these colors are equal, there is a bijection $\sigma : V_G \to V_H$ such that $\chi_{\psi_{d,G}}^{(1)}(v) = \chi_{\psi_{d,H}}^{(1)}(\sigma(v))$ for all $v \in V_G$. In particular, this implies that $\{ (D_{P_G})_{uw} : w \in V_G \} = \{ (D_{P_H})_{xv} : x \in V_H \}$ for all $v \in V_G$. Therefore, $P_G$ and $P_H$ have the same multiset of distances, and $\frac{1}{2n^2} \sum_{v \in V_G} \sum_{w \in V_G} (D_{P_G})_{uw} = \frac{1}{2n^2} \sum_{y \in V_H} \sum_{z \in V_H} (D_{P_H})_{yz}$. These two observations and Lemma B.5 imply the lemma. □

Proposition B.7 (Forward Direction of Lemma B.4). Let $\psi_d$ and $\psi_g$ be RPEs such that, for any graph $G$, $\psi_{d,G}$ and $\psi_{g,G}$ are the squared distance and Gram matrix of a centered point set $P_G \subset \mathbb{R}^d$. Let $(G, X_G)$ and $(H, X_H)$ be featured graphs. Let $u \in V_G$ and $x \in V_H$. If $\chi_{\psi_{d,G}}^{(2)}(u) = \chi_{\psi_{d,H}}^{(2)}(x)$, then $\chi_{\psi_{g,G}}^{(1)}(u) = \chi_{\psi_{d,H}}^{(2)}(x)$. Moreover, if $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\psi_d$-WL, then $(G, X_G)$ and $(H, X_H)$ are indistinguishable by $\psi_g$-WL.

Proof. We prove this by induction on $t$. For $t = 0$, this is obvious as $\chi_{\psi_{g,G}}^{(2)}(u) = \chi_{\psi_{g,H}}^{(2)}(x)$ implies $\chi_{\psi_{g,G}}^{(0)}(u) = X_G(u) = \chi_{\psi_{g,H}}^{(0)}(x)$.

Now suppose the proposition is true for a natural number $t$, and let $u \in V_G$ and $x \in V_H$ such that $\chi_{\psi_{d,G}}^{(t+3)}(u) = \chi_{\psi_{d,H}}^{(t+3)}(x)$. By induction, we know that $\chi_{\psi_{d,G}}^{(t+2)}(u) = \chi_{\psi_{d,H}}^{(t+2)}(x)$ implies $\chi_{\psi_{g,G}}^{(t)}(u) = \chi_{\psi_{g,H}}^{(t)}(x)$, so the first coordinates of $\chi_{\psi_{g,G}}^{(t+1)}(u)$ and $\chi_{\psi_{g,H}}^{(t+1)}(x)$ are equal.

We now show the second coordinates are equal. The fact that $\chi_{\psi_{d,G}}^{(t+3)}(u) = \chi_{\psi_{d,H}}^{(t+3)}(x)$ implies there is a bijection $\sigma : V_G \to V_H$ such that $(\chi_{\psi_{d,G}}^{(t+2)}(v), (D_{P_G})_{uw}) = (\chi_{\psi_{d,H}}^{(t+2)}(\sigma(v)), (D_{P_H})_{xv})$ for all $v \in V_G$. As $\chi_{\psi_{d,G}}^{(t+2)}(v) = \chi_{\psi_{d,H}}^{(t+2)}(\sigma(v))$ implies $(G_{P_G})_{uv} = (G_{P_H})_{\sigma(v)\sigma(v)}$ by Lemma B.6, then we know that:

$$(G_{P_G})_{uv} = \frac{1}{2} \left( (G_{P_G})_{uv} + (G_{P_G})_{uw} - (D_{P_G})_{uw} \right) = \frac{1}{2} \left( (G_{P_H})_{\sigma(v)\sigma(v)} + (G_{P_H})_{xx} - (D_{P_H})_{xx} \right) = (G_{P_G})_{\sigma(v)\sigma(v)}.$$

Moreover, $\chi_{\psi_{d,G}}^{(t+2)}(v) = \chi_{\psi_{d,H}}^{(t+2)}(\sigma(v))$ implies $\chi_{\psi_{g,G}}^{(t)}(v) = \chi_{\psi_{g,H}}^{(t)}(\sigma(v))$ by the inductive hypothesis. Therefore, as $\sigma$ is a bijection, the second coordinates of $\chi_{\psi_{g,G}}^{(t+1)}(u)$ and $\chi_{\psi_{g,H}}^{(t+1)}(x)$ are equal:

$$\{ (\chi_{\psi_{g,G}}^{(t)}(v), (G_{P_G})_{uv}) : v \in V_G \} = \{ (\chi_{\psi_{g,H}}^{(t)}(y), (G_{P_H})_{xy}) : y \in V_H \}. □$$

Proposition B.8 (Backward Direction of Lemma B.4). Let $\psi_d$ and $\psi_g$ be RPEs such that, for any graph $G$, $\psi_{d,G}$ and $\psi_{g,G}$ are the squared distance and Gram matrix of a centered point set $P_G \subset \mathbb{R}^d$. Let $\psi_g = (\psi_g, I)$ be the diagonal augmentation of $\psi_g$. Let $(G, X_G)$ and $(H, X_H)$ with featured graphs. Let $u \in V_G$ and $x \in V_H$. If $\chi_{\psi_{g,G}}^{(t+1)}(u) = \chi_{\psi_{g,H}}^{(t+1)}(x)$, then $\chi_{\psi_{d,G}}^{(t)}(u) = \chi_{\psi_{d,H}}^{(t)}(x)$. In particular, $\psi_g$-WL with diagonal augmentation is at least as strong as $\psi_d$-WL.

Proof. We prove this by induction on $t$. For $t = 0$, this is obvious as $\chi_{\psi_{g,G}}^{(1)}(u) = \chi_{\psi_{g,H}}^{(1)}(x)$ implies $\chi_{\psi_{g,G}}^{(0)}(u) = X_G(u) = X_H(v) = \chi_{\psi_{g,H}}^{(0)}(x)$.

Now suppose the proposition is true for a natural number $t$, and suppose that $\chi_{\psi_{g,G}}^{(t+2)}(u) = \chi_{\psi_{g,H}}^{(t+2)}(x)$. By induction, we know that $\chi_{\psi_{g,G}}^{(t+1)}(u) = \chi_{\psi_{g,H}}^{(t+1)}(x)$ implies $\chi_{\psi_{d,G}}^{(t)}(u) = \chi_{\psi_{d,H}}^{(t)}(x)$, so the first coordinates of $\chi_{\psi_{d,G}}^{(t+1)}(u)$ and $\chi_{\psi_{d,H}}^{(t+1)}(x)$ are equal.

We now show the second coordinates are equal. As $\chi_{\psi_{g,G}}^{(t+2)}(u) = \chi_{\psi_{g,H}}^{(t+2)}(x)$, then there is a bijection $\sigma : V_G \to V_H$ such that $(\chi_{\psi_{g,G}}^{(t+1)}(v), (G_{P_G}, I)_{uv}) = (\chi_{\psi_{g,H}}^{(t+1)}(\sigma(v)), (G_{P_H}, I)_{\sigma(v)v})$ for all $v \in V_G$. The diagonal augmentation implies that
Lemma B.9. Let $G$ and $H$ be graphs. Let $u \in V_G$ and $v \in V_H$ such that $N^{(1)}_{L^+_G}(u) = N^{(1)}_{L^+_H}(v)$. Then $L^+_G(u, u) = L^+_H(v, v)$.

The proof is based on several auxiliary results.

Lemma B.10. Let $G$ be a connected graph with more than 1 vertex and let $L$ denote its graph Laplacian. Then, for any $u \neq v \in V$, we have that $L^+(v, v) > L^+(u, v)$.

Proof. By the fact that $RD(u, v) = L(u, u) + L(v, v) - 2L(u, v)$, we have that

$$L^+(v, v) - L^+(u, v) = \frac{1}{2} (RD(u, v) + L^+(v, v) - L^+(u, v)).$$

Therefore, to prove that $L^+(v, v) > L^+(u, v)$, it suffices to prove that

$$RD(u, v) > L^+(u, u) - L^+(v, v).$$
By Lemma B.5, we have that
\[ L^1(u, u) - L^1(v, v) = \frac{1}{n} \left( \sum_{w \in V} RD(u, w) - \sum_{w \in V} RD(v, w) \right) \]
\[ = \frac{1}{n} \sum_{w \in V} RD(u, w) - RD(v, w) \]
\[ = \frac{1}{n} \sum_{w \in V \setminus \{u,v\}} RD(u, w) - RD(v, w) \]
\[ \leq \frac{1}{n} \sum_{w \in V \setminus \{u,v\}} RD(u, v) \quad \text{(Triangle inequality.)} \]
\[ = \frac{n-2}{n} RD(u, v) < RD(u, v). \]

Lemma B.11. Let \( G \) be a graph and let \( L \) denote its graph Laplacian. Let \( u \in V \). Then either

1. \( L^1(u, u) > L^1(u, v) \) for all \( v \in V \), or
2. \( L^1(u, u) = 0 \) for all \( v \in V \).

Proof. Let \( G_1, \ldots, G_k \) denote the connected components of \( G \). Then, we have that \( L = L_1 \oplus \cdots \oplus L_k \) and thus \( L^1 = L^1_1 \oplus \cdots \oplus L^1_k \). For each connected component \( G_l \), if it contains more than 1 vertex, then by Lemma B.10, \( L^1_l \) satisfies the condition that the diagonal entries are strictly larger than all other entries in the corresponding rows. If \( G_l \) contains only 1 vertex, then \( L^1_l = 0 \) and hence the corresponding row and column in \( L^1 \) is always 0. This concludes the proof.

Now, we finish the proof of Lemma B.9.

Proof of Lemma B.9. By the definition of the \( L^1 \)-WL test, \( \chi^{(1)}_{L^1_H} (u) = \chi^{(1)}_{L^1_H} (v) \) implies that \( \{ L^1_H(u, w) : w \in V_G \} = \{ L^1_H(v, x) : x \in V_H \} \). By Lemma B.11, we know that either the multisets \( \{ L^1_G(u, w) : w \in V_G \} = \{ L^1_H(v, x) : x \in V_H \} \) are all 0s, in which case \( L^1_G(u, u) = 0 = L^1_H(v, v) \), or they have the same maximal element, which is \( L^1_G(u, u) = L^1_H(v, v) \).

B.3. SPE APE-GT is Stronger than RD-RPE-GT

Background. First, we provide the definition of SPE (Huang et al., 2024). Denote the eigenvalues and eigenvectors of the Laplacian as \( \lambda_1 \leq \ldots \leq \lambda_{|V|} \) and \( z_1, \ldots, z_{|V|} \). Let \( A := [\lambda_1, \ldots, \lambda_{|V|}] \in \mathbb{R}^{|V|} \) and \( V := [z_1|\cdots|z_{|V|}] \in \mathbb{R}^{|V| \times |V|} \), so \( L = V \text{ diag}(A)V^T \).

Stable and expressive positional encoding (SPE) is the APE
\[ \text{SPE}(V, A) = g(V \text{ diag}(f(A))V^T), \]
where \( f : \mathbb{R}^n \to \mathbb{R}^n \) is a permutation-equivariant function like an elementwise MLP or DeepSets (Zaheer et al., 2017) and \( g : \mathbb{R}^{n \times n} \to \mathbb{R}^n \) is any graph neural network. In our context, we assume that \( f \) is a DeepSets network and \( g \) is a 2-EGN.

By removing the final layer of 2-EGN from SPE, one obtains a natural RPE that we call the relative-SPE (RSPE): RSPE\((V, A) = V \text{ diag}(f(A))V^T \).

Lemma B.12. If a chosen RSPE is diagonally-aware (or diagonally augmented), then there exists a 2-EGN \( g \) such that RSPE-RPE-GT is equivalent to SPE-APE-GT in terms of distinguishing power.

Proof. This follows from Theorem 3.10.

Notice that when \( f \) is an elementwise function, RSPE reduces to a spectral kernel and we hence have the following result; however, RSPE is more general than spectral kernels as \( f(A)_i \) may be a function of all the eigenvalues, not just the \( i \)th eigenvalue. Accordingly, we have the following lemma.
Lemma B.13. RSPE can compute any spectral kernel.

Based on the lemma, we are able to prove our main result in this section.

Theorem 4.4. For unfeatured graphs, diagonally augmented SPE-APE-GT is at least as strong as RD-RPE-GT.

Proof. The precise statement of the result is that there exists a choice of RSPE with the diagonal augmentation such that its corresponding SPE-APE-GT is at least as strong as RD-RPE-GT.

By Lemma B.12, we know that there exists a 2-EGN $g$ such that RSPE-RPE-GT is equivalent to SPE-APE-GT in terms of distinguishing power. Therefore, it suffices to show that RSPE-RPE-GT is at least as strong as RD-RPE-GT. Since the pseudoinverse of the Laplacian $L^\dagger$ is a spectral kernel, by Lemma B.13 RSPE can be chosen so that its corresponding RSPE-WL is at least as strong as $L^\dagger$-WL. Since the extra diagonal augmentation of the two RPEs will not change the relative distinguishing power of their RPE-augWL test, by Lemma 3.6 and the fact that RD is diagonally-aware, we conclude the proof. 

B.4. Powers of Matrices and Spectral Kernels: Proofs from Section 4.3

We want to show that the multidimensional RPE $(I, L, \ldots, L^k)$ is equivalent to spectral kernels in distinguishing power. To prove this, we will use a basic result from the interpolation literature showing that any function on $k$ points can be fit exactly by a $(k-1)$-degree polynomial $p$.

Lemma B.14. Let $f : \mathbb{R} \to \mathbb{R}$ be any function and let $\{x_1, \ldots, x_n\} \subset \mathbb{R}$. Then there exists an $(n-1)$-degree polynomial $p : \mathbb{R} \to \mathbb{R}$ such that $p(x_i) = f(x_i)$ for all $1 \leq i \leq n$.

Theorem 4.6. $(I, L, \ldots, L^{2n-1})$-WL is at least as strong as $K^f$-WL on graphs with at most $n$ nodes.

Proof. Let $G$ and $H$ be graphs such that $K^f$-WL distinguishes $G$ and $H$. Let $\{\lambda_{G,1}, \ldots, \lambda_{G,n}\}$ and $\{\lambda_{H,1}, \ldots, \lambda_{H,n}\}$ be the spectra of the Laplacians $L_G$ and $L_H$ respectively, and denote their union $\{\lambda_{G,1}, \ldots, \lambda_{G,n}\} \cup \{\lambda_{H,1}, \ldots, \lambda_{H,n}\} = \{\lambda_0, \ldots, \lambda_{2n} \}$ (without loss of generality, we assume these elements are distinct). Let $p(x) = \sum_{i=0}^{2n-1} c_i x^i$ be the polynomial guaranteed by Lemma B.14 for the point cloud $\{x_0, \ldots, x_{2n-1}\}$ and for the function $f$ in defining $K^f$. Let $p_l : \mathbb{R}^{2n} \to \mathbb{R}$ be the linear function with the same coefficients as $p$, i.e. $p_l(x) = \sum_{i=0}^{2n-1} c_i x_i$. By linearity, if we apply $p_l$ elementwise on the tensor $(I, L_G, \ldots, L_G^{2n-1})$, we find that it equals $K^f$ for $G$:

$$p_l(I, L_G, \ldots, L_G^{2n-1}) = \sum_{i=0}^{2n-1} c_i L^i_G = \sum_{i=0}^{2n-1} \sum_{j=2}^n c_i \lambda_{G,j} z_j z_j^T = \sum_{j=2}^n p(\lambda_{G,j}) z_j z_j^T = \sum_{j=2}^n f(\lambda_{G,j}) z_j z_j^T = K_G^f$$

The same calculation holds for $H$. Therefore, as $K^f$-WL distinguishes $G$ and $H$, then $p_l \circ (I, L, \ldots, L^{2n-1})$-WL distinguishes $G$ and $H$.

Moreover, Proposition B.1 implies $(I, L, \ldots, L^{2n-1})$-WL distinguishes $G$ and $H$. As the above argument can be repeated (using different polynomials $p$) to show that $(I, L, \ldots, L^{2n-1})$ can distinguish any pair of graphs that $K^f$ can, then $(I, L, \ldots, L^{2n-1})$-WL is as strong as $K^f$-WL on graphs with $n$ nodes.

The following theorem uses normalized versions of the adjacency matrix and Laplacian. Recall that $D$ denotes the degree matrix, $A$ denotes the adjacency matrix, and $L$ denotes the graph Laplacian. The symmetrically-normalized adjacency matrix is $A = D^{-1/2} A D^{-1/2}$, and its symmetrically-normalized Laplacian is $L = D^{-1/2} A D^{-1/2} = I - A$. We let $\mu_1 \leq \cdots \leq \mu_n$ denote eigenvalues of $A$ and let $\nu_1 \leq \cdots \leq \nu_n$ denote eigenvalues of $\hat{L}$.

Note that $\nu_n = 1 - \mu_n$. Moreover, $\hat{A}$ and $\hat{L}$ they have the same set of eigenvectors $\{x_1, \ldots, x_n\}$ (up to choice of orthonormal basis). For a function $f : \mathbb{R} \to \mathbb{R}^+$, we define the normalized spectral kernel as $\hat{K}^f = \sum_{i=2}^n f(\nu_i) x_i x_i^T$.

Theorem 4.8. $(I, \hat{A}, \ldots, \hat{A}^{2n-1})$-WL is at least as strong as $\hat{K}^f$-WL on graphs with at most $n$ nodes.

Proof. This theorem follows as the eigenvalues $\mu_i$ of $\hat{A}$ and $\nu_i$ of $\hat{L}$ can be matched as $\mu_i = 1 - \nu_i$. The rest of the proof is the same as Theorem 4.6 by using polynomials to fit the function $\hat{f}(x) = f(1 - x)$.

Theorem 4.9. $(I, H^{(1)}, \ldots, H^{(2n-1)})$-WL is at least as strong as $K^f$-WL on graphs with at most $n$ nodes.
Proof. This theorem follows as the eigenvalues of $H^{(t)}$ are $e^{-t\lambda_i} = (e^{-\lambda_i})^t$, so the proof is the same as the proof of Theorem 4.6 by using polynomials to fit the function $\hat{f}(x) = f(-\log(x))$.

B.5. Common Matrices: Proof of Proposition 4.10

Proposition 4.10. $A, \tilde{A}, \hat{A}, L, \tilde{L}$ and $\bar{L}$ induce equivalent RPE-augWL tests. In particular, all of these RPE-augWL tests are equally strong as the WL test.

Proof. By Proposition B.16 below, we know that $A$-WL is equivalent to the WL test. Hence, we only need to show that all other RPE-augWL tests are equivalent to $A$-WL.

Choose any featured graphs $(G, X_G)$ and $(H, X_H)$. Pick $u \in V_G$ and $v \in V_H$. First of all, we observe the following fact.

Fact 4. $\chi_G^{(1)}(u) = \chi_H^{(1)}(v)$ implies that $\deg_G(u) = \deg_H(v)$.

$A$: We inductively prove that $\chi_G^{(t)}(u) = \chi_H^{(t)}(v)$ if $\chi_G^{(1)}(u) = \chi_H^{(1)}(v)$. The case when $t = 0$ trivially holds. Assume that the statement holds for some $t \geq 0$. Then, we first assume that $\chi_G^{(t+1)}(u) = \chi_H^{(t+1)}(v)$. This implies that $\chi_G^{(t+1)}(u) = \chi_H^{(t+1)}(v)$.

By Fact 4, we have that $\deg_G(u) = \deg_H(v)$. By induction, we have that $\chi_G^{(t)}(u) = \chi_H^{(t)}(v)$ and

$$\{ (\chi_G^{(t)}(x), \tilde{A}G(u,x)) : x \in V_G \} = \{ (\chi_H^{(t)}(y), \tilde{A}H(v,y)) : y \in V_H \}.$$ 

Hence, we have that

$$\{ (\chi_G^{(t)}(x), A_G(u,x) / \deg_G(u)) : x \in V_G \} = \{ (\chi_H^{(t)}(y), A_H(v,y) / \deg_H(v)) : y \in V_H \},$$

and thus $\chi_G^{(t+1)}(u) = \chi_H^{(t+1)}(v)$.

Conversely, assume that $\chi_G^{(t+1)}(u) = \chi_H^{(t+1)}(v)$. This implies that $\chi_G^{(1)}(u) = \chi_H^{(1)}(v)$. Similarly to Fact 4, we have that $\deg_G(u) = \deg_H(v)$. Then, the above argument can be repeated to show that $\chi_G^{(t+1)}(u) = \chi_H^{(t+1)}(v)$.

Therefore, $\tilde{A}$-WL is equivalent to $A$-WL.

$\hat{A}$: We prove that $\hat{A}$-WL is equivalent to $\tilde{A}$-WL and hence $A$-WL by showing that for any $u \in V_G$ and $v \in V_H$, one has for all $t \geq 0$ that

$$\chi^{(t)}(u) = \chi^{(t)}(v) \implies \chi^{(t)}(u) = \chi^{(t)}(v) \text{ and } \chi^{(t+1)}(u) = \chi^{(t+1)}(v) \implies \chi^{(t)}(u) = \chi^{(t)}(v).$$

The case when $t = 0$ holds trivially.

Now assume that the statement holds for any $t \geq 1$. $\chi^{(t+1)}(u) = \chi^{(t+1)}(v)$ implies that

$$(\chi^{(t)}(u), \{ (\chi^{(t)}(x), A_G(u,x) / \sqrt{\deg_G(u) \deg_G(x)}) : x \in V_G \})$$

$$= (\chi^{(t)}(v), \{ (\chi^{(t)}(y), A_H(v,y) / \sqrt{\deg_H(v) \deg_H(y)}) : y \in V_H \}).$$

By counting the number of non-zero elements on both sides, we have that $\deg_G(u) = \deg_H(v)$. Hence,

$$(\chi^{(t)}(u), \{ (\chi^{(t)}(x), \deg_G(u), A_G(u,x) / \sqrt{\deg_G(x)}) : x \in V_G \})$$

$$= (\chi^{(t)}(v), \{ (\chi^{(t)}(y), \deg_H(v), A_H(v,y) / \sqrt{\deg_H(y)}) : y \in V_H \})$$

and thus

$$(\chi^{(t)}(u), \{ (\chi^{(t)}(x), \deg_G(u), A_G(u,x)) : x \in V_G \})$$

$$= (\chi^{(t)}(v), \{ (\chi^{(t)}(y), \deg_H(v), A_H(v,y)) : y \in V_H \}).$$
Finally, by the inductive hypothesis we have that
\[
\chi_{A_G}^{(t+1)}(u) = (\chi_{A_G}^{(t)}(u), \{ (\chi_{A_G}^{(t)}(x), \bar{A}_G(u,x)) : x \in V_G \}) \\
= (\chi_{A_H}^{(t)}(v), \{ (\chi_{A_H}^{(t)}(y), \bar{A}_H(v,y)) : y \in V_H \}) = \chi_{A_H}^{(t+1)}(v).
\]

For the other direction, assume that \( \chi_{A_G}^{(t+2)}(u) = \chi_{A_H}^{(t+2)}(v) \). This implies that
\[
(\chi_{A_G}^{(t+1)}(u), \{ (\chi_{A_G}^{(t+1)}(x), \bar{A}_G(u,x)) : x \in V_G \}) \\
= (\chi_{A_H}^{(t+1)}(v), \{ (\chi_{A_H}^{(t+1)}(y), \bar{A}_H(v,y)) : y \in V_H \}).
\]

It is obvious that \( \text{deg}_G(u) = \text{deg}_H(v) \). Let \( \sigma : V_G \to V_H \) denote a bijection such that \( (\chi_{A_G}^{(t+1)}(x), \bar{A}_G(u,x)) = (\chi_{A_H}^{(t+1)}(\sigma(x)), \bar{A}_H(v,\sigma(x))) \) for all \( x \in V_G \). Then, we have that \( \text{deg}_G(x) = \text{deg}_H(\sigma(x)) \). Hence,
\[
(\chi_{A_G}^{(t+1)}(x), \bar{A}_G(u,x)) = (\chi_{A_H}^{(t+1)}(\sigma(x)), \bar{A}_H(v,\sigma(x))).
\]
By the inductive hypothesis, we have that \( (\chi_{A_G}^{(t)}(x), \bar{A}_G(u,x)) = (\chi_{A_H}^{(t)}(\sigma(x)), \bar{A}_H(v,\sigma(x))) \). Therefore,
\[
\chi_{A_G}^{(t+1)}(u) = (\chi_{A_G}^{(t)}(u), \{ (\chi_{A_G}^{(t)}(x), \bar{A}_G(u,x)) : x \in V_G \}) \\
= (\chi_{A_H}^{(t)}(v), \{ (\chi_{A_H}^{(t)}(y), \bar{A}_H(v,y)) : y \in V_H \}) = \chi_{A_H}^{(t+1)}(v).
\]

\( L, \hat{L}, \tilde{L} \): Note that the graph Laplacian \( L \) is combinatorially-aware. Hence by Theorem 4.16, \( L \)-WL is at least as strong as the WL test and hence \( A \)-WL test. For the other direction, we prove the stronger result that \( \chi_{A_G}^{(t)}(u) = \chi_{A_H}^{(t)}(v) \) implies that \( \chi_{L_G}^{(t)}(u) = \chi_{L_H}^{(t)}(v) \) for any \( u \in V_G \) and \( v \in V_H \).

The statement trivially holds when \( t = 0 \). Assume that the statement holds for some \( t \geq 0 \). Then, we assume that \( \chi_{A_G}^{(t+1)}(u) = \chi_{A_H}^{(t+1)}(v) \). This implies that \( \chi_{A_G}^{(t)}(u) = \chi_{A_H}^{(t)}(v) \). By Fact 4, we have that \( \text{deg}_G(u) = \text{deg}_H(v) \). By definition, \( \chi_{A_G}^{(t)}(u) = \chi_{A_H}^{(t)}(v) \) and hence by induction hypothesis, \( \chi_{L_G}^{(t)}(u) = \chi_{L_H}^{(t)}(v) \). Now, from the fact that \( \{ (\chi_{A_G}^{(t)}(x), A_G(u,x)) : x \in V_G \} = \{ (\chi_{A_H}^{(t)}(y), A_H(v,y)) : y \in V_H \} \), we obtain a bijection \( \sigma : V_G \to V_H \) such that \( (\chi_{A_G}^{(t)}(x), A_G(u,x)) = (\chi_{A_H}^{(t)}(\sigma(x)), A_H(v,\sigma(x))) \) for all \( x \in V_G \). We assume that \( \sigma(u) = v \) (otherwise we can modify \( \sigma \) so that the assumption holds). Then, by inductive hypothesis we have that \( \chi_{L_G}^{(t)}(x) = \chi_{L_H}^{(t)}(\sigma(x)) \) for all \( x \in V_G \). Furthermore, from the fact that \( A_G(u,x) = A_H(v,\sigma(x)) \), \( \sigma(u) = v \) and \( \text{deg}_G(u) = \text{deg}_H(v) \), we have that \( L_G(u,x) = L_H(v,\sigma(x)) \) for all \( x \in V_G \).

Hence, \( \{ (\chi_{L_G}^{(t)}(x), L_G(u,x)) : x \in V_G \} = \{ (\chi_{L_H}^{(t)}(y), L_H(v,y)) : y \in V_H \} \). Therefore, \( \chi_{L_G}^{(t)}(u) = \chi_{L_H}^{(t)}(v) \). This concludes the proof.

Therefore, \( L \)-WL is equivalent to \( A \)-WL. Similarly, \( \hat{L} \)-WL is equivalent to \( \hat{A} \)-WL and \( \tilde{L} \)-WL is equivalent to \( \tilde{A} \)-WL. Hence, all of these RPE-aug-WL tests are equivalent to the WL test.

\( \square \)

B.6. Combinatorial-Awareness: Proof of Theorem 4.16

**Theorem 4.16.** Let \( \psi \) be a combinatorially-aware RPE. Then, \( \psi \)-WL is at least as strong as WL.

For any two featured graphs \( (G, X_G) \) and \( (H, X_H) \), we prove the following stronger lemma that immediately implies Theorem 4.16.

**Lemma B.15.** Let \( \psi \) be a combinatorially-aware RPE. Let \( u \in G \) and \( v \in H \). If \( \chi_{\psi_G}^{(t)}(u) = \chi_{\psi_H}^{(t)}(v) \), then \( \chi_{G}^{(t)}(u) = \chi_{H}^{(t)}(v) \).

**Proof.** We prove this by induction on the iteration. The case \( t = 0 \) holds trivially by definition of the two WL tests.

Now inductively suppose the theorem is true for iteration \( t \). Let \( u \in G \) and \( v \in H \) such that \( \chi_{\psi_G}^{(t+1)}(u) = \chi_{\psi_H}^{(t+1)}(v) \).

First, by definition, \( \chi_{\psi_G}^{(t)}(u) = \chi_{\psi_H}^{(t)}(v) \). This and the inductive hypothesis imply \( \chi_{G}^{(t)}(u) = \chi_{H}^{(t)}(v) \).
Next, by definition, there is a bijection $\sigma : V_G \to V_H$ such that $(\chi_G^{(t)}(w), \psi_G(u, w)) = (\chi_H^{(t)}(\sigma(w)), \psi_H(v, \sigma(w)))$ for all $w \in V_G$. This implies $\psi_G(u, w) = \psi_H(v, \sigma(w))$ if and only if both $\{u, w\}$ and $\{v, \sigma(w)\}$ are edges or non-edges; therefore, $\{\chi_G^{(t)}(w) : \{u, w\} \in E_G\} = \{\chi_H^{(t)}(x) : \{v, x\} \in E_H\}$. This and the inductive hypothesis imply $\{\chi_G^{(t)}(w) : \{u, w\} \in E_G\} = \{\chi_H^{(t)}(x) : \{v, x\} \in E_H\}$. This and the observation from the previous paragraph imply $\chi_G^{(t+1)}(u) = \chi_H^{(t+1)}(v).$

Note that the adjacency matrix $A$ is trivially combinatorially-aware and hence $A$-WL is at least as strong as the WL. In fact, the other direction also holds and hence we have that the $A$-WL and WL are equally strong.

**Proposition B.16 (RPE-augWL generalizes WL).** Consider the RPE given by the adjacency matrix $A$. Given two graphs $G$ and $H$, then $\chi(G) = \chi(H)$ iff $\chi_A(G) = \chi_A(H)$.

**Proof.** We only need to prove the direction that the WL is at least as strong as the $A$-WL. Let $(G, X_G)$ and $(H, X_H)$ be two featured graphs. We prove the following stronger statement:

**Lemma B.17.** Assume that $\{\chi_G^{(t)}(u) : u \in V_G\} = \{\chi_H^{(t)}(v) : v \in V_H\}$. Let $u \in G$ and $v \in H$. If $\chi_G^{(t)}(u) = \chi_H^{(t)}(v)$, then $\chi_A^{(t)}(u) = \chi_A^{(t)}(v)$ and hence $\{\chi_A^{(t)}(u) : u \in V_G\} = \{\chi_A^{(t)}(v) : v \in V_H\}$.

**Proof of Lemma B.17.** We prove this by induction on the iteration. The case $t = 0$ holds trivially by definition of the two WL tests.

Now inductively suppose the theorem is true for iteration $t$. Let $u \in G$ and $v \in H$ such that $\chi_G^{(t)}(u) = \chi_H^{(t)}(v)$. By definition, $\chi_G^{(t)}(u) = \chi_H^{(t)}(v)$ and $\{\chi_G^{(t)}(w) : \{u, w\} \in E_G\} = \{\chi_H^{(t)}(x) : \{v, x\} \in E_H\}$. By induction assumption, we have that $\chi_G^{(t)}(u) = \chi_H^{(t)}(v)$. Therefore, there is a bijection $\sigma : N_G(u) \to N_H(v)$ such that $\chi_G^{(t)}(w) = \chi_H^{(t)}(\sigma(w))$ for all $w \in N_G(u)$. Now, since $\{\chi_G^{(t)}(x) : x \in V_G\} = \{\chi_H^{(t)}(y) : y \in V_H\}$, we have that $\{\chi_G^{(t)}(x) : x \in V_G \setminus N_G(u)\} = \{\chi_H^{(t)}(y) : y \in V_H \setminus N_H(v)\}$. Hence there exists a bijection $\tau : V_G \setminus N_G(u) \to V_H \setminus N_H(v)$ such that $\chi_G^{(t)}(x) = \chi_H^{(t)}(\tau(x))$ for all $x \in V_G \setminus N_G(u)$. Now, we define a bijection $\Phi : V_G \to V_H$ as the union of $\sigma$ and $\tau$. In this way, we have that for any $x \in V_G$, $A_G(u, x) = A_H(v, \Phi(x))$ and $A_G^{(t)}(x) = \chi_A^{(t)}(\Phi(x))$. Hence, we have that

$$(\chi_A^{(t)}(u), \{\chi_A^{(t)}(x), A_G(u, x) : x \in V_G\}) = (\chi_A^{(t)}(v), \{\chi_A^{(t)}(y), A_H(v, y) : y \in V_H\}).$$

This implies that $\chi_A^{(t+1)}(u) = \chi_A^{(t+1)}(v)$ and we hence concludes the proof.

This concludes the proof.

**B.7. Resistance Distance is not Combinatorially-Aware**

In Figure 6, we show a graph $G$ so that $RD(1, 3) = RD(4, 5) = 1$ but $\{4, 5\} \in E_G$ and $\{1, 3\} \notin E_G$. This proves that the resistance distance is not combinatorially-aware.

![Figure 6](image.png)

Figure 6. RD(1, 3) = RD(4, 5) = 1.
B.8. Resistance Distance and Block Cut-Edge Component Trees

For a connected graph \( G \), a cut edge is an edge \( e \in E_G \) such that \( G \setminus \{ e \} \) is disconnected. An (edge-)biconnected component of \( G \) is a maximal subset \( U \subset V_G \) such that the subgraph of \( G \) induced by \( U \) is connected and has no cut edges. The block cut-edge tree of \( G \) is the tree whose vertices are the edge-biconnected components \( BCC(G) \) of \( G \) and its edges are \( \{ \{ C_1, C_2 \} : C_1 \neq C_2 \in BCC(G), \exists \{ u, v \} \in E_G \text{ such that } u \in C_1 \text{ and } v \in C_2 \} \), i.e. the edges of the block cut-edge tree correspond to cut edges in \( G \) that connect two edge-biconnected components.

Similarly, a cut vertex is a vertex \( v \in V_G \) such that \( G \setminus \{ v \} \) is disconnected.

In this section, we prove the following theorem.

Theorem B.18. Let \( G \) and \( H \) be unfeatured graphs.

1. Let \( \{ u, v \} \in E_G \) and \( \{ x, y \} \in E_H \). If \( \| \chi_{RD_G}^{(t)}(u), \chi_{RD_G}^{(t)}(v) \| = \| \chi_{RD_H}^{(t)}(x), \chi_{RD_H}^{(t)}(y) \| \) for all \( t \geq 0 \), then \( \{ u, v \} \) is a cut edge if and only if \( \{ x, y \} \) is a cut edge.

2. If \( \chi_{RD}(G) = \chi_{RD}(H) \), then the block cut-edge trees of \( G \) and \( H \) are isomorphic.

Background The following are well-known facts about effective resistance that will be useful for proving this theorem.

Lemma B.19. Let \( G \) be a graph with \( \{ u, v \} \in E_G \). Then \( RD_G(u, v) \leq 1 \). Moreover, \( RD_G(u, v) = 1 \) if and only if \( \{ u, v \} \) is a cut edge.

Lemma B.20. Let \( G \) be a graph with \( u, v, w \in V \). Then \( RD_G(u, v) + RD_G(v, w) = RD_G(u, w) \) if and only if \( v \) is a cut vertex such that \( u \) and \( w \) are disconnected in \( G \setminus \{ v \} \).

Notation For any pair of vertices \( u \) and \( v \) of a graph \( G \), their resistance distance is denoted by \( RD_G(u, v) \); however, we may drop the subscript \( G \) when it is clear from the context.

Recall that the notation \( \chi_{RD}(G) = \chi_{RD}(H) \) means that two graphs \( G \) and \( H \) have the same multisets of the RD-WL colorings of their vertices for all \( t \geq 0 \), i.e. \( \{ \chi_{RD_G}^{(t)}(v) : v \in V_G \} = \{ \chi_{RD_H}^{(t)}(v) : v \in V_H \} \), where \( \chi_{RD_G} \) and \( \chi_{RD_H} \) are RD-WL colorings of \( G \) and \( H \), respectively. Similarly, we define \( \chi_{RD_G}(u) \) as the ordered tuple \( (\chi_{RD_G}^{(0)}(u), \chi_{RD_G}^{(1)}(u), \ldots) \).

In other words, \( \chi_{RD_G}(u) = \chi_{RD_H}(v) \) if and only if \( \chi_{RD_G}^{(t)}(u) = \chi_{RD_H}^{(t)}(v) \) for all \( t \geq 0 \). We call these the colors of the graphs and nodes, respectively. We prove the following lemma about this new notation.

Lemma B.21. Let \( u \in V_G \) and \( u' \in V_H \) be such that \( \chi_{RD_G}(u) = \chi_{RD_H}(u') \). Then \( \{ \chi_{RD_G}(v), RD_G(u, v) \} : v \in V_G \} = \{ \chi_{RD_H}(v'), RD_H(u', v') \} : v' \in V_H \}. \)

Proof. If not, then there is some iteration \( t \) such that \( \{ \chi_{RD_G}^{(t)}(v), RD_G(u, v) \} : v \in V_G \} \neq \{ \chi_{RD_H}^{(t)}(v'), RD_H(u', v') \} : v' \in V_H \}. \) In this case, clearly \( \chi_{RD_G}^{(t+1)}(u) \neq \chi_{RD_H}^{(t+1)}(u') \). \)

Lemma B.22. Let \( C \) be any set of colors. Let \( u \in V_G \) and \( u' \in V_H \) be such that \( \chi_{RD_G}(u) = \chi_{RD_H}(u') \). Let \( D(u) \) (respectively, \( D(u') \)) be the multisets of the resistance distances of all vertices of \( G \) (respectively, \( H \)) with color \( C \) from \( u \) (respectively, \( u' \)), i.e. \( D(u) = \{ RD_G(u, v) : v \in V_G, \chi_{RD_G}(v) \in C \} \) and \( D(u') = \{ RD_H(u', v') : v' \in V_H, \chi_{RD_H}(v') \in C \} \). Then \( D(u) = D(u') \). In particular, the mean, minimum, and maximum of the multisets \( D(u) \) and \( D(u') \) are equal.

Proof. If these sets are not the same, then by Lemma B.21, it cannot be the case that \( \chi_{RD_G}(u) = \chi_{RD_H}(u') \). \)

Lemma B.23. Let \( \{ u, v \} \) be a cut edge in \( G \), and let \( S_u \) and \( S_v \) be the vertex sets of the connected components of \( G \setminus \{ u, v \} \) such that \( u \in S_u \) and \( v \in S_v \). Let \( C_{uv} \subset V \) be the subset of all vertices that have RD-WL-color \( \chi_{RD_G}(u) \) or \( \chi_{RD_H}(v) \). Then \( S_u \cap C_{uv} = \{ u \} \) or \( S_v \cap C_{uv} = \{ v \} \).

Proof. Let \( x \) be the farthest vertex of \( C_{uv} \) (with respect to the resistance distance) from the set \( \{ u, v \} \) in \( G \). Assume \( x \neq u \) and \( x \neq v \), otherwise the statement of the lemma trivially holds. Without loss of generality assume \( x \in S_u \). We show that \( C_{uv} \cap S_v = \{ v \} \).
Let \( y \in S_v \), and \( y \neq v \). Let \( m_y, m_u \), and \( m_v \) be the maximum (resistance) distance of \( y \), \( u \) and \( v \) from any vertex in \( C_{uv} \). Note \( m_u = RD(u, x) \), and \( m_v = RD(v, x) = 1 + RD(u, x) \) because of the choice of \( x \). Further, we have \( m_y \geq RD(y, v) + RD(v, x) = RD(y, v) + m_v > m_u \), and that \( m_y \geq RD(y, u) + RD(u, x) = RD(y, u) + m_u = RD(y, v) + 1 + m_y > m_u \) as \( \{ u, v \} \) is a cut edge. Thus, \( m_y \neq m_u \) and \( m_y \neq m_v \). In particular, the list of distances of both \( v \) and \( u \) to vertices in \( C_{uv} \) are different from the list of distances of \( y \) to these vertices. Hence, by Lemma B.22, the color \( \chi_{RD_G}(y) \) is different from both of the colors \( \chi_{RD_G}(u) \) and \( \chi_{RD_G}(v) \).

**Theorem B.24.** Let \( G \) and \( H \) be two graphs with the same RD-WL colorings. Let \( \{ u, v \} \in E_G \) be a cut edge, and let \( \{ u', v' \} \in E_H \) be such that \( \chi_{RD_G}(u) = \chi_{RD_H}(u') \) and \( \chi_{RD_G}(v) = \chi_{RD_H}(v') \). Then, \( \{ u', v' \} \) is a cut edge in \( H \).

**Proof.** Let \( S_u \) and \( S_v \) be the vertex sets of the connected components of \( G \setminus \{ u, v \} \) such that \( u \in S_u \) and \( v \in S_v \). Also, let \( C_{uv}^G \) (respectively, \( C_{uv}^H \)) be the set of all vertices that are colored \( \chi_{RD_G}(u) \) or \( \chi_{RD_G}(v) \) in \( G \) (respectively, in \( H \)). By Lemma B.23, and without loss of generality, we assume \( C_{uv}^G \cap S_v = \{ v \} \). Therefore, the closest vertex of \( C_{uv}^G \) to \( u \), which is at distance 1 to \( v \) since \( \{ u, v \} \) is a cut edge; the vertex \( u \) is the closest to \( v \) as there are no other vertices besides \( v \) in \( C_{uv}^G \cap S_v \), and any vertex in \( C_{uv}^G \cap S_u \) is at distance at least 1 from \( v \) via the series formula of the resistance distance.

Since \( \chi_{RD_G}(v) = \chi_{RD_H}(v') \), the closest vertex in \( C_{uv}^H \) to \( v' \) has distance 1 from \( v' \)—otherwise \( \chi_{RD_H}(v') \) would be different from \( \chi_{RD_G}(v) \) by Lemma B.22. Moreover, \( RD_H(u', v') \leq 1 \) as \( \{ u', v' \} \in E_H \). Thus, \( RD_H(u', v') = 1 \) and, by Lemma B.19, \( \{ u', v' \} \) is a cut edge.

**Lemma B.25.** Let \( G \) and \( H \) be two graphs with the same RD-WL colorings. Let \( \{ u, v \} \) be a cut edge in \( G \) and \( S_u, S_v \) be the partitions of \( G \setminus \{ u, v \} \). Let \( \{ u', v' \} \) be a cut edge in \( H \) such that \( \chi_{RD_G}(u) = \chi_{RD_H}(u') \) and \( \chi_{RD_G}(v) = \chi_{RD_H}(v') \), and let \( S'_u, S'_v \) be partitions of \( H \setminus \{ u', v' \} \). Let \( C \) be any subset of colors used in these equivalent colorings. Let \( D_v = \{ d_1, \ldots, d_k \} \) be the list of distances of vertices with color \( C \) in \( S_v \) from \( v \) and let \( L_u = \{ \ell_1, \ldots, \ell_t \} \) be the list of distances of vertices with color \( C \) in \( S_u \) from \( u \). Similarly, let \( D'_v = \{ d'_1, \ldots, d'_k \} \) be the list of distances of vertices with color \( C \) in \( S'_v \) from \( v' \) and let \( L'_u = \{ \ell'_1, \ldots, \ell'_t \} \) be the list of distances of vertices with color \( C \) in \( S'_u \) from \( u' \). Then, we have \( D_v = D'_v \) and \( L_u = L'_u \). In particular, \( |D_v| = |D'_v| \) and \( |L_u| = |L'_u| \).

**Proof.** Without loss of generality, by permuting indices, let \( D_1 = D_v \cap D'_v = \{ d_1, \ldots, d_p \} = \{ d'_1, \ldots, d'_p \} \), and \( L_1 = L_u \cap L'_u = \{ \ell_1, \ldots, \ell_q \} = \{ \ell'_1, \ldots, \ell'_q \} \). Hence,

\[
D'_v = \{ d_1, \ldots, d_p, d_{p+1}, \ldots, d_k \},
\]

and

\[
L'_u = \{ \ell_1, \ldots, \ell_q, \ell_{q+1}, \ldots, \ell_t \}.
\]

By the definition of \( D_1 \),

\[
\{ d_{p+1}, \ldots, d_k \} \cap \{ d_{p+1}, \ldots, d_k \} = \emptyset,
\]

and

\[
\{ \ell_{q+1}, \ldots, \ell_t \} \cap \{ \ell_{q+1}, \ldots, \ell_t \} = \emptyset.
\]
Again, Equations (3) and (4) imply

\[ \{ d_1, d_2, \ldots, d_k, \ell_1 + 1, \ldots, \ell_t + 1 \} = \{ d_1', d_2', \ldots, d_k', \ell_1' + 1, \ldots, \ell_t' + 1 \} \]

Therefore, removing \( D_I \) and \( L_I \) from these multisets, we conclude

\[ \{ d_{p+1}, \ldots, d_k, \ell_{q+1} + 1, \ldots, \ell_t + 1 \} = \{ d_{p+1}', \ldots, d_k', \ell_{q+1}' + 1 \ldots \ell_t' + 1 \} \]

Equations (3) and (4) imply

\[ \{ d_{p+1}, \ldots, d_k \} = \{ \ell_{q+1} + 1 \ldots \ell_t + 1 \}, \]

and

\[ \{ \ell_{q+1} + 1, \ldots, \ell_t + 1 \} = \{ d_{p+1}', \ldots, d_k' \}. \] (5)

On the other hand, since the list of distances of vertices with color \( C \) from \( u \) in \( G \) is the same as the list of vertices with color \( C \) from \( u' \) in \( H \), i.e. \((D_u + 1) \cup L_u = (D_{u'} + 1) \cup L_{u'}\). Specifically,

\[ \{ d_1 + 1, \ldots, d_k + 1, \ell_1, \ldots, \ell_t \} = \{ d_1' + 1, \ldots, d_k' + 1, \ell_1', \ldots, \ell_t' \} \]

\[ \quad = \{ d_1 + 1, \ldots, d_p + 1, d_{p+1} + 1, \ldots, d_k + 1, \ell_1, \ldots, \ell_{q+1}, \ell_{q+2}, \ldots, \ell_t \}. \]

Therefore,

\[ \{ d_{p+1} + 1, \ldots, d_k + 1, \ell_{q+1}, \ldots, \ell_t \} = \{ d_{p+1}', \ldots, d_{k'+1}, \ell_{q+1}' \ldots \ell_t' \}. \]

Again, Equations (3) and (4), imply

\[ \{ d_{p+1} + 1, \ldots, d_k + 1 \} = \{ \ell_{q+1}' \ldots \ell_t' \}, \]

and

\[ \{ \ell_{q+1}, \ldots, \ell_t \} = \{ d_{p+1}', \ldots, d_{k'+1} \}. \] (6)

Combining Equations (5) and (6), we conclude

\[ \{ \ell_{q+1}, \ldots, \ell_t \} = \{ d_{p+1}', \ldots, d_{k'+1} \} = \{ \ell_{q+1} + 2, \ldots, \ell_t + 2 \}. \]

Thus, \( \{ \ell_{q+1}, \ldots, \ell_t \} \) is empty, implying \( L_u \subset L_{u'} \), and \( D_v = D_{v'} \), as desired. \( \square \)

**Lemma B.26.** Let \( G \) and \( H \) be two graphs with the same RD-WL colorings. Let (i) \( \{ u, v \} \) be a cut edge in \( G \), (ii) \( u' \in V_H \) such that \( \chi_{RD_G}(u) = \chi_{RD_H}(u') \), (iii) \( v' \in V_H \) such that \( \chi_{RD_H}(v') = \chi_{RD_G}(v) \), and \( RD_H(u', v') = 1 \). Then, \( \{ u', v' \} \) must be a cut edge in \( H \).

Note that the lemma does not trivially follow from Lemma B.19 since \( \{ u', v' \} \) is not assumed to be an edge a priori.

**Proof.** Let \( C_{uv} \) be the set of all vertices that are colored \( \chi_{RD_G}(u) \) or \( \chi_{RD_G}(v) \) in \( G \). By Lemma B.23, \( S_u \cap C_{uv} = \{ u \} \) or \( S_v \cap C_{uv} = \{ v \} \). Assume that \( S_u \cap C_{uv} = \{ v \} \); the other case is similar.

Suppose, to derive a contradiction, that \( \{ u', v' \} \) is not a cut edge. Let \( w' \) be a neighbor of \( v' \) that resides in the same connected component as \( u' \) in \( H \setminus \{ v' \} \). (In particular, if \( v' \) is not a cut vertex \( w' \) can be any neighbor of \( v' \).) Such a \( w' \) exists and is distinct from \( u' \), otherwise \( \{ u', v' \} \) would be a cut edge. We know that \( RD_H(w', u') < RD_H(w', v') + RD_H(v', u') = RD_H(w', v') + 1 \); the triangle inequality implies the inequality, and it is a strict inequality because, in the case of equality, \( v' \) would a cut vertex separating \( w' \) and \( u' \), contradicting the choice of \( w' \). Let \( \ell = RD_H(w', v') \), and note that \( \ell < 1 \), as otherwise \( \{ w', v' \} \) is a cut edge between \( v' \) and \( u' \) implying that \( RD_H(u', v') > 1 \).

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Since \( \chi_{RD_G}(v) = \chi_{RD_H}(v') \), there must exist a vertex \( w \in V_G \) such that \( \chi_{RD_G}(w) = \chi_{RD_H}(w') \) and \( RD_G(v, w) = \ell < 1 \). Since all vertices in \( S_u \) are at a distance at least one from \( v \), we have \( w \in S_v \). Let \( L_w \) be the list of distances of vertices in \( C_{uv} \) from \( w \). Since \( S_v \cap C_{uv} = \{v\} \), the smallest distance in \( L_w \) is \( \ell \) and the second smallest distance in \( \ell + 1 \), to \( v \) and \( u \), respectively.

Let \( C_{u',v'} \) be the set of all vertices in \( H \) that are colored \( \chi_{RD_H}(u') = \chi_{RD_H}(v') = \chi_{RD_H}(v) \). Then, let \( L_{u'} \) be the list of all distances of \( u' \) to vertices in \( C_{u',v'} \). Since \( \chi_{RD_H}(u') = \chi_{RD_G}(v) \), then \( L_{u'} = L_w \) by Lemma B.22. In particular, the smallest two numbers in \( L_{u'} \) are \( \ell \) and \( \ell + 1 \). We know \( RD_H(u', v') = \ell \), and by the triangle inequality \( RD_H(u', v') + 1 = \ell + 1 \). Since, the second smallest number in the list is \( \ell + 1 \), and not smaller, the inequality must be tight, i.e. \( RD_H(u', v') = RD_H(v', u') + 1 = RD_H(H, v') + RD_H(v', u') \). Therefore, \( v' \) is a cut vertex separating \( u' \) and \( v' \), contradicting the choice of \( u' \).

**Lemma B.27.** Let \( G \) and \( H \) be two graphs with the same RD-WL colorings. Let \( u, v \) be a cut edge in \( G \) and \( \{u', v'\} \) a cut edge in \( H \) such that \( \chi_{RD_G}(u) = \chi_{RD_H}(u') \) and \( \chi_{RD_G}(v) = \chi_{RD_H}(v') \). Furthermore, let \( B_v \) (resp. \( B_{v'} \)) be the biconnected component of \( v \) (resp. \( v' \)) in \( G \) (resp. \( H \)). Finally, let \( K \) (resp. \( K' \)) be the set of all cut edges except \( \{u, v\} \) (resp. \( \{u', v'\} \)) with one endpoint in \( B_v \) (resp. \( B_{v'} \)). Then there exists a bijection between \( f : K \to K' \), such that for any \( \{x, y\} \in K \) and \( \{w, z\} = f(\{x, y\}) \), if \( x \) in on \( v \)'s side in \( G \setminus \{x, y\} \) and \( w \) is on \( v' \)'s side in \( H \setminus \{w, z\} \), then \( \chi_{RD_G}(x) = \chi_{RD_H}(w) \) and \( \chi_{RD_G}(y) = \chi_{RD_H}(z) \).

**Proof.** Let \( S_v \) (resp. \( S_{v'} \)) be the vertex set of the connected component of \( G \setminus \{u, v\} \) (resp. \( H \setminus \{u', v'\} \)) that contains \( v \) (resp. \( v' \)).

Let \( X = \{x_1, \ldots, x_k\} \) be the set of endpoints of \( K \) that are in \( B_v \) ordered such that \( RD(v, x_1) \leq \ldots \leq RD(v, x_k) \). (Note that each \( x_i \) may be connected to multiple cut edges of \( K \).)

By Lemma B.25, there exists \( X' = \{x_1', \ldots, x_k'\} \subset S_{v'} \) such that for every \( i \in [k] \)

1. \( \chi_{RD_G}(x_i) = \chi_{RD_H}(x_i') \) and
2. \( RD_G(v, x_i) = RD_H(v', x_i') \).

(Let \( C_X \) be the set of all vertices that are colored by the colors \( \{\chi_{RD_G}(x_1), \ldots, \chi_{RD_G}(x_k)\} \) in \( S_v \). Note, \( C_X \) is a (possibly proper) superset of \( \{x_1, \ldots, x_k\} \). Therefore, by Lemma B.25, there exists a set \( C_X' \subseteq S_{v'} \) such that there is a one-to-one correspondence between \( C_X \) and \( C_X' \) with corresponding pairs have the same color and distance to \( v \) and \( v' \). The existence of \( X' \) with the aforementioned properties follows as \( X \subseteq C_X \).)

For each \( i \in [k] \), let \( Y_i \) be the set of all vertices that are adjacent to \( x_i \) with a cut edge in \( K \). Since \( \chi_{RD_G}(x_i) = \chi_{RD_H}(x_i') \), by Lemma B.26, for each \( i \in [k] \), there exists \( Y_i' \) such that (1) for all \( y' \in Y_i' \), \( \{x_i', y'\} \) is a cut edge, and (2) the multisets \( \{\chi_{RD_G}(y)\}_{y \in Y_i} = \{\chi_{RD_H}(y)\}_{y' \in Y_i'} \).

Next, we show for every \( i \in [k] \) and every \( y' \in Y_i' \), \( RD_H(v', x_i') < RD_H(v', y_i') \), or equivalently, \( v' \) is in the connected component of \( x_i' \) in \( H \setminus \{x_i', y_i'\} \). We prove this by induction on \( i \).

For each \( i \in [k] \), and each \( y \in Y_i \), let \( S_y \) be the set of all vertices on the \( y \) side in \( G \setminus \{x_i, y\} \), and let \( S_i = \bigcup_{y \in Y_i} S_y \). For all \( h < i \), and each \( y' \in Y_i' \), let \( S_{h,y}' \) be the set of all vertices on the \( y' \) side in \( H \setminus \{x_h', y_i'\} \), and \( S_h' = \bigcup_{y' \in Y_i'} S_{h,y}' \). Note \( S_v \setminus \bigcup_{h < i} S_h \) contains \( v \) and, by the induction hypothesis, \( S_{v'} \setminus \bigcup_{h < i} S_{h'} \) contains \( v' \).

By Lemma B.25 and that \( RD_G(v, x_i) = RD_H(v', x_i') \), \( S_h \) and \( S_{h'} \) induce the same set of color/distance pairs from \( v \) and \( v' \), respectively; i.e. there is a one-to-one map \( f \) from \( S_h \) to \( S_{h'} \) such that for each pair \( (q, f(q)) \), (i) \( q \) and \( f(q) \) have the same color, and (ii) \( RD_G(v, q) = RD_H(v', f(q)) \). Thus, \( B_{v,i} = S_v \setminus \bigcup_{h < i} S_h \) and \( B'_{v,i} = S'_{v'} \setminus \bigcup_{h < i} S_{h'} \) induce the
same set of color/distance pairs from \( v \) and \( v' \), respectively. Let \( C \) be the set of colors of vertices that are incident to cut edges. The \( i \)th smallest distance with color from \( C \) in \( B_v \) corresponds to \( x_i \). We know \( x_i' \) has the same color as \( x_i \), and \( RD_G(v, x_i) = RD_H(v', x_i') \). If there exists \( y' \in Y'_i \) such that the \( RD_H(v', y') < RD_H(v', x_i) \) then the \( i \)th smallest number in \( B'_{v,i} \) would be smaller than \( RD_G(v, x_i) \) which is a contradiction. Hence, \( RD_H(v', x_i') < RD_H(v', y') \) for all \( y' \in Y'_i \), as desired.

Therefore, \( B'_{v'} = S'_{v'} \setminus \bigcup_{i \in [k]} S_i' \) is connected, and it has the same set of colors as \( B_v = S_v \setminus \bigcup_{i \in [k]} S_i \). So, it must be the biconnected component that contains \( v' \).

\[ \text{Theorem B.28.} \] If two graphs \( G \) and \( H \) have the same RD-WL colorings, then their block cut-edge trees are isomorphic.

\[ \text{Proof.} \] Let \( \{u, v\} \) be a cut edge in \( G \) such that \( S_u \) is a biconnected component. Let \( \{u', v'\} \) be an edge in \( H \) with \( \chi_{RD_G}(u) = \chi_{RD_H}(u') \) and \( \chi_{RD_G}(v) = \chi_{RD_H}(v') \). By Lemma B.27, \( S'_{u'} \) is a biconnected component of \( H \). Root the block cut-edge tree of \( G \) at \( S_u \) and the block cut-edge tree of \( H \) at \( S'_{u'} \), so all cut edges are directed away from \( S_u \) and \( S'_{u'} \).

For a directed cut edge \( u \to v \), define \( T_G[v] \) the be the block cut-edge subtree rooted at the biconnected component of \( v \). We use induction on the size of \( T_G[v] \) to show that for two same colored edges with the same direction \( u \to v \) and \( u' \to v' \), \( T_G[v] \) and \( T_H[v'] \) are isomorphic.

Let \( B_v \) and \( B'_{v'} \) be the biconnected components of \( v \) in \( G \) and \( v' \) in \( H \) respectively. For the base case that \( B_v = S_v \), then by Lemma B.27, \( B'_{v'} = S'_{v'} \) and the statement holds. Alternatively, also by Lemma B.27, the outgoing directed edges of \( B_v \) and \( B'_{v'} \) are in one-to-one correspondence with matching head and tail colors. Let these sets of edges be \( K \) and \( K' \), respectively, and let \( f \) be the bijection between them that preserves colors. For any \( x \to y \in K \), and its image \( f(x) \to f(y) = w \to z \in K' \), by the induction hypothesis, the block cut-edge subtrees \( T_G[y] \) and \( T_H[z] \) are isomorphic. Therefore, \( T_G[v] \) and \( T_H[v'] \) are isomorphic.

### C. Experiments

In this section, we carry out experiments to validate our two main results Theorem 3.8 and Theorem 3.10. Our code is adapted from the GraphGPS module (Rampášek et al., 2022) and subsequent fork from Müller et al. (2024).

#### C.1. Graph Isomorphism: CSL

<table>
<thead>
<tr>
<th>CSL Dataset: Classification Accuracy (( \uparrow ))</th>
<th>HKdiagSE</th>
<th>RWSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>APE-GT</td>
<td>100 ± 0.00</td>
<td>100 ± 0.00</td>
</tr>
<tr>
<td>DeepSet RPE-GT</td>
<td>100 ± 0.00</td>
<td>100 ± 0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CSL Dataset: Classification Accuracy (( \uparrow ))</th>
<th>RSPE Powers of Adjacency</th>
<th>RD</th>
<th>SPD</th>
<th>Adjacency</th>
</tr>
</thead>
<tbody>
<tr>
<td>RPE-GT</td>
<td>100 ± 0.00</td>
<td>100 ± 0.00</td>
<td>90 ± 0.00</td>
<td>10 ± 0.00</td>
</tr>
<tr>
<td>EGN APE-GT</td>
<td>100 ± 0.00</td>
<td>100 ± 0.00</td>
<td>90 ± 0.00</td>
<td>10 ± 0.00</td>
</tr>
<tr>
<td>GIN</td>
<td>10 ± 0.00</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

We consider the graph classification task on the Circular Skip Links (CSL) dataset (Dwivedi et al., 2023). The goal of the CSL dataset is to classify graphs according to their isomorphism type. This is classified as a “Hard” task by Müller et al. (2024).

To validate Theorem 3.8, we consider two different APEs: Random Walk Structural Encoding (RWSE) and Heat Kernel Diagonal Structural Encoding (HKdiagSE) from the GraphGPS Library (Rampášek et al., 2022). For both APEs, we used
times \{1, \ldots, 20\}. We test these APEs with APE-GTs and their corresponding RPEs by applying a DeepSet and the result GTs are denoted DeepSet RPE-GTs.

To validate Theorem 3.10, we consider four different RPEs: RSPE (Huang et al., 2024), a stack of 20 powers of the adjacency matrix (inspired by RRWP (Ma et al., 2023)), the resistance distance (RD), the shortest-path distance (SPD), and the adjacency matrix. We then consider their corresponding APEs by applying a 2-EGN and the result GTs are denoted EGN APE-GTs. We ran the RPE-GT and APE-GT for 1000 epochs each. Our results are averaged over 5 random seeds. See Table 1 and Table 2 for the results.

As our theoretical results (Theorems 3.8 and 3.10) predict, RPE-GTs and EGN APE-GTs have the same classification accuracy when using the same RPE. Likewise, APE-GT and DeepSets RPE-GT have the same classification accuracy when using the same APE. This validates our main theorems.

Moreover, note that the accuracy of Adjacency-RPE-GT and GIN are equal, which agrees with Corollary 4.17.

### C.2. Graph Isomorphism: BREC

Table 3. Performance of different RPEs on the BREC dataset. Basic, Regular, Extension, and CFI are subsets of the BREC dataset. Results are shown in the form of mean ± standard deviation. Experiments are averaged over 5 runs.

<table>
<thead>
<tr>
<th>BREC Dataset: Pair-Distinguishing Accuracy (†)</th>
<th>Basic</th>
<th>Regular</th>
<th>Extension</th>
<th>CFI</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>RPE: Resistance Distance (RD)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RPE-GT</td>
<td>100.00 ± 0.00</td>
<td>35.71 ± 0.00</td>
<td>100.00 ± 0.00</td>
<td>7.60 ± 1.14</td>
<td>54.40 ± 0.29</td>
</tr>
<tr>
<td>EGN APE-GT</td>
<td>100.00 ± 0.00</td>
<td>35.71 ± 0.00</td>
<td>100.00 ± 0.00</td>
<td>7.00 ± 1.23</td>
<td>54.25 ± 0.31</td>
</tr>
<tr>
<td>RPE: Shortest-Path Distance (SPD)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RPE-GT</td>
<td>26.67 ± 0.00</td>
<td>9.29 ± 0.00</td>
<td>40.8 ± 0.45</td>
<td>6.8 ± 0.11</td>
<td>19.15 ± 0.22</td>
</tr>
<tr>
<td>EGN APE-GT</td>
<td>26.67 ± 0.00</td>
<td>9.42 ± 0.28</td>
<td>41.00 ± 0.00</td>
<td>11.80 ± 0.45</td>
<td>20.50 ± 0.18</td>
</tr>
<tr>
<td>RPE: Stable Positional Encoding (SPE)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RPE-GT</td>
<td>97.00 ± 2.17</td>
<td>34.71 ± 0.57</td>
<td>96.00 ± 1.87</td>
<td>3.2 ± 4.47</td>
<td>51.5 ± 0.73</td>
</tr>
<tr>
<td>EGN APE-GT</td>
<td>0.97 ± 2.17</td>
<td>33.14 ± 0.97</td>
<td>98.80 ± 0.84</td>
<td>8.80 ± 1.30</td>
<td>53.05 ± 0.54</td>
</tr>
<tr>
<td>RPE: Stack of Powers of Adjacency Matrix</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RPE-GT</td>
<td>100.00 ± 0.00</td>
<td>35.00 ± 0.00</td>
<td>94.60 ± 0.00</td>
<td>9.80 ± 0.84</td>
<td>53.55 ± 0.28</td>
</tr>
<tr>
<td>EGN APE-GT</td>
<td>8.00 ± 1.39</td>
<td>32.86 ± 0.00</td>
<td>88.20 ± 1.79</td>
<td>3.00 ± 0.00</td>
<td>46.75 ± 0.47</td>
</tr>
<tr>
<td>RPE: Adjacency Matrix</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RPE-GT</td>
<td>0.00 ± 0.00</td>
<td>0.00 ± 0.00</td>
<td>0.00 ± 0.00</td>
<td>0.00 ± 0.00</td>
<td>0.00 ± 0.00</td>
</tr>
<tr>
<td>EGN APE-GT</td>
<td>0.00 ± 0.00</td>
<td>0.00 ± 0.00</td>
<td>0.00 ± 0.00</td>
<td>0.00 ± 0.00</td>
<td>0.00 ± 0.00</td>
</tr>
</tbody>
</table>

Table 4. Performance of different APEs on the BREC dataset. Basic, Regular, Extension, and CFI are subsets of the BREC dataset. Results are shown in the form of mean ± standard deviation. Experiments are averaged over 5 runs.

<table>
<thead>
<tr>
<th>BREC Dataset: Pair-Distinguishing Accuracy (†)</th>
<th>Basic</th>
<th>Regular</th>
<th>Extension</th>
<th>CFI</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>APE: Heat Kernel Diagonal Structural Encoding (HKdiagSE)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>APE-GT</td>
<td>56.00 ± 4.50</td>
<td>26.00 ± 0.57</td>
<td>38.00 ± 3.16</td>
<td>3.00 ± 0.00</td>
<td>27.75 ± 1.43</td>
</tr>
<tr>
<td>DeepSets RPE-GT</td>
<td>59.00 ± 4.01</td>
<td>18.86 ± 1.84</td>
<td>59.60 ± 6.11</td>
<td>1.2 ± 1.30</td>
<td>30.65 ± 1.57</td>
</tr>
<tr>
<td>APE: Random Walk Structural Encoding (RWSE)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>APE-GT</td>
<td>84.33 ± 3.65</td>
<td>31.29 ± 0.83</td>
<td>62.40 ± 4.39</td>
<td>1.00 ± 0.00</td>
<td>39.45 ± 1.10</td>
</tr>
<tr>
<td>DeepSets RPE-GT</td>
<td>69.67 ± 5.32</td>
<td>21.29 ± 2.73</td>
<td>63.80 ± 2.39</td>
<td>0.4 ± 0.55</td>
<td>33.95 ± 1.81</td>
</tr>
</tbody>
</table>

We consider the graph isomorphism benchmark dataset BREC (Wang & Zhang, 2024). The BREC dataset tests a graph neural network architecture’s ability to distinguish pairs of non-isomorphic graphs. Unlike the CSL dataset which poses the graph isomorphism problem as a graph classification problem, the BREC dataset considers pairs of non-isomorphic graphs and tests whether a graph neural networks can learn different representations for the two graphs. The graph neural network is trained via contrastive learning on sets of graphs pairs with randomly permuted node indices. The graph neural network
Comparing Graph Transformers via Positional Encodings

is then evaluated using the $T_2^2$ test on the learned features for each of the two graphs. The exact training and evaluation procedures can be found in the original BREC dataset paper (Wang & Zhang, 2024).

We compared several RPEs on the BREC dataset. We found that RD, SPE, and a stack of 20 powers of the adjacency matrix all perform similarly well and perform better than SPD in terms of total accuracy. Moreover, the adjacency matrix achieves 0% accuracy, which matches the theoretical results of Proposition 4.10 as all pairs of graphs in the BREC dataset are WL indistinguishable.

We also compared two APEs on the BREC dataset: RWSE and HKdiagSE from the GraphGPS library (Rampášek et al., 2022). For both APEs, we used times \{1, ..., 20\}. We found that RWSE slightly outperformed HKdiagSE.

Finally, for the most part, both RPEs and APEs achieved similar performance for their different architectures, i.e. RPE-GT and EGN APE-GT or APE-GTs and DeepSets RPE-GT. This matches our theoretical results (Theorems 3.8 and 3.10).

However, one interesting thing we found is that there are several graph pairs in the CFI subset that SPD-GTs were able to learn to distinguish while RD-GTs did not. This suggests that SPD-WL and RD-WL may be incomparable. Zhang et al. (2023) show there are graphs that RD-WL can distinguish that SPD-WL cannot; this suggests the converse is true too, although it is not a definitive proof of this fact and should not be interpreted as such. A question for future research would be to prove that these pairs of graphs are indistinguishable by RD-WL or to find a RD-GT that could distinguish these pairs of graphs.

Hyperparameter search was performed for each pair of PE and architecture.

C.3. Graph Regression: ZINC

Table 5. Test performance on the Small ZINC dataset. Results are shown in the form of mean ± standard deviation. Experiments are averaged over 3 runs.

<table>
<thead>
<tr>
<th>ZINC Dataset: MAE (↓)</th>
<th># Parameters</th>
<th>RD</th>
<th>SPD</th>
<th>SPE</th>
</tr>
</thead>
<tbody>
<tr>
<td>RPE-GT</td>
<td>573922</td>
<td>0.096 ± 0.002</td>
<td>0.130 ± 0.010</td>
<td>0.132 ± 0.007</td>
</tr>
<tr>
<td>EGN APE-GT</td>
<td>520514</td>
<td>0.196 ± 0.004</td>
<td>0.217 ± 0.011</td>
<td>0.200 ± 0.007</td>
</tr>
<tr>
<td># Parameters</td>
<td></td>
<td>RD+EF</td>
<td>SPD+EF</td>
<td>SPE+EF</td>
</tr>
<tr>
<td>RPE-GT</td>
<td>696226</td>
<td>0.069 ± 0.004</td>
<td>0.092 ± 0.010</td>
<td>0.092 ± 0.001</td>
</tr>
<tr>
<td>EGN APE-GT</td>
<td>664818</td>
<td>0.110 ± 0.003</td>
<td>0.132 ± 0.004</td>
<td>0.126 ± 0.003</td>
</tr>
</tbody>
</table>

Although our theoretical results are for the distinguishing power of graph transformers and apply most directly to graph classification/isomorphism tasks, we would also like to compare RPEs and APEs on real-world tasks beyond those. In this experiment, we compare RPE-GTs and EGN APE-GTs for graph regression on the small ZINC dataset containing 12k graphs (Dwivedi et al., 2023). We consider the RPEs resistance distance (RD), shortest-path distance (SPD), and SPE (Huang et al., 2024). See Table 5 for the results.

We test the models both with and without the use of edge features of graphs in the ZINC dataset. Edge features are distinct from RPEs as they are not dependent on the graph structure and are associated to edges and not a pairs of vertices. For the ZINC dataset, the features are one-hot encodings of the bond type (e.g. single, double, triple). When we include edge features, we concatenate them to the RPE and pass the concatenated tensor to the model in place on the RPE. This use of edge features is not captured by our theoretical results, and it is not clear if this is the best or most natural way of including edge features in a graph transformer. Other papers have proposed different ways of incorporating edge features into a graph transformer (Ma et al., 2023; Jin et al., 2023).

From Table 5, we see that the performance of EGN APE-GT is worse than the corresponding RPE-GT. This could be partially explained by Theorem 3.10, which states that RPE-GTs have stronger distinguishing power than EGN APE-GTs for graphs with node features (as the graphs in ZINC do). Additionally, we suspect that the training of the extra EGN layer introduces additional difficulty in the training process, leading to worse performance of APE-GT compared to RPE-GT. This result aligns with our expectations, suggesting that instead of converting an RPE into an APE, it may be better to use the RPE directly in a RPE-GT.
**Hyperparameters & experimental setup.** Our results are averaged over 3 random seeds. We ran the RPE-GT and APE-GT for 1000 epochs each.

Following Zhang et al. (2023), the functions $f_1$ and $f_2$ in the RPE-GT head are embeddings into Gaussian kernels followed by an MLP.

Hyperparameter search was performed for RPE-GTs and EGN APE-GTs. We chose the final hyperparameters for each architecture to have similar numbers of parameters. Hyperparameters involved in our models are listed in Table 6.

<table>
<thead>
<tr>
<th></th>
<th>RPE GTs</th>
<th>EGN APE GTs</th>
<th>SPE</th>
</tr>
</thead>
<tbody>
<tr>
<td># Transformer Layers</td>
<td>14</td>
<td>8</td>
<td>3</td>
</tr>
<tr>
<td># Transformer Heads</td>
<td>8</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td># Gaussian Kernels</td>
<td>16</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td># MLP Layers</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MLP Hidden Dimension (No Edge Features)</td>
<td>16</td>
<td>EGN Hidden Dim (No Edge Features)</td>
<td>48</td>
</tr>
<tr>
<td>MLP Hidden Dimension (Edge Features)</td>
<td>16</td>
<td>EGN Hidden Dim (Edge Features)</td>
<td>64</td>
</tr>
<tr>
<td>APE Type</td>
<td>Add</td>
<td></td>
<td></td>
</tr>
<tr>
<td># DeepSets Layers</td>
<td>3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DeepSets Hidden Dimension</td>
<td>64</td>
<td></td>
<td></td>
</tr>
<tr>
<td># Parameters</td>
<td>17217</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**C.4. Code**

Code for all experiments can be found at [https://github.com/blackmit/comparing_graph_transformers_via_positional_encodings](https://github.com/blackmit/comparing_graph_transformers_via_positional_encodings)